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Three-phase numerical simulations of solidification with natural convection in a vertical cylindrical annulus

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ABSTRACT

We present numerical simulations of solidification in a vertical cylindrical annulus with temporal evolution of three interfaces, i.e., solid–liquid, solid–gas, and liquid–gas, and with the presence of natural convection. The numerical technique used is an axisymmetric front-tracking/finite difference method in which the interface separating two phases is represented by connected elements moving on a stationary grid. The governing Navier–Stokes and energy equations are solved in the entire domain with the no-slip and isothermal boundary conditions treated by interpolation techniques. A simple tri-junction condition 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 of the liquid θ_0, and the density ratio of the solid to liquid phases ρ_{sl} are investigated. The effect of the tri-junction in terms of the growth angle ϕ_{gr} is also considered. 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 U-shaped top surface while shrinkage ($\rho_{sl} > 1.0$) forms a cavity near the outer wall of the annulus. An increase in ϕ_{gr} results in an increase in its slope near the outer wall. Without volume change ($\rho_{sl} = 1.0$), the top surface of the solidified phase becomes more curved with an increase in *Pr* or *We*. In contrast, varying *St* in the range of 0.01–1.0, *Ra* in the range of 10^3–10^6 or θ_0 in the range of 1.0–2.0 has only a very minor effect on the top surface. Concerning the circulation flows induced by natural convection, the remarkable effects are yielded by variation of *Ra* and θ_0: increasing *Ra* or θ_0 results in an increase in the strength and the number of circulations. The circulations along with the interfacial tension force are the sources of the top front and solidification interface deformation. In addition, the effects of these parameters on the solidification rate are also investigated.

1. Introduction

The phase change problem including moving boundary during outward phase change from a cooled cylinder appears in many engineered systems such as thermal energy storage systems, food processing and others, and has thus received much attention (Mahdaoui et al., 2014; Padmanabhan and Murthy, 1986; Sablani et al., 1990).

For solidification in an annulus, Sinha and Gupta (1982) carried out experimental and numerical investigations for radial outward solidification of water in a horizontally concentric cylindrical annulus. Sugawara et al., (2010) used the PHOENICS code to analyze freezing of water around a coolant tube immersed horizontally inside an adiabatic rectangular cavity. Ezan et al., (2013) numerically investigated the freezing process of water fully filled in a horizontal cylindrical annulus. The effect of the initial temperature of water was examined. Other numerical predictions for the phase change process in a horizontal annulus can be found in Zhang and Faghri (1997) and Wang et al., (2013). However, in these above-mentioned works, volume change upon solidification was neglected, i.e., three phases have not been considered. In consideration of volume change, Avci and Yazici (2013) and Yazici et al., (2014) left an air gap at the top of the horizontal annulus during their experiments.

Concerning vertical annuli, Akgün et al., (2007) experimentally studied melting and solidification characteristics of paraffin in a vertical tube-in-shell unit. Solomon et al., (2013) investigated the subcooling effect in a vertical concentric tube by experiments. Jesumathy et al., (2012) experimentally studied heat transfer characteristics of paraffin wax during phase change processes in a vertical annulus. To allow the material to expand freely, 10% of the whole volume was left unfilled. Even though there have been many experimental studies concerning vertical annuli, there are a few numerical studies related to this problem. Ismail et al., (2014) used a boundary immobilization method to study solidifica-

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Table 1
Literature summary.

Source	Method		Material (*Prandtl number*)	Horizontal annulus	Vertical annulus	Volume change (Three phases)
	Experiment	Simulation				
Sinha and Gupta (1982)	x	x	Water ($Pr \cong 7$)	x		
Ezan et al. (2013)	x	x	Water ($Pr \cong 7$)	x		
Zhang and Faghri (1997)		x		x		
Wang et al. (2013)		x	*n*-octadecane ($Pr \cong 50$)	x		
Avci and Yazici (2013)	x		Paraffin ($Pr \cong 100$)	x		x
Yazici et al. (2014)	x		Paraffin ($Pr \cong 100$)	x		x
Akgün et al. (2007)	x		Paraffin ($Pr \cong 100$)		x	
Solomon et al. (2013)	x		Paraffin (RT 21) ($Pr \cong 100$)		x	
Jesumathy et al. (2012)	x		Paraffin ($Pr \cong 100$)		x	x
Ismail et al. (2014)	x	x	Water ($Pr \cong 7$)		x	
Kim et al. (1993) [a]		x	Water ($Pr \cong 7$)		x	x
Present study [b]		x	$Pr=0.01–10$		x	x

[a] Flow and temperature fields in the gas phase, and the tri-junction effect have not been considered.
[b] Fully resolved flow and temperature fields in three phases, and the tri-junction effect are investigated with the effects of some other parameters such as interfacial tension and initial temperature of the fluid x: available.

tion external to a long tube. The physical domain was transformed to a computational domain to ease the calculations. However, only the cases of equal densities of solid and liquid were examined. Accounting for density difference, Kim et al., (1993) investigated the icing process of water in an annulus with the presence of three phases: ice, water and air. The method used was that proposed by the authors for axisymmetric problems (Charn-Jung et al., 1993). However, the condition at the tri-junction was not reported, and the interfacial tension effect on the free surface has not been considered. In addition, the results were only for water. To our knowledge, solidification in an annulus applies for not only water but also some other materials such as metals and phase change materials for the latent heat thermal energy storage (Agyenim et al., 2010).

Concerning of three phase computations, recently we have used the front-tracking method (Tryggvason et al., 2001; Al-Rawahi and Tryggvason, 2002) with modification to account for the presence of three phases with volume change upon phase change [see Vu et al., (2013, 2015) for drop solidification on a cold plate, and Vu (2016) for inward solidification in a cooled circular cylinder]. In these works, we used an indicator function to set the velocity within the solid phase to zero. We then combined the method with interpolation techniques to deal with no-slip and constant isothermal boundary conditions for solidification around circular cylinders with forced convection (Vu et al., 2016; Vu and Wells, 2017). This method is used in the present study.

It appears that detailed numerical calculations on the solidification process in a vertical annulus, which includes volume change upon solidification, are still lacking in the literature (see Table 1). 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 annulus during solidification. These gaps motivate our present study on this problem, which is extremely important both academically and in its industrial applications. In this study, we apply the front-tracking method for three-phase computations of solidification combined with interpolation techniques to simulate the solidification of a pure phase change material in the annulus. The front tracking technique is used to represent the solidification interface and the interpolation techniques are to deal with the no-slip and constant isothermal temperature boundary conditions (Vu et al., 2016; Vu and Wells, 2017). We examine the effects of various parameters on the process in terms of the top surface profile, flow and temperature fields, and evolution of the solid phase.

2. Mathematical formulation and numerical method

Fig. 1a shows the investigated problem. A liquid at temperature T_0 is placed in a vertical annulus. The radii of the inner and outer walls of the annulus are R_i and R_o, respectively. The fusion temperature of the liquid is T_m ($T_m \le T_0$). At time $t=0$, the inner wall temperature is suddenly lowered to T_c below T_m, i.e., $T_c < T_m$, and is kept at that temperature for $t>0$, while the outer wall is insulated. A solid layer forms near the cold inner wall, and then the solidification front propagates outward. A gas phase is introduced at the top of the domain. 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 not to flow over the top solid surface (Kim et al., 1993). Accordingly, the governing equations are given by

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

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

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

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. κ is twice the mean curvature, and $\mathbf{n}_f$ is the unit normal to the interface denoted by f. $\mathbf{f}$ 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 boundary (Vu et al., 2016; Vu and Wells, 2017). 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

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