Multiscale modeling for the prediction of casting defects in investment cast aluminum alloys

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Abstract

Macroscopic modeling of heat transfer and fluid flow is now routinely used for the prediction of macroscopic defects in castings, while microscopic models are used to investigate the effects of alloy changes on typical microstructures. By combining these two levels of modeling it is possible to simulate the casting process over a wider range of spatial and temporal scales. This paper presents a multiscale model where micromodels for dendrite arm spacing and microporosity are incorporated into a macromodel of heat transfer and in order to predict the as cast microstructure and prevalence of microscopic defects, specifically porosity. The approach is applied to aluminum alloy (L169) investment castings. The models are compared with results obtained by optical image analysis of prepared slices, and X-ray tomography of volume samples from the experiments. Multiscale modeling is shown to provide the designer with a useful tool to improve the properties of the final casting by testing how altering the casting process affects the final microstructure including porosity.

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1. Introduction

Competition in many industries, especially the automotive and aerospace industries, is becoming increasingly intense. As suppliers and manufacturers of components strive to maintain profit margins whilst reducing cost, it is evident that the manufacturing processes involved should be more productive and higher quality. The reduction in processing involved by casting parts, rather than using forging or other techniques, has encouraged the use of cast parts in applications where previously other techniques were the only way of meeting exacting mechanical properties.

In order to achieve the required mechanical specification, the casting process should be controlled to ensure that the parts produced are reliably free from defects. It is now common to simulate the filling and basic solidification of aluminum castings, allowing the prediction of macrostructural defects such as incomplete filling [1] or hotspots due to restricted flow [2]. However, to improve standards still further, the microstructure must be considered. Microporosity in particular has been shown to have a marked effect on fatigue and tensile properties of material [3,4].

A number of models predicting the formation of microporosity during solidification have been developed. Recently, Lee et al. have published an in depth review of Al–Si alloy microporosity models [5]. The review categorizes existing models as (i) analytic solutions, (ii) criteria function models, (iii) Darcy’s law numerical solutions, coupled with mass and energy balances, (iv) diffusion-controlled pore growth in three phase systems, or (v) continuum diffusion models with stochastic pore nucleation and pore/microstructure interactions. These modeling approaches vary in mathematical complexity ranging from the simplest category (i) analytic solutions, requiring minimal calculation, to the highly complex, computationally-intensive category (v) stochastic continuum diffusion models.
None of the existing models can completely describe the formation of microscopic porosity under all industrial conditions, but in general, the comprehensive applicability and quantitative predictive ability of the models is proportional to their computational cost. For example, many analytic solutions yield correct trends for shrinkage-driven average pore growth for only highly constrained physical conditions (rarely encountered in industry), whilst stochastic continuum models can predict individual pore nucleation and growth of an entire population of pores under temperature and diffusion gradients and evolving solidification structures, but only within a very small volume (The volume has to be small because the model is so computationally demanding). Again, although for different reasons, this makes the model difficult to apply to large-scale industrial castings). However, by coupling an existing microscopic porosity model to a macrostructural heat-flow model, a hybrid multiscale model can be created which optimizes the predictive ability of the model and minimizes the computational cost. The purpose of the work presented in this paper is to test the hybrid modeling approach by using a relatively simple category (iv) (diffusion-controlled pore growth in three phase systems) microporosity model with a microscopic dendrite arm spacing model and a commercial macroscopic model.

This paper briefly outlines the theory used in the commercial macroscopic model, followed by a detailed presentation of a microscopic model for the prediction of gas porosity. These models are then used to simulate a series of simple aluminum alloy (L169) investment castings with a range of shapes and casting conditions. For comparison, experimental measurements have been made using optical image analysis of the resulting microstructure. A pair of samples was also examined with X-ray tomography. The resulting 3-dimensional dataset gives a better idea of pore shape and allows a further comparison with the model predictions. The range of conditions allows the importance of shrinkage versus gas porosity to be elucidated.

2. Macromodeling approach

The casting process was simulated using, CAP\textsuperscript{1}, a commercial package which solves for heat transfer using a finite element method. The macromodel solves the Fourier equation for heat transfer, taking into account latent heat of fusion:

\[ \rho C_p \frac{\partial T}{\partial t} = k \nabla^2 T + \frac{\partial f_s}{\partial t} L \]  

where \( T \) is the temperature, \( t \) is the time, \( \rho \) is the density, \( C_p \) is the specific heat capacity, \( k \) is the thermal conductivity, \( L \) is the latent heat and \( f_s \) is the fraction solid.

Eq. (1) was solved using a fully implicit scheme for the initial time steps, followed by a Crank–Nicolson scheme for increased accuracy. A preconditioned conjugate-gradient iterative solver was used to minimize computational cost. Although the filling can also be simulated with this software by solving the Navier–Stokes equations, it was assumed not to have a large influence upon the microstructure of the simple shapes used in the experiments.

The casting was meshed with 92,000 quadrilateral elements (Fig. 1) using AMESH which is a semi-automated meshing program that produces meshes suitable for use in subsequent analysis.

2.1. Material properties

The alloy of interest, L169, is a hypoeutectic Al–Si alloy similar in composition to LM25, therefore, the material property values used for L169 in the macromodel were based upon the recommended values given by Mills [6]. Unfortunately, no appropriate data for the properties of the shell mould were found in the literature. Therefore, starting with values based upon

\footnote{CAP and AMESH, registered by EKK Inc, 2065 West Maple, Walled Lake, MI 48390, USA.}

Fig. 1. FEM rendering of the two investment moulds used: (a) geometry A; (b) geometry B.
similar materials, a series of runs was made to determine the sensitivity of the micromodel results to changes in these values. Based upon the results of this study (which are presented later), measurements were performed to characterize the most sensitive properties: heat capacity, density and thermal conductivity.

The heat capacity was measured with a differential scanning calorimeter (DSC) under static air conditions over a temperature range of 100–675 °C. Pulverized samples of mould material (ca. 50 mg) were placed in new Pt crucibles and the furnace temperature was increased at a rate of 20 °C min⁻¹. The system was calibrated with an empty Pt crucible and a standard z-sapphire reference disc. Density of the investment casting mould was determined using a finely powdered sample of the investment mould, a relative density bottle and a single pan balance. The thermal conductivity was measured by using a modified Lee’s Disc method [7].

The temperatures obtained from the thermocouples placed in the actual castings were used as the initial conditions. The model proved to be insensitive to the casting mould heat transfer coefficient; however, it was very sensitive to heat loss between the mould and the surroundings. The heat transfer coefficient between the mould and its surroundings was calculated by solving for both the convective and radiative heat losses.

3. Micromodeling approach

Two different microstructural features are compared in this paper, secondary dendrite arm spacing (DAS) and microporosity. The DAS is governed by the amount of time that ripening of the arms has to occur, termed the local solidification time, $t_s$ [8]. The secondary dendrite arm spacing is related to approximately the cube root of $t_s$. In this paper, the following empirically relationship was used:

$$ \text{DAS} = 7.7t_s^{0.38} \text{ (µm)} $$

The formation of microporosity is a complex phenomenon that depends upon the local pressure, insoluble gases and nucleation and growth phenomena. A model for the formation of microporosity is presented below that is based upon the growth of pores due to the presence of insoluble gases, specifically hydrogen in aluminum alloys.

3.1. Microscale pore growth model

The microscale pore growth model predicts the proportion of the total porosity formed in the melt due to hydrogen diffusion and the temperature dependence of hydrogen solubility. Although aluminum L169 contains significant quantities of Mg, Cu, and Fe, the primary alloying element is Si [9]. Therefore, for computational simplicity, the model treats L169 as a pseudo-binary Al–7wt. % Si alloy. The model is not coupled in both directions; although the inputs to the micromodel derive from the macromodel, there is no feedback from the micromodel into the macromodel.

3.1.1. Model system

The model system consists of a spherical hydrogen pore centered within a spherical volume of Al–7wt. % Si alloy. Initially, the system is in equilibrium and contains three phases (solid, liquid, and gas) and three components (aluminum, silicon, and hydrogen). The phases consist of (i) liquid alloy with dissolved atomic hydrogen, (ii) solid alloy with dissolved atomic hydrogen, and (iii) gaseous molecular hydrogen. Fig. 2 shows a schematic of the model system.

The starting concentration of hydrogen in the system is calculated from a specified initial pore size and the equilibrium solubility of hydrogen in the alloy. The solubility of hydrogen in liquid aluminum is much greater than that in the solid and the solubility diminishes with decreasing temperature [10]. As a result, when the initial equilibrium is perturbed by reducing temperature linearly with time, the newly-formed solid rejects its excess hydrogen into the liquid alloy and the concentration of hydrogen in the liquid–solid alloy increases, becoming supersaturated. When this occurs, a diffusion gradient forms within the liquid–solid alloy in the direction of the hydrogen pore. The pore becomes larger as the diffusing hydrogen reaches it.

Within this simplified system, the growing pore is assumed not to be distorted by the equiaxed grain formation around, retaining its spherical shape. At the eutectic temperature, the entire volume of the alloy is considered to become instantaneously solid, effectively ‘locking in’ the gas pore diameter.
Table 1
Material property constants used in the microscale pore growth model

<table>
<thead>
<tr>
<th>Constant</th>
<th>Symbol</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen equilibrium coefficient</td>
<td>$k_{H}$</td>
<td>0.10</td>
<td>Estimated</td>
</tr>
<tr>
<td>Silicon equilibrium coefficient</td>
<td>$k_{Si}$</td>
<td>0.13</td>
<td>[11]</td>
</tr>
<tr>
<td>Liquidus slope</td>
<td>$m_{L}$</td>
<td>$-7.12$ K per wt.%</td>
<td>Calculated</td>
</tr>
<tr>
<td>System pressure</td>
<td>$P_{m}$</td>
<td>$1.013 \times 10^9$ Pa</td>
<td>Set</td>
</tr>
<tr>
<td>Alloy liquidus temperature</td>
<td>$T_{liq}$</td>
<td>889.9 K</td>
<td>Calculated</td>
</tr>
<tr>
<td>Alloy eutectic temperature</td>
<td>$T_{Al\text{eut}}$</td>
<td>939.7 K</td>
<td>Calculated</td>
</tr>
<tr>
<td>Adjusted melting temperature of pure Al</td>
<td>$T_{Al\text{eff}}$</td>
<td>850.2 K</td>
<td>[11]</td>
</tr>
<tr>
<td>Initial wt.% of Si in the alloy</td>
<td>$W_{Si}$</td>
<td>7.0 wt.%</td>
<td>Set</td>
</tr>
<tr>
<td>Surface tension</td>
<td>$G$</td>
<td>856 mJ m$^{-2}$</td>
<td>[21]</td>
</tr>
<tr>
<td>Liquid density</td>
<td>$\rho_l$</td>
<td>2390 kg m$^{-3}$</td>
<td>[11]</td>
</tr>
<tr>
<td>Solid density</td>
<td>$\rho_s$</td>
<td>2550 kg m$^{-3}$</td>
<td>[11]</td>
</tr>
</tbody>
</table>

3.1.2. Model theory and assumptions

The model assumes that the system being simulated is closed, spherical, and spatially isothermal; the hydrogen pore is located in the center of the system and is of a known initial radius; a mixture of solid and liquid alloy surrounds the pore symmetrically; the liquid alloy is continuous; and no hydrogen concentration gradients exist in the solid alloy (because the solid particle size is small). In physical terms, this corresponds to a system of equally sized pores, evenly distributed throughout the alloy.

3.2. Material properties

Values for the material property constants used in the model are listed in Table 1. The model assumes that the evolution of fraction solid is given by the Scheil equation after the dendrite tips have impinged on each other [11]. The silicon concentration in the interdendritic liquid is also determined using a Scheil equation. The volume of liquid and solid alloy were described in terms of density, fraction solid, and total alloy mass, assuming that there were no spatial thermal gradients on a local level (i.e. on the scale of the system) and that the mass of the system is conserved.

The volume of the pore was calculated assuming that the ideal gas law holds, and that the vapor pressures of aluminum and silicon are negligible. The total pressure within the pore can be determined by summing the applied pressure on the system, metallostatic pressure, and the Gibbs–Thompson curvature effect due to surface tension at the gas–liquid interface [12].

The equilibrium solubility of hydrogen in silicon–silicon alloys, $S_1$, (in units of ml H$_2$ STP per 100 g alloy) was determined using an expression for pure aluminum given to account for the effect of silicon on hydrogen solubility [13]. The effective hydrogen diffusivity was calculated by combining the solid and liquid diffusivities given by Eichenauer and Markopoulos [14] with an improvement on the law of mixtures suggested by Markworth [15].

3.3. Hydrogen mole balance in the liquid alloy

By starting with the general equation of continuity for a dilute constituent in a spherical system [16] and assuming that the liquid alloy is effectively stationary; hydrogen diffusion occurs only in the r-direction; and the binary diffusivity may be approximated by an effective diffusivity; the mole balance for dissolved hydrogen in the liquid alloy becomes:

$$\frac{\partial C_i}{\partial t} = D \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C_i}{\partial r} \right) + R_H$$

(3)

where $C_i$ is the molar concentration of atomic hydrogen in the liquid alloy and $R_H$ is the rate of hydrogen entering the liquid.

Assuming conservation of mass, the rate of hydrogen entering the liquid phase from the solid phase may be calculated from the rate of change of the number of moles of atomic hydrogen per unit volume of liquid:

$$R_H = \frac{d(n_{Si}/V_l)}{dr}$$

(4)

where $n_{Si}$ is the moles of atomic hydrogen in the solid alloy and $V_l$ the volume of liquid. The hydrogen in the liquid and solid alloy are assumed to be related by an equilibrium condition:

$$C_s \equiv k_{H} C_l$$

(5)

where $k_{H}$ is the partition coefficient.

Using Eqs. (5) and (4) may be rearranged in terms of concentration yielding:

$$R_H = \frac{d(k_{H} C_l V_s/V_l)}{dr}$$

(6)

By applying the product and quotient rules to Eq. (6) and substituting in the fraction solid expression for the volume of the solid, the final form of the hydrogen mass
balance in liquid aluminum is:

$$\frac{\partial C_l}{\partial t} = \frac{D_e}{(1 - k_H) V_S / V_l} \frac{\partial C_l}{\partial r^2} + \frac{D_e}{(1 - k_H) V_S / V_l} \frac{2}{r} \frac{\partial C_l}{\partial r} + \frac{C_{m_{\text{alloy}}} m_{\text{alloy}}}{V_l} \frac{\partial f_s}{\partial t} \left[ k_H + \frac{V_S}{\rho S} \right]$$

(7)

3.4 Initial and boundary conditions

Initially, the system was in three-phase equilibrium and had a constant hydrogen concentration throughout the liquid–solid volume. The gas pore–liquid alloy interface is assumed to be at equilibrium at all times. Since no hydrogen leaves or enters the model system, a zero flux boundary condition was selected for the outer boundary of the system. The initial condition is consistent with the boundary conditions.

4. Experimental methods

A series of castings, designed to yield varying levels of shrinkage and gas porosity, was made. The aluminum was cast under four different conditions, produced sequentially from the same molten charge, ranging from low to high gas levels, with and without grain refiner. Thus a wide range of solidification conditions was studied. Table 2 shows the conditions discussed in this paper.

As shown in Fig. 1, both shapes of casting are made up from three flat rectangular sections. In type A, the sections reduce in thickness from 15 to 4 mm in two steps and in type B, the middle section is thinner (7 mm) than the first (18 mm) and the last (11 mm). The castings were produced using alloy L169. Table 3 shows the composition as determined by spark emission spectroscopy. Wax assemblies were constructed to yield castings of the required dimensions. The assemblies were shelled using a water-based colloidal silica binder with an alumino-silicate refractory and an alumino-silicate stucco (molochite). Sufficient coats were applied to achieve a nominal shell thickness of 5 mm. After drying, de-waxing and firing, the shells were preheated to a temperature of 500 ± 10 °C, in preparation for the casting. Two of the castings were set up with thermo-

Table 2
Experimental conditions

<table>
<thead>
<tr>
<th>Casting</th>
<th>Ref</th>
<th>Shape</th>
<th>H₂ level</th>
<th>Grain Refiner</th>
<th>Other Additions</th>
<th>Pouring Temp.(°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Condition 1</td>
<td>1A</td>
<td>De-gassed</td>
<td>No</td>
<td>Sodium</td>
<td>740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>1B</td>
<td></td>
<td></td>
<td>Flux</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Condition 2</td>
<td>2A</td>
<td>De-gassed</td>
<td>Yes</td>
<td>Metallic</td>
<td>740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>2B</td>
<td></td>
<td></td>
<td>Sodium</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Condition 3</td>
<td>3A</td>
<td>100g gas</td>
<td>Yes</td>
<td>Sodium</td>
<td>740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3B</td>
<td>tablet</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Condition 4</td>
<td>4A</td>
<td>450g gas</td>
<td>Yes</td>
<td>Sodium</td>
<td>740</td>
<td></td>
</tr>
<tr>
<td></td>
<td>4B</td>
<td>tablet</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Table 3
Composition of L169, as determined by spark emission spectroscopy

<table>
<thead>
<tr>
<th>Element</th>
<th>Si</th>
<th>Mg</th>
<th>Ti</th>
<th>Fe</th>
<th>Cu</th>
<th>Al</th>
</tr>
</thead>
<tbody>
<tr>
<td>wt.%</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Si</td>
<td>6.8±0.1</td>
<td>0.59±0.02</td>
<td>0.15±0.02</td>
<td>0.08±0.01</td>
<td>0.026±0.01</td>
<td>Balance</td>
</tr>
</tbody>
</table>

2 Calder Aluminium Ltd, Derbyshire UK.
3 02 B/5 ppm, Cryoservice Ltd, Worcester, UK.
4 London & Scandinavian Metallurgical Co Ltd, South Yorkshire, UK.
5 Foseco (FS) Ltd, Staffordshire, UK.
6 Foseco (FS) Ltd, Staffordshire, UK.
Tablets were plunged in the charge prior to the moulds being poured at 740 °C.

4.1. Measurement of microstructure by optical image analysis

Specimens were taken from a slice through the middle of the test casting, such that the plane observed was perpendicular to the y-axis, as shown in Fig. 3 for the two geometries. In this direction the entire specimen was well away from the edges of the casting and therefore, any variation due to surface effects was avoided. The specimens were ground flat and then polished for optical microscopy.

The microporosity was measured on these specimens at 9X on an optical microscope coupled to a CCD camera for eight adjacent frames totaling an area of 104 mm². The resulting images were analyzed using a commercial image analysis package, allowing the pore dimensions (Ferret lengths), equivalent circular diameters, areal density and distributions to be obtained.

The secondary dendrite arm spacing (DAS) measurements were obtained using a linear intercept method for a total of at least 30 spacings per result.

4.2. Measurement of porosity by X-ray tomography

Tomography was carried out on cylindrical specimens 3 mm in diameter by 10 mm long. The sample was mounted in an X-ray tomography machine, with an accelerating voltage of 90 kV, spot size of 5 μm and set up to give a geometric magnification of about 2.5 × and calibrated using an Aluminium wedge. The image was detected on a moving CCD camera as the sample was rotated. The output from the CCD was fed through a reconstruction algorithm [17], and beam hardening was also corrected computationally, to produce a series of

<table>
<thead>
<tr>
<th>Casting</th>
<th>Sample location</th>
<th>H2 level</th>
<th>t₀ (s)</th>
<th>Experimental pore diameter (μm)</th>
<th>Predicted pore diameter (μm)</th>
<th>Experimental% (P)</th>
<th>Predicted% (P)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 A 2</td>
<td>Degassed</td>
<td>337</td>
<td>60</td>
<td></td>
<td></td>
<td>0.2</td>
<td></td>
</tr>
<tr>
<td>1 A 4</td>
<td>Degassed</td>
<td>176</td>
<td>68</td>
<td></td>
<td></td>
<td>0.3</td>
<td></td>
</tr>
<tr>
<td>1 A 7</td>
<td>Degassed</td>
<td>77</td>
<td>64</td>
<td></td>
<td></td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>2 A 2</td>
<td>Low</td>
<td>337</td>
<td>78</td>
<td></td>
<td></td>
<td>0.7</td>
<td></td>
</tr>
<tr>
<td>2 A 4</td>
<td>Low</td>
<td>176</td>
<td>58</td>
<td></td>
<td></td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>2 A 7</td>
<td>Low</td>
<td>77</td>
<td>64</td>
<td></td>
<td></td>
<td>0.4</td>
<td></td>
</tr>
<tr>
<td>3 A 1</td>
<td>Medium</td>
<td>450</td>
<td>397</td>
<td></td>
<td></td>
<td>0.6</td>
<td>0.6</td>
</tr>
<tr>
<td>3 A 2</td>
<td>Medium</td>
<td>336</td>
<td>338</td>
<td></td>
<td></td>
<td>2.6</td>
<td>0.5</td>
</tr>
<tr>
<td>3 A 3</td>
<td>Medium</td>
<td>217</td>
<td>347</td>
<td></td>
<td></td>
<td>1.6</td>
<td>0.6</td>
</tr>
<tr>
<td>3 A 4</td>
<td>Medium</td>
<td>176</td>
<td>205</td>
<td></td>
<td></td>
<td>1.7</td>
<td>0.5</td>
</tr>
<tr>
<td>3 A 5</td>
<td>Medium</td>
<td>144</td>
<td>386</td>
<td></td>
<td></td>
<td>3.6</td>
<td>0.5</td>
</tr>
<tr>
<td>3 A 6</td>
<td>Medium</td>
<td>115</td>
<td>383</td>
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<td></td>
<td>5.0</td>
<td>0.5</td>
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<tr>
<td>3 A 7</td>
<td>Medium</td>
<td>77</td>
<td>280</td>
<td></td>
<td></td>
<td>2.8</td>
<td>0.4</td>
</tr>
<tr>
<td>4 A 1</td>
<td>High</td>
<td>450</td>
<td>492</td>
<td></td>
<td></td>
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<td>1.3</td>
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<td>4 A 2</td>
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<td>442</td>
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<tr>
<td>4 A 3</td>
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<td>144</td>
<td>401</td>
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<td>4 A 6</td>
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<td>4 A 7</td>
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<td>77</td>
<td>279</td>
<td></td>
<td></td>
<td>2.0</td>
<td>1.2</td>
</tr>
</tbody>
</table>


7 Zeiss KS400, Imaging Associates Ltd, Oxon, UK.
slices through the sample, which can be assembled to give a three-dimensional image [18]. The difference in gray-scale between the pores and the aluminum alloy is clear, and by thresholding it is possible to find the boundary surface and thence number of pores as well as volume and size for each individual pore.

5. Results and discussion

5.1. Experimental results

The measured porosity characteristics and dendrite arm spacing are listed in Table 4 at several locations for each of the four casting conditions. The results and typical micrographs (Fig. 4) show clearly that there is very little pore formation in the de-gassed samples (conditions 1 and 2, see Table 2). For this reason the analysis concentrates mainly on the samples from the medium and highly gassed castings (conditions 3 and 4, see Table 2). The micrographs of type A castings (Fig. 5) can be contrasted with those from type B (Fig. 6). Clearly the casting geometry has had an effect, and there is an increase in the amount of porosity in the thick end of the type B castings when compared with the thin end of type A. It can also be seen that the nature of the porosity has changed, becoming much more irregular compared with other sections from the same cast.

The two-dimensional metallographic measurements only give a number density per unit area; however, a volume number density of pores is required to determine the model system volume. The Johnson–Saltykov method [19], which assumes spherical pores, was used to approximate a volume density from the volume data. As can be seen from the tomography results, the assumption that the pores are spherical is reasonable (see Fig. 7).

5.2. Tomography results

The reconstructed 3D images of the tomography specimens (Fig. 7) illustrate the difference between the medium and high gas conditions (3 and 4, respectively); medium gas produces many fine pores while high gas gives fewer larger pores. The overall percentage porosity is greater in the high gas level (condition 4) sample, as given in Table 5.

The resolution of the tomography is 29.1 μm per voxel, which is sufficient for pores of the size measured (≈ 5% error). A small specimen size was used to allow faster measurement and analysis. However, it resulted in a small number of pores being measured. This is especially true in the high gas case where 14 pores are found compared with 43 metallographically. Despite the reduced number of pores counted, tomography provides some unique advantages over metallography. Firstly, no assumptions of the sphericity of the pores is required to obtain the number density per unit volume. Secondly, the full-interconnected pore shape is visible for tortuous pores. Thirdly, tomography can be performed non-
destructively. Finally, with metallographic image analysis it is often difficult to distinguish automatically between pores and other features, such as silicon flakes or intermetallics; that distinction is easier with tomography.

5.3. Macromodel results

The thermal conductivity, density and specific heat of the mould were measured experimentally for the mould material used. For the aluminum, the experimental measurements of the latent heat evolution of the aluminum provided by Mills [6] were employed. A comparison of the solidification model results to the experimentally measured solidification times is shown in Fig. 8. The agreement is excellent, except at location one, which is directly below the pouring basin. The pouring basin acts as a riser, feeding hot molten metal

<table>
<thead>
<tr>
<th>Location</th>
<th>$R_{ps}$ (mm)</th>
<th>$N_p$ (mm$^{-3}$)</th>
<th>Number of pores counted</th>
<th>$R_{ave}$ (μm)</th>
<th>%P</th>
</tr>
</thead>
<tbody>
<tr>
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<td>39A1</td>
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<td></td>
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<td></td>
<td>Tomography</td>
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<td></td>
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<td>0.397</td>
<td>3.814</td>
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<td>102</td>
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<td></td>
<td>Micromodel</td>
<td></td>
<td></td>
<td></td>
<td>91.9</td>
</tr>
<tr>
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<td>49A1</td>
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<td>14</td>
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<tr>
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<td>0.979</td>
<td>43</td>
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<tr>
<td></td>
<td>Micromodel</td>
<td></td>
<td></td>
<td></td>
<td>152</td>
</tr>
</tbody>
</table>
into this region as shrinkage occurs, increasing the local solidification time. This phenomenon is not included in the model, explaining the under-prediction of the local solidification time at this location.

Although the macromodel cannot predict the exact amount of shrinkage or the porosity characteristics within a region, areas that are underfed can be identified. Fig. 9 illustrates that there are no isolated, unfed, regions in type A castings, whilst type B castings show that region farthest from the pouring basin becomes isolated from the feeder (Fig. 10) since the thin central section of casting type B cools much faster than the thicker tip. This is confirmed by the experimental results (Fig. 6), which show more porosity in positions where the model predicts insufficient feeding. In the well-fed areas, pores are fewer, whereas, in the poorly fed areas pores are irregular in shape and the total amount of porosity is greater, which suggests that this section is poorly fed as predicted by the model.

5.4. DAS micromodel

Once it was established that the macromodel predicted the solidification conditions satisfactorily it was possible to progress to the microstructure modeling. The results of applying Eq. (2) to the macromodel results for...
the prediction of secondary dendrite arm spacing is shown for the two casting geometries in Fig. 9b, Fig. 10b. The correlation to the experimental measurements is good, as illustrated in Fig. 11 for geometry A.

5.5. Porosity micromodel

The porosity micromodel was solved numerically on a Pentium II PC by implementing a moving-boundary, explicit finite difference technique [20]. Simulations were made using each of the seven experimental cooling rates at two levels of initial hydrogen concentration. Initial hydrogen concentrations at the casting temperature of 740 °C were estimated to be 0.20 ml H₂ STP per 100 g for the medium level of dissolved hydrogen (3A and 3B samples) and 0.30 ml H₂ STP per 100 g for the high level of dissolved hydrogen (samples 4A and 4B).

The predicted values for the average final pore diameter are shown with the measured average pore diameter in Table 4. The model correctly predicts all the trends in the data; however, the average pore size is consistently under-predicted. The accuracy of the predictions improved for the castings with a higher initial hydrogen concentration. The tomography results suggest that a small part of the error may lie with the optical microscopy measurements; however, the single data point does not allow a full comparison across the range of conditions. The increased deviation at lower hydrogen levels may be explained in the following manner.

In the measured samples, porosity is formed due to gas evolution and shrinkage effects. Because the micromodel does not account for shrinkage porosity, it seems logical that the predicted pore sizes would be less than the measured value. Because the 3A and 4A moulds have essentially identical cooling curves, the amount of porosity formed due to shrinkage should be the same in both, regardless of their dissolved hydrogen concentrations. It follows that the porosity predictions for samples with a medium hydrogen concentration (3A) would deviate more from the measured values than predictions for high concentration samples (4A), since the percentage of shrinkage porosity (relative to the total porosity) is greater in the 3A samples. Fig. 12 shows the correlation of the model predictions to the measured values and, although there is a fair amount of scatter, the correlations follow the expected trends. Predictions for the medium concentration samples (3A) have an average deviation of −43% from the experimental values. For the high hydrogen samples (4A), the average deviation from experimental values is −28%.

Although the macromodel can predict hotspots, it cannot predict any porosity characteristics within the hotspot. In order to approximate the phenomenon of shrinkage porosity within the micromodel, the system pressure (Pₘₐₓ, a model input variable), was reduced. This allows a comparison of the two factors causing porosity: hydrogen gas and shrinkage. The casting condition of sample 4A, location 2, was selected since this point corresponded closely to the linear correlation of experimental and predicted values shown in Fig. 12, and give the extreme case of high gas.

At a reduced system pressure of 0.43 atmospheres, the predicted pore diameter for the 4A location 2 sample is equal to the experimental value. Therefore, even at high initial hydrogen levels, shrinkage is providing a driving force that creates about half the volume of porosity. For cases where the gas level is lower, shrinkage will become even more important. Clearly reducing the system pressure is an approximation, as the growth of the pore will alter the local pressure; however, it does provide a first order solution appropriate for this computationally very fast micromodel. To describe the feeding behavior properly, the porosity micromodel system pressure should be coupled to a shrinkage pressure predicted in a macromodel. Furthermore, the model would have to allow a change in geometry, to cope with the less spherical pores found in poorly fed regions.

The porosity micromodel correctly predicts all the trends in the data, providing a tool that can be used to determine the effect of altering processing conditions upon the final average pore radius. The predictions are fast and give reasonable, order-of-magnitude approximations of the average final pore size. However, they are limited in accuracy since shrinkage pressure is not included.

6. Conclusions

A multiscale modeling approach was implemented to predict the microstructure and the distribution of microporosity within a series of castings. The model
predictions were compared with data obtained by optical analysis of sections from the respective castings. As a further check on the accuracy of the optical image analysis, two samples were also analyzed by X-ray tomography.

With accurate thermophysical data, which was obtained by experiment, the finite-element macromodel coupled with the DAS micromodel gave an excellent prediction of secondary dendrite arm spacing. The macromodel alone was also able to predict the likelihood of porosity forming due to poor feeding and shrinkage, which is of considerable benefit as it allows moulds to be redesigned or configured before prototypes need to be built.

The micromodel predicted the correct correlations of processing parameter to final pore size, but illustrated a systematic quantitative inaccuracy. This inaccuracy was shown to be caused by not including the shrinkage pressure. Therefore, the model may be used as a qualitative tool to determine how changes in casting practice (especially degassing) will affect final properties.

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References