



A finite element formulation for macrosegregation during alloy solidification using a fractional step method and equal-order elements



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ARTICLE INFO

Keywords:

Macrosegregation
Solidification
Finite element
Fractional step
Equal-order

ABSTRACT

A finite element formulation of the “minimal” solidification model is presented for the prediction of macrosegregation during two-dimensional (2D) columnar solidification of binary alloys. A fractional step method is extended to solve the thermosolutal convection that has a damping in the mushy zone during solidification. Using this method, the velocity and pressure are decoupled and interpolated by linear equal-order triangular elements, resulting in decoupled systems that can be solved simply and efficiently. For convection-diffusion equations of energy, solute and momentum, the consistent streamline upwind Petrov-Galerkin (SUPG) method and the second-order Crank-Nicolson scheme are used for the discretization and integration over the spatial domain, respectively. A solution procedure is designed to couple the resolutions of conservations of energy, solute and momentum, as well as the macrosegregation model at an overall computational efficiency and accuracy. The formulation is first validated and then applied to predict macrosegregation during solidification of Pb-18 wt%Sn and Sn-10 wt%Pb alloys in a rectangular mold. The formation of macrosegregation is investigated, and comparisons with another finite element method (FEM) based code are made.

1. Introduction

Macrosegregation, i.e., chemical heterogeneities at macroscopic scale, is a challenge in many solidification processes, because it deteriorates microstructure and mechanical properties of the final products, causing increased economic and environmental costs. It has been acknowledged that the macrosegregation is caused by relative movements of solid and liquid phases, which are related to the transport phenomena that take place over several characteristic length scales [1–3]. Numerical models were originally concentrated on the effect of solute redistribution, and included only buoyancy-driven convection in the interdendritic liquid [4–9]. Subsequently, transport equations accounting for different length scales were derived by a volume averaging technique [10–12] or mixture theory [13]. Using the two methods, a single set of conservation equations can be derived for the whole domain (including the liquid, solid and mushy zones), with the mushy zone treated as a porous medium. After that, multiphase models [14–16] that couples multiple sets of conservation equations for different phases were developed. Nevertheless, the coupling of global multiphase transport phenomena with microscopic solidification kinetics is extremely complex and requires large amount of computation resources. As a consequence, the one-domain model based on the

volume averaging technique [10–12] or mixture theory [13] is still fundamental and inevitable in practice.

The major advantage of FEM is the flexibility of mesh discretization, and arbitrarily shaped domains can be easily approximated by unstructured meshes with high accuracy. The disadvantage is that larger computation amount and higher memory are required than other numerical methods, such as the finite volume method. In the case of solidification, more seriously, the efficiency is lower further due to another range of reasons. Firstly, a coupled system of equations resulting from conservations of energy, mass, momentum and solute must be solved. Nonlinearities in these equations should be dealt with carefully, and a specific solution procedure is needed to couple different transport phenomena efficiently. In particular, the thermosolutal natural convection is difficult to be simulated with a good accuracy due to the low Prandtl number (~ 0.01) and the great Lewis number ($\sim 10^4$) of liquid metals [17]. Secondly, the numerical solution of incompressible flows is inherently difficult, because the velocity and pressure are coupled by the incompressibility constraint implicitly. It has been demonstrated that a fractional step method or projection method [18–20] is efficient for this problem, but their use in solidification remains very limited [21–24]. Thirdly, for all fully coupled methods and most fractional step methods, the approximation spaces for velocity and pressure must a

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<https://doi.org/10.1016/j.commatsci.2018.08.009>

Received 22 May 2018; Received in revised form 1 August 2018; Accepted 4 August 2018

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priori satisfy a compatibility condition known as the *inf-sup* condition or LBB condition [25]. In order to improve the computational efficiency, it is of great significance to use various methods [26–32] to circumvent the LBB restriction in the case of solidification.

Recently, contributions were called to verify and validate a “minimal” solidification model and numerical codes for ingot solidification of binary metallic alloys, and two reference cases for 2D columnar solidifications of Pb-18 wt%Sn and Sn-10 wt%Pb alloys were proposed [17]. Some comparisons between the results obtained by different computer codes have been made by Combeau et al. [33,34], where most of those codes were based on the finite volume method, and one finite element code provided by CEMEF (France) was included. Therefore, more contributions based on FEM are needed for reference solutions of this important problem.

The present work is a contribution dedicated to develop a simple and efficient finite element formulation for the numerical simulation of macrosegregation during solidification of metallic alloys. As a first step for practical application, the “minimal” solidification model [17] for 2D columnar solidification of binary alloys is considered. The numerical principle based on FEM and fractional step method is first described in detail. Then validation of the in-house code is given based on the experiments performed by Hebditch and Hunt [35]. Finally, application in the two reference cases proposed by Bellet et al. [17] is presented, and the results and comparisons with those obtained by the FEM code of CEMEF [33,34] are discussed.

2. Numerical principle

2.1. Mathematical model

The “minimal” model proposed by Bellet et al. [17] for solidification of binary alloys is implemented in present work. It assumes that the liquid flow is laminar and Newtonian, that the solid phase is fixed and non-deformable, and that the mushy zone is treated as a porous medium with isotropic permeability defined by the Carman-Kozeny relation [36]. In addition, local thermodynamic equilibrium holds at the solid/liquid interface, with perfect solute diffusion in both solid and liquid phases (lever rule). All properties in both phases are equal and constant, except the density in the buoyancy term, which is determined by the Boussinesq approximation. The conservation equations of mass, momentum, energy and solute are written as follows:

Total mass conservation:

$$\nabla \cdot \mathbf{V} = 0 \quad (1)$$

where \mathbf{V} is the average liquid velocity vector.

Momentum conservation for liquid phase:

$$\rho \frac{\partial \mathbf{V}}{\partial t} + \frac{\rho}{g_l} (\nabla \mathbf{V}) \mathbf{V} = \nabla \cdot (\mu_l \nabla \mathbf{V}) - g_l \nabla p - \frac{\mu_l}{K} g_l \mathbf{V} + g_l \rho_b \mathbf{g} \quad (2)$$

where p is the pressure, t the time, ρ the reference density, ρ_b the density in the buoyancy term, g_l the liquid fraction, μ_l the dynamic viscosity of the liquid, K the permeability in the mushy zone, and \mathbf{g} the gravity vector.

Energy conservation:

$$\rho \frac{\partial H}{\partial t} + \rho c_p \nabla T \cdot \mathbf{V} - \nabla \cdot (\lambda \nabla T) = 0 \quad (3)$$

where H is the volume averaged specific enthalpy, T the temperature, λ the average thermal conductivity, and c_p the specific heat.

Solute conservation:

$$\frac{\partial w}{\partial t} + \nabla w_l \cdot \mathbf{V} = 0 \quad (4)$$

where w and w_l are the average mass concentration and the average mass concentration in liquid, respectively.

The supplementary relations are given by:

Permeability of the mushy zone:

$$K = \frac{\lambda_2^2}{180} \frac{g_l^3}{(1-g_l)^2} \quad (5)$$

where λ_2 is the secondary dendrite arm spacing.

Density in the buoyancy term:

$$\rho_b = \rho [1 - \beta_T (T - T_{ref}) - \beta_w (w_l - w_{ref})] \quad (6)$$

where β_T is the thermal expansion coefficient, β_w the solutal expansion coefficient, T_{ref} the reference temperature, and w_{ref} the reference mass concentration.

Volume averaged enthalpy:

$$H = c_p T + g_l L \quad (7)$$

where L is the latent heat of fusion.

Microsegregation model (lever rule):

$$w_s = k_p w_l \quad (8)$$

$$w = g_l w_l + g_s w_s \quad (9)$$

$$g_l + g_s = 1 \quad (10)$$

$$T = T_m + m_l w_l \quad (11)$$

where w_s is the average mass concentration in solid, k_p the partition coefficient (< 1), g_s the solid fraction, T_m the melt temperature of pure solvent, and m_l the liquidus slope (< 0).

2.2. Fractional step method

In order to circumvent the difficulty of solving a large system obtained by mixed finite element methods, a fully implicit four-step fractional method [28] originally used for Navier-Stokes equations is extended to solve the thermosolutal convection which has a damping in the mushy zone during solidification. Using this method, the coupled system of conservation equations of mass and momentum is split into several decoupled systems of much smaller size, which can be solved easily with much less computational cost. The time derivative is discretized by a fully implicit Euler backward method. The terms of convection, diffusion, pressure gradient, Darcy drag, and buoyancy are integrated using the Crank-Nicolson scheme which has second-order accuracy in time. The resulting time-discrete equations of the decoupled systems corresponding to Eqs. (1) and (2) are written as follows:

$$\frac{\rho}{g_l} \frac{\hat{\mathbf{V}} - \mathbf{V}^n}{\Delta t} + \frac{1}{2} \frac{\rho}{g_l^2} [(\nabla \hat{\mathbf{V}}) \hat{\mathbf{V}} + (\nabla \mathbf{V}^n) \mathbf{V}^n] = \frac{1}{2} \frac{\mu_l}{g_l} (\nabla^2 \hat{\mathbf{V}} + \nabla^2 \mathbf{V}^n) - \nabla p^n - \frac{1}{2} \frac{\mu_l}{K} (\hat{\mathbf{V}} + \mathbf{V}^n) + \rho_b \mathbf{g} \quad (12)$$

$$\frac{\rho}{g_l} \frac{\mathbf{V}^* - \hat{\mathbf{V}}}{\Delta t} = \frac{1}{2} \nabla p^n \quad (13)$$

$$\nabla^2 p^{n+1} = \frac{2\rho}{\Delta t} \nabla \cdot \mathbf{V}^* \quad (14)$$

$$\frac{\rho}{g_l} \frac{\mathbf{V}^{n+1} - \mathbf{V}^*}{\Delta t} = -\frac{1}{2} \nabla p^{n+1} \quad (15)$$

where superscript n denotes the time level, and Δt the time step. The liquid fraction g_b , permeability K and density ρ_b are all evaluated at time level $n + 1/2$. As the permeability is highly nonlinear with the liquid fraction and unable to be integrated accurately, the Darcy drag term is included only in Eq. (12) to improve the computational efficiency. With the pressure gradient term treated explicitly, an intermediate velocity $\hat{\mathbf{V}}$ is first solved by Eq. (12), and substituted to Eq. (13) to calculate another intermediate velocity \mathbf{V}^* . Then, the pressure is obtained by the pressure Poisson equation Eq. (14) derived from the incompressibility

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