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Numerical modeling of equiaxed structure forming in the cast during alloy solidification

Elzbieta Gawronska[a,*], Norbert Sczygiol[a], Eugeniusz Dubow[b]

[a]*Czestochowa University of Technology, Faculty of Mechanical Engineering and Computer Science, Dabrowskiego 69, 42201 Czestochowa, Poland*

[b]*Altaj Technical University I.I. Polzonow, Lenin Str. 46, 656015 Barnaul, Russia*

Abstract

In this study, we assumed that only the equiaxed structure created in the cast and the characteristic dimension is the final radius of grain. Because of the difference between the initial temperature of the molten metal and of the mold, there are significant differences in the average cooling rate when the liquidus temperature is achieved. The cooling rates vary within the range of 0.78 $K.s^{-1}$ to 29.88 $K.s^{-1}$. Since the average radius of grain is a function of the cooling rate, the radii of the smallest grains are 17.71 m, while the radii of the biggest grains are 366.22 m.

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Keywords: numerical modeling; solidification; equiaxed structure; characteristic dimension; grain radius

1. Introduction

The casting process is the most direct and shortest route from a component design to final product. This makes casting one of the major manufacturing processes, while casting alloys are some of the most widely used materials. One of the main reasons for the versatility of the casting process is the wide range of mechanical and physical properties covered by casting alloys. They may be of complex equipment and they are used in 90% of all manufactured goods [1]. Solidification is an inherent part of casting process. The structure of the casting is generated during the solidification and also is often the final structure of the casting. It also follows that the

* Corresponding author. Tel.: +48 34 3250589.
E-mail address: gawronska@icis.pcz.pl

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mechanical properties of the casting, which are a direct consequence of the microstructure, are controlled through the solidification process [2, 3]. Solidification models often analyze solidification events at a micro-, a macro- and an intermediate scale (the meso-scale) [4, 5]. The intermediate scale allows for the description of the microstructure features at grain level, without resolving the grain boundary. On this level solid-liquid interface appears in three regions: liquid, mushy (containing both liquid and solid phase), and solid. The macro scale relates the (growing) solid phase as a whole and allows for the description of certain parameters such as dimension of the grains or the extent zones of particular types of structures.

The casting solidification is the heterogeneous process, so it is differently in each point of the casting. The course of solidification can be described by a cooling curve or by a solidification curve – curve between the liquidus and solidus lines in the phase diagram (Fig. 1A). The first case describes the variation of the temperature within the time and allows for the designate of the cooling rate at any time during the process. Whereas the second case is characterized by the quantitative changes of the part of solid and liquid phase in function of temperature. All possible solidification curves (e.g. line no. 3 in Fig. 1A) take place between two extreme cases i.e. equilibrium solidification (line no. 1 in Fig. 1A) and non-equilibrium solidification (line no. 2 in Fig. 1A). The first of them describes homogeneous distribution of solute concentration both of in liquid and solid phase of the casting. The second of them describes significant pushing out of solute to liquid phase and lack of diffusion of solute in solid phase. During the indirect solidification (line no. 3 in Fig. 1A) there is no alignment of the distribution of solute concentration in solid phase but is significant diffusion of solute. In the real castings, except the rapidly solidifying layers adjoining to the mold and the slowly solidifying central areas of the massive castings, the indirect solidification occurs.

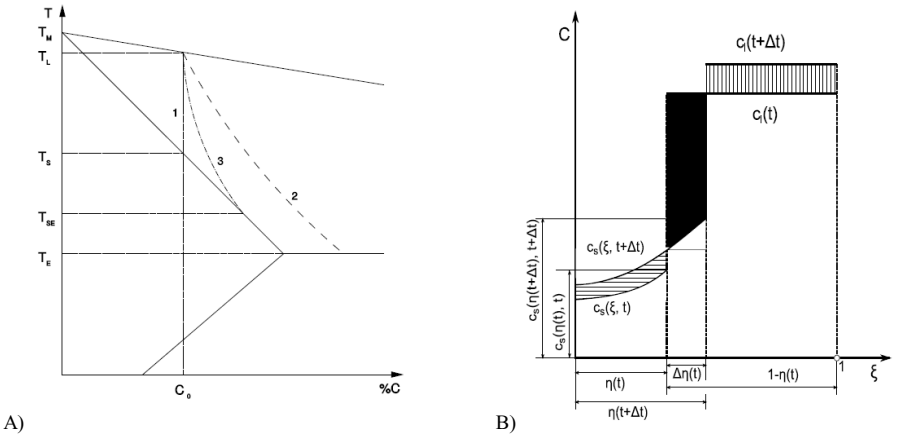


Fig. 1. A) Models of solid phase growth in binary alloys (T – temperature, C –chemical composition of the alloy; T_M – solidification temperature of the base component, T_l – liquidus temperature, T_s – solidus temperature for equilibrium solidification T_{SE} – solidus temperature for indirect solidification); B) The momentary distribution of solute concentration in the grain.

Numerical simulations are used for optimization of casting production. In many cases they are a unique possible technique for carrying out of the experiments which real statement is complicated. Computer modeling allows defining the major factors for a quality estimation of alloy castings. Simulations help to investigate interaction between solidifying casting and changes of its parameters or initial conditions [6]. In order to the efficient performance of large series of computational studies using reasonable resources, the framework needs to be not only accurate but also computationally efficient. Increasing capacity of computer memory makes it possible to consider growing problem sizes. At the same time, increasing of the precision of simulations triggers even greater load. There are several opportunities to tackle this kind of problems. For instance, one can use parallel computers [7, 8], the other can use accelerated architectures such as GPUs [9] or FPGAs [10], and the other can use special organization of computations [11–14].

In paper we concern only part of the numerical modeling of thermo-mechanical phenomena occurring during the production of castings, i.e. the solidification and the formation of structure. We focus on the enthalpy formulation of solidification which is characterized by high efficiency in connecting with the finite elements method [15]. We have described the traditional models of equilibrium and non-equilibrium solidification and we have proposed own model of indirect solidification. We assumed that in the casting there can be formed only one type of structure, namely the equiaxed structure. The grain size was dependent on the cooling rate. We carried out the numerical simulations of solidification for the alloy solidifying in the metal mold. The results are showed as distributions of the cooling rates and the average radii of the equiaxed grains.

2. Models of solid phase growth

A solid phase growing is directly associated with the latent heat of solidification released, whereas the start and the end of this process is connected with the achievement of the liquidus and solidus temperature, respectively (Fig. 1A). For example the binary alloy with eutectic transformation, for each solidification model can build appropriate numerical model of the solid phase growth. In the case of non-equilibrium solidification, described by Scheil equation, the eutectic temperature is always reached. This means that the final portion of metal solidifies at a constant temperature. In the equilibrium model of solidification, the final solidification temperature is dependent on the chemical composition of alloy. Only for alloys with the solute concentration greater than the maximum its solubility in the solid phase, the final solidification temperature is equal to the eutectic temperature. In the indirect solidification, the course of solidification is depended on the path of solute diffusion, and thus on the size of grains in the casting structure. In turn, the average grain size is related to the cooling rate. The complete distribution of the solute in the liquid phase and its diffusion in solid phase of the future grain assumes in the indirect solidification (Fig. 1B).

The obtained solution connects the solute concentration on the solidification surface with the part of phase fraction. Next, using the relationship between concentration and temperature (phase diagram) can finally obtain a function binding the part of solid phase with temperature. The mass balance of solute in the single grain area is:

$$m\eta^{m-1}(t)\frac{d\eta(t)}{dt}C_s(\eta(t),t)+m\frac{1}{r_z}D_s\eta^{m-1}(t)\frac{\partial C_s(\eta(t),t)}{\partial\xi}+\left(1-\eta^m(t)\right)\frac{dC_l}{dt}-m\eta^{m-1}(t)\frac{d\eta(t)}{dt}C_l(t)=0 \quad (1)$$

where subscript *s* refers to solid phase, subscripts *l* refers to liquid phase, *m* is the grain dimension factor (*m* = 1 – planar grain, *m* = 2 – cylindrical grain, *m* = 3 – spherical grain), *C* is the solute concentration, η is the current thickness or radius of the solid phase grain, r_z is the final radius of the grain, D_s is the coefficient of the solute diffusion in solid phase and ξ designates the current coordinate. Since the equilibrium and nonequilibrium solidification models are extreme cases of the indirect solidification, the mass balance of solute in both instances can be obtained from Eq. (1).

Introducing the notion of a local solidification time t_f, the part of solid phase can be defined as:

$$f_s=\sqrt{\frac{t}{t_f}} \quad (2)$$

For parabolic growth the Brody-Flemings equation is:

$$C_s=kC_0[1-(1-2\alpha k)f_s]^{\frac{k-1}{1-2\alpha k}} \quad (3)$$

where α is the dimensionless back-diffusion coefficient (vel Brody-Flemings coefficient), calculated as:

$$\alpha=\frac{D_s t_f}{r_z^2} \quad (4)$$

and the product $D_s t_f$ can be regarded as material parameter, and the solute partition coefficient is:

$$k = \frac{C_S^*}{C_l^*} \tag{5}$$

wherein C^* designates the solute concentration on solidification surface.

By making additional assumptions (Ω – amendment of α coefficient) and necessary transformations Eq. (3) can be written as:

$$f_s(T) = \frac{1}{1-2\Omega k}\left(1 - \left(\frac{T_M - T}{T_M - T_l}\right)^{\frac{1-2\Omega k}{k-1}}\right) \tag{6}$$

where:

$$\Omega(\alpha) = \alpha(1 - \exp(-1/\alpha)) - 1/2\exp(-1/(2\alpha)) \tag{7}$$

If the numerical model of solidification assumes the possibility of forming the grains of different sizes and the solute concentration is lower than its maximum solubility in the solid phase, then, in according to Eq. (7), the portion of grains can gain the eutectic temperature and the portion of ones can solidify above that temperature during solidification process. It is crucial to the grain size in this case. If the solute concentration is equal to or larger than its maximum solubility in solid phase, then all grains gain the eutectic temperature.

3. Modeling of equiaxed structure

Numerical modeling of structure formed in the casting is one of the most difficult problems in computer simulations of solidification. Extent of the zones of the different types of structure and the characteristic dimensions of the grains in these zones depend on the undercooling at the start of solidification. Undercooling, on the other hand, depends on the cooling rate. All the possible values of the cooling rates are between the infinitely large ($\dot{T} \to \infty$) and infinitely small ($\dot{T} \to 0$) value of the cooling rate.

Velocity of the grain growth in solid phase is exponential function of undercooling (kinetic, curvature or constitutional) of liquid metal alloy. Velocity of the grain growth is:

$$v = K(\Delta T)^n \tag{8}$$

where K is the alloy constant (obtained from measured solidification curves and the final grain radii in structure), ΔT is undercooling and n takes value from 1.3 to 2.3, but is often equal to 1, too. Assuming that only the equiaxed grains formed in the casting, the velocity of their growth can be written as:

$$v = \frac{dr}{dt} \tag{9}$$

Substituting Eq. (9) to Eq. (8) and integrating in the range of 0 to r_z and of 0 to t_f, the final grain radius is:

$$r_z = K(\Delta T)^n t_f \tag{10}$$

Since the maximum grain radius in structure is r_b, thus if $t_f \to \infty$ then $r_z \to r_b$, and if $t_f \to 0$ then $r_z \to 0$.

In paper we assumed that the characteristic dimension is the final grain radius which is depend on the cooling rate:

$$r_z = r_b[1 - \exp(-1/\dot{T})] \tag{11}$$

where $\dot{T}$ is the average cooling rate calculated from the beginning of the process until the liquidus temperature is reached. It can be noticed that if $\dot{T} \to 0$ then $t_f \to \infty$ and $r_z \to r_b$; and if $\dot{T} \to \infty$ then $t_f \to 0$ and $r_z \to 0$. In Eq. (11) the maximum grain radius in structure is depend on used the casting alloy and it should be determined experimentally. For very large values of undercooling the fine-grain structure is obtained, in this the zone of frozen grains. In the inner areas of the casting, where the undercooling is much lower and less differentiated than the undercooling of the layer in contact with the mold, the equiaxed grains radii are more or less the same and relatively large.

4. Results of numerical experiments

We have conducted numerical experiments with the usage of the our software called NuscaS [14]. We have used finite element method to solve enthalpy formulation of solidification supplemented by Newton and continuity boundary conditions. We used indirect model of solid phase growth for binary alloy (Eq. (6)). We depict the geometry and dimensions of the considered system in Fig. 2A. The computational mesh consists of the triangular finite elements. In the further analysis we focus on selected nodes (n166, n1153, n2541, n2750, n3668) that we denote in the Fig. 2A.

We performed series of numerical simulation of solidification for Al–2wt.%Cu alloy casting solidifying in the metal form. The values of material properties of liquid phase, solid phase and mold are given in Table 1.

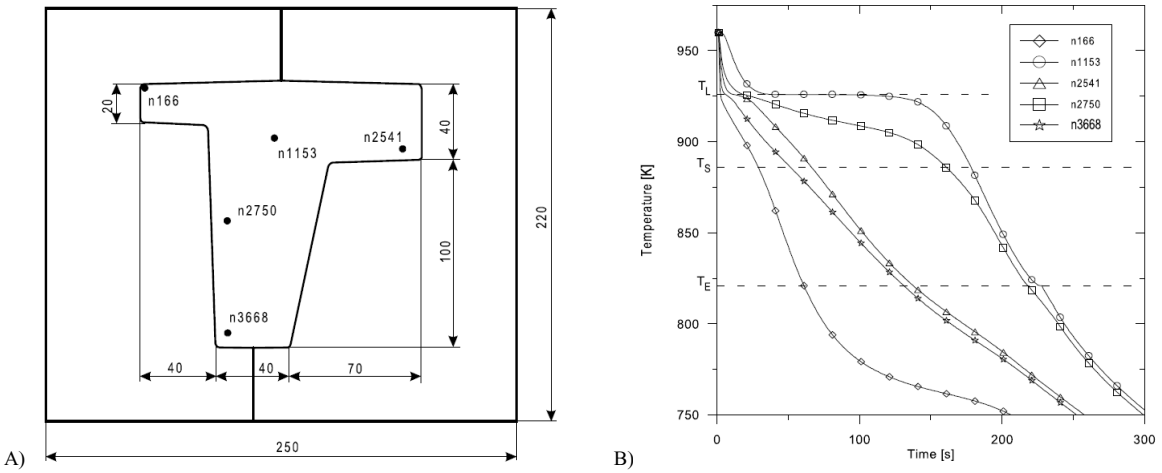


Fig. 2. The analyzed casting in mold with the selected nodes (A) and the cooling curves in selected nodes (B).

Table 1. Physical properties of cast and mold material using during computer simulation of Al–2wt.%Cu alloy solidification.

Quantity	Unit symbol	Liquid phase	Solid phase	Mold
density	$kg.m^{-3}$	2498	2824	7500
specific heat	$J.kg^{-1}.K^{-1}$	1275	1077	620
thermal conductivity	$W.m^{-1}.K^{-1}$	104	262	40
latent heat of solidification	$J.kg^{-1}.K^{-1}$	390 000		–
solute partition coefficient	–	0.125		–

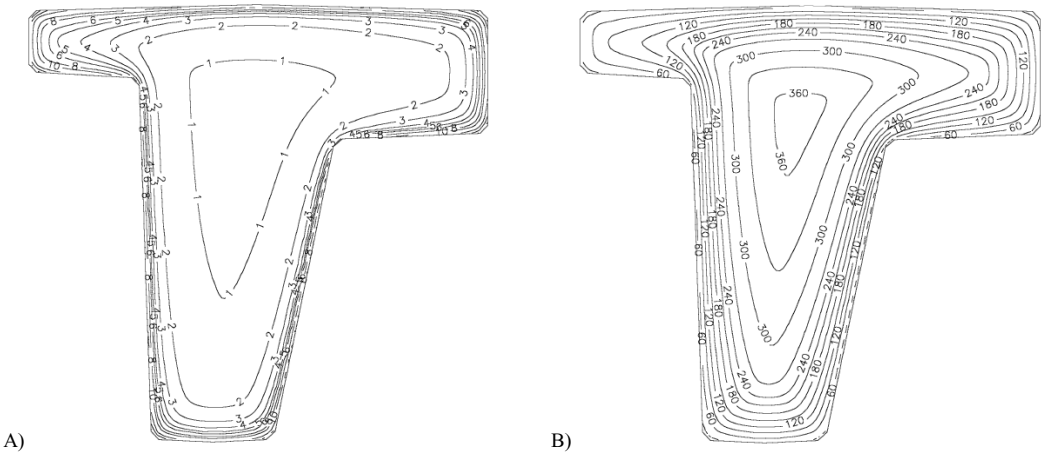
Between liquidus and solidus temperature we assumed linear variation thermal conductivity coefficient with temperature. In order to carry out the numerical simulations the needed temperatures were read from phase diagram and T_M = 933 K, T_l = 926 K, T_s = 886 K and T_l = 821 K. The maximal grain radius is equal to $3.5 \cdot 10^{-5}$.

Since the average grain radius depends on the cooling rate hence significantly differences the grain size in the casting (Fig. 3). The smallest grains radii, calculated in the nodes near the mold, are 17.71 μm, whereas the largest grains radii, calculated in the inner of the casting, are 366.22 μm.

All the characteristic values related to the course of solidification in chosen nodes of mesh are shown in Table 2.

Table 2. Characteristics of solidification in the selected nodes.

Number of nodes	T_{SE} (K)	Ω (–)	f_s^E (–)	r (μm)	$\dot{T}$ (K.s^{-1})
166	876.0	0.4872	1	17.71	29.88
3668	863.6	0.3708	1	63.51	7.48
2541	827.0	0.2114	1	130.07	3.33
2750	821.0	0.1360	0.9867	195.55	2.02
1153	821.0	0.0447	0.9672	366.22	0.78



A) B)

Fig. 3. Distribution of the cooling rates (K.s^{-1}) (A) and the average grains radii (μm) (B).

5. Remarks and conclusions

Numerical modeling has been developed to predict the solidification microstructure quantitatively in general and grain size in particular. Mechanical properties of castings are dependent on their microstructure. A model of equiaxed solidification, coupled with a macroscopic model for thermal description of solidification has been developed. The model is able to predict time-dependent thermal field and undercooling during the liquid and solid phase growth. The relationship between grain radii and the cooling conditions were also investigated. The modeling was applied for calculation of the grain radii. It significantly enhances the understanding of solidification processing such as the behavior of solute Cu in aluminum alloys and the formed structure.

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