NUMERAL SIMULATION APPLICATION IN MICROPOROSITY PREVISION IN ALUMINUM ALLOY CASTINGS

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ABSTRACT

The porosity formation in castings is very important due to its frequency and its correspondent deleterious effects in the cast parts mechanical properties. In special the presence of porosity has a dramatic effect on the fatigue life in cast aluminum alloys. The objective of this paper is to apply a numerical method based on finite difference to understand dissolved gases and solidification parameters roles in the porosity formation in aluminum alloys during the solidification. The model predictions are compared with experimental results unidirectional upward solidification of Al 4.5 wt % Cu.

1. INTRODUCTION

In order to reduce vehicle weight, many automotive components have been redesigned to take advantage of materials such as lightweight and polymers [1,2]. To this end, aluminum castings alloys are being widely used for many automotive components. These alloys have good casting characteristics, reasonable mechanical properties, and are heat treatable. [3] However, the performance requirements of structural castings, particularly chassis or suspension components, place granter requirements on their mechanical properties. An important factor that leads to a decrease in castings mechanical properties (notably ductility and fatigue life) is the presence of microporosity [4].

Most metallic materials for engineering structural applications will undergo a dendritic solidification process, no matter whether these materials are the final-part forms, as various castings, or in the middle-stage forms as various ingots for the subsequent mechanical processing. The dendritic solidification behaviors are critical in determining the properties of the formed parts/materials [5]. These properties are governed mainly by such factors as porosity, presence of a second phase, grain size, and dendrites spacing [6]

Porosity, which occurs in almost all aluminum alloy castings, is detrimental to mechanical properties and pressure-tightness of the casting [7]. As a result, research has been conducted on the porosity formation for almost half a century. Microporosity may occur during solidification of castings either due to rejection of gas from the liquid metal or to the inability to feed through interdendritic channels to compensate for the shrinkage [8-23].

Demanding application in the automotive industry call for aluminum castings to be mass-produced without casting defects. Predictive models for heat and fluid flow has being used in components and casting processes design, but the ability of those models predicts quantitatively casting defects such as porosity and hot tearing, still limited. As far as the solidification parameters are concerned, the variables that control porosity may be narrowed down to the thermal gradient, the rate of solidification, the cooling rate and the solidification time. Based on these, various approaches have been suggested to predict casting porosity, the oldest being the empirical criteria derived from experimentation [23]. Semi-empirical criteria based on thermal parameters have also been formulated [24-27]. Many of these criteria are based on Darcy's law, which brings near the mushy zone to a porous medium. The pressure drop in the mushy zone is then expressed in terms of thermal criteria functions to predict the onset porosity. The current modeling practice is to calculate these criteria functions using the solidification model to predict porosity [8,13,28,29]. Some of these functions are quite successful in predicting porosity in short freezing range alloys, though there are many difficulties in applying them for long-freezing alloys.

The primary limitation of the thermal parameter- based models, however, is that they do not account for the dissolved gases role in the metal; in effect, they account for the porosity resulting from the shrinkage alone. It has been clearly established that porosity in castings is often the result of a gas presence combination and shrinkage effects. Extensive theoretical and experimental work has been carried out to analyze the micro porosities formation during the solidification [8-22].

As the porosity absence has a dramatic effect on the fatigue live in cast aluminum alloys, several studies [29,30] show that the porosity elimination can increase the average fatigue life up to a factor of 10 [3]. Therefore, the aim of this work is to examine numerical and experimental models to

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understand the dissolved gases and solidification parameters roles.

2. MICROPOROSITY FORMATION MODELING

Considering that alloys solidification is primarily governed by heat diffusion, the basic continuity equation at macroscopic scale is the energy conservation equation given by [32]:

$$\rho \cdot c_p \cdot \frac{\partial T}{\partial t} = \nabla \bullet \left(k \cdot \nabla T \right) + Q \tag{1}$$

where

 ρ = solid metal density, c_p = solid metal specific heat, k = solid metal thermal conductivity, Q = heat liberated during solidification, T = temperature, t = time.

The heat liberated during solidification may be written as:

$$Q = \rho \cdot L_m \cdot \frac{\partial f_s}{\partial t}$$
(2)
where

 L_m = solidification latent heat, f_s = solid fraction.

From equations 1 and 2:

$$\rho \cdot c_p \cdot \frac{\partial T}{\partial t} - \rho \cdot L_m \cdot \frac{\partial f_s}{\partial T} \cdot \frac{\partial T}{\partial t} = \nabla \bullet \left(k \cdot \nabla T \right) \quad (3)$$

As enthalpy (*H*) is given by: T_{T}

$$H = \int_{0}^{r} \rho \cdot c_{p} \cdot dT + \rho \cdot L_{m} \cdot (1 - f_{s}) \quad (4)$$

and

$$\frac{\partial H}{\partial T} = \rho \cdot c_p - \rho \cdot L_m \cdot \frac{\partial f_s}{\partial T} \qquad (5)$$

From equations 3 and 5:

$$\frac{\partial H}{\partial t} = \nabla \bullet \left(k \cdot \nabla T \right) \tag{6}$$

For unidirectional heat flow, equation 6 takes the form of:

$$\frac{\partial H}{\partial t} = k \cdot \frac{\partial^2 T}{\partial x^2} \tag{7}$$

Considering a chilled (cooled) mold, a balance of energy in the metal/mold interface gives:

$$-k \cdot \frac{\partial T}{\partial x} - h \cdot (T_i - T_0) = 0 \qquad (8)$$

where

- h = heat transfer coefficient at metal/mold interface
- T_i = temperature at metal/mold interface
- T_0 = coolant temperature

The solid fraction as temperature function is determined using the Scheil equation [33] and the enthalpy variation curve versus temperature can be calculated.

Following a suitable discretization of the metal/mold system, the differential equations are solved using finite difference method. The temperatures are determined from enthalpy values, using the enthalpy variation curve versus temperature, and the solidus and liquidus isotherms positions during solidification are obtained. From these parameters it is possible to calculate the dendrites tip movement rate, the local solidification time and thermal gradients ahead of dendrite tips and then predict dendrite arms spacing variation during solidification. The following equations, proposed respectively by Hunt [34] and Bower [35], are applied to estimate the primary (λ_1) and secondary (λ_2) arms spacing:

$$\lambda_1 = 2.83 \cdot \sqrt[4]{\frac{D_l \cdot \Gamma \cdot k_e \cdot \Delta T_0}{v_l \cdot G_l^2}}$$
[9]

and

$$\lambda_2 = 7.5.10^{-6} (t_l)^{0.39} \quad [10]$$

where

 D_l = diffusion coefficient in liquid

 G_l = liquidus temperature gradient

 k_e = distribution coefficient

 $t_l =$ local solidification time

- v_l = liquidus isotherm movement rate
- $\Delta T_0 =$ liquidus-solidus range

Favorable conditions for microporosity formation are inefficient liquid feed; difficulty in interdendritic flow, low energy for pore nucleation; low pressure acting on the liquid metal or due to surface tension and gases at high pressure, that is, a high gas content and low solubility in the solid phase [36]. These conditions for the porosities formation, expressed in terms of pressures predict the thermodynamic condition for porosity formation in castings by the equation [7-11,17,18,20-22]:

$$P_G + \Delta P \ge P_A + P_M + P_\sigma \tag{11}$$

where P_G is the dissolved gases pressure in the melt, ΔP is the pressure drop in interdendritic channels, P_A is the atmospheric pressure, P_M is the metalostatic pressure and P_{σ} is the necessary pressure to overcome surface tension.

During solidification, gas rejection at the solid/liquid interface leads to an increased gas concentration in the liquid. If this concentration reaches a critical value, based on the net solubility of gas in the liquid, then pores can nucleate and grow [10-12,21]. In the case of aluminum alloys, hydrogen is the highest interest gas [16,33] and Sievert's law can be applied [13-15]:

$$P_{gas} = 10^5 \left(\frac{H_{liq}}{S}\right)^2 \tag{12}$$

where H_{liq} is the gas weight percentage (hydrogen) dissolved in the liquid and *S* is the solubility in cm³ of H₂(g) per 100g of alloy, in equilibrium with 1 atm pressure of H₂(g).

As the interdendritic channels are very small for typical dendrite arms spacing, the flow through this fine mesh can be treated as a flow through a finely porous media and thus Darcy's law can be applied, and the pressure drop is given by [8]:

$$\Delta P = -\int_{0}^{L} \frac{v_i \cdot \mu \cdot g_l}{K} \cdot dx \qquad (13)$$

where

 g_l = liquid volumetric fraction K = permeability L = interdendritic channel length v_i = flow rate μ = liquid viscosity ΔP = pressure drop $v_i = -\beta \cdot v_s$

where

 v_s = solidus isotherm movement rate

(14)

 β = shrinkage

The interdendritic channels permeability (K) is given by the following equation proposed by one of the authors of this paper [19]:

$$K = \frac{\lambda_1^2 \cdot f_l^2}{8 \cdot \pi \cdot \tau^3} \tag{15}$$

where

 f_l = the liquid fraction

 τ = the channel tortuosity given by:

$$\tau = 1 + \sum_{n=1}^{3} \left(\frac{\lambda_2}{\lambda_1} \right)^{f_l^n} \tag{16}$$

Pressure caused by surface tension of the liquid/gas interface represents an initial resistance to the gas bubble formation, varying with many factors and nucleation mechanisms [38]. A bubble cannot be established with a very small radius, for a radius tending to zero, the pressure due to tension would tend to an infinite value. But there is a critical size of bubble, under which it is not able to survive and over which it tends to grow [7]. To calculate this pressure, Lapace's equation is being used, which relates the pressure difference along the interface with the surface tension and the principal curvature radii of this interface at the point considered [7-11,16,17,39]. This equation is given by:

$$P_{\sigma} = \frac{\sigma_{\rm lg}}{r_p} \tag{17}$$

where

 σ_{lg} = surface tension of the liquid/gas interface, in N/m r_p = curvature radii of the pore, in m, which depend upon the interdendritic space volume and its geometry and the contact angle at the junction among gas, solid and liquid.

Following a suitable discretization of the metal/mould system, the differential equations are solved using a finite difference method. According to equation 17, when gas pressure, added to the pressure drop in interdedrtic channels, exceed metalostatic and atmospheric presures sum plus the pressure due to surface tension, the pore can nucleate. A pore with a large radius of curvature can nucleate at moderate gas pressure, it means, low gas concentration in the interdendritic liquid, because the contribution to pressure due to surface tension is low [40].

3. EXPERIMENTAL PROCEDURE

Experiments were performed to validate model results with unidirectional upward the Al 4.5 wt %Cu. Fig.1 shows a experimental apparatus schematic illustration used to solidify unidirectionally. Temperature profiles in the casting and in the mould during solidification were measured by using chromel-alumel thermocouples and a computational data acquisition system. The initial hydrogen concentration was measured by a Telegas apparatus [41].



Figure 1 – Schematic casting arrangement and thermocples position in ceramic mold and metal.

The microstructure was analysed through optical microscopy. The transverse and longitudinal sections of the samples were polished and attacked with Keller's reagent to measure the primary and secondary dendrite arm spacing. Transversal samples were used to measure the primary dendrite arm spacing and longitudinal samples were used to measure the secondary dendrite arm spacing [42]. Pore fraction was measured by image analysis.

4. **RESULTS AND DISCUSSION**

In the case of the experimental apparatus used, upward directional solidification, of the Al 4.5 wt % Cu alloy, there was a columnar structure formation in almost the entire sample. Figures 2 and 3 show, respectively, typical microstructure of Al- 4.5 wt Cu ingots.

The dendritric structure formed by the alloy shapes the porosity interdendritic located between two primary spacings.



Figure 2 – Unidirectionally solidified Al 4.5 wt % Cu alloy micrographs, longitudinal section at a distance of 40mm from the metal/chill mold interface showing the microporosities. Magnification 19.2x.



Figure 3 – Unidirectionally solidified Al 4.5 wt % Cu alloy micrographs, transverse section at a distance of 14mm from the metal/chill mold interface showing the microporosities. Magnification 60x.

Figure 4 shows the liquidus and solidus isotherms evolution during solidification predicted by the numerical model compared with experimental data. Good agreement is observed.

Heat transfer coefficient variation at metal/mould interface was estimated through the experimental casting temperature adjustment close to the interface and in the numerical method. The coefficient varies from about 4,000 to 1,000 $(W/m^2 K)$ during the solidification process. Figure 5 shows the heat transfer coefficient at the chilled interface estimated by the model.



Figure 4 – Solidus and liquidus isotherms evolution compared with experimental results.

Figure 6 compares primary and secondary arm spacing experimental results with the models proposed by Hunt [34] (primary) and Brower (secondary) [35]. It suggests that Brower's model describes well the secondary arm spacing variation found in the present work but Hunt underestimates the primary arm spacing variation.



at metal/mould.

Fig. 7 also compares radius and pores position experimental results with model predictions for an initial gas concentration of 0.10 cc/100g Al, showing a good agreement. For a better comparison it is defined, for experimental results, an equivalent average pore radius (radius of a circle with area equivalent to the measured average pore area) [43].

Since the developed mathematical model results showed good agreement when compared with the experimental results, one can use the model to evaluate other variables process. As an example, some numerical model simulation results developed for the case of the Al-4.5%Cu alloy are presented below.



Figure 6 - Primary and secondary dendrite arm spacing experimental results compared with predictions by Hunt [34] and Brower's [35] models.



Figure 7 – Porosity radius variations predicted by the numerical model, compared to experimental results obtained from the directionally solidified Al 4.5 wt %Cu alloy, as cooling rate function.

Figure 8 presents the pores radius variation predicted by the developed numerical model, considering different initial hydrogen concentrations as cooling rate function. Figure 8 shows that for the same thermal condition and for the same alloy, pore radius increases directly with the initial hydrogen content. This occurs due to the gas pressure (Pgas) and exceeds the acting pressure much more easily with the increase in hydrogen concentration. It can also be seen that the porosity formation can be avoided for certain hydrogen concentrations through the increase in cooling rate.



Figure 8 - Pore radius variation considering the cooling rate for different initial hydrogen concentrations as cooling rate function.

Figures 9 and 10 show pore radius position and primary arm spacing predicted by the model for different initial hydrogen concentrations (0.10, 0.05 and 0.00 cc/100g Al) respectively, adopting a constant value for the heat transfer coefficient (2,200 W/m²K) and the variable coefficient estimated in this work. For primary arm spacing calculation, Hunt's [34] equation is applied. Adopting the constant coefficient, pore formation is seen in the casting entire extension, for hydrogen concentrations of 0.10 and 0.05. Supposing that no gas is dissolved until 0.08 m from the chilled interface, the pores can be induced by shrinkage (Figure 9).

Adopting the variable coefficient and the other conditions remaining the same, the primary arm spacing and the pore radius also increase, for hydrogen concentrations of 0.10 and 0.05. Supposing no initial gas is dissolved there is practically no pore formation in the casting. From the results, the importance of an accurate heat transfer coefficient is evident to predict pore formation.

Figure 11 shows microporosity dimensions variation formed under two conditions: with and without dissolved hydrogen and considering the following parameters: heat transfer coefficient in metal/mould interface as a constant and equal to 4.000 W/m²K; the use of Hunt's [34] and Bower's [35] equations to predict the interdendritic primary and secondary spacing, respectively. It is noted that for high cooling rates (over 1°C/s) the porosity formation by shrinkage is favored, influenced by smaller spacing, which diminishes permeability and, on the other hand, increases the pressure gradient inside the channels. Diminishing the cooling rate (less than 1°C/s), the microporosity formation by gases is favored.



Figure 9 - Pore radius position predicted by a constant heat transfer coefficient numerical model of different gas







Figure 11 – Microporosity dimensions variations formed under two conditions: with and without dissolved hydrogen.

Microporosity formation during solidification can be properly predicted by this numerical model. This model is able to analyse the conditions for pore formation by shrinkage and/or dissolved gas.

Applying the model it is possible to estimate the pore position and its size. It is also evident the importance of proper equations to estimate primary and secondary arm spacing variation and heat transfer coefficient variation during solidification to obtain correct predictions from the numerical model.

For the case of the experimental apparatus used (unidirectional upward solidification) and for the Al 4.5 wt% Cu alloy, in which a columnar structure was formed in almost the entire extension of the samples, a limit situation was observed, as interdendritic feeding is strongly favored, because the primary arm spacing increases with the distance from the chill mould, making permeability increase as solidification progresses. Considering this, for these test conditions, the pressure drop was always less than the acting pressure, indicating that there is no pore formation due to shrinkage and that the pores formed are related to the presence of gases.

For a given initial hydrogen content, the pores volumetric fraction and its size diminish with the increasing in the cooling rate; for rates below 1°C/s, the volume of porosity by gases has an abrupt increase, since the primary spacing increases drastically.

For a certain cooling rate, the pores volumetric fraction and their size increase with the initial hydrogen content and these increases are larger, the smaller the cooling rates.

Therefore, the reduction of initial hydrogen content and/or the cooling rate increase, it decreases the volume of porosity and pore size. Consequently, it increases the fatigue life, because pore size appears to be a dominant factor in the fatigue life of aluminum alloys.

The practical implications of these results are considerable. With an accurate predictive models set, component designers will be able to conduct the majority of the build/ test /redesign cycle simulation. The predictive models would reduce the need for multiple sets of casting to achieve an optimum design, ultimately saving time and cost while ensuring durable cast components.

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