A 3-phase model for mixed columnar-equiaxed solidification in DC casting of bronze

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Abstract. A three-phase Eulerian approach is used to model the columnar-to-equiaxed transition (CET) during solidification in DC casting of technical bronze. The three phases are the melt, the solidifying columnar dendrites and the equiaxed grains. They are considered as spatially interpenetrating and interacting continua by solving the conservation equations of mass, momentum, species and enthalpy for all three phases. The so defined solidification model is applied to a binary CuSn6 DC casting process as a benchmark to demonstrate the model potentials. Two cases are studied: one considering only feeding flow and one including both feeding flow and equiaxed sedimentation. The simulated results of mixed columnar and equiaxed solidification are presented and discussed including the occurrence of CET, phase distribution, feeding flow, equiaxed sedimentation and their influence on macrosegregation.

1. Introduction
A common defect that occurs in direct-chill (DC) casting of bronze is macrosegregation: an inhomogeneous distribution of alloy composition that exists over the entire casting [1-3]. The main mechanism that leads to formation of macrosegregation is a relative motion between liquid and solid in the mushy zone, caused by i.e. feeding flow, thermal-solutal convection, forced convection, grain sedimentation, etc. Some modeling works for two phases solidification (liquid and columnar) considering binary and ternary alloys have been carried out by the authors [4-6]. The corresponding simulation results are in qualitatively good agreement with experimentally obtained macrosegregation profiles for small castings, which are usually made at the laboratory scale.

In recent years, a 3-phase model for mixed columnar-equiaxed solidification was developed for ingot casting by the authors [7-9]. In this model the competitive growth of columnar and equiaxed phase, melt convection, equiaxed grain sedimentation, and their influence on the species transport and macrosegregation are taken into account. In the present study, this model is adapted and applied to the benchmark DC casting of bronze. Two cases are studied: one considering only feeding flow and the other including both feeding flow and equiaxed sedimentation. The simulated results are presented and some important findings are raised.

2. Benchmark definition and model description
The presented model is applied to a benchmark simulation of DC casting process as displayed in figure 1. Here ① gives the position of the inlet where a pressure inlet and a casting temperature of T_{cast} = 1523 K are taken, ② marks the upper part of the mold which is assumed to be insulating, ③ shows the lower part of the graphite mould surrounded by a copper mold with h = 3000 Wm^{-2}K^{-1} and

$T_{lower—mold}$ = 550 K, ④ indicates a water cooling system with h = 3000 Wm^{-2}K^{-1} and T_{water} = 300 K, and ⑤ displays the position of the outlet with a casting velocity of $\vec{u}_{cast}$ = 1.44 mm s^{-1}. Calculations were done for the binary alloy CuSn6. A 2D symmetric simulation has been performed.
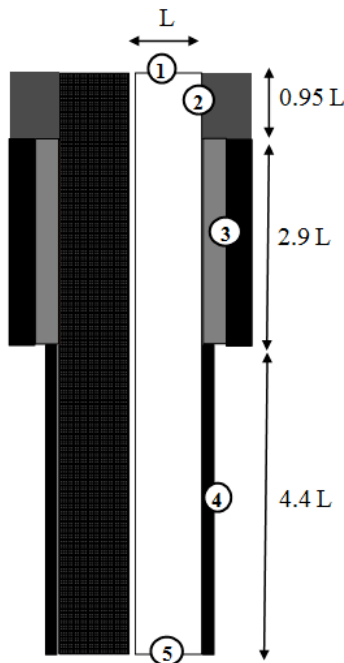

Figure 1. Configuration of the benchmark

The main assumptions of the 3-phase model are:

- The considered three phases are: the melt (*l*), the columnar dendrite trunks (*c*), and the equiaxed grains (*e*) with corresponding volume fractions f_l, f_c and f_e.

- Columnar dendrites are approximated by growing cylinders starting from the mould wall towards the casting center.

- Equiaxed grains are approximated as spheres. A constant number density of 10^{12} m^{-3} is initialized.

- Growth of the columnar and equiaxed is governed by diffusion.

- The permeability in the columnar mush is modeled according to Blake-Kozeny, while the drag law between the melt and equiaxed phase is modeled according to Kozeny-Carman [10].

- The columnar primary dendrite tips grow with the isotherm of an undercooling ΔT of 4 K.

- Growth of columnar primary tips is stopped when the volume fraction of equiaxed phase in front of them reaches to 0.49 (hard blocking criterion) [11].

- The equiaxed phase is not allowed to grow if its diameter is larger than the inter-columnar space.

- Packing limit for the equiaxed phase is set as $f_e + f_c \geq 0.637$ [12], and [13] the equiaxed crystals are trapped and forced to move with the columnar phase when the trapping limit of $f_c \geq 0.2$ is reached.

- The Boussinesq approach is used to model the grain sedimentation. The momentum exchange due to drag is modeled by using the Blake-Kozeny approach [13].

3. Results and discussion

3.1. Case A: Feeding flow

In this case only feeding flow due to solidification shrinkage is considered. Figure 2a shows the temperature distribution including the isolines of zero liquid-to-equiaxed mass transfer rate M_{le} = 0 ① and zero liquid-to-columnar mass transfer rate M_{lc} = 0 ②. The isoline ① envelops a region where equiaxed crystals grow, while the isoline ② envelopes a region where columnar trunks grow. Figure 2b shows the distribution of the two solid phases. It can be seen that the equiaxed phase starts to grow in front of the columnar phase. As soon as the undercooling ΔT = 4 K is reached, the columnar phase is allowed to grow. Because the growth of columnar is limited by ΔT = 4 K, equiaxed phase growing from the casting surface can reach to the volume fraction about 30% till the transition region between the two phases. In reality the equiaxed grains formed near the casting surface would grow along the heat flux direction and change into columnar phase. But for analyzing the simulation results, we keep the volume fraction of the equiaxed phase as it forms. In the center of the casting the growth of columnar phase is stopped by the large amount of equiaxed grains and only equiaxed phase is present till the end of solidification.

Figure 2c shows the relative velocity between the liquid and the columnar phase (v_{lc}). The region of ③ displays the mushy zone including both columnar and equiaxed, and the gray line ④ indicates the

packing limit of $f_e + f_c = 0.637$. 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. This speed-up is caused by the solidification-induced shrinkage of the whole stand. Close to the columnar tip front the relative motion turns so that v_{lc} is now perpendicular to the solid fraction isolines and points from the dendrite tip towards their roots. Note that right at the center v_{lc} increases heavily below the packing limit (gray line ④ in figure 2c). This is caused by the fact that in the totally equiaxed region solidification-induced feeding above the packing limit happens by a collective motion of liquid and equiaxed grains. At the packing limit the equiaxed grains are stopped and so mass flow conservation accelerated the liquid. A similar phenomenon happens at the limit where the equiaxed grains are stopped by the presence of $f_c \geq 0.2$ of columnar dendrites (trapping limit).

The predicted macrosegregation, based on the 3-phase model with only feeding flow, is shown in figure 3. Figure 3a displays the macrosegregation pattern in the region marked by the rectangle domain in figure 2a. Figure 3b shows the macrosegregation plotted along the outlet. It can be seen that there is a positive macrosegregation appearing at the casting surface and a negative one in the center, as it is already discussed in literature for the two phase simulation [14]. The remarkable difference is that in the columnar-to-equiaxed transition (CET) region a strong negative macrosegregation peak is predicted in the present case. This is caused by the difference in the drag force of the columnar and the equiaxed region. The melt being sucked into the mush by solidification-induced feeding is locally choosing the path with the smaller resistance. Thus, a slight change of liquid velocity is induced for the flow along the vertical CET line, leading to the formation of a negative macrosegregation peak in this region.
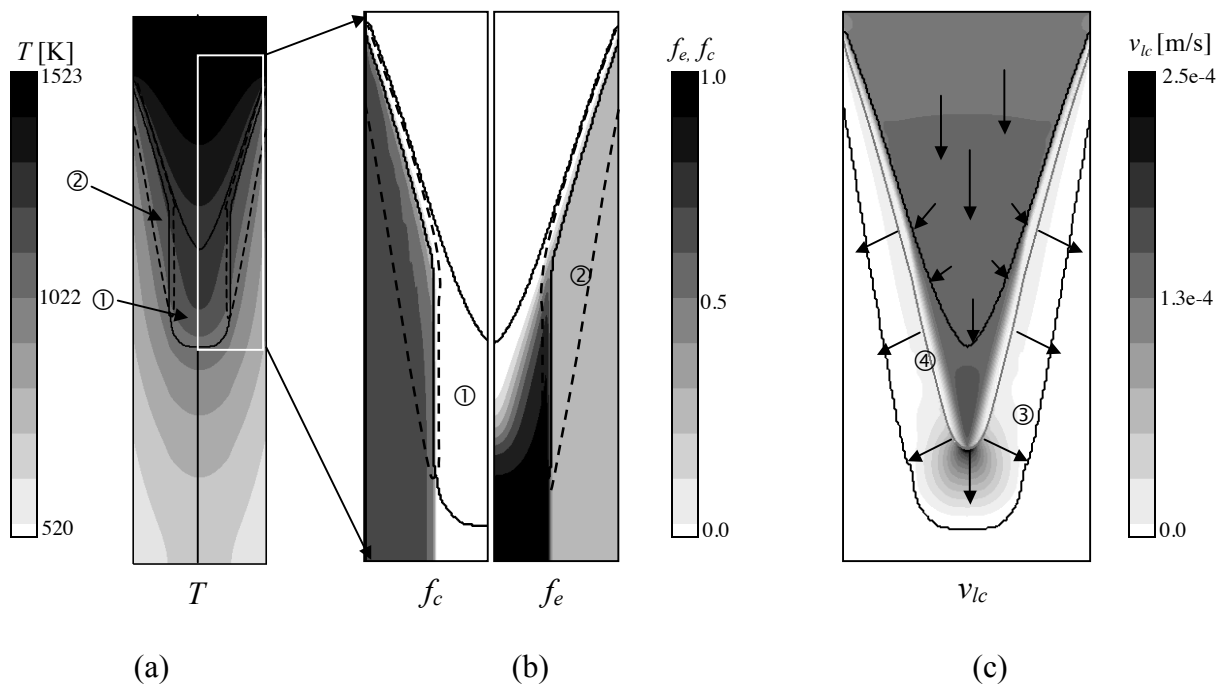

Figure 2. Simulation result of Case A: (a) temperature distribution and (b) volume fraction of equiaxed f_c (left) and columnar f_e (right) in the rectangle domain marked in (a). The solid line ① shows isoline of $M_{le} = 0$, and broken line ② shows $M_{lc} = 0$. (c) Relative velocity v_{lc} between the liquid and the columnar phase. Magnitude of v_{lc} is displayed in gray scale. The direction is shown by arrows. The region marked with number ③ is the mushy zone of both columnar and equiaxed within the two black lines, and the gray line ④ marks the packing limit $f_e + f_c = 0.637$.

3.2. Case B: Feeding flow and grain sedimentation
In Case B sedimentation of equiaxed grains is added to the model assumptions of Case A. Figure 4a shows the temperature distribution including the isolines of $M_{le} = 0$ ① and $M_{lc} = 0$ ②. The isoline ① envelops a region where equiaxed crystals grow, while the isoline ② envelopes a region where columnar trunks grow. Figure 4b shows the distribution of the two solid phases. It can be seen that when sedimentation of equiaxed is added in this specific benchmark, no columnar-to-equiaxed transition (CET) occurs and both, the columnar and equiaxed, grow in the whole casting domain. The volume fraction of equiaxed cannot reach the hard blocking criterion 0.49 before the columnar tips are present. The reason of less equiaxed forming in the casting center in comparison to the Case A is that the sedimentation of equiaxed is bringing Sn-rich liquid from the mushy zone into the bulk melt, resulting in the increased liquid concentration in the bulk melt. This will lead to a lower liquidus temperature and hence the growth of equiaxed and columnar is delayed. As the hard blocking criterion for CET is not met, columnar growth can now extend to the casting center.
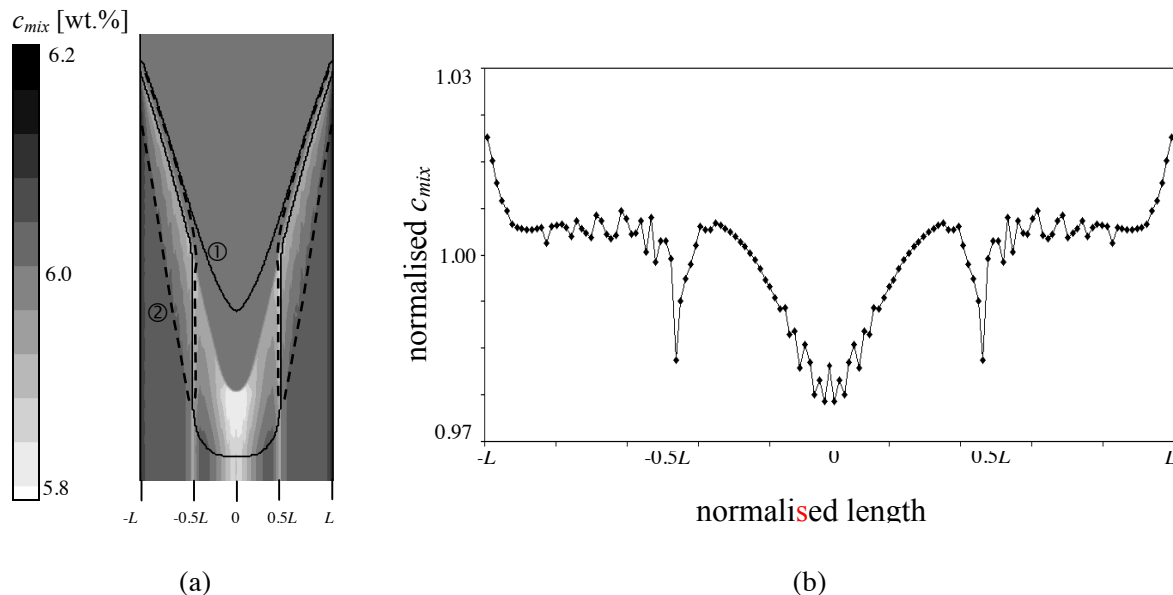

(a)   (b)

Figure 3. Predicted macrosegregation (c_{mix} of Sn in wt.%) of Case A: (a) macrosegregation pattern and (b) c_{mix} plotted along the outlet. Solid line ①: $M_{le} = 0$, dash line ②: $M_{lc} = 0$.

Figure 4c shows the relative velocity, v_{lc}, between the liquid and the columnar with arrows indicating its direction, and the magnitude of v_{lc} is shown by the grey scale. 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. Therefore, additional fluid is needed to fulfill the mass conservation, which induces a first small vortex.

Afterwards (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 centre (III) again a vortex forms transporting smaller grains upwards. In the area of columnar growth (enveloped by line ②) 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.
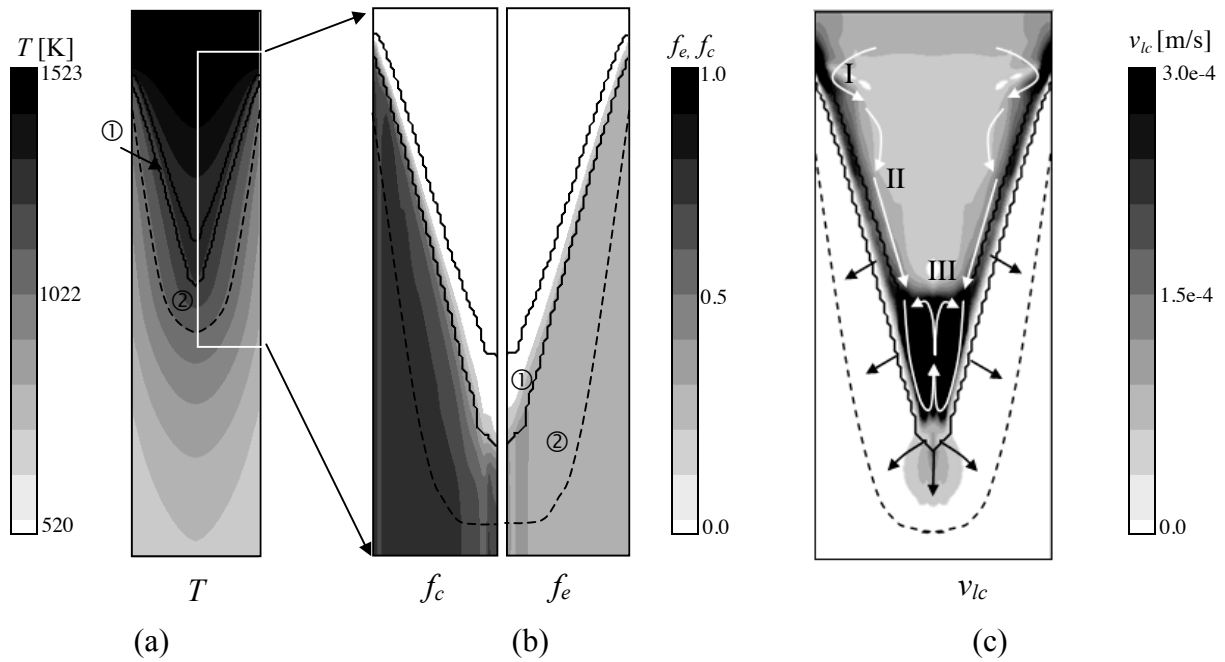
Figure 4. Simulation result of Case B: (a) temperature distribution and (b) volume fraction of equiaxed f_c (left) and columnar f_e (right) in the rectangle domain marked in (a). The solid line ① shows isoline of $M_{le} = 0$, and broken line ② shows $M_{lc} = 0$. (c) Relative velocity v_{lc} between the liquid and the columnar phase. Magnitude of v_{lc} is displayed in grey scale; the arrows indicate the direction.
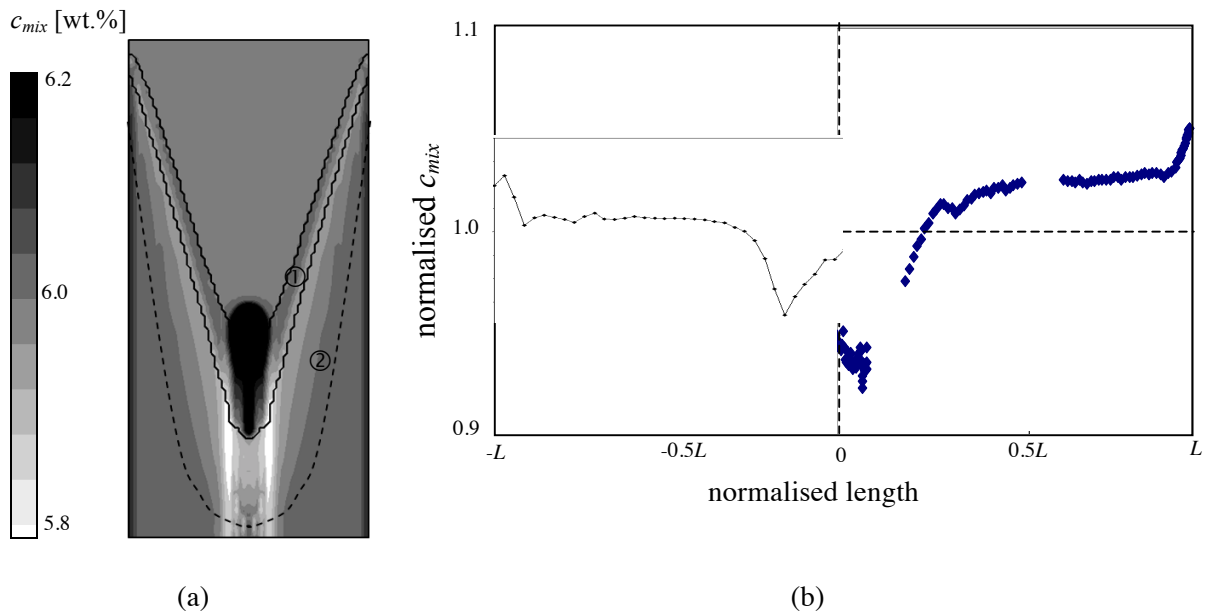

Figure 5. Predicted macrosegregation (c_{mix} of Sn on wt.%) of Case B: (a) macrosegregation pattern and (b) comparison of the calculated c_{mix} along the outlet (left) with the measured c_{mix} in a CuSn7.6P0.022 round strand (right). Solid line ①: $M_{le} = 0$, dash line ②: $M_{lc} = 0$.

Figure 5a shows the predicted macrosegregation distribution in the strand and plotted along the outlet. It can be seen that the liquid is enriched in solute in the center of the casting indicated by the black region in figure 5a. This is caused by the sedimentation induced vortex motion of liquid, which brings Sn-enriched liquid from the mushy zone into the bulk melt. Another interesting phenomenon is

the W- type macrosegregation profile as shown in figure 5b. This is due to the fact the most equiaxed grains are settled down not at the casting center, but at the locations slightly off-center where the negative macrosegregation is reduced by their deposition, leading to the formation of W-type macrosegregation profile. The typically measured Sn profile in the casting process shown in the left part of figure 5b is very similar to the simulation results, which hints that the reasons behind the W-type macrosegregation might be the vortex movement caused by the equiaxed sedimentation.

4. Conclusions

A three-phase Eulerian solidification model was applied to simulate a binary CuSn6 benchmark for a DC casting process. Two cases were studied: one with feeding flow, and one with feeding flow and sedimentation of equiaxed grains. Following conclusions are made:

1. The developed model can be used to simulate the competing growth of columnar and equiaxed during continuous casting process of bronze. In the case of only feeding flow, a phase transition from columnar to equiaxed (CET) is predicted.

2. Near the CET region there is a strong negative c_{mix} induced by the different drag laws in the columnar and the equiaxed region.

3. The sedimentation of equiaxed induces a vortex motion of both liquid and equiaxed in the center of the casting. The typically measured Sn profile in the casting process is very similar to the simulation results, which hints that the reasons behind the W-type c_{mix} might be the vortex movement caused by the equiaxed sedimentation. Further experimental evidences are sought to support the proposition.

Acknowledgements

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