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Front tracking based macroscopic modeling of equiaxed and columnar zones in a binary alloy solidification

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Abstract

The Front Tracking based computer simulation model of solid-liquid phase transition driven by diffusion and thermo-solutal natural convection is presented, and its predictions are verified and validated by comparison with the data obtained from the other available numerical solution and the experimental study. The front tracking approach, based on local dendrite tip kinetics, is capable of distinguishing zones of columnar mush and of equiaxed grains and, thus, provides means for more precise modeling of binary alloy solidification.

Keywords: Front Tracking, binary alloy, solidification.

1. Introduction

Solidification of a binary alloy is a very complex multi-scale phenomenon where a two-phase solid-liquid region (referred to as a mushy zone) develops. It consists of two different grain structures, i.e.: columnar dendrites in the form of a dense anisotropic crystalline-like matrix immersed in an inter-dendritic liquid and equiaxed grains, which can freely grow in the under-cooled liquid, impinge and float in the liquid phase or drop down due to both density differences of the solid and liquid phases and thermo-solutal buoyancy forces. The distinct morphologies of these two grain structures cause problems in the numerical modeling of binary alloy solidification – as it requires both: special techniques to distinguish the columnar and equiaxed zones and application of different simulation models in each of these regions. In the commonly used enthalpy-porosity model of transfer phenomena in the mushy zone [1, 2] the interface between the columnar dendrites region, growing from the cooled walls into the superheated melt, and the equiaxed grain region developing in the under-cooled and solute reach liquid, is not directly tracked. These two different structures are distinguished by checking the solid volume fraction [3, 4]. When it exceeds a characteristic value, called the coherency point and known from theoretical and/or experimental analysis, the structure is treated as a stationary columnar mush and modeled as a Darcian porous medium [4]. Otherwise, an equiaxed grain structure forms and is modeled by a dispersed slurry of crystals in a liquid phase [3, 4].

Recently, a special Front Tracking (FT) method on a fixed control-volume grid was developed, [5–7] where local dendrite tip kinetics (known from theory and experiments) is used to track a set of mass-less marker particles, which approximates the current shape of the columnar dendrite tips curve. Thus, this FT approach is potentially capable of directly dis-

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tinguishing between the columnar mush and the under-cooled liquid/equiaxed region developing ahead of the dendrite tip curve. Having identified both these regions at any point in the solidification process, different computational models can be used in each of them.

The paper presents the modified FT application in macroscopic modeling of non-equilibrium solidification of a metallic binary alloy driven by conduction and thermo-solutal natural convection, where the columnar mush and equiaxed zone are identified through the front tracking procedure. The main modification issue lies in the use of the macroscopic Front Tracking algorithm to detect one of the porous or slurry zones, to implement a proper flow model. Additionally, the front displacement dependent source terms in the energy equation, responsible for the energy generation due to solidification and characteristic for the Front Tracking method [5–7], were exchanged to source terms characteristic for the enthalpy model. This new numerical model, called Enthalpy Porosity & Front Tracking model (EP-FT), is further verified and validated for the case of solidification of alloy Pb-48 wt.% Sn by comparing its predictions with the other available numerical solution [8] and experimental data [9].

2. Mathematical model and computer simulation

The mathematical model, based on the volume averaging theory [10, 11], consists of mass, momentum and energy conservation equations for the solid-liquid mixture, and for species mass fraction in the mixture [11]. Following [12], two different forms of the mixture momentum equation are used, respectively, in the columnar mush and the completely solid phase (Eq. 1), and in the liquid and the slurry regions (Eq. 2), where x_i, V, u_i, p, T, C, ρ, μ_L, g_i, f, r, β_T, β_C and K stand respectively, for the *i-th* Cartesian coordinate, mixture velocity vector, component of the velocity in the *i-th* direction, pressure, temperature, solute (tin) mass fraction, density, dynamic viscosity of liquid, component of the gravity vector, mass solute fraction, volumetric solute fraction, thermal expansion coefficient, the solutal expansion coefficient and the permeability coefficient of a porous medium model. Subscripts i, S and L refer to *i-th* component of the vector, the solid phase and the liquid phase, respectively.

The conservation equations are supplemented with closure assumptions: local thermodynamic equilibrium at the interface, linking between the $T - C_L - g_s$ fields in a way supplied in [13], the Carman-Kozeny model of porosity, equal phase velocities [12] and density described by the relation taken from [12] in the slurry region.

To distinguish the zones of columnar and equiaxed dendrites at any point in the solidification process, the front tracking procedure on a fixed control volume grid, recently developed [5–7], is adopted. Details of the front tracking technique are available elsewhere [5–7]. A crucial issue in the FT approach is the proper choice of dendrite tip kinetics, which can be obtained experimentally and/or through a theoretical analysis based on an assumed shape of the dendrite tip and on the solution of transport equations in the vicinity of the dendrite tip [5, 14, 15]. In the calculations presented lather in this paper, the marker velocity w, is assumed, according to the KGT dendrite tip kinetics [15], in the approximated polynomial form

$$w = 1.6891 \cdot 10^{-7} \triangle T^2 + 1.21745 \cdot 10^{-7} \triangle T^3 \quad (3)$$

The macroscopic conservation equations are discretised on a fixed control-volume grid with the power-law *upwinding* scheme [16]. Mutually linked pressure and velocity fields are iteratively computed with the SIMPLE algorithm [16]. The fully implicit time marching scheme is used and the inner iteration loop, matching temperature and species mass fraction fields (linked through the *phase diagram*), is based on the algorithm given in [13].

3. Model verification and validation

To verify the presented numerical model, an example problem of the Pb-48 wt.% Sn solidification in a rectangular cavity was calculated. Details of mould geometry, boundary conditions and physical properties of the alloy can be found in [8]. For the purpose of comparison, the classical Enthalpy-Porosity

$$\frac{\partial}{\partial t}(\rho u_i) + \nabla \cdot (\rho V u_i) = \nabla \cdot (\mu_L \nabla u_i) - \frac{\mu_L}{K}\left[u_i - (u_S)_i\right] - r_L \rho_L g_i \left[\beta_{T,L}\left(T - T_{ref}\right) + \beta_{C,L}\left(C_L - C_{ref}\right)\right] - g_L \frac{\partial p}{\partial x_i} \tag{1}$$

$$\begin{aligned}\frac{\partial}{\partial t}(\rho u_i) + \nabla \cdot (\rho V u_i) = {} & \nabla \cdot (\mu_L \nabla u_i) - \nabla \cdot \left[u_L f_S \nabla (u_S)_i\right] \\ & + \nabla \cdot \left[u_S r_S \nabla (u_s)_i\right] - \nabla \cdot \left[\left(\frac{\rho f_S}{f_L}\right)(V - V_S)\left(u_i - (u_S)_i\right)\right] \\ & - r_S \rho_S g_i \left[\beta_{T,S}\left(T - T_{ref}\right) + \beta_{C,S}\left(C_S - C_{ref}\right)\right] \\ & - r_L \rho_L g_i \left[\beta_{T,L}\left(T - T_{ref}\right) + \beta_{C,L}\left(C_L - C_{ref}\right)\right] - \frac{\partial p}{\partial x_i}\end{aligned} \tag{2}$$

(EP) model [1] was used primarily, where the momentum equation, (Eq. 1), was valid in the whole analyzed domain. Next, calculations were performed using the proposed Enthalpy Porosity & Front Tracking (EP-FT) approach, where the momentum transfer was described by both (Eq. 1) and (Eq. 2), in the columnar mush and in the rest of the domain respectively. The EP model predictions were compared with the numerical results of Ahmad et al. [8] and a very similar streamlines pattern was obtained.

Next, the EP and EP-FT models were validated by comparison of the calculated 2D macro-segregation pattern for the Pb-48 wt.% Sn alloy with the pertinent experimental data presented in [9].

Fig. 1 shows the relative tin mass fraction changes in a completely solidified alloy along horizontal lines at six selected heights measured from the bottom of the cavity (shown in meters above the plots in Fig. 1) and the length is measured from the left cooling surface. Slightly better agreement with the experiments is observed in the proposed EP-FT model. The relative tin mass fraction $\overline{C}$ was defined with the formula $(C - C_o)/C_o \cdot 100\%$, where C_o was the nominal mass fraction of tin.

Finally, to address the relevance of the slurry flow in front of the columnar dendrite tips and its impact on the flow pattern and macro-segregation in the solidifying alloy, two different models of the mushy zone (relate to the EP and EP-FT models) were used in calculations of the Pb-48 wt.% Sn solidification in a rectangular cavity. The comparison of the relative solute (tin) mass fraction field after 150 s. of the solidification for both EP and EP-FT simulations are shown in Fig. 2. Similarly, the calculated streamlines pattern with both models is shown in Fig. 3. The calculations performed show considerable differences in the flow structures and in the tin mass fractions and, in effect, the significance of the proper choice of the porous/slurry model in the two-phase zone.

Convective flow is much stronger in the presence of floating dendrites – the EP-FT model (compare $|\psi_{max}|$values in the Fig. 3 caption). This is caused by the assumption of stationary dendrites in the whole mushy zone (the EP model), which implies the development of a large porous region weakening the strength of the natural convection.

The presence of the slurry region in front of columnar dendrites radically changes the flow pattern in the mould and the resulting macro-segregation picture. The fluid flow field obtained with the EP model is mainly thermally driven, but in the EP-FT model the flow is solute driven in the columnar dendrites zone and thermally driven in the mushy/liquid zone. A good solute mixing in the slurry region, as predicted by the EP-FT model, is observed. It is evident this phenomenon promotes high values of the final solute fraction in an upper part of the cavity, where the liquid solidifies last, and is a probable reason for the higher values of relative tin mass fraction predicted by the EP-FT

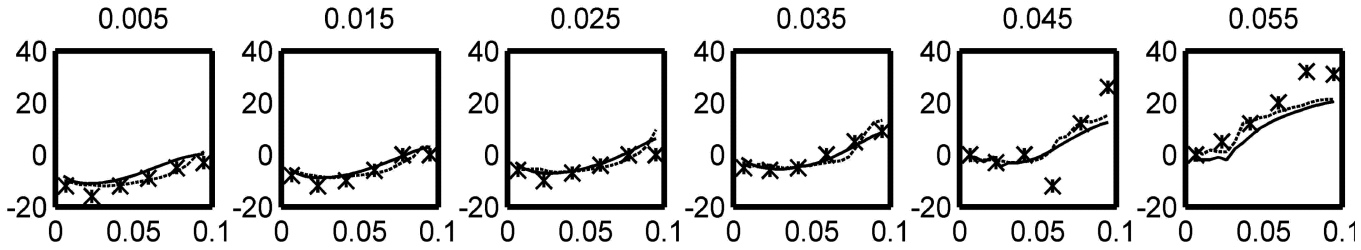

Figure 1: Relative tin mass fraction $\overline{C}$ distributions in the completely solidified alloy Pb-48 wt.% Sn along several horizontal lines distributed in the longitudinal symmetry plane of the ingot. Solid line – the EP model, dashed line – the EP-FT model, crosses – experimental data [9]

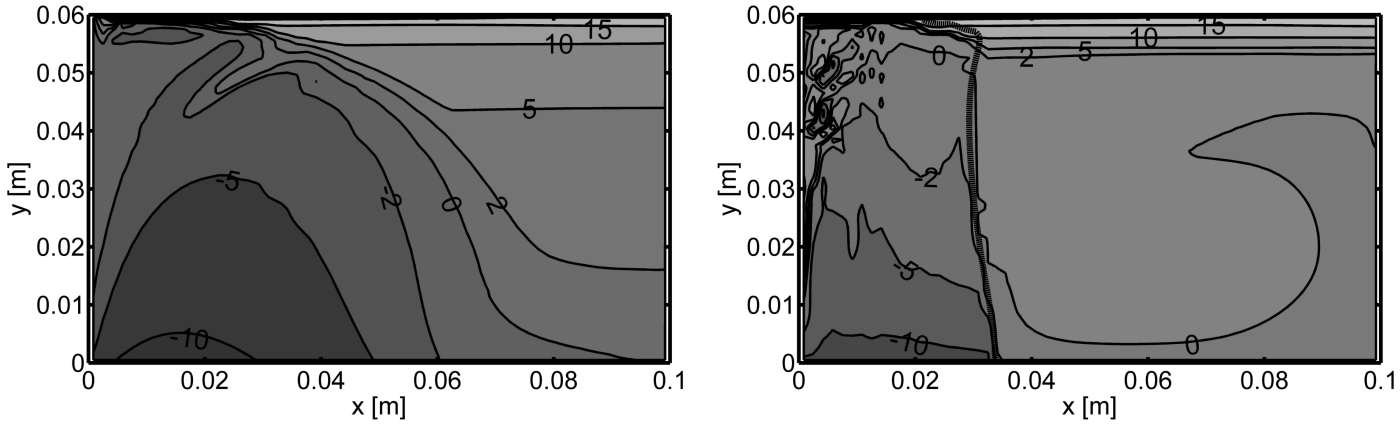

Figure 2: Relative tin mass fraction $\overline{C}$ after 150 s. of solidification: left – the EP model, right – the EP-FT model

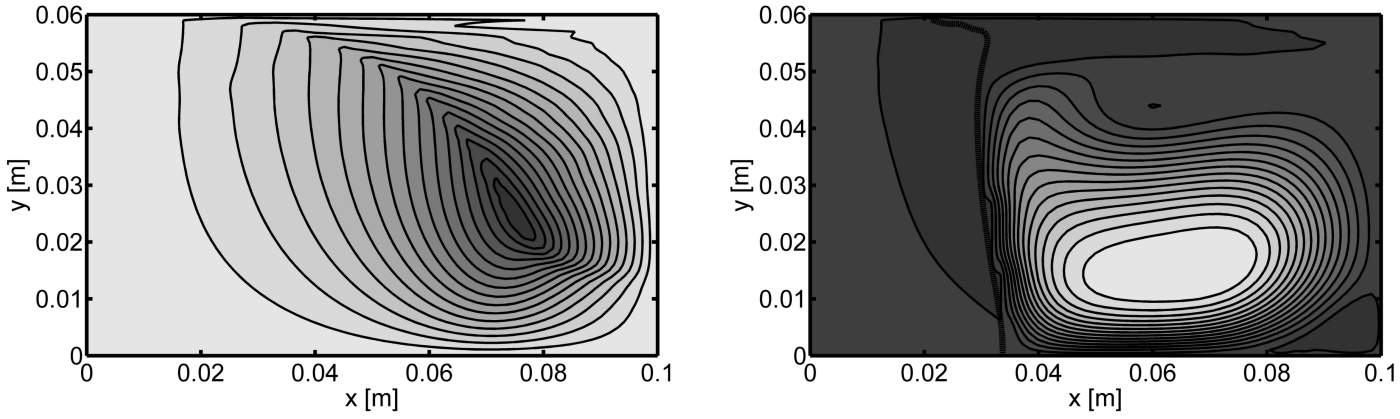

Figure 3: Streamlines after 150s of Pb-48 wt.% Sn solidification: left – the EP model, $\left(|\psi_{max}| = 8.8 \cdot 10^{-6}\left[m^2/s\right]\right)$, right – the EP-FT model, $\left(|\psi_{max}| = 1.4 \cdot 10^{-4}\left[m^2/s\right]\right)$

model.

4. Concluding remarks

The computer simulation model proposed in the paper, for macroscopic calculations of binary alloy solidification, differs from others available in the literature by the coupling of the simplified classical model based on the volume averaging method with the special technique of front tracking on a fixed spatial grid. This combination is capable of distinguishing the interface between two different dendrite structures developing in the mushy zone, i.e. the columnar mush and the equiaxed grain region. In each of these zones different models have been developed, Darcy's porous medium was used to mimic the inter-dendritic liquid flow in the stationary dendrite region and the model of slurry with floating dendrites was adopted in the equiaxed part of the mushy zone. Validation of the presented models with experiment [9] shows that the EP-FT model gives a slightly better match to the experimental data, especially in the upper and bottom parts of the cavity, when compared with the classical model of stationary solid phase inherent in the EP approach. The comparison of the relative tin mass fraction and stream functions patterns highlights the crucial importance of the proper choice of the porous/slurry model in the two-phase zone.

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