

PREDICTION OF ROOM TEMPERATURE MECHANICAL PROPERTIES IN ALUMINIUM CASTINGS

Zhanli Guo, Nigel Saunders, Peter Miodownik, Jean-Philippe Schillé

Sente Software Ltd., Surrey Technology Centre, Guildford GU2 7YG, U.K.

1 Introduction

Cast aluminium alloys have widespread applications for structural components in the automotive industry. For example, in power-train applications, including engine blocks, cylinder heads and transmission cases. However, to achieve the maximum impact on fuel efficiency, the application of cast aluminium alloys needs be extended to more critical structural parts, such as brake valves and callipers which are traditionally made of cast iron and steels. The most significant barrier to the acceptance of cast aluminium in many structural applications has been its reputation for variability in mechanical properties. Anything that may help predict and/or control the results of casting variables would be of great benefit to industry.

Mechanical properties are linked to the microstructure in the material, which is determined by the chemical composition (trace elements and alloying elements) and casting conditions (solidification rate and casting defects). In practice, solidification occurs under non-equilibrium conditions which can be modelled using the so-called Scheil-Gulliver approach. This approach has proved to yield excellent results for phase evolution in aluminium alloys [1] and will be adopted in the present study.

Typical casting microstructural features consist of primary phases (dendritic Al phase or primary silicon particles), eutectics (Al-Si, Al-Al₂Cu, Al-Al₃Mg₂ etc.) and intermetallics (AlFeSi, Al₅Cu₂Mg₈Si₆ etc.), all of which are considered in the strength model. The model developed here differs from previous work on mechanical properties [2,3,4], in that it can be applied to a wide range of commercial aluminium alloys and the calculations are carried out in an automatic fashion.

2. Calculation of Microstructural Features

2.1 Phase Evolution During Solidification

The phase evolution in aluminium alloys during casting can be modelled straightforwardly via the so-called Scheil-Gulliver approach [1], which can be carried out using thermodynamic calculations [5]. It provides the necessary information for further property modelling, such as phase fractions and composition. For instance, the information for hypoeutectic Al-Si alloys includes the fractions of primary Al phase, the Al-Si eutectic and the percentages of the Al and Si phases in the Al-Si eutectic. The fractions of other possible eutectics, as well as secondary intermetallics formed during solidification, can also be calculated.

2.2 Secondary Dendrite Arm Spacing Calculation

It has been proposed [6] that secondary dendrite arm spacing (SDAS) can be related to the cooling rate using the equation

$$\lambda = AV_c^{-n} \quad (1)$$

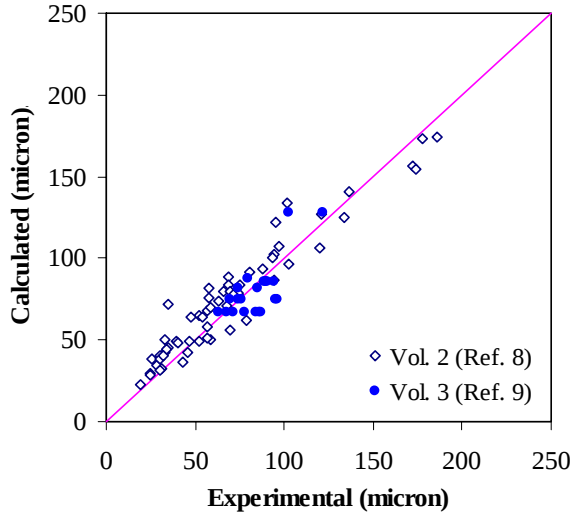


Fig. 1. Comparison between experimental and calculated SDAS for a variety of commercial aluminum alloys. (See Appendix for alloys used in the comparison)

where λ is the secondary dendrite arm spacing, A is an alloy-dependent parameter and n is an exponent whose value is close to $1/3$. Different values for A and n in Eq. 1 are reported in literature for different aluminium alloys [7]. Their values can vary even within the same alloying system. For the great majority of cases, it has been shown that dendrite arm spacing decreases with increasing concentration of alloying elements [8,9,10], although there are studies reporting no composition effect [11].

In the present work, a composition effect needs to be considered so as to make the relationship between cooling rate and dendrite arm spacing accurate enough for practical use in multi-component

alloys. To this end, we have made the material constant A composition dependent and Eq. 2 is then written as:

$$\lambda = A_0 / \left(\sum_i c_i x_i + \sum_{i,j} c_{ij} x_i x_j \right) V_c^{-n} \quad (2)$$

Where x_i and x_j are the atomic fractions of element i and j , c_i , c_{ij} are, respectively, the corresponding coefficients and A_0 is a constant independent of alloy chemistry. The values for these coefficients have been empirically fitted against experimental data [12,13] and n given a value of $1/3$. Comparison between calculation and experimental data is shown in Fig. 1, which covers a wide range of cast aluminium alloys and a wide range of cooling rates.

3. Strength Calculation

Based on the microstructural information calculated using the Scheil-Gulliver model, the next step is to quantify the contribution from each constituent to mechanical properties. Typical contributions to the strength of cast aluminium includes solid solution strengthening and precipitation hardening due to intermetallics. The properties to be calculated are yield and tensile strength.

3.1 Primary Phases

The first requirement is to calculate the strength contribution from the dendritic structure of the primary Al phase. First solid solution strengthening is calculated, and then the effect of secondary dendrite arm spacing on strength will be added. The methodology adopted for solid solution strengthening of one phase is described by the following equation:

$$\sigma_0 = \sum_i x_i \sigma_i^0 + \sum_i \sum_j x_i x_j \Omega_{ij} + \dots \quad (3)$$

where σ_0 is the total strength, σ_i^0 is the strength of pure element i , x_i and x_j are the atomic fractions of elements i and j , and the values of Ω_{ij} are solute interaction coefficients evaluated from information in ref.14.

A Hall-Petch type equation is used to describe the strength variation due to change in secondary dendrite arm spacing:

$$\sigma_{den} = \sigma_0 + k_{den} \lambda^{-0.5} \quad (4)$$

where σ_{den} and k_{den} are the flow stress and the “Hall-Petch coefficient” for the dendritic phase. As the grain size in the as-cast condition is usually very large for aluminium alloys, its effect on strength is not considered in the present study. Different values of k_{den} have been reported for different alloys [4,15,16]. However, the values reported may not be appropriate if not all the strengthening mechanisms are considered when estimating k_{den} . In the present study, k_{den} is set as a constant value of $0.25 \text{ MPa.m}^{-1/2}$ for simplification.

3.2 Strength of the Silicon Eutectic Structure

The strength of the silicon eutectic structure consists of a contribution from (i) the two co-precipitating phases Al and Si, as well as (ii) the possible strengthening due to the silicon particles. The particle size is affected by the cooling rate and can be fibrous or platelike. The eutectic strength is a function of the fibrosity of these particles in that a fibrous structure leads to higher resistance to yield [17,18]. The fineness of the eutectic microstructure is closely related to the secondary dendrite arm spacing and we have related the strength of the Al-Si eutectic to λ using the following equation:

$$\sigma_{eut} = (f_{Al} \sigma_{Al} + f_{Si} \sigma_{Si}) / f_{eut} + k_{eut} \lambda^{-0.5} \quad (5)$$

where f_{Al} and f_{Si} are the fractions of Al, Si in the Al-Si eutectic, respectively, and σ_{Al} and σ_{Si} are the strength of Al, Si in the Al-Si eutectic. σ_{Al} is effectively the σ_0 in Eq. 5 and σ_{Si} is set as a constant. f_{eut} is the fraction of the eutectic ($f_{eut} = f_{Al} + f_{Si}$), and k_{eut} the Hall-Petch coefficient.

Such a treatment reflects the observed effect of cooling rate on the strength of the eutectic, in that faster cooling results in a finer eutectic and in turn higher strength. The Hall-Petch coefficient is obtained through fitting against experimental data for alloys Al-6.5Si [19], Al-7Si and Al-12.6Si [20] where no interference from intermetallics or the dendritic Al phase exists.

3.3 Precipitation Strengthening due to Intermetallics

Many types of intermetallics can form during solidification. In the present study, these precipitates are assumed to be unshearable and their contribution to strength is modelled via the Orowan looping mechanism as used by [21], where

$$\sigma_{ppt} = 0.84M \left(\frac{1.2Gb}{2\pi L} \right) \ln \frac{r}{b} \quad (6)$$

where σ_{ppt} is the strength contribution from precipitates, M is the Taylor factor (normally close to 3), r is the particle radius, b the Burger's vector, G the shear modulus and L the inter-particle spacing. Assuming the precipitates are spherical, it is straightforward to calculate L from r if the volume fraction of the precipitate is known [22], which is the case here as we are using results for phase evolution from the Scheil-Gulliver calculation described in 2.1.

Assuming the change in size follows a coarsening law, r can be assumed to be proportional to $t^{1/3}$ [23,24,25]. As time t is inversely proportional to the cooling rate, it is also reasonable to assume the particle size to be proportional to $V_c^{-1/3}$.

$$r = r_0 V_c^{-1/3} \quad (7)$$

where r_0 is a constant, independent of alloy chemistry, obtained by fitting against experimental data. This assumption is supported by experimental observations [26,27], though the value of the exponent is not exactly equal to -1/3. It is possible to calculate the strength contribution from each precipitate type individually, but to simplify the situation, all the precipitates were considered as one group of the same size.

3.4 Calculation of Overall Strength and Validation

The eutectics formed in aluminium alloys can be of types other than Al-Si, such as Al-Al₂Cu and Al-Al₃Mg₂. Their strength can be modelled using equations similar to Eq. 5 and the overall yield strength of an casting alloy can be calculated using the formula

$$\sigma_y = f_p \sigma_p + \sum_i f_i \sigma_i + \sigma_{ppt} \quad (8)$$

where f_p and σ_p are the fraction and strength of the primary phase, i.e. the dendritic phase in this study, and f_i and σ_i correspond to various types of eutectics.

The model developed has been tested extensively against experimental data and a comparison plot is shown in Fig. 2, where each data point represents one commercial alloy, either from sand casting or permanent mold casting. It can be seen that it covers all types of cast aluminium alloys except the 7xx series (Al-Mg-Zn alloys), where low temperature precipitation during cooling may harden the alloy.

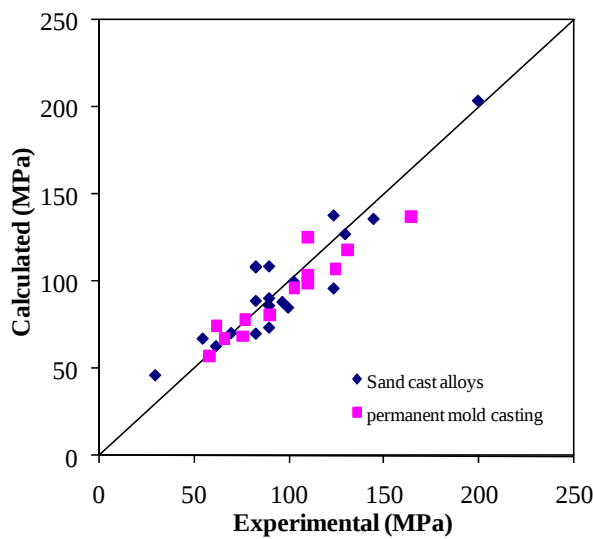


Fig.2 Comparison between experimental and calculated yield stress of various cast alloys. (See Appendix for alloys used in the comparison)

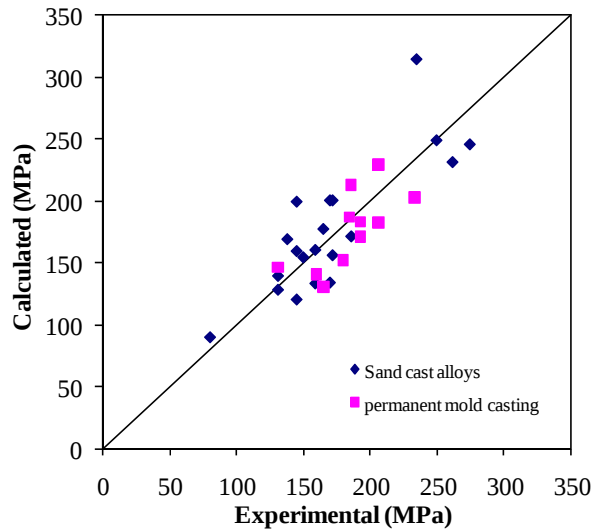


Fig.3 Comparison between experimental and calculated tensile stress of various cast alloys. (See Appendix for alloys used in the comparison)

The model described in the previous section allows the calculation of the yield stress. But, it is also possible to calculate other useful mechanical properties such as tensile stress [28,29,30] using relationships developed by Tabor [31]. Such work has been undertaken here and tensile strengths calculated from σ_y are compared with experiment in Fig.3.

It is also possible to calculate stress strain curves using this approach, and such work will be included in future development so that generalised mechanical properties, including high temperature flow stress can be modelled.

4. Summary

A model has been developed for the calculation of strength of cast aluminium alloys. The model can be applied to a wide range of casting aluminium alloys and casting methods. With only chemical composition and cooling rate as inputs, the model calculates microstructural constituents, cooling curve, dendrite arm spacing and strength, including yield and tensile strength for a wide range of aluminium castings. The strengthening mechanisms considered are solid solution strengthening, precipitation hardening and the effect of secondary dendrite arm spacing. The phases that contribute to strengthening include primary phases, various types of eutectics and intermetallics. The model should be a useful tool for tailoring mechanical properties by correct choice of chemical composition and casting parameters. It can also be used to help analyse the consequences of unintended processing or property variations, and identify potential improvements.

APPENDIX

Alloys used in Fig. 1 for comparison of experiment with calculation for secondary dendrite arm spacing

201, 204, 206, 319, B319, 332, 339, C355, 356, A356, A357, A380
B380, B390, 413, 512, 518, 713

Alloys used in Figs. 2 and 3 for comparison of experiment with calculation for strength

Sand casting

Pure Al, 208, 213, 240, 319, 355, 356, A356, 357, 443, A444, 511, 512, 513, 535
A535, B535, LM4, LM5, LM6,

Permanent mold casting

238, 308, 319, 324, 333, 356, 357, 443, A444, 513, Al-6.5Si, Al-7Si, Al-12.6Si

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