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Numerical study of solid-liquid phase change by phase field method

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ABSTRACT

The phase field method is developed to solve free boundary problems (e.g., solid-liquid phase change) without tracing phase interface positions in microscope and mesoscope based on the Ginzburg–Landau theory. Besides, different from the classical Stefan problem, surface tension allowing for the possibility of undercooling (or superheating) effect is introduced for the more realistic physics in the phase field method. In the present study, a phase field model is established and a feasibility study of the phase field model on the macro scale is done through two classical problems: the conduction solid-liquid phase change problem and the convection melting problem. Some results are obtained and model validation is carried out by comparing the results with the Neumann solutions and the classical correlations, respectively. It is found that the results obtained by the phase field model agree well with those of the benchmark solutions on the whole, but some differences, for example, delay of interface moving and undercooling (or superheating) effect, exist if the effect of surface tension is obvious. It's concluded that the phase field method is a reliable method to simulate more realistic solid-liquid phase change problems no matter whether natural convection is considered or not on the macro scale.

1. Introduction

Solid-liquid phase change problems are a kind of free boundary problems and have been studied extensively in mathematics, physics, material science and other research areas for more than a century. The governing equations for general solid-liquid phase change problems are as follows [1]:

$$\rho c_p \frac{\partial T}{\partial t} = k\nabla^2 T \qquad \text{in } \Omega \tag{1}$$

$$\rho L V_n = k[\nabla T \cdot \mathbf{n}]_+^- \qquad \text{on } \Gamma \tag{2}$$

$$s(T - T_m) = -\sigma(\kappa + \alpha V_n) \quad \text{on } \Gamma \tag{3}$$

The Eqs. (1)–(3) together are well known as the modified Stefan problem. When σ is set to be zero, Eq. (3) is reduced to

$$T = T_m \tag{4}$$

The Eqs. (1) and (2) together with (4) are then called the classical Stefan problem.

In recent years, as the demand for efficient latent energy storage and advanced material casting technology increases, the research on solid-liquid phase change problems is still of great significance, which then promotes the development of relevant numerical computation methods further. At present, the numerical computation methods of solid-liquid phase change problems are mainly divided into four categories: the front tracking method [2–4], the level set method [5–7], the enthalpy method [8–10] and the phase field method [11–13]. In the front tracking method, the solid-liquid interface is treated explicitly by a distinguished representation, while each phase is modeled separately. However, the interface morphology that can be treated in the front tracking method is usually relatively simple. Different from the front tracking method, the solid-liquid interface can be treated implicitly in the level set method, the enthalpy method and the phase field method by which the interface with complex morphology can be treated more easily. In the level set method, interface normals and curvatures are still needed to be calculated accurately. As for the enthalpy method, a key feature of it and its variants is that the distinguishability of phases is based on the temperature alone. That is to say, the enthalpy method is derived from the classical Stefan problem and surface tension that causes undercooling (or superheating) effect is not taken into consideration.

The phase field method is a relatively new modeling method for phase change problems and has experienced an increasing interest in material science and other areas because of its fundamental origins and advantages. Originated from the Ginzburg-Landau theory, an ordered parameter is introduced to separate solid and liquid phases. Asymptotic analyses have been done rigorously to demonstrate that as interface thickness approaches zero, solutions to the

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Nomenclature

T	Temperature, °C
c_p	Specific heat capacity, J kg^{-1} K^{-1}
K	Thermal conductivity, W m^{-1} K^{-1}
V_n	Interface velocity, m s^{-1}
n	Unit vector normal to the interface (positive if directed toward the liquid)
L	Latent heat per mass, J kg^{-1}
S	Entropy density difference between solid and liquid, J m^{-3} K^{-1}
H	Height/width of the cavity, m
X	Cartesian axis direction, m
y	Cartesian axis direction, m
u	Velocity along x direction, m s^{-1}
v	Velocity along y direction, m s^{-1}
p	Pressure, Pa
g	Gravitational acceleration, m s^{-2}
t	Time, s
a	Thermal diffusivity, m^2 s^{-1}
Ste	Stefan number
Fo	Fourier number
Ra	Rayleigh number
Nu	Nusselt number
Pr	Prandtl number
h	Heat transfer coefficient, W m^{-2} K^{-1}

Greek Symbols

Ω	Bulk domain
Γ	Solid-liquid interface
ρ	Density, kg m^{-3}
σ	Surface tension, J m^{-2}
κ	Curvature, m^{-1}
ξ	Characteristic length, J$^{1/2}$ m$^{-1/2}$
α	Kinetic coefficient, s m^{-2}
μ	Dynamic viscosity, Pa s
ν	Kinematic viscosity, m^2 s^{-1}
β	Thermal expansion coefficient, K^{-1}
ϕ	Ordered parameter
ε	Interface thickness, m
τ	Dimensionless time
λ	Root of the transcendental equation

Subscripts

m	Melting point
n	Normal to the interface
c	Reference point
l	Liquid phase
s	Solid phase

phase field equations formally approach those of the modified Stefan problem expressed in Eqs. (1)–(3) so that a more realistic solid-liquid phase change process can be modeled by the phase field method [14]. However, the application of the phase field method is largely limited to the meso and micro scale, for example, dendrite growth, because the interface thickness is usually on the atomic scale and this will result in enormous and unrealistic computation burdens on the macro scale, especially for 2D and 3D computation.

In addition, fluid flow plays an important role in the melting and solidification process, because it can influence interface morphology and temperature distribution. Several excellent trial studies on the phase field method coupled with convection have already been done during the past few years. Tong et al. [15], Beckermann et al. [16] and Boettinger et al. [17] proposed phase field models to investigate the dendrite growth under forced convection, considering the effect of convection velocity, flow direction and anisotropy on dendrite morphology and growth behavior. Tönhardt and Amberg [18] performed a 2D simulation of succinonitrile (SCN) dendrite growth in a natural convection environment. Chen and Lan [19] further explored the effect of natural convection on three dimensional dendrite growth. However, the previous studies on the phase field method coupled with convection are still limited to the meso and micro scale and the relatively systematic study coupled with convection on the macro scale hasn't been carried out yet.

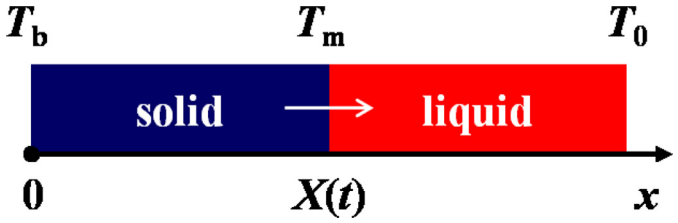

Fig. 1. Schematic diagram of the two-region solidification process in a semi-infinite space.

In this paper, a two dimensional phase field model for solid-liquid phase change problems in which natural convection can be taken into consideration is established to study the feasibility of the phase field method on the macro scale through two classical problems: the conduction solid-liquid phase change problem and the convection melting problem. Some results obtained by the phase field model, including interface position evolution, temperature distribution, average Nusselt number evolution and so on are compared with the Neumann solutions of the classical Stefan problem and the classical scaling correlations of Nusselt number of melting with natural convection in a square cavity, respectively.

2. Physical problem description

2.1. Conduction solid-liquid phase change problem

The conduction solid-liquid phase change problem is to solve the interface position evolution and temperature distribution in melting or solidification without convection. The initial conditions for pure phase change materials determine whether the problem will be classified into one- or two-region problems further [20]. The analytical solutions to the classical Stefan problem exist in a limited number of idealized situations involving semi-infinite or infinite regions, simple boundary and initial conditions, and so on. Such analytical solutions are also called the Neumann solutions. Here, the two-region solidification process in a semi-infinite space is taken as an example to study the feasibility of the phase field model on the macro scale. The schematic diagram is shown in Fig. 1.

The liquid at a uniform temperature T_0 ($T_0 > T_m$) is confined to a half-space $x > 0$. At time $t = 0$, the boundary surface at $x = 0$ is lowered to a temperature T_b ($T_b < T_m$) and maintained at T_b in the following time. As a result, the solidification starts at the surface $x = 0$ and the solid-liquid interface propagates in the positive x direction. The Neumann solutions of the two-region solidification process in a semi-infinite space are given as follows.

Interface evolution:

$$X(t) = 2\lambda\sqrt{a_s t} \tag{5}$$

Temperature distribution in solid phase:

$$T_s(x,t) = \frac{erf\left(\frac{x}{2\sqrt{a_s t}}\right)}{erf\lambda}(T_m - T_b) + T_b \tag{6}$$