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Full Length Article

Effect of thermodiffusion on the fluid flow, heat transfer, and solidification of molten metal alloys

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ABSTRACT

In this paper, a transient Finite Element (FE) method has been employed to solve the transport equations to investigate the heat transfer and fluid flow and the effect of thermodiffusion on vertical solidification of a binary molten metal alloy, forming a rod. The binary system considered in this study is Sn—Bi composed of 65% Sn and 35% Bi subjected to bottom cooling. It is found that the flow of molten metal at the boundary of the mushy region plays an important role in the shape and geometry of the zone. The presence of thermodiffusion shows considerable difference in the composition of the solidified rod, compared with the one without considering the effect of thermodiffusion. Thermodiffusion also causes a faster solidification and a more uniform concentration distribution. The results of this study may be extended to similar binary and multicomponent systems in which a temperature gradient exists and the Soret coefficient is large enough so as to affect the fluid flow and concentration of the species.

1. Introduction

Solidification process plays an important role in metallurgy as it determines the physical and mechanical properties of the solidified parts. Solidification is present in several industrial processes, such as casting, welding, crystal growth, metallurgy, energy conservation, refrigeration, and polymer crystallization. In most industrial processes, materials solidify within a temperature interval, where they experience a phase transition. The solidification process starts from heating the solid precursor to achieve a complete phase change, then it undergoes a partial solidification, in a liquid–solid two phase region, which is called the mushy zone, and ends after complete solidification. The fluid flow in the mushy zone strongly affects the formation of crystal micro-structures in the final solidified components.

In the past, experimental and numerical studies have been carried out on solidification of metals, semiconductors, etc. Some numerical models have been developed to account for the fluid flow and heat transfer, as well as solidification kinetics, e.g. see Reference 1. The front part of the solidification growth zone (mushy zone) is more important for research purposes than other zones. However, the knowledge about the fluid flow and its effects on the development of the mushy zone is quite limited. Some studies have considered bottom-cooled vertical solidification, experimentally and theoretically, some of which concerning the fluid flow are reviewed here. Tewari and Shah [2] have investigated the effect of the growth rate on the evolution of macro-segregation in Pb—Sn alloys. Directional solidification was carried out by lifting and lowering the furnace past a stationary crucible, wherein convection occurred due to solute build up ahead of a growing solid-liquid interface in Pb-Sn alloys. In another study, Felicelli et al. [3] conducted mathematical simulation of convection and segregation for the case of vertical solidification of Pb-Sn alloys using a volume-averaged, single-domain model. Sazarin and Hellawell [4] conducted experiments on Pb-Sn alloys, where the details of experimental procedure, data and analyses have been presented by Singh et al. [5]. They suggested that one of the central features of the mathematical modeling of convection is the representation of the mushy region. Both isotropic and anisotropic models of permeability have been used. It is important to note that experimental data on permeability are limited to the middle portion of the mushy region.

Kawaguchi et al. [6] simulated the growth of Cd—Zn—Te crystals by the vertical gradient freezing (VGF) method from a non-dilute melt. It was found that the zinc segregation is dependent on the convective flows. In a similar study, Okano et al. [7] studied crystal growth of In—P by the liquid encapsulated VGF method. The directional solidification of molten In—Sb in a silica ampoule was studied, where different thermal conditions were considered to simulate temperature and velocity distributions [8]. Celentano et al. [9] performed a comparative assessment of the finite volume and finite

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element methods in problems involving natural convection. They evaluated the thermally induced fluid flow patterns, the modified temperature field, and the heat transfer conditions. Rady and Mohanty [10] applied an enthalpy-porosity fixed-grid method to the melting and solidification of pure metals in a rectangular cavity. They found that during solidification, recirculation cells vanish with time. The cell near the interface affects the local solidification rate at the cavity top.

Voller and Prakash [11] and Voller et al. [12] developed an enthalpy formulation based fixed grid methodology for the numerical solution of convection–diffusion in the mushy zone using an alternative approach to that used by Gartling [13]. Considering the effect of other external forces, Eckert et al. [14] studied directional solidification in cylindrical samples of Sn—Pb exposed to a rotating magnetic field (RMF), where the direct impact of the local flow structure on the formation of the mushy zone was demonstrated. Also, several other investigations reveal a significant impact by convection occurring in the liquid phase on the kinetics of the solidification process, as well as on the resulting macro- and micro-structures. For instance, Wu et al. [15] addressed the importance of considering the melt flow, laminar and turbulent, in the mushy zone, where the flow patterns in and near the mushy zone were found to play an important role in the formation of the mushy zone.

In a study, Nikrityuk et al. [16] studied the influence of an external magnetic field on the solidification processes of two component materials in a cylindrical mould with adiabatic walls and cooled bottom. The magnetic field was found to provoke a convex shape in the mushy zone front. It has been found that the motion of the melt depends on the particular type of the magnetic field applied to the molten metal alloy, e.g. see References 17,18. Numerical simulation of complex multiphase flow systems, such as the solidification of systems with a free surface, such as molten droplets, have been carried out as well, using the level set or volume of fluid methods, e.g. see Reference 19. There are other works that consider the transport phenomena, instability and other related flow characteristics of solidification, e.g. see References 20–25. The mixture solidification model, used for the current study, has been verified theoretically and experimentally, e.g. see References 26–28, where the evolution of the solid shell thickness of a continuous cast steel slab was numerically predicted and was compared with the experimental data on the breakout shell.

In solidification processes, since the liquid temperature gradients are often high, thermodiffusion is not necessarily negligible. Thermodiffusion, also in molten metals and semiconductors called thermomigration, is the mass diffusion of a component with respect to others in a multicomponent fluid, induced by a temperature gradient in the mixture [29–31]. Thermodiffusion is a mechanism, beside regular diffusion, that is caused by a concentration gradient. The diffusion fluxes determine the solute gradients in the liquid at a given growth rate. In some cases, thermodiffusion may have a considerable or significant influence on the composition of the liquid and the final solidified product. For dilute solutions, the mass flux is proportional to the concentration and temperature gradients as follows [32]:

$$\vec{J} = -D_m \nabla C - D_T(\beta_0 + \beta_1 C)\Delta T \tag{1}$$

Generally, the diffusion coefficient is not independent of temperature. As the first approximation, it may be written as the following linear form [33]:

$$D_m(T) = D_0 + \frac{\partial D_m}{\partial T}(T - T_m) \tag{2}$$

Mathematical models and numerical procedures to study solidification processes have been improved over the past years. Here in our solidification model, the thermodiffusion and temperature dependent diffusion are considered, where the domain is subjected to cooling from below. At present, in spite of the extended history of study of solidification, many aspects of the physics of this phenomenon remain unclear. The fluid flow in the mushy region is driven by flow in the bulk liquid, which considering all driving forces is crucial for obtaining realistic simulations results. In this paper, we study the solidification of a model binary alloy, Sn—Bi, in a cavity by solving the heat transfer, the fluid flow and the species equations using the finite element (FE) method in the presence of thermodiffusion or thermomigration effect, where the flow patterns and unprecedented details and results on the effect of thermodiffusion on solidification of binary molten metals are presented and elucidated.

2. Governing equations

To obtain accurate results, the mathematical model must include heat transfer, phase change, momentum, continuity and mass transport equations. Also, variations of physical properties with temperature and the thermodiffusion effect must be considered. In the present study, axisymmetric geometry is adopted to simulate formation of a cylindrical rod. The governing equations of mixture given by Eqs. (3) through (15) are used to model the mushy zone (Fig. 1). This mixture combines liquid and solid that are quantified by their volume fractions, f_l and f_s, respectively. The liquid molten metal changes from a pure liquid to complete solid. Solidification occurs in front of the cold zone such that the solid phase becomes immobile as it sticks to the cold surface. The geometrical model is a cylindrical cavity containing 35% Bi and 65% Sn. Our model for the vertical solidification accounts for the solidification of the liquid phase, including convection and conduction heat transfer within the mushy region. The continuum model has been adopted for

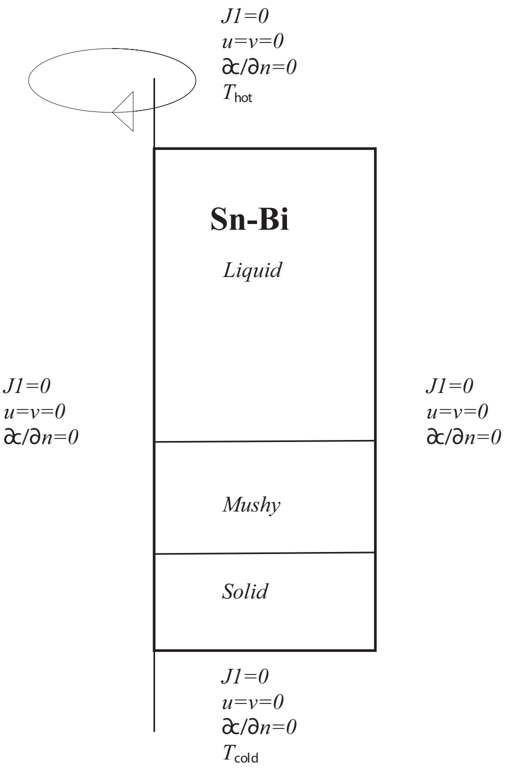

Fig. 1. Schematic diagram of the computational domain and boundary conditions.