Advanced Materials Research Vols. 154-155 (2011) pp 1415-1418
Online available since 2010/Oct/27 at www.scientific.net
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doi:10.4028/www.scientific.net/AMR.154-155.1415

Numerical study of the thermosolutal convection induced macrosegregation during columnar solidification

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Keywords: macrosegregation, convection, solidification, modelling

Abstract. As a response to "call for contribution to a numerical problem for 2D columnar solidification of binary alloys" [Bellet et al., Int. J. Therm. Sci., Vol. 48(11)(2009), p. 2013], the macrosegregation in a Pb-18wt.%Sn benchmark casting is numerically studied with a two-phase columnar solidification model developed by the current authors. The studies were done with 2D calculations in response to the call, and a 3D calculation was performed to confirm the consistency with the 2D case. A grid-sensitivity study was done to ensure the reliability and accuracy of the present results. The segregation mechanism due to thermosolutal convection was analyzed and the uncertainties resulting from the inaccurate thermophysical properties, modelling and process parameters are discussed. The numerical model was evaluated by comparison with experiments.

Introduction

Macrosegregation, a measureable inhomogeneity of concentration in the scale of a casting, is often occurring in metal casting. Macrosegregation has a certain impact on the final mechanical properties of the castings and its prediction is of high relevance. The origin of this defect is due to different bulk and interdendritic flow phenomena caused by thermosolutal convection, feeding of the solidification shrinkage, grain sedimentation, or thermal/mechanical deformation of the solidified skeleton. The appearance of macrosegregation in the cast products is also diverse, due to the complexity of the above mentioned flow phenomena, which is still challenging for the research in this field. With the enhanced computational power, many numerical models have been developed, trying to predict the macrosegregation quantitatively. As the macrosegregation is extremely sensitive to the model assumptions and the resolution of the flow details, quantitative evaluation of those modelling approaches is expected. Therefore, a benchmark problem was proposed recently by Bellet et al. [1] to verify and valid the mathematical models and numerical codes. The benchmark focuses on the macrosegregation induced by thermosolutal convection. This paper presents a contribution to that call with a columnar solidification model developed by the authors [2-4].

The Benchmark Problem and Numerical Model

The benchmark configuration together with necessary boundary and initial conditions are shown in Fig. 1a [1]. A two-phase columnar solidification model [2-4] is used. The model simplifications and process conditions are summarized as follows:

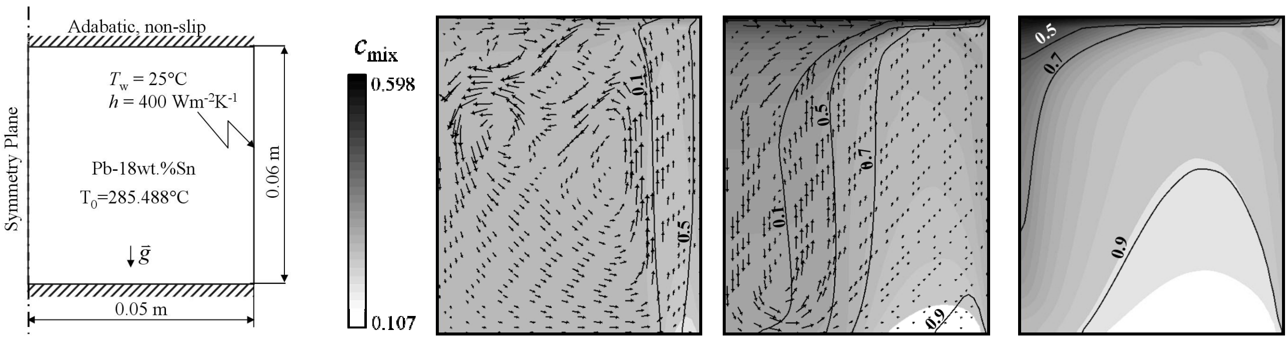
- Mold filling is ignored. Solidification starts with an initial temperature of 285.5 °C and a melt concentration of Pb-18 wt.%Sn;
- Two phases are considered, namely the melt and columnar phase. No equiaxed grains nucleate in the calculation domain;
- The columnar dendrite morphology is approximated by step-wise growing cylinders with constant (primary arm) spacing and the growth rate of the columnar phase is governed by diffusion around the cylindrical trunk;

- The columnar trunks start to grow from the right side of the wall, the columnar tip front is assumed to be coincided with the liquidus temperature isotherm;
- Solidification shrinkage is ignored and the Boussinesq approach is used for thermosolutal convection;
- Thermophysical properties and thermodynamic parameters are given in literature [1].

Results

Solidification Sequence. The solidification sequence of the benchmark is shown in Fig. 1b-d. The final macrosegregation (c_{mix}) pattern predicted is shown in Fig. 1d: a small region with positive c_{mix} is found in the upper surface area and in the lower part a large negative one is predicted.

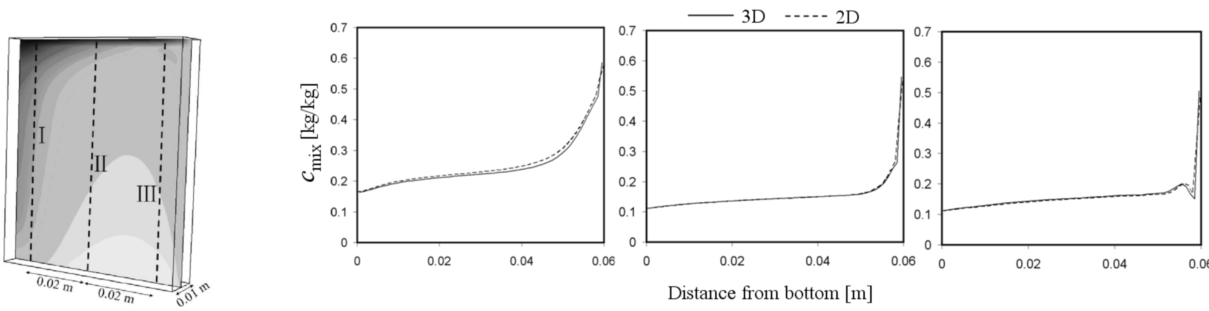
The solidification sequence shows that the volume fraction of the columnar phase (f_c-isolines) moves from the cold wall towards the bulk melt region. The solute (Sn)-enriched interdendritic melt has a lower density, and thus rises upwards in the two-phase mushy zone, while the bulk melt in front of the mushy zone sinks downwards. The melt near the columnar tip with lower temperature might sink and thus partially compensate or reverse the above mentioned convection pattern. However, with the given temperature and solute gradient, the solutal buoyancy dominates over the thermal buoyancy. The upward flow in the mushy zone and the downward flow in the bulk melt are the primary phenomena leading to the final macrosegregation.



(a) (b) at 15 s (c) at 150 s (d) at 430 s

$v_{\ell,\,max}$ = 5.5 mm/s, c_{mix}: 0.134 ~ 0.252 | $v_{\ell,\,max}$ = 0.82 mm/s, c_{mix}: 0.110 ~ 0.505 | $v_{\ell,\,max}$ = 0, c_{mix}: 0.107 ~ 0.598

Fig. 1 (a) Configuration of the benchmark problem [1]. (b-d) Solidification sequence at 15 s, 150 s and 430 s. The evolution of macrosegregation c_{mix} is shown in gray scale, liquid velocity v_ℓ in vectors and f_c in iso-lines.

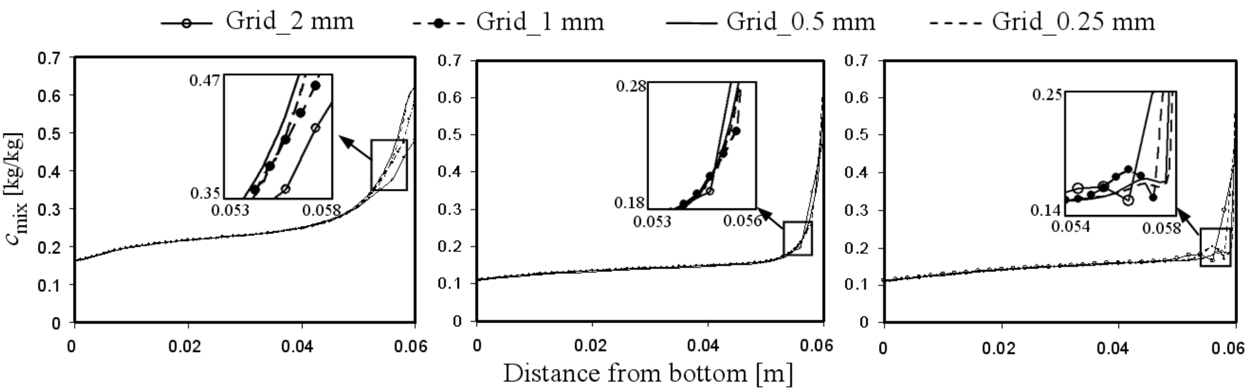


(a) (b) Position I (c) Position II (d) Position III

Fig. 2 Comparison of 2D and 3D calculations. (a): Predicted c_{mix} at the mid-cross section in the 3D domain. (b-d): Comparison of the c_{mix} profiles of the 2D and 3D results along lines I to III marked in (a).

3D Simulation. Although 2D calculation is requested by the call [1], the real situation of the experiment is 3D, which may have more complex flow and result in different c_{mix} pattern. For this reason, we have done a 3D calculation and compared it with the 2D case. The predicted c_{mix} in 3D is displayed on the mid-cross section of the benchmark (Fig. 2a). Comparisons between 2D and 3D simulation results are shown in Fig. 2b-d taken along lines I to III marked in Fig. 2a. It can be seen that 2D and 3D results show minor differences. Therefore it can be concluded that 3D flow does not affect the c_{mix} for the current case and the 2D calculation is suitable for this study.

Grid Study. The effect of mesh size on the segregation prediction is studied. Simulations are made with different mesh sizes: 2, 1, 0.5 to 0.25 mm. In Fig. 3, c_{mix} profiles along lines I to III (marked in Fig. 2a) with different mesh sizes are plotted. In most region the mesh size has almost no influence on the c_{mix} profile, while in the upper part (close to the top surface) significant difference of c_{mix} is seen, especially when coarse grid (>1 mm) is used. This study suggests that it is enough to resolve the current problem with a mesh size less than 0.5 mm.



(a) Position I (b) Position II (c) Position III

Fig. 3 Comparison of c_{mix} calculated with a grid size varying from 2 mm to 0.25 mm plotted along lines I to III marked in Fig. 2a.

Discussion

Mechanism. According to our previous work [5], with the assumption of stationary solid and no solidification shrinkage, the evolution of the c_{mix} in the mushy zone can be expressed as:

$$\frac{\partial c_{mix}}{\partial t} = -f_\ell \vec{u}_\ell \cdot \nabla c_\ell \, . \tag{1}$$

The evolution of c_{mix} depends on the flux of the interdendritic melt flow $f_\ell \vec{u}_\ell$ and the gradient of the liquid concentration ∇c_ℓ. If both vectors $f_\ell \vec{u}_\ell$ and ∇c_ℓ point in the similar directions (the angle between the two vectors is smaller than 90°), it leads to decrease in the local c_{mix}, i.e. $\partial c_{mix} / \partial t < 0$. As shown in Fig. 4, this occurs in the lower part of the cavity. In other words solute-poor melt replaces the solute-rich melt in this region, and thus, leads to negative macrosegregation. In the opposite situation, if $f_\ell \vec{u}_\ell$ and ∇c_ℓ point in the opposite direction, it leads to an increase in c_{mix}, and this mechanism operates in the upper part of the cavity.

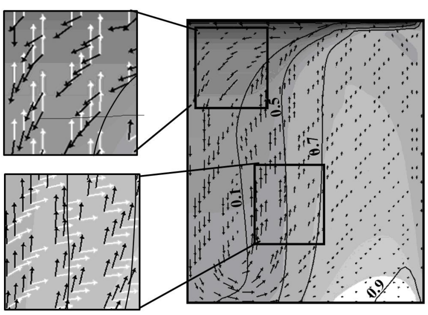


Fig. 4 Analysis of the formation of c_{mix} at 150 s. Black arrows: $\vec{u}_\ell$. White arrows: ∇c_ℓ.

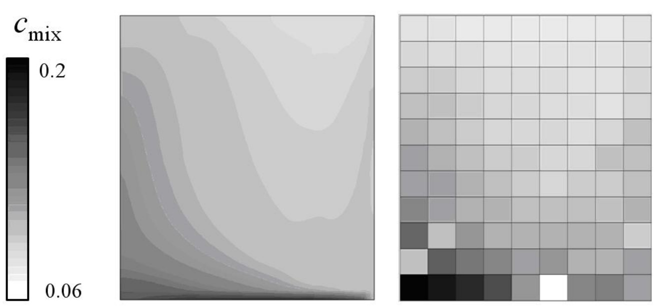


Fig. 5 Simulation of the c_{mix} in a Sn-10wt.%Bi casting (left) and compared with the experimental result (right) [6].

Uncertainties and Further Experimental Evaluation. Although the accuracy of the calculation was controlled to ensure that the presented numerical results represent the converged solution of the benchmark as defined by the call [1], these results can only be an approximation of the reality. The difference between the model and the real casting is thought to be caused by two aspects: first the benchmark is limited to thermosolutal convection and, second there are uncertainties regarding to the applied physical properties, permeability law of the mushy zone and process conditions. For example, people found stripe-like channel segregates in the experimental Pb-Sn castings with the similar configuration as the current benchmark [6-8] which are also predicted by some models [8,9]. However, no such kind of segregation is observed in the current benchmark, because the liquid velocity field, especially in the liquid-solid two-phase region, is quite stable and no remelting phenomenon is predicted.

Some additional parameter studies were made intentionally to enhance the flow intensity and instability, e.g. with artificially increased permeability of the mush zone. In this case instable flow near the front of the mush zone was obtained, and the similar stripe-like segregates were predicted. It implies that the channel segregation can also be predicted by the current model when the process conditions and physical parameters are in favor of instable flow.

It is worth mentioning that the current model has predicted similar c_{mix} distribution as Quillet et al. observed in the experiment [6]. The simulated c_{mix} is compared with the experimental result for Sn-10wt.%Bi in Fig. 5. For this alloy, the solute enriched interdendritic melt has a higher density, and thus flows downwards, resulting in positive c_{mix} in the lower part and negative one in the upper part.

Conclusions

The macrosegregation in a Pb-18wt.%Sn benchmark [1] is numerically simulated with a two-phase columnar solidification model. The macrosegregation pattern from the lower cold corner (negative segregation) towards the upper hot corner (positive segregation) is predicted. The segregation caused by thermosolutal convection can be analyzed by $\partial c_{\mathrm{mix}} / \partial t = -f_\ell \vec{u}_\ell \cdot \nabla c_\ell$, that is, when $f_\ell \vec{u}_\ell$ and ∇c_ℓ point in the same direction negative segregation tends to form, and when they point in opposite directions positive segregation tends to form. With a mesh size less than 0.5 mm grid-independency of the numerical result is verified for the current benchmark. 3D calculation is consistent with the 2D calculation. Some uncertainties caused by thermophysical properties, modelling and process parameters in this benchmark problem are discussed. Finally a Sn-10wt.%Bi casting is simulated, and predicted segregation shows a reasonable agreement with the experiment [6].

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Materials Processing Technologies
doi:10.4028/www.scientific.net/AMR.154-155

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