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Modelling of macrosegregation in direct chill casting considering columnar-to-equiaxed transition using 3-phase Eulerian approach

J Hao[1], Y J Lin[1], Y Nie[1], M Wu[2] and A Ludwig[2]

[1] Department of Mechanical, Materials and Manufacturing Engineering, University of Nottingham Ningbo China, China

[2] Chair for Modelling and Simulation of Metallurgical Processes, University of Leoben, Austria

E-mail: jane.hao@nottingham.edu.cn

Abstract. A 3-phase Eulerian approach is used to model the macrosegregation during solidification in direct chill (DC) casting of binary bronze (Cu-Sn). The three phases are the melt, the solidifying columnar dendrites and the equiaxed grains. The thermodynamic information of Cu-Sn is included based on published thermodynamic data, which are coupled with the 3-phase solidification model. The occurrence of columnar-to-equiaxed transition (CET), phase interactions, feeding flow, equiaxed sedimentation and their influence on macrosegregation are considered in the model. The model is applied to a laboratory DC casting process of bronze as a benchmark to demonstrate the model potentials. The simulation results of mixed columnar and equiaxed solidification as well as the formation of macrosegregation are presented. The focus of this work is to analyze and discuss the macrosegregation mechanisms by different flow including feeding flow and crystal sedimentation.

1. Introduction

Bronzes (Cu-Sn) are among the oldest engineering materials, and nowadays are still used in many different applications with which high quality materials are required for example electronics. Due to the fact that bronzes have a rather large mushy zone (with the solidification interval of about 200°C), macrosegregation often appears in direct chill (DC) casting process of bronze. Macrosegregation is an inhomogeneous distribution of alloy composition that exists over the entire casting [1]. It decreases the workability of the product and thus has to be removed. Macrosegregation is known to be caused by a combination of microsegregation and relative motion between liquid and solid in the mushy zone, induced by different flow phenomenon of forced convection, thermo-solutal convection, feeding flow, equiaxed sedimentation, etc [2]. Since diffusion in the solid is too slow to remove macrosegregation by heat treatment, it has to be minimized during solidification by choosing appropriate casting parameters.

Several macrosegregation models have been developed by researchers [3-7]. Flemings et al.[3] developed a model to predict the formation of channel-type segregation for multicomponent systems.

The model considered heat, mass and momentum transport in the mushy zone. Beckermann et al.[4] applied a coupled multicomponent solidification model with melt convection to a large industry-scale ingot. Their simulation results qualitatively agreed with the positive segregation observed in the ingot. Ludwig et al. [5] presented a model coupling the ternary phase diagram with the multiphase solidification simulation and apply it to a DC casting of bronze. Goyeau et al.[6] developed a macroscopic model by using a volume averaging technique with local closure, taking into account the spatial variation of the pore-scale geometry within the mushy zone. Combeau et al. [7] presented a two-phase model to study the influences of both motion and morphology of equiaxed grains on a steel ingot. However, these models did not distinguish between the columnar phase and the equiaxed phase; the two phases are presented as one solid phase during solidification.

Wu et al. [8] developed a mixed columnar-equiaxed solidification model, which considered the competitive growth of columnar and equiaxed phase, melt convection, equiaxed grain sedimentation, together with their influence on the species transport and macrosegregation. This model successfully predicted the conic negative segregation in the lower region of the ingot and the columnar-to-equiaxed-transition (CET) [9]. The authors have modified and applied the model to study macrosegregation in a laboratory DC casting of bronze [10]. Based on that study this paper presents an insight investigation on the formation mechanisms of macrosegregation by different flow phenomena, especially the effects of equiaxed crystal sedimentation are discussed in details.

2. Model Description

2.1. General Assumptions.

Ternary and binary simulation work on different continuous casting processes have been published and discussed during the last years by the authors [5,8]. The presented simulation results for a binary CuSn DC casting takes into account three phases: the liquid phase, the columnar phase, and the equiaxed phase. The thermodynamic information of Cu-Sn is included based on thermodynamic data [11] and coupled with the multiphase model. Details of the three-phase mixed columnar-equiaxed solidification model can be found in the literature [8,9]. Here, only a brief outline of the model assumptions is given.

- Columnar dendrites, approximated by growing cylinders, start to grow at the mold wall only if the local temperature drops below the liquidus temperature.
- The diffusion field around the columnar cylinder induces a shell-like growth around the cylinder. The growth of columnar is controlled by specific model assumptions as described in the next part.
- Homogenuous nucleation is modelled by initialising a certain number of nucleus in each cell. No further nucleation is allowed after the growth of crystals start.
- Growth of equiaxed grains is included by a diffusion driven growth around a spherical crystal and controlled by specific model assumptions as described in the following.
- Feeding flow is considered by taking into account the density difference between liquid and solid.
- Mechanical interaction between the mush and the flow is calculated via Darcy's low.
- The mushy permeability is modelled by the Blake-Kozeny permeability approach [12].

2.1.1. Blocking Mechanism.

Based on the fact that during solidification the columnar and equiaxed phase grow competing with each other, the solidification model is performed by allowing each phase growing simultaneously with the following blocking mechanisms to ensure physical growth conditions:

(i) The columnar phase is not allowed to grow if the undercooling of the liquid (ΔT) is smaller than 4K [12]. The applied undercooling allows the growth of the equiaxed phase in front of the columnar dendrite tips.

(ii) The columnar phase is not allowed to grow if the equiaxed volume fraction (f_e) exceeds 0.49. Experimental observations [13] indicate that the columnar front is blocked by a certain amount of equiaxed crystals in front of it. Therefore, this condition ensures that the columnar cannot overgrow the equiaxed phase when it has already a certain amount of volume fraction.

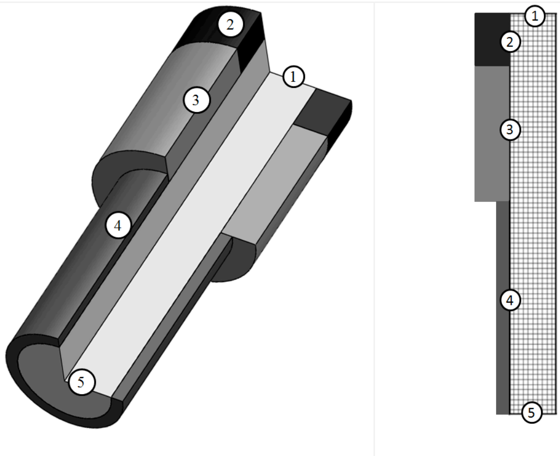
(iii) The equiaxed phase cannot grow if its diameter (d_e) is bigger than the space between the primary dendrite arm spacing (λ_1) of the columnar phase and the diameter of the columnar dendrite trunk (d_c) [13]. This condition models the growth of the equiaxed phase within the dendrite trunks; it is thought that an equiaxed crystal is not able to grow further if it's sticking within two dendrite trunks.

(iv) The equiaxed phase is blocked in its movement when the sum of the volume fraction of the equiaxed phase and the columnar phase reaches the packing limit of $f_e + f_c >= 0.637$ [14].

(v) The equiaxed is trapped and forced to move with the columnar when the volume fraction of columnar reach to a certain value, that is, trapping limit of $f_c >= 0.2$ is reached [14].

3. Benchmark Configuration

The presented model is applied to a benchmark simulation of a laboratory DC casting process as displayed in figure 1. For the process simulation a casting velocity of $\vec{u}_{cast} = 1.44$ mm□s^{-1} and a casting temperature of T_{cast} = 1523 K are used. Calculations were done for the binary alloy CuSn6. Since the mold is of a round shape, a 2D axis-symmetric simulation has been performed. Figure 1a displays the configuration of the benchmark, and figure 1b displays the geometry and grid for the simulation. The grid size is 3 mm with quadrilateral mesh. The boundary conditions used in the simulation are marked in the figure: ① indicates the position of the inlet where a pressure inlet is taken, ② assigns the upper part of the mold which is assumed to be insulating, ③ shows the lower part of the graphite mold where h = 3000 W□m^{-2}□K^{-1} and T_{lower_mold} = 550 K, and ④ displays a water cooling system with h = 3000 W□m^{-2}□K^{-1} and T_{water} = 300 K, and ⑤ shows the position of the outlet with a casting velocity of $\vec{u}_{cast} = 1.44$ mm□s^{-1}. The mold wall is considered to move with casting velocity, therefore a non-slip condition for the columnar phase is applied. As initial conditions, hot melt (T_{init} = 1523 K) at the casting velocity ($\vec{u}_{cast} = 1.44$ mm□s^{-1}) is assumed. The presented results are taken after reaching steady state.



(a) (b)

Figure 1. (a) Configuration of benchmark. (b) Geometry and grid for calculation. The grid size is 3 mm. ① marks the position of the inlet, ② and ③ mark the upper and lower part of the mold, ④ indicates a water cooling system, and ⑤ displays the position of the outlet.

4. Result and Discussion

Two simulation settings have been applied in the study, namely (i) Case A: just feeding flow has been considered to model the shrinkage during solidification induced by the density difference between solid and liquid, and (ii) Case B: in addition to the feeding flow, the flow induced by the settling effect of the equiaxed phase is taken into account by including gravity force. In the following the two cases are first presented in each own and afterwards compared. The temperature field, the volume fraction of the equiaxed and columnar phase, the relative velocity between phases and the macrosegregation are shown and discussed.

4.1 Case A: Feeding Flow

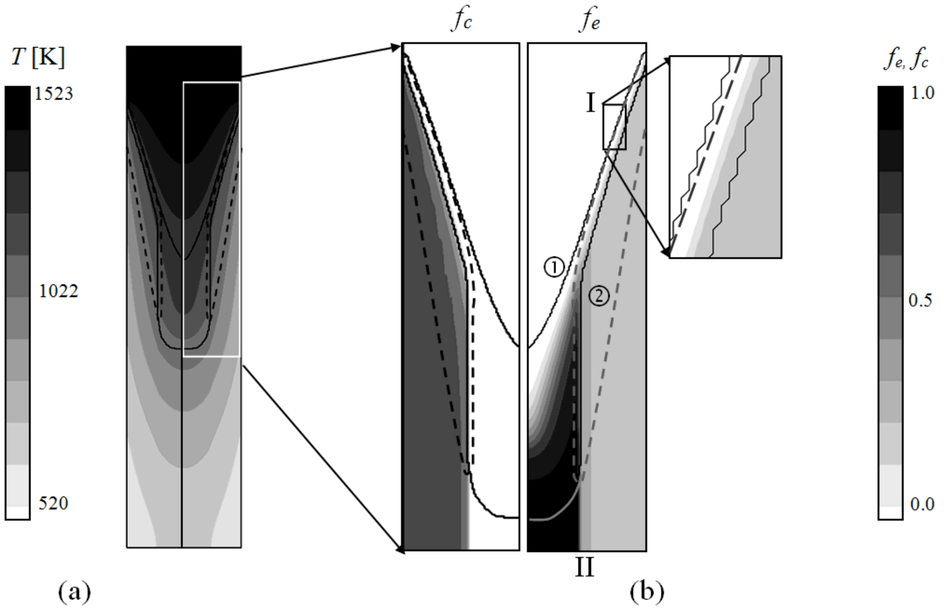


Figure 2. (a) Temperature distribution in the casting. (b) Volume fraction of columnar (left) and equiaxed (right) in the rectangle marked in (a). The solid iso-surface ① shows equiaxed grow region, and dashed iso-surface ② shows columnar grow region.

In this case study only feeding flow due to solidification shrinkage caused by density differences between liquid and solid is considered in the model. figure 2 shows the simulation results of temperature distribution and volume fraction of equiaxed (f_e) and columnar (f_c), including the equiaxed growth region marked by the solid iso-surface ① and the columnar growth region marked by the dashed iso-surface②. In figure 2b it could be seen that at the mold surface where the solidification process starts, the volume fraction of equiaxed can reach about 30%. This is due to the above stated blocking mechanism (i), which delays the growth of columnar phase with 4K undercooling, creating space for equiaxed growth. The competing growth between the two phases can be seen more clearly from the zoomed region (I) that equiaxed starts to grow earlier than columnar. Figure 2b shows that that the volume fraction of equiaxed is kept at 30% from the casting surface to columnar-to-equiaxed transition (CET) marked by (II); this is due to the blocking mechanism (iii) with which the equiaxed growth stops when the its diameter (d_e) is larger than the space between the primary dendrite arm spacing (λ_1) and the diameter of the columnar dendrite trunk (d_c). It should be noted that in reality the equiaxed grains formed near the casting surface would grow along the heat flux direction and change into columnar phase; but in the simulation the equiaxed formed is kept not changed, which is convenient for analyzing the results. In the simulation columnar-to-equiaxed transition (CET) occurs at location (II) marked in figure 2b, where the columnar growth stops because the undercooling is less than 4K again, and thus equiaxed can grow to reach volume fraction 0.49 to block the columnar dentrite tip till the end of solidification; therefore there is only equiaxed growing in the center of the casting.

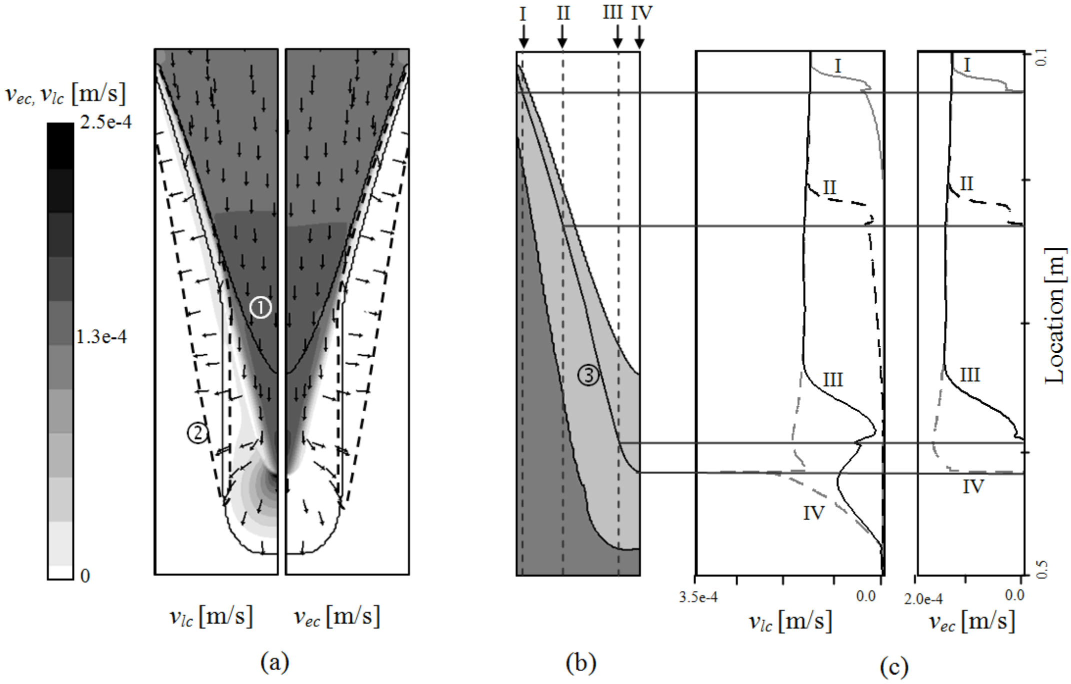


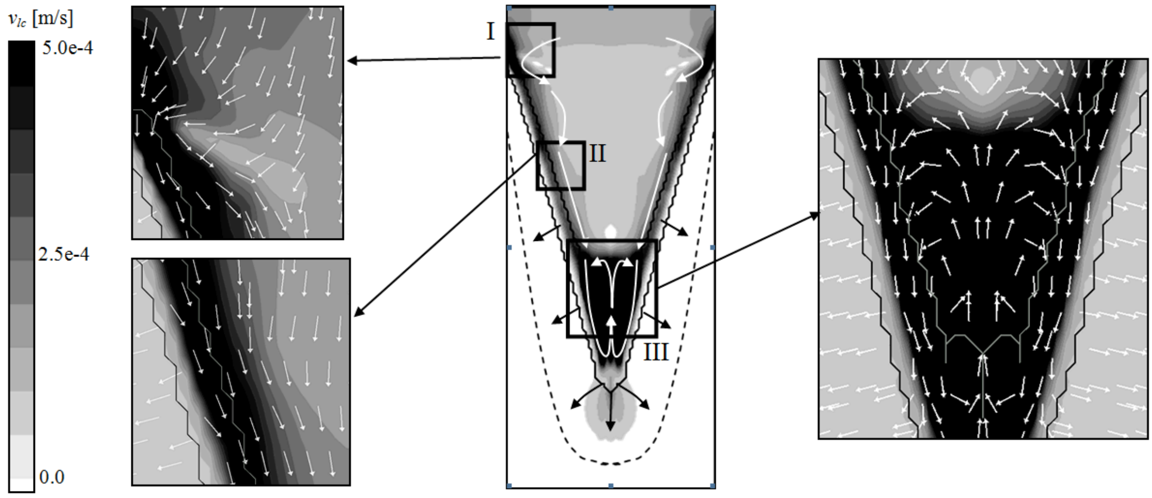
Figure 3. (a) Relative velocity between liquid and columnar v_{lc}, and between equiaxed and columnar v_{ec} in the region marked by the white rectangle in figure 2a. The magnitudes of the relative velocity are shown by the contours and the black vectors display the directions. The solid iso-surface ① shows equiaxed grow region, and dashed iso-surface ② shows columnar grow region. (b) Sketch of the liquid zone (white color), mush zone (light gray), and solid zone (dark gray). ③ marks the iso-surface of packing limit f_e+f_c = 63.7%. (c) Relative velocity plotted from top to bottom in the casting at 4 locations (marked by label I to IV).

Studying the relative velocity fields between the liquid and the solid phases, the different flow behaviour is getting obvious as shown in figure 3. In figure 3a it could be seen that the relative velocity between columnar and liquid (v_{lc}) shows the same flow pattern with the relative velocity between equiaxed and columnar (v_{ec}); this is due to the fact that the equiaxed moves with the melt before they are settled. In the upper part of the casting where no columnar phase exists the relative motion v_{lc} represents the melt flow speed-up compared to the casting speed, which is caused by the solidification-induced shrinkage of the whole casting. In reality there is no equiaxed phase in the upper part of the casting, yet in the simulation it is assumed a certain number of nucleus in each cell so the relative motion v_{ec} is presented. Close to the columnar tip front the relative motion turn directions so that v_{lc} and v_{ec} are now perpendicular to the solid fraction iso-surface and point from the dendrite tip towards their roots; this is induced by that the liquid and equiaxed try to feed the solidifying columnar region.

In figure 3b three different colored regions are displayed: the white area is the region where only liquid presents; the light grey zone shows the mushy zone where all the three phases exist; the dark grey region is full solidified without any liquid left so only columnar and equiaxed phase present. The iso-surface ③ marks the packing limit of $f_e + f_c \geq 0.647$ in blocking mechanism (iv). In figure 3c relative velocities are plotted from top to bottom in the casting at 4 locations marked by (I) to (IV). The curves plotted in figure 3c show that there are some peaks of relative velocity v_{lc} and v_{ec} as marked by the horizontal lines, which shows that the locations of peaks correspond to iso-surface③, the packing limit. These peaks can be explained as following: the mixture of liquid and equiaxed are being sucked into the mushy zone to feed the shrinkage of columnar phase before the packing limit is fulfilled; when the packing limit is reached the equiaxed grains must stop moving, but the solidification still goes on, so the liquid is accelerated to feed the reduced volume. Therefore in figure 3c it could be seen that when the packing limit is reached v_{ec} is reduced to zero, while at the same time v_{lc} shows a positive peak. It also can be observed that v_{ec} has a small peak shortly before reduced to zero; this is because that the sudden increase of liquid velocity gives the equiaxed some momentum.

4.2 Case B: Feeding Flow and equiaxed sedimentation

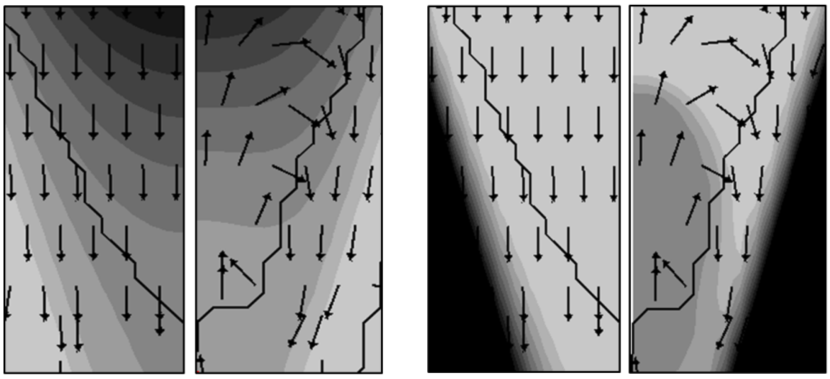
In this case study both feeding flow and equiaxed grains sedimentation are considered in the model. Figure 4 shows the flow pattern of relative velocity between the liquid and the columnar v_{lc}. Here only v_{lc} is displayed because Case A already shows that the relative velocity v_{lc} and v_{ec} has the same flow pattern. Three zoomed regions (I to III in figure 4a and figure 4c) display the detailed flow pattern with vectors showing velocity directions and contours of magnitudes. It can be seen that the movement of liquid in the equiaxed growth area is mainly influenced by the grain sedimentation. At the beginning of solidification (marked by I), equiaxed starts to grow and settle; thus additional fluid is needed to fulfill the mass conservation, which induces a first small vortex there. Afterwards (marked by II) due to grain sinking the equiaxed crystals are moving along the solidification front at the columnar dendrite tip area and continue to drag the liquid downwards. In the casting centre (marked by III) again a vortex forms transporting smaller grains upwards. In the area of columnar growth (enveloped by iso-surface②) the movement of liquid has the same pattern as in Case A, flowing from the dendrite tips towards the dendrite roots to feed the solidification shrinkage. It can be seen from the magnitude of the velocity field that the effect of sedimentation on liquid motion is remarkable stronger than that of feeding flow.



(a) (b) (c)

Figure 4. Relative velocity between liquid and columnar v_{lc} in the region marked by the white rectangle in figure 4a. The magnitudes of the relative velocity are shown by the contours with flow patterns indicated by arrows (middle). Three zoomed regions (I to III) display the detailed flow pattern with vectors showing directions (left and right).

Figure 5 compares the relative velocity v_{lc}, temperature and liquid concentration Sn for Case A and Case B at the casting center. This is to explain the simulation results in [10] that less equiaxed formed when sedimentation is included in the model and columnar can grow to the casting center. In figure 5a, it can be seen that the temperature field in Case B is lifted up compared to Case A; this is caused by the upwards movement of liquid which is induced by the vortex of equiaxed grains in casting center. Therefore the temperature is colder in Case B than in Case A in the casting center, which is one of the reasons that the growth of equiaxed is delayed. Another reason is that the vortex of equiaxed grains brings Sn-enriched liquid from the mushy zone into the bulk melt in the casting center, as shown in figure 6b; such increased liquid concentration leads to a lower liquidus temperature, which also delays the growth of equiaxed. Therefore the equiaxed starts to grow at the same time with columnar, and in the center of the casting equiaxed volume fraction is less than 0.49 so columnar is not blocked by the equiaxed.



(a) Temperature

(1000 ~ 1050 [°C])

(b) Liquid Concentration Sn

(6.01 ~ 7.00 [wt. %])

Figure 5. Comparison of (a) temperature and (b) liquid concentration for Case A and Case B at the casting center. Quantities are shown by gray levels with black for maximum and white for minimum with the ranges shown in the brackets. Vectors display directions of relative velocity between liquid and columnar. The black curve shows the start of solidification.

The predicted macrosegregation distribution of Sn in the casting was presented in the previous study [10], which showed that a positive macrosegregation formed in the center of the casting. This is caused by the equiaxed sedimentation induced vortex motion as displayed in figure 5, which brings Sn-enriched liquid from the mushy zone into the bulk melt. The study [10] also showed the macrosegregation along the outlet of the casting; a W-type macrosegregation profile was seen in both the simulation and measurement. In the simulation it is observed that most of the equiaxed grains are settled down not at the casting center, but at the locations slightly off-center where the mixture concentration is strongly reduced by their deposition, leading to the formation of W-type macrosegregation profile. The typically measured Sn profile in the measurements shows the similar macrosegregation pattern; this hints that the reasons behind the W-type macrosegregation might be the vortex movement caused by the equiaxed grains sedimentation. This proposition will be investigated by experiments in future.

5. Conclusion

A three-phase Eulerian solidification model was applied to simulate a binary CuSn6 DC casting process, which has shown the model's potential of calculating the mixed columnar and equiaxed solidification. Two cases were studied: one with feeding flow, and one with both feeding flow and sedimentation of equiaxed grains. The following conclusions are stated:

1. The developed model can be used to simulate the competing growth of columnar and equiaxed during solidification of DC casting process of bronze. Columnar grows from the mold wall towards the center of the casting, while equiaxed grow between the dentrite arms, ahead of the columnar front, and also in the bulk melt. With feeding flow the phase transition CET is predicted.
2. The simulation results show a peak of liquid velocity at the point where the movement of equiaxed grains is stopped. The phenomena behind this are: the mixture of liquid and equiaxed are being sucked into the mushy zone to feed the solidification shrinkage of columnar dentrite; as soon as the movement of equiaxed is stopped, liquid is accelerated to feed the shrinkage.
3. When sedimentation of equiaxed is added to the model, the volume fraction of equiaxed in the center of the casting is not large enough to block the columnar tip growth. The reason of less

equiaxed forming is that the sedimentation of equiaxed brings Sn-enriched liquid from the mushy zone into the bulk melt; such increased liquid concentration in the bulk melts leads to a lower liquidus temperature and hence the growth of equiaxed is delayed.

4. The sedimentation of equiaxed induces a vortex motion of both liquid and equiaxed in the center of the casting. The equiaxed grains are settled down not at the casting center, but at the locations slightly off-center where the mixture concentration would be strongly reduced by their deposition, leading to the formation of W-type macrosegregation profile. Further experiments are expected to support the proposition.

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