International Journal of Heat and Mass Transfer 111 (2017) 398–409

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Three-phase computation of solidification in an open horizontal circular cylinder

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ARTICLE INFO

Article history:
Received 16 February 2017
Received in revised form 29 March 2017
Accepted 4 April 2017

Keywords:
Front-tracking
Three-phase simulation
Interpolation
Solidification
Open horizontal cylinder

ABSTRACT

We present numerical simulations of solidification in an open vertical circular cylinder with the presence of a gas phase and natural convection. The numerical technique used is a two-dimensional front-tracking method combined with an interpolation method. A simple tri-junction condition, in terms of the growth angle ϕ_{gr}, is included due to the presence of three phases. Effects of various dimensionless parameters such as the Prandtl number *Pr*, the Stefan number *St*, the Rayleigh number *Ra*, the Weber number *We*, the dimensionless initial temperature θ_0, the density ratio of the solid to liquid phases ρ_{sl} and the thermal expansion coefficient ratio of the gas to liquid phases β_{gl} are investigated. Numerical results show that, the shape of the solidified phase is strongly affected by ρ_{sl} and ϕ_{gr}. Volume expansion ($\rho_{sl} < 1.0$) produces a "cone-like" top surface while shrinkage ($\rho_{sl} > 1.0$) forms a cavity at the center of the cylinder. An increase in ϕ_{gr} in the range of 0–15° results in an increase in the slope of the top solid interface near the center. Decreasing *St* in the range of 1.0–0.01, with the presence of volume expansion, results in a steeper solid interface near the center. Without volume change ($\rho_{sl} = 1.0$), the top surface of the solidified phase becomes more curved with an increase in *Pr* in the range of 0.01–10, *Ra* in the range of 10^3–5×10^5, or *We* in the range of 10^{-5}–4×10^{-3}. In contrast, varying θ_0 (in the range of 1.0–2.5) or β_{gl} (in the range of 5×10^{-4}–5×10^{-1}) has a very minor effect on the top surface. In addition, the effects of these parameters on the evolution of the solidification front are also investigated.

1. Introduction

The phase change problem including moving boundary during inward solidification from a cooled cylinder appears in many engineered systems such as thermal energy storage systems, food processing, metallurgy and others, and has thus received much attention [1–3]. Experimental investigations can be found in Patel et al. [2] and Stewart and Smith [4]. Simplified analytical solutions of this problem have been presented by Riley et al. [1] and by Guenigault and Poots [5]. Numerically, Tao [6] developed a numerical method for the solidification problem of a saturated liquid contained in a cylindrical or spherical container. Voller and Cross [7] presented an explicit technique based upon the enthalpy method to obtain the solidification and melting time for two-dimensional regions with cylindrical symmetry. Bilir and İlken [3] used the enthalpy method with control volume approach to study the inward solidification in cylindrical and spherical containers with an initial temperature different from the fusion value.

However, in these above-mentioned works, volume change upon solidification was neglected, i.e., three phases have not been considered, even though it has been recognized as a major problem, e.g., in casting [8–10] or in the design of the latent heat thermal storage [11]. In consideration of volume change upon solidification in a tube, 10% of the whole shell volume was left unfilled to allow the phase change material to expand freely during the experiments of Jesumathy et al. [12]. Similarly, Avci and Yazici [13] and Yazici et al. [14] left an air gap at the top of the horizontal annulus during their experiments.

Even though there have been many studies concerning solidification in a cylinder, numerical investigations accounting for volume change in the problem are rather limited. Viskanta and Gau [15] adopted the integral and finite difference methods for the inward solidification in a horizontal tube. The authors also accounted for the effects of density difference on the solidification process. However, the effect of the tri-junction, i.e., presence of three phases, was not included. Liu et al. [16] used a volume-shrinkage-based method to study inward solidification within a spherical capsule in consideration of volume shrinkage. The method was verified through the comparison with the experimental result. However, fully resolved flow fields have not been

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http://dx.doi.org/10.1016/j.ijheatmasstransfer.2017.04.011
0017-9310/

reported in their results. Kim et al. [17] numerically investigated the icing process of water in an annulus with the presence of three phases: ice, liquid and air. However, the condition at the tri-junction was not reported, and the interfacial tension effect on the free surface has not been considered. Vu [18] used the front-tracking method to investigate solidification in a vertical cylinder with the presence of three phases. The study considered only the effects of volume change and tri-junction conditions. Solomon et al. [19] performed two-dimensional simulations of solidification and melting in a cylindrical capsule with the presence of a void at the top. The effect of the void on the solidifying front and the isotherms within the capsule was analyzed. However, no flow was reported, and the effects of the tri-junction and some other parameters have not been considered. Assis et al. [20] numerically and experimentally investigated the solidification process in a spherical shell with an opening at the top. Their results were applied only for paraffin since it was used as a working material. To our knowledge, solidification in a horizontal cylinder applies for not only water or paraffin, but also some other materials such as metals and phase change materials for the latent heat thermal energy storage [21,22]. Some other numerical works, e.g., Assis et al. [23] and Solomon et al. [24], included the third fluid, i.e., the gas phase, but applied for melting processes in spherical containers, and have not revealed the flow field and the effect of the tri-junction. For inward solidification in rectangular containers, numerical investigations with density difference can be found in [25–27]. However, these works have not shown in details the flow field in the gas [25,26] or liquid [25,27] phases, as well as the effects of some parameters such as the tri-junction, surface tension, and thermal expansion coefficients.

It appears that detailed numerical calculations on the solidification process in a horizontal cylinder with the presence of three phases are still lacking in the literature. Our literature search, summarized above, has not turned up systematic information on how volume change, tri-junction, natural convection, surface tension and so on affect the process. In addition, no simulations have considered three phases with the detailed flow and temperature fields within the cylinder during solidification. These gaps motivate our present study on this problem, which is extremely important both academically and in its industrial applications [9,21]. In this study, we apply the front-tracking method for three-phase computations of solidification [18,28,29] combined with interpolation techniques [30,31] to simulate the solidification of a pure phase change material in an open horizontal cylinder. The front-tracking technique is used to represent the interfaces and the interpolation techniques are to deal with the no-slip and constant isothermal temperature boundary conditions. We vary many parameters such as the Prandtl number, the Stefan number, the Rayleigh number, the interfacial tension (in terms of the Weber number), the initial temperature of the liquid, and the thermal expansion coefficient ratio of the gas to liquid to examine their effects on the process. In addition, the effects of volume change (in terms of the density ratio) and tri-junction (in terms of the growth angle) are also investigated. Such a careful investigation in this paper has not been reported before.

2. Mathematical formulation and numerical method

Fig. 1a shows the investigated problem. A liquid at temperature T_0 is placed in a horizontal circular cylinder of radius R. The top of the cylinder is open with a width of $0.2R$. The fusion temperature of the liquid is T_m ($T_m \le T_0$). At time $t = 0$, the cylinder wall temperature is suddenly lowered to T_c below T_m, i.e., $T_c < T_m$, and is kept at that temperature for $t > 0$. A solid layer forms near the cold wall, and then the solidification front propagates inward. A gas phase with the initial temperature T_0 is introduced at the top of the domain to account for volume change upon solidification. Initially, the liquid occupies the cylinder with a height H_l. We assume that the fluids are incompressible, immiscible and Newtonian. We treat all phases as one fluid with variable properties such as density ρ, viscosity μ, thermal conductivity k and heat capacity C_p. In addition, volume change is assumed to occur only at the solidification front. In the case of volume expansion, the liquid is assumed to not flow over the top solid surface [17,18,28,29]. Accordingly, the governing equations are given by:

$$\frac{\partial(\rho\mathbf{u})}{\partial t} + \nabla\cdot\rho\mathbf{u}\mathbf{u} = -\nabla p + \nabla\cdot[\mu(\nabla\mathbf{u} + \nabla\mathbf{u}^T)] + \int_f \sigma\kappa\delta(\mathbf{x} - \mathbf{x}_f)\mathbf{n}_f dS + \rho\mathbf{f} + \rho\mathbf{g}\beta(T - T_m) \quad (1)$$

$$\frac{\partial(\rho C_p T)}{\partial t} + \nabla\cdot(\rho C_p T\mathbf{u}) = \nabla\cdot(k\nabla T) + \int_f \dot{q}_f\delta(\mathbf{x} - \mathbf{x}_f)dS + \rho C_p h \quad (2)$$

$$\nabla\cdot\mathbf{u} = (1/\rho_s - 1/\rho_l)\int_f \delta(\mathbf{x} - \mathbf{x}_f)\dot{q}_f dS/L_h \quad (3)$$

Here, $\mathbf{u}$ is the velocity vector, p is the pressure, $\mathbf{g}$ is the gravitational acceleration. T and the superscript T denote the temperature and the transpose. $\mathbf{f}$ is the momentum forcing used to impose no-slip condition on the solid–fluid interface. h is the energy forcing used to impose constant temperature at the cylinder wall [30,31]. The Dirac delta function $\delta(\mathbf{x} - \mathbf{x}_f)$ is zero everywhere except for a unit impulse at the interface $\mathbf{x}_f$. L_h is the latent heat. $\dot{q}$ is the heat flux at the solidification interface, given as:

$$\dot{q} = k_s\frac{\partial T}{\partial n}\Big)_s - k_l\frac{\partial T}{\partial n}\Big)_l = -\rho_s V_n L_h \quad (4)$$

where the subscripts s and l represent solid and liquid, respectively. V_n is the velocity normal to the solidification front. Eq. (3) accounts for volume change at the solidification front due to density difference between the solid and liquid [18,28,29]. The last term in Eq. (1) is the Boussinesq approximation for density changes due to thermal gradients [32] with β denoting the volumetric expansion coefficient. The effect of the temperature on the interfacial tension coefficient σ acting on the gas–liquid interface [33] is given by:

$$\sigma = \sigma_0 - \sigma_T(T - T_m) \quad (5)$$

Here σ_0 and σ_T are the surface tension coefficient at a reference temperature T_m and the Marangoni tension coefficient, respectively.

We use here a front-tracking/finite difference method for the presence of three phases, phase change and volume change combined with interpolation techniques [29–31]. The interface is represented by connected elements that move on a fixed, rectangular grid (Fig. 1b). The three phases and their properties are specified using the indicator functions that are determined from the known positions of the interface points: the points of the solidification and solid–gas fronts are used to construct the indicator I_s ($I_s = 0$ in solid and $I_s = 1$ in liquid and gas) while the indicator I_l ($I_l = 0$ in liquid and solid and $I_l = 1$ in gas) is built from the points on the solid–gas and liquid–gas interfaces. Accordingly, the values of the material property fields at every location are then given by:

$$\varphi = I_l\varphi_g + (1 - I_l)[I_s\varphi_l + (1 - I_s)\varphi_s] \quad (6)$$

$$\beta = I_l\beta_g + (1 - I_l)\beta_l \quad (7)$$

Here φ stands for ρ, μ, C_p, or k. The subscript g in Eqs. (6) and (7) denotes the gas phase. The solidification front propagates with the normal velocity V_n, $V_n = -\dot{q}_f/(\rho_s L_h)$, while the liquid–gas front is advected by the velocity interpolated from the fixed grid velocities. At the tri-junction, i.e., the triple point in 2D (Fig. 1), we correct the position of this point by applying a constant growth angle