Modelling and Simulation of Globular Equiaxed Eutectic Solidification in a Direct Chill Casting of Aluminium Binary Alloy Systems

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Abstract
A comprehensive modelling of globular equiaxed eutectic solidification in a direct chill casting of aluminium binary alloy systems has been presented. The modelling applies the finite volume method in a diffusion dominated 2D axisymmetric domain. The model couples the macroscopic heat transfer equation with solidification kinetics model to predict total solidification time, actual solidification time, grain size, undercooling, and grain growth rate in the two binary aluminium alloy systems namely; Al-Cu system and Al-Si system. The linearization of the solidification kinetics source term coupled to the heat transfer equation ensures robust and converged computation of the numerical model. The results obtained show that under the same cooling conditions at the billet surface, Al-Cu alloy system solidifies faster than Al-Si alloy system. In addition higher undercooling, grain size and growth rate are evident in the former than the later.

Key words: Dc, solidification, kinetics, macroscopic, grain

1. Introduction
Direct Chill (DC) casting is the main process for producing aluminium shapes suitable for subsequent processing in extrusion and rolling operations. DC casting produces ingots/billets (ingot is rectangular in shape while billet is cylindrical in shape) of uniform cross section. The liquid metal is initially held in a water cooled mould. After some delay to ensure proper solidification of shell thickness, the solidified shell is lowered to the pit by hydraulic mechanism. At the exit of the mould, a direct water jet is impinging on the surface of the solid shell to further the cooling process of the billet. Almost universally, the cooling medium is water, both for the mould cooling (primary cooling) and the direct water cooling (secondary cooling). Higher percentage of heat extraction in DC casting is during the secondary cooling process, thus, ensures the formation of globular equiaxed grains.

During metal solidification, there are two typical microstructures: columnar dendrites and equiaxed grains [1]. At the start of solidification, equiaxed grains are preferentially formed at the solid walls where heat extraction is highest. Depending on the cooling condition and heat transfer mechanism, next is columnar dendrites which grow inward toward the central part of the casting. Due to instabilities at the dendritic columnar tip, equiaxed grains may form at the dendrite tip thereby, mechanically blocking the columnar tip [1], leading to columnar-equiaxed competitive growth. But in DC casting processes, due to large heat extraction process, equiaxed grains are generally expected to be predominately formed in the solidified billet.

The first attempt to predict solidification microstructure through computational modelling and to validate such a model against cooling curves was carried out by Oldfield [2]. Rappaz [3] introduces the basic concept of macroscopic and microscopic phenomena. The model he [3] developed can be adapted to any solidification process. Other methods of coupling of macro-transport and micro-transport or solidification kinetics techniques are; the Micro-Latent Heat Method (MLHM) by...
Nastac and Stefanescu [4], the Micro-Enthalpy Method (MEM) by Rappaz and Gandin [5] and the Latent Heat Method (LHM) [6,7]. In all of these works [2-7], it appears that no direct numerical quantification of nucleation kinetics coupling in DC casting system has been reported in literature. In addition, the LHM method originally proposed by Kanetkar et al. [7] and also improved by Stefanescu [6] did not comprehensively present the linearization of the source term which represents the coupling of the solidification kinetics in the macroscopic heat transfer equation. In the present work, a model for globular equiaxed solidification in DC casting of aluminium binary alloy is presented. The model also includes comprehensive linearization of the solidification kinetics source term in the macroscopic heat transfer equation.

2. Model Description
In modelling solidification kinetics during the Al-alloy solidification in DC casting, we assumed the following;
1. Macroscopic transport is controlled by diffusion only; this is a reasonable approximation because microstructural evolution of metal alloy solidification is within diffusion length scale.
2. 2D axisymmetric model.
3. Grain morphology is modelled as spheres and the grain size is modelled with a volume average diameter.
4. Globular equiaxed eutectic solidification is considered; the assumption of equiaxed grains is reasonable due to high heat extraction in DC casting. Therefore, dendritic columnar grains are not considered.
5. The problem is in an unsteady state with respect to the fixed coordinate system.
6. Material properties are constant but different in the respective phases.
7. Instantaneous nucleation model is assumed (i.e. all the nuclei or grains are formed at an instant of solidification)

Continuum formulation of Bennon and Incropera [8] is employ to present the model equations in this work. In the continuum model, it is taken that the solid and liquid phases can occupy each finite volume simultaneously [9].

The mixture diffusion coefficient, thermal conductivity and specific heat capacities are defined as follows;

\[ k = k_l g_l + k_s g_s, \quad c = c_l f_l + c_s f_s, \quad g_l + g_s = 1, \quad f_l + f_s = 1, \quad f_s = \frac{\rho_s \rho}{c_p}, \quad f_l = \frac{\rho_l}{\rho} \]

where \( k \) is the thermal conductivity, \( c \) is the specific heat capacity, \( f \) is the liquid mass fraction, \( g \) is the volume fraction and subscript \( l \) and \( s \) denote liquid and solid respectively.

Macro Heat Transfer Equation;

\[ \rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial y} \left( k \frac{\partial T}{\partial y} \right) + \frac{1}{r} \frac{\partial}{\partial r} \left( r k \frac{\partial T}{\partial r} \right) + S_T \]

where \( S_T = \rho L \frac{\partial f_s}{\partial t} \),

\( c_p \) is the specific heat capacity, \( \rho \) is the density, \( k \) is the thermal conductivity, \( L \) is the latent heat and \( f_s \) is the local volume solid fraction.

2.1 Solidification Kinetics Model
The source term \( S_T \) expression in Eq. (3) contains the latent heat, density and the volume solid fraction terms. The method of evaluating the source term is what differentiates macro-modelling that utilizes the Scheil or Lever rule solidification model and the micro-macro model that uses nucleation kinetics modelling. The Scheil or Lever rule solidification models assume a
solidification path, but in real metallurgical system the solidification path is not known priori. Therefore, the models presented below for handling the solid fraction evolution is those suggested by Kanetkar et al. [7] and Stefanescu [10].

\[ \frac{\partial f_S}{\partial t} = 4\pi R^2 (t) NV (1 - f_S) \]  

where \( N \) is the number of grain per unit volume, or grain density, \( R \) is the grain radius and \( V \) is the growth velocity.

\[ V = \frac{\partial R}{\partial t} = \mu \Delta T^2 \]  

where \( \Delta T \) is the undercooling; \( \Delta T = T_e - T \), \( T_e \) = eutectic temperature, and \( \mu \) is a growth constant

\[ f_S = 1 - \exp[-(4/3)\pi N R^3 (t)] \]  

Equation (2) is discretized using the Finite Volume Method (FVM) [11], the discretized equations are presented as follows;

\[ a_p T_p = a_E T_E + a_W T_W + a_N T_N + a_S T_S + a_p^0 T_p^0 + S_u \]  

where, \( a_p = a_E + a_W + a_N + a_S + a_p^0 - S_p \), \( a_E = a_W = \frac{k_{pA_w}}{\Delta x}, a_N = a_S = \frac{k_{pA_e}}{\Delta y}, a_p = \frac{\rho c_{pA_p} \Delta V}{\Delta t} \),

\[ \Delta V = \Delta r \Delta y, A_e = A_w = \Delta y, A_n = A_s = \Delta r. \]

2.2 Treatment of the Source Term

To ensure a converged numerical solution and improvement in the computational time, the source term is linearized as outline below. Combining Eqs. (4) and (5) and substituting them in Eq. (3) gives;

\[ S_T = [\rho L A \pi R^2 (t) N \mu (T_e - T_p)^2 (1 - f_S)] r_p \Delta V \]  

The source term \( S \) in Eq. (2) is linearized as suggested in Reference [11];

\[ S_T = \left[ S_T^{old} + \left( \frac{\partial S_T}{\partial T} \right)^{old} (T_p - T_p^{old}) \right] r_p \Delta V \]  

Thus,

\[ \frac{\partial S_T}{\partial T} = -\rho L B \pi R^2 (t) N \mu (T_e - T_p) (1 - f_S) \]  

Therefore,

\[ \frac{\partial S_T}{\partial T}^{old} = -\rho L B \pi R^{old2} (t) N \mu (T_e - T_p^{old}) (1 - f_S^{old}) \]  

Substituting Eq. (10) in Eq. (9) gives;

\[ S_T = \rho L A \pi R^{old2} (t) N \mu (T_e - T_p^{old})^{2} (1 - f_S^{old}) r_p \Delta V - \rho L B \pi R^{old2} (t) N \mu (T_e - T_p^{old}) (1 - f_S^{old}) (T_p - T_p^{old}) r_p \Delta V \]  

Eq. (11) can be further rearranged to gives;

\[ S_T = -\rho L B \pi R^{old2} (t) N \mu (T_e - T_p^{old}) (1 - f_S^{old}) r_p \Delta V T_p + \left[ \rho L A \pi R^{old2} (t) N \mu (T_e - T_p^{old})^{2} (1 - f_S^{old}) r_p \Delta V T_p^{old} \right] \]  

Following Patankar’s [12] Linearization expression;

\[ S_T = S_T^p T_p + S_u \]  

comparing Eqs. (12) and (13);

\[ S_p = -\rho L B \pi R^{old2} (t) N \mu (T_e - T^{old}) (1 - f_S^{old}) r_p \Delta V, \]

\[ S_u = \rho L A \pi R^{old2} (t) N \mu (T_e - T^{old})^{2} (1 - f_S^{old}) r_p \Delta V + \rho L B \pi R^{old2} (t) N \mu (T_e - T^{old}) (1 - f_S^{old}) r_p \Delta V T^{old} \]  

2.3 Boundary Conditions and Numerical Implementation

The physical boundary is shown in Figure 1 and the casting is taught to be filled in the domain instantaneously from the hot top. The initial temperature at the start of solidification is 969 K. The
boundary conditions for the energy equation is that; at the hot top the casting temperature is kept at 969 K, an adiabatic boundary condition is applied at the bottom, the vertical walls of the hot top is also adiabatic. The primary extraction of heat at the chill mould, the air gap, the water impingement zone and the downstreaming zone are as given by Suyitno et al. [13], represented by Nzebuka et al. [14] and presented in Table 1. The thermodynamic and physical properties of the material (Al-4\%Cu alloy) are given in Nzebuka et al. [14] and Kanetkar et al. [7].

The discretized energy equation (Eq. 7) is numerically solved using the Gauss-Seidel iterative method. The source term \( S_T \) is coupled directly to the discretized equation. To ensure grid independent solution, the discretized grid size is divided into 1 x 1 mm\(^2\) and the choosing time step size is 0.1 second for the instantaneous nucleation model. The time step is choose in such a way as to capture the recalescence period during microscopic solidification. For each time step, 500 iterations are performed to ensure convergence. The macro heat transfer equation is solved first at every iteration level, and a condition is tested to decide whether the bulk macroscopic temperature and the solid fraction at every node within the computational domain are less than the eutectic temperature \( T_e \) and 1 respectively.

![Computational domain and the boundary conditions](image)

Figure 1: Computational domain and the boundary conditions

If the tested condition is satisfy at any nodes the micro nucleation kinetics equation (Eq. 14) is coupled for that node and solved. The solutions are iterated until a convergence is reached.

| Boundaries | Boundary conditions |
|------------|---------------------|
| Mould      | \(-k \frac{\partial T}{\partial x} = h(T - T_{\text{water}})\) Where \( h = h_c (1 - f_s) + h_{\text{gap}} f_s \), \[14\], \( h_c = 5000 \text{W/m}^2/\text{K} \) |
| Air Gap    | \(-k \frac{\partial T}{\partial x} = h_{\text{gap}}(T - T_{\text{ambient}})\) |
| Water jets | \( k \frac{\partial T}{\partial x} = 27300T - 1,273,088.915 \) if \( T < 120^\circ\text{C} \) |
|            | \( k \frac{\partial T}{\partial x} = 94,252.48T - 9,240,434.453 \) if \( 120^\circ\text{C} \leq T < 150^\circ\text{C} \) |
|            | \( k \frac{\partial T}{\partial x} = 12,259.18T - 3,058,560.867 \) if \( T > 150^\circ\text{C} \), \[14\] |
3. Result and Discussions

In order to justify the assumption of instantaneous nucleation applied in the current work, Figure 2a is plotted for the case of continuous nucleation model for Al-Cu alloy system. It should be noted that the reference point for plotting all the quantities versus time figures in this work is at the centre of the casting. The continuous nucleation model is described by Gaussian distribution [1] to account for the characteristics variation of the nucleation rate. Thus, as represented by Wu and Ludwig [1], the following expression is used in evaluating the nucleation rate;

\[
\frac{dn}{dt} = \frac{n_{\text{max}}}{\sqrt{2 \pi \Delta T_{\text{n}}}} \exp\left(-\frac{(\Delta T - \Delta T_{\text{crit}})^2}{2(\Delta T_{\text{n}})^2}\right),
\]

where the nucleation parameters is taken to be \( n_{\text{max}} = 10^{14} \text{ m}^{-3} \), \( \Delta T_{\text{n}} = 10 \text{ K} \), and \( \Delta T_{\text{crit}} = 4 \text{ K} \). From Figure 2a it is evident that the nucleation time is less than 20 seconds, which is lower than the total solidification time as shown later. Figure 2b is a cooling curve for Al-Si and Al-Cu binary alloy system. The cooling curves depict eutectic solidification system, and aid in estimating the total solidification time. It is evident from the Figure 2a that the total solidification time (from zero point to the end of the horizontal section of the curves) for Al-Cu is about 100 seconds while that of Al-Si alloy is approximately 160 seconds. Comparing the total solidification time to the nucleation time of approximately 20 seconds, it is immediately seen that the nucleation time is short. Thus, it is safe to say that the assumption of instantaneous nucleation can be reasonable to some casting system.

![Figure 2](image-url)

Figure 2: Computed (a) nucleation rate vs time; (b) cooling curves for Al-Si, and Al-Cu alloy

The end of the eutectic solidification of Al-Cu alloy is almost the start of the eutectic solidification of Al-Si binary alloy system. The major reason while there is different solidification time in the two binary alloy systems is due to different thermodynamic and physical properties of the constitutional alloying elements. The undercooling and recalescence phenomena are clearly seen in the two curves. The undercooling and recalescence phenomena cannot be evaluated or obtained in the macro-heat transfer modelling that couples tradition temperature liquid fraction relation (i.e. Scheil and Lever rule).

Figure 3-4 shows a general trend for the evolution of solid fraction, grain size, growth rate and undercooling with time at the central part of the billet for the two binary alloy systems. Figure 3a
demonstrates that the evolution of solid fraction for Al-Cu alloy system is faster than the Al-Si alloy system; thus, solidification rate of the former is faster than the later. For the grain size evolution (Figure 3b) it should be noted that the same growth constant $\mu$ ($5 \times 10^{-8}$ m/s.K$^2$) and grain density $N$ of $(10^{14}$ m$^{-3}$) were used in computing the grain size (Eq. 5) for both alloy systems.

Figure 3: (a) Solid fraction evolution with time and (b) Grain size evolution with time

The grain size for Al-Cu alloy after solidification is higher than the grain size for Al-Si alloy. One can argue that since the former solidifies faster than the later, from metallurgical point of view the later (Al-Cu) will have smaller grain size than the former (Al-Si). To clarify any doubt, it should be recalled that the density of copper is higher than the density of silicon, therefore the density of Al-Cu alloy is higher than the density of Al-Si alloy. In addition the eutectic temperature for Al-Si (850 K) used in the computation is higher than the eutectic temperature for Al-Cu alloy (821 K). These and many other physical properties of the binary alloy systems can contribute to the variation in the grain size, growth rate, and undercooling seen in Figure 3-4. The undercooling and growth rate (Figure 4) for Al-Cu alloy is much higher than the undercooling in Al-Si alloy system under the same cooling conditions at the billet surface. The end of lower horizontal portion of the graphs (3-4) indicates the actual start of the solidification and the start of the top horizontal portion of the graphs indicates the end of the solidification. Conclusively the actual solidification time for Al-Cu alloy is approximately 50 seconds and that for Al-Si alloy is approximately 60 seconds. At the beginning of solidification the actual size of grains is in the range of $10^{-7}$-10$^{-6}$m which is seen as zero in the vertical section of Figure 3b. Figure 5 is plotted in the scale of $\mu$m for Al-Cu alloy system.
Figure 5: Grain size vs time for Al-Cu alloy system.
It is worth noting that the predicted grain size (Figure 5) in the DC casting is within the range of the experimentally predicted grain size for Al-Cu alloy by Eskin et al. [15].

Figure 6 is an illustration of solidification progress in the entire casting domain as depicted in the colour legend for Al-Cu alloy. At 50 seconds (Figure 6a), it is obvious from the contour plot that sufficient liquid metal is still present at the central part of the billet.

![Temperature Contours](image.png)

Figure 6: Temperature contours (K) for (a) 50 seconds (b) 100 seconds (c) 120 seconds (d) 150 seconds
This conclusion is made base on the fact that the colour legend indicates that the temperature at the billet centre is above 850 K which is greater than the eutectic temperature of 821 K. The width of the central liquid region reduces as the solidification time increases (Figure 6b). At 120 seconds (Figure 6c) the liquid band has significantly disappear from the central part of the billet and the temperature range is between 700 K and 800 K. Finally at 150 seconds (Figure 6d) the temperatures at the central part of the billet are within 450 K to 500 K which indicates that major part of billet is completely solid at that region. It is instructive to note that there is large thermal gradient from the cooling zones to the billet centre as seen in the Figure 6, which further indicates that solidification and heat transfer is from the billet periphery to the billet centre.

4. Conclusion
A detailed modelling of globular equiaxed eutectic solidification in a direct chill casting of aluminium binary alloy systems has been presented. The linearization of the solidification kinetics source term coupled to the heat transfer equation ensures robust and converged computation of the numerical model. The model couples the macroscopic heat transfer equation with the solidification kinetics model to predict total solidification time, actual solidification time, grain size, undercooling, and grain growth rate in two binary aluminium alloy systems.
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