Comparison of two-phase and three-phase macroscopic models of equiaxed grain growth in solidification of binary alloy with electromagnetic stirring

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Abstract. Simulations of equiaxed solidification using two-phase and three-phase models are performed for the experimental benchmark AFRODITE with electromagnetic stirring. A three-phase model presented by authors elsewhere accounts for solid phase, inter- and extradendritic liquid phases. With respect to that model, the two-phase approach can be considered as reduced or simplified, yet, this implies also less number of assumptions regarding closure relations. In simulations, as expected, final segregation obtained with two–phase model is stronger, yet, it is qualitatively similar to the segregation pattern obtained with three-phase model.

1. Introduction
In industrial casting production, a large equiaxed grain region is often expected because it is supposed to provide better homogeneity than the structure consisting of columnar grains [1]. Both industrial and laboratory experiments indicate that forced convection may promote formation of equiaxed grains. Yet, it is also known that interaction between convection and solidifying structure may lead to appearance of channels, freckles and zones of macrosegregation. Post-mortem analysis of sample provides information only about the final state of solidification and can be rather puzzling since evolution of various processes in time remains unclear. As far as in-situ experiments are concerned, they often deal with rather weak convective flow because of small sizes of samples, therefore, these observations could not be easily transposed to large-scale solidification processes. Consequently, numerical modelling is needed to understand how emerging columnar or equiaxed solid structure affects convection and solute transport during solidification process. Numerical simulation of solidification with equiaxed grains is more challenging than with columnar ones because such phenomena as nucleation, grains’ drag by liquid phase, and their packing due to interaction with walls and other grains have to be considered. Currently, volume averaged method makes simulation of equiaxed solidification under forced convection at macroscale possible [2]. However, despite the variety of existing equiaxed solidification models [3–7], reliability of results obtained with their use remain uncertain mainly because of two reasons. First, these
models rely on various physical assumptions used to close system of equations and contain lots of empirical parameters to which numerical results are quite sensitive [8–13]. Second, there is a lack of experimental data which could help to validate model of solidification in a purely equiaxed regime in presence of convection. Consequently, it is important to perform numerical studies of a particular solidification problem using different parameters or closure relations or even models based on different approaches. For example, in the simulation of 2.45 ton ingot solidification by Li et al. [9], it was found that the presence of equiaxed grains cause severe negative segregation at the bottom, however, if maximum nuclei density is larger than some critical value, the segregation will be relieved. With a two-phase equiaxed model, Krane et al. [13] simulated a benchmark solidification case using different packing limit fraction. They concluded that for a two-phase model the packing limit fraction had to be very likely smaller than 0.637, which is the value traditionally used in three-phase model. Wang et al. [8] demonstrated crucial effect of solute diffusion length on the calculation results of macrosegregation in Hebditch-Hunt case using three-phase model. Wu et al. [3] found that in solidification of Al–4.7 wt.% Cu alloy two-phase globular equiaxed model predicts heavier segregation than three-phase dendritic one. Plotkowski et al. [11] compared three different grain attachment models. Cited studies helped to understand role of various parameters and assumptions in equiaxed solidification modelling, yet, none of them used experimental results to validate their models.

Present works deals with comparison of three-phase and two-phase modelling of equiaxed solidification of a binary Sn–10wt%Pb alloy under the action of electromagnetic convection. The modelling is based on data issued from the experiment, referred hereafter as AFRODITE, which is briefly described below while details and results of the experiment can be found elsewhere [14-15]. Application of a three-phase model to this experimental case using two-dimensional description was also reported previously [16]. In the present study we are interested if a two-phase model which can be considered reduced (or simplified) compared to three-phase provides similar results regarding grain growth, their motion and segregation pattern.

2. Description for solidification case

The experiment under consideration presents solidification of a binary Sn–10wt%Pb alloy in a rectangular cavity with inner size of 100×60×10 mm (figure 1). In the experiment a constant difference of 40 K is imposed for temperatures at the heaters adjacent to the lateral walls of the cavity, and cooling rate of CR = 0.03 K/s is applied to solidify the sample [17], other walls are regarded as adiabatic. Thermal resistance between heaters and the solidifying volume makes the temperature differences across the latter smaller and equal to nearly 15 degrees [15] that is taken as initial condition in calculations. A travelling magnetic field created with a linear motor placed horizontally along the cavity and below gave rise to Lorentz force acting mainly along the bottom and rapidly decreasing in the vertical direction. An analytical expression for the resulting Lorentz force presented in [18] was used in numerical simulations. Since Lorentz force counteracts the buoyancy, convection in the cavity is less intense compared to the case without the stirring [19], and there is no need to introduce additional damping force to account for front and back walls.

![Figure 1. Scheme of the experimental set-up. Initial condition T_d(t)-T_c(t)=15°C is used in simulations.](image-url)
However, simulations of the melt flow performed with laminar approach, both for 2D and 3D configurations, could not be converged because of the interaction of two unstable vortices existing in the fluid. The vortex appeared due to the electromagnetic stirring cannot overcome the thermal convection near the hotter boundary. Consequently, for further simulations a realizable $k$-$\varepsilon$ turbulent model is used while calculated turbulent viscosity is rather low that indicated weak turbulence.

3. Model description

The shape of equiaxed grain depends on cooling condition and grain size. Generally, equiaxed grains prefer to grow as globular ones when they are still small [7]. In most conditions, transition from globular shape to dendritic one happens due to triggering of faster velocity of dendrite tip compared to diffusion-controlled velocity [3]. In present work, similar to other ones [5, 20], we assume dendritic shape of grains for three-phase model and globular one for two-phase mode (figure 2). In three-phase model, the liquid phase is divided into inter- and extradendritic parts. The interdendritic liquid in the model is united with solid “skeleton” thus giving grain phase surrounded by an imaginary envelope. Details of three-phase model can be found elsewhere [8, 16], below only a two-phase model is shortly presented with its governing equations given in table 1. Major differences of two models are described at the end of this section and summarized in table 2.

![Figure 2. Schematic figure of an equiaxed grain with dendritic shape (a) and globular solid grain (b).](image)

In two-phase model, the volume fraction of solid phase $f_s$ and liquid phase $f_l$ satisfy the constraint $f_s + f_l = 1$. Both phases have their proper velocities, temperatures $T_s$ and $T_l$, and concentrations of the solute $c_s$ and $c_l$. Initial state of the model is supposed to be pure melt of a nominal concentration $c_0$, whose temperature is above the liquidus temperature. With condition of thermal equilibrium between solid and liquid phases, an infinitely fast heat transfer between the phases is assumed which is provided in the model with a large value of heat transfer coefficient (table 1). Once the constitutional undercooling somewhere in the volume is larger than critical value, the nucleation happens with the nucleation rate $N_n$ giving rise to grains number density (concentration of grains) $n$. It is supposed that nucleation can happen throughout the process if liquid fraction exists, conditions of constitutional undercooling are satisfied, and total number of grains is below of maximal one defined with $n_{\text{max}}$. Although assumption regarding importance of dendrites’ fragmentation as a source of nuclei can be found elsewhere [21], this phenomenon is not taken into account in the models presented here to limit uncertainty of the latter. The transport equation is solved for $n$ thus defining the local number of grains which is related to the size of grains. It is supposed that $n$ is transported with the velocity of the solid phase whose small amount appears simultaneously with nucleation and whose growth occurs according to local undercooling, i.e. to the distribution of the concentration in surrounding liquid. In the vicinity of grain, the latter is defined by convective transport but also by diffusion of the solute rejected by the solid phase according to the phase diagram. Similar to [7] and based on our experience [8] we suppose that the solute diffusion length in the liquid $l_i$ depends on intensity of liquid flow around the grain. The back diffusion in solid is neglected as well as shrinkage phenomenon, i.e. all densities in the conservation equations are constant and equal to the reference density: $\rho_s = \rho_l = \rho_{\text{ref}}$. Similar to Založnik and Combeau [5], to model the sedimentation (here the floating) phenomenon, in the buoyancy term, a constant difference between the solid phase density and a reference density is introduced. The Boussinesq approximation accounts for solutal and thermal convection in the liquid phase. To calculate the drag force in two-phase model we use Happel model [22] for a low solid fraction and when grains are packed the Kozeny-Carman model.
[23] is applied. Note that in three-phase model the approach is similar but the drag force is calculated with grain fraction since it is applied to grains. Regarding grains packing, we choose to block those grains whose fraction is above a critical one and which are situated either near the wall or near already packed neighbouring grain. This allows us to avoid unphysical situation with blocking of grains brought to the cavity centre by forced convection.

**Table 1.** Conservation equations, source terms, and auxiliary expressions

| 1. Conservation equations |
|---------------------------|
| Mass: $\frac{\partial (f_1 \rho_l)}{\partial t} + \nabla (f_1 \rho_l \vec{u}_l) = M_{sl} - M_\Phi$; $\frac{\partial (f_3 \rho_s \vec{u}_s)}{\partial t} + \nabla (f_3 \rho_s \vec{u}_s) = M_{ls} + M_\Phi$ |
| Momentum: $\frac{\partial (f_1 \rho_l \vec{u}_l)}{\partial t} + \nabla (f_1 \rho_l \vec{u}_l \vec{u}_l) + \frac{\mu_l}{\rho_l} (\nabla \vec{u}_l + (\nabla \vec{u}_l)^T) = \vec{u}_l M_{sl} + \vec{F}_{bl} + \vec{U}_{st} + f_l \vec{F}_{ems}$ |
| $\frac{\partial (f_3 \rho_s \vec{u}_s)}{\partial t} + \nabla (f_3 \rho_s \vec{u}_s \vec{u}_s) - f_s \nabla \rho_s + \nabla \mu_s f_s (\nabla \vec{u}_s + (\nabla \vec{u}_s)^T) = \vec{u}_s M_{ls} + \vec{F}_{bs} + \vec{U}_{st} + f_s \vec{F}_{ems}$ |
| Energy: $\frac{\partial (f_1 \rho_l h_1)}{\partial t} + \nabla (f_1 \rho_l h_1 \vec{u}_l) = \nabla (k_1 f_1 \nabla T) + L M_{ls} f_1 + M_{sl} h_1 + Q_{st}$ |
| $\frac{\partial (f_3 \rho_s h_s)}{\partial t} + \nabla (f_3 \rho_s \vec{u}_s h_s) = \nabla (k_s f_s \nabla T) + L M_{ls} f_s + M_{ls} h_s + Q_{ls}$ |
| $\text{where } h_1 = \int_{r_1}^{r_2} c_p^1 dT + h_1^{ref}, h_s = \int_{r_1}^{r_2} c_p^2 dT + h_s^{ref}$ |
| Solute: $\frac{\partial (f_1 \rho_l c_l)}{\partial t} + \nabla (f_1 \rho_l c_l \vec{u}_l) = \nabla (D_{sl} f_1 \nabla c_l) + J_{st}$ |
| $\frac{\partial (f_3 \rho_s c_s)}{\partial t} + \nabla (f_3 \rho_s \vec{u}_s c_s) = J_{ls}$ |

| Grain number density: $\frac{\partial}{\partial t} n + \nabla (\vec{u}_s n) = N_\Phi$ |

| 2. Source terms |
|-----------------|
| Mass: $M_{ls} = -M_{sl} = \rho_l \cdot S_s \cdot v_{ls}$; $M_\Phi = N_\Phi \rho_l \cdot \frac{1}{6} \pi d_0^3$ |
| Momentum: $\vec{F}_{bl} = f_l \rho_l \vec{g} \left[ \beta_T (T_{ref} - T_l) + \beta_c (c_{ref} - c_l) \right]; \vec{F}_{bs} = f_s (\rho_s^b - \rho_{ref}) \vec{g}$ |
| $\vec{U}_{ls} = -\vec{U}_{st} = K_{ls} (\vec{u}_l - \vec{u}_s)$ |
| Energy: $Q_{ls} = -Q_{st} = H' (T_l - T_s), H' = 1 \times 10^9 W m^{-3} K^{-1}$ |
| Solute: $J_{ls} = -J_{st} = (M_{ls} + M_\Phi) \cdot c_s$ |
| Grain number density: $N_\Phi = \{ f_l (n_{max} - n) / \Delta t \}, \text{ if } (\Delta T > \Delta T_{nuc}) \text{ or } (n < 1)$ |

| Auxiliary expressions |
|-----------------------|
| $c_l^* = \frac{T_l - T_0}{m}$; $c_s^* = k \cdot c_l^*$; $S_s = f_1 \cdot (36 \pi \cdot n)^{1/3} \cdot f_s^{2/3}$ |
| $v_{ls} = \frac{D_{ls}}{l_i} \cdot c_l^* - c_l^*$; $K_{ls} = \begin{cases} \frac{4 f_s^2 \beta^2 \mu_l}{d_s^2}, & \text{if } f_s < f_{sp} \\ \frac{180 \mu_s f_s^2}{f_l d_s^2}, & \text{if } f_s > f_{sp} \end{cases}$ |
| $l_i = \frac{d_s}{2} \left( \frac{1}{1 - f_s^3} + \frac{1/3 Re^a}{3 f_l} \right)^{-1}$ |
| $\beta = \begin{cases} \frac{9}{2} f_s \frac{2 + 4/3 f_s^{5/3}}{2 - 3 f_s^{1/3} + 3 f_s^{5/3} - 2 f_s^2} \end{cases}^{1/2}$ |
The main difference between the three-phase and two-phase models is related to the phase transition mechanism that is governed by solute and heat transport, in kinematic interaction between the phases and in treatment of grain packing, each item is discussed below.

1. In two-phase model the phase transition occurs between two phases, solid and liquid, and is controlled by solute distribution in the surrounding liquid, rejection of the solute happens into liquid surrounding the grain. In three-phase model solidification can be regarded as strong coupling of two processes. The first one, noted in the Table 2 as $l\rightarrow d$, consists of grain enlargement that is related to the tip growth and is seen as expansion of the grain envelope with the velocity $v_{\text{env}}$. This process is governed by the solute undercooling ahead of tips and results in transformation of liquid surrounding the grain into interdendritic liquid. The second stage (notated as $d\rightarrow s$) is actually transition of the interdendritic liquid to the solid skeleton, which is governed by the solute undercooling in the interdendritic liquid. Rejection of the solute happens at the interface between the solid and interdendritic liquid and further the solute is transported to the liquid surrounding the grain via molecular diffusion. Consequently, in three-phase model interdendritic phase plays role of “buffer” which defines difference in growth rate of grain and solid phase. Therefore, one can expect that solid fraction in the two-phase model will increase faster compared to the three-phase model. On the other hand, increase of grain fraction in three-phase model should be more intense than increase of the solid fraction in two-phase model.

### Table 2. Phase transfer rate between phases in models

| Surface area concentration | Interface movement velocity | Phase transfer rate |
|---------------------------|----------------------------|---------------------|
| Two phase model<br>$l\rightarrow s$ $S_s = f_t \cdot (36\pi \cdot n)^{1/3} \cdot f_s^2$ | $v_{ls} = \frac{D_t \cdot c_i^* - c_i}{l_t} \cdot \frac{c_i^* - c_s^*}{l_s}$ | $M_{ls} = S_s \cdot v_{ls}$ |
| Three phase model<br>$l\rightarrow d$ $S_e = f_t \cdot (36\pi \cdot n)^{1/3} \cdot f_e^2$ | $v_{\text{env}} = \Phi_M \cdot m_i \cdot (\kappa - 1) \cdot c_i^*$ | $M_{ld} = S_e \cdot v_{\text{env}}$ |
| $d\rightarrow s$ $S_{ds} = f_e \cdot \rho_s \cdot 2 \cdot f_{e}^e$ | $v_{ds} = \frac{D_t \cdot c_i^* - c_d}{l_d} \cdot \frac{c_i^* - c_s^*}{l_s}$ | $M_{ds} = S_{ds} \cdot v_{ds}$ |

Note: $\Phi_M = 0.683$ is growth shape factor assuming an octahedral grain envelope shape [10].

2. In two-phase model liquid and solid phase are moving independently and exchange momentum. In three-phase model we assume that the interdendritic liquid and solid phase share the same velocity field, and momentum interaction happens between grain and surrounding liquid. Consequently, accounting of the first item, we assume stronger kinematic interaction between phases in three-phase model. Yet, further discussion depends on properties of material and solidification conditions: whether only natural convection is involved and what is the density relation between liquid and solid phases.

3. It is of high importance at which fraction grains are getting packed since it determines intensity of the convective transport between the packed grains and the latter, at large extent, defines final segregation pattern. In three-phase model the packing is applied to grains while solid fraction inside can be rather small, i.e. the region of interdendritic liquid can be large that assumes growth of grains with further enrichment of the interdendritic and extradendritic liquid. In two-phase model the packing is applied to the solid phase that means that to have similar situation with large amount of liquid between blocked solid the packing has to be performed earlier. It is widely accepted that the packing fraction limit for the grain phase is 63.7% [10, 12, 24], that corresponds to the packing fraction of randomly arranged monodisperse spheres. This value is kept in simulations with three-phase model. The packing limit for solid phase in two-phase models is generally accepted to be in range $f_{s,p} = 0.1 - 0.5$ [13, 25, 26], large dispersion is related to the type of the solid grain, dendritic or globular. In present simulations for
a two-phase model a value of \( f_{s,p} = 0.3 \) is defined, similar to the work [27]. It should be underlined that in two-phase model all liquid between grains can move while in three-phase it applies only to extradendritic liquid, that means that whatever is adjustment of the packing limit, behaviour of systems composed of three and phases will be different.

4. Results and discussion

To understand results presented below one should remember that solid phase is supposed to be lighter than liquid and this difference increases with enrichment of fluid by rejected solute. This means that growing grains float in the liquid instead of been sediment. Simulations start with overheated liquid in order to have the temperature and flow field installed before solidification is started. First nuclei appear nearly at 180 s of calculations at the upper corner of the colder boundary. The solid (in 2-phase model) and equiaxed (in 3-phase model) phase which starts to appear is brought to the centre of the cavity where it is remelted. Solidification along the whole colder wall begins at \(-400\) s of calculations. Then, the grains which nucleate closer to the bottom first travel along the cold wall that allows them to grow till the fraction at which they are packed while some of them can travel along the upper wall without been remelted. Since that time the solid grains in two-phase model and equiaxed grains in three-phase model start to fill the cavity. After 540 s of calculations temperature fields obtained with two-phase and three-phase models are different because of difference in convective flow (figure 3(a) and (b)). In two-phase model the packed grains completely occupy the upper boundary and damp their convection flow which otherwise would consist of interacting vortices due to natural and forced convection (figure 3(a) and (c)). The forced flow is concentrated in the lower part of the cavity where fraction of the solid phase is low. Liquid from the cold boundary is brought to the cavity centre by forced convection that creates a region of low temperature in the bottom half of the cavity. Also, forced convection defines transport of rejected solute, a part of which is captured in the centre of its vortex.

**Figure 3.** Results obtained at 540 s of simulations: temperature distribution in two-phase (a) and three-phase (b) model, the black line on these picture correspond to the edge of the zone of packed grains defined with \( f_{s,p} = 0.3 \) in two-phase model and \( f_{s,p} = 0.637 \) in three-phase model, velocity field in the liquid is superposed over temperature distribution; map of the average concentration and contours for solid fraction in two-phase model (c) and grain fraction for three-phase model (d).

In three-phase model two vortices with different direction still exist in the cavity at 540 s. The vortex generated by Lorentz force is located only at a lower half and a vortex related to thermal-solute effect
occupies the upper half of the cavity (figure 3(b)). While equiaxed grains exist almost everywhere their growth mainly at the colder side, consequently, the packed zone is located there.

In final macrosegregation maps (figure 4), both models show negative segregation at the top and positive in the lower part of the cavity that can be explained as follows. At early stage of solidification grains are brought to the top by buoyancy and forced convection where they solidify taking less value of solute and rejecting the excess to the liquid which becomes heavier. Rejected solute is captured by the forced convection which redistributes it along the bottom but also drag slightly upward. At the same time heavier fluid tends to sediment throughout the process and mostly at the final stage of solidification, when the grains are packed yet liquid continues to move between them.

![Figure 4](image)

**Figure 4.** Final macrosegregation map obtained with two-phase (a) and three-phase (b) model.

Although the general character of the macrosegregation patterns is similar for two models, discrepancies are seen in details and some of them can be explained by different assumptions used in the models. In two-phase model both drag force and buoyancy are related to the solid fraction while in three-phase model the buoyancy is applied to the solid fraction and the drag force is related to the grain fraction. That means that at the beginning of solidification globular grains in two-phase model are subjected to stronger buoyancy force and weaker drag force hence grains in two phase model show stronger tendency to float up to the top of cavity and get packed there (figure 3(a)). At the end of solidification, the liquid flow between packed grains in two-phase model is more intense than in three-phase model, due to smaller value of packing fraction and since in three-phase model the interdendritic liquid is attached to the solid skeleton. Because of this in two-phase model solute rejected by grains descents and has time to be redistributed over the whole bottom. An interesting phenomenon which cannot be presented here because of a short format of the paper is the interaction of forced and buoyancy flow which is responsible for the shape of the zone of negative segregation at the upper part of the cavity.

It can be believed that through appropriate adjustment of parameters of both models it is possible to obtain results in the two-phase model closer to those of the three-phase model. To our opinion, results should become more similar if interdendritic fraction is kept as small as possible because, as we stated above, it serves as a buffer between the solid and the extradendritic liquid. In principle, this can be done by adjustment of solute transport through the interdendritic liquid via modification of two diffusion lengths and calculation of the surface concentration, i.e. using various form factors. The critical packing fraction should be modified accordingly.

5. Summary
A two-phase and three-phase equiaxed solidification models are applied to simulations of AFRODITE experiment on solidification of a binary Sn–10wt%Pb alloy under the forced convective flow driven by electromagnetic force. With chosen set of parameters both models provide qualitatively similar results which resemble final distribution of Pb in the sample obtained via X-Ray imaging (figure 12(c) in [15]). Analysis of results show that fraction at which grains are getting packed is one of the crucial parameters since it defines regions of action of forced and buoyancy convection in the case under consideration. Evolution of the convective flow is different in two models because it is subjected to the interaction with solid phase (in two-phase model) and grain phase (in three-phase). Different flow field leads to different temperature evolutions during the process. Surprisingly, despite these differences throughout the
process, calculated final macrosegregation maps shows qualitatively similar results. In both cases negatively segregated layer at top is formed and positive segregation zone is observed at bottom similar to the experimental case. This indicates probably that final segregation is largely defined by residual flow through rigid solid network.

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