Numerical prediction of water-ice phase-change with natural convection including density inversion region

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Abstract. This study proposes a computational method for water-ice phase-change with natural convection including density inversion region. In the proposed method, orthogonal structured grids are used for all computations. The Stefan conditions are calculated while approximately taking into account positions of water-ice interfaces in each computational cell. After the confirming the basic applicability of the proposed method to the natural convection including density inversion region in a square cavity, a numerical experiment of freezing and melting problems is performed. As a result, freezing of water and melting of ice, which are enhanced by complex circulating flows due to the density inversion in the water, are simultaneously predicted.

Keywords: fluid-solid interaction, water-ice phase-change, Stefan condition, natural convection, density inversion

1. Introduction

Phase changes between water and ice are often seen in natural phenomena and engineering problems, such as freezing of water pipes and melting of frozen soil. The flows of water near ice surfaces have a significant influence on freezing and melting processes. The main objective of this study is the development of a computational method based on MICS (Multiiphase Incompressible flow solver with Collocated grid System) [1] to treat water convection, heat conduction in ice, and water-ice phase-change on orthogonal structured grids. To estimate the water-ice phase-change, the method proposed by Tago et al. [2] is improved so that the position of the water-ice interface in each computational cell can be approximately taken into account.

In this study, the propose method is first applied to the natural convection including density inversion region in a square cavity, and the characteristics of the velocity and temperature distributions are compared with the reference numerical results. Then, the proposed method is applied to the numerical experiment in which the freezing of water and the melting of ice simultaneously occur. Note that this study assumes that the volume change associated with the phase change is negligible.

2. Numerical method

Governing equations of the proposed method consist of incompressible condition, momentum equations for fluid phases, temperature equation, and Stefan condition. Incompressible condition and momentum equations for fluid phases are the same as those in the previous study using MICS [1]. In the first computational step of MICS, solid phases are assumed to be fictitious fluids and fluid flows are calculated for the entire computational domain. After that, flow velocities are updated with phase-averaging operation based on the volume fraction of the solid phase in each computational cell.

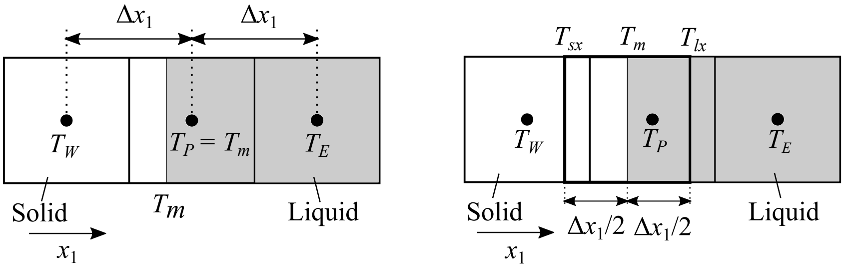
The temperature equation and Stefan condition used in this study are as follows:

$$\frac{\partial T}{\partial t}+\frac{\partial (Tu_j)}{\partial x_j}=\frac{1}{(\rho c_p)_m}\left\{\frac{\partial}{\partial x_j}\left(\lambda\frac{\partial T}{\partial x_j}\right)+\rho_s h_L\frac{\partial f_s}{\partial t}\right\}, \tag{1}$$

$$\lambda_s\frac{\partial T_s}{\partial x_i}-\lambda_l\frac{\partial T_l}{\partial x_i}=\rho_s h_L\frac{\partial \xi_i}{\partial t}, \tag{2}$$

where t is the time, x_i is the i-th Cartesian coordinate, T is the phase-averaged temperature, u_i is the component of phase averaged velocity, ρ_s is the density of the solid, and h_L is the latent heat of melting. λ_s and λ_l are the thermal conductivity of solid and fluid phases. Similarly, T_s and T_l are the temperature of solid and fluid phases. f_s is the volume fraction of solid in each computational cell. Phase-averaged physical properties $(\rho c_p)_m$ and λ are calculated by $(\rho c_p)_m = f_s\rho_s c_{p,s} + (1-f_s)\rho_l c_{p,l}$ and $\lambda = f_s\lambda_s + (1-f_s)\lambda_l$ where ρ_l is the density of the fluid, $c_{p,s}$ is the specific heat at constant pressure of the solid, and $c_{p,l}$ is that of the fluid. To simply treat deformation of water-ice interface on the Cartesian coordinate, Stefan conditions are separately considered for each direction and the ice-layer width ξ_i in the computational cell which contains water-ice interface is updated using Eq. (2).

Figure 1 shows temperature variables on cell center used in computations of Eq. (2). The subscript P represents the computational cell which contains the water-ice interface, and furthermore the subscripts W and E represent neighboring cells of that. The temperature of the water-ice interface is assumed to be fixed at the freezing temperature T_m. In the conventional method [2], T_P calculated from Eq. (1) is replaced by T_m in the computations of Eq. (2) as shown in Fig. 1 (a). On the other hand, intermediate temperatures T_{sx} and T_{sl}



(a) Tago et al. [2] model (b) present model

Figure 1: Temperature variables on cell center used in computations of Stefan condition

are set in the proposed method as shown in Fig. 1 (b), and they are used in the computations of Eq. (2) to consider the position of water-ice interface in each computational cell.

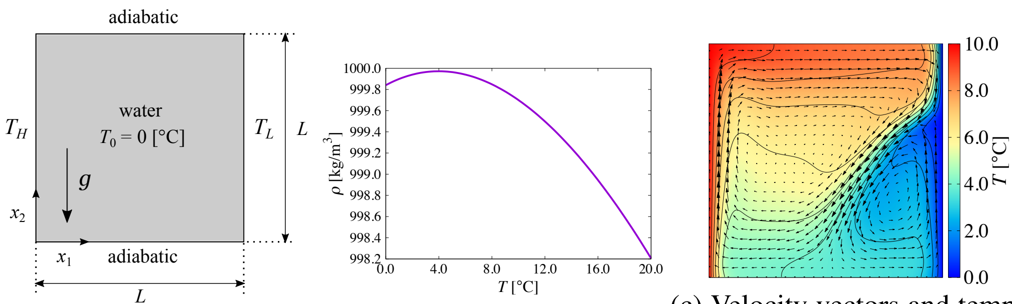
In our previous study [3], it was confirmed that the proposed method can improve the mesh convergence and can reasonably predict the freezing of water in a square cavity [4] and the melting of ice-layer [5]. In this study, the program code for the calculation part of Eq. (2) is restructured so that it can be applied to problems in which the freezing of water and the melting of ice occur simultaneously.

3. Applications

3.1. Natural convection including density inversion region in a square cavity

To confirm the basic characteristics of the fluid computation, the proposed method is applied to the natural convection including density inversion region in a square cavity [6]. The computational domain is shown in Fig. 2 (a), where L is 38 [mm]. The temperatures T_H and T_L are fixed at 10 [°C] and 0 [°C]. Physical properties of fluid are set assuming water. The relationship between fluid density and temperature is given by Fig. (b) [6]. Figure 2 (b) indicates that the fluid density reaches a maximum around 4 [°C] in this study.

Figure 2 (c) shows the calculated velocity vectors and temperature distribution in the steady state. Since the fluid density reaches a maximum around 4 [°C], clockwise and counterclockwise circulating flows are formed in the regions with temperatures higher and lower than 4 [°C], respectively. These results are in good agreement with the reference numerical results [6].



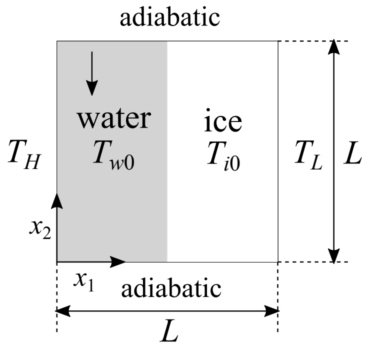
(a) Computational domain (b) $\rho_l - T$ relationship (c) Velocity vectors and temperature distribution (steady state)

Figure 2: Computational conditions and results of natural convection including density inversion region in a square cavity

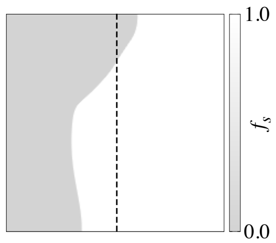
3.2. Freezing and melting problem with natural convection including density inversion region

Figure 3 (a) shows the computational domain for freezing and melting problem with natural convection including density inversion region. In this numerical experiment, both water and ice phases are initially exist in the computational domain. Computational conditions are set as follows: $L = 38$ [mm], $T_H = 10$ [°C], $T_L = -10$ [°C], and $T_{w0} = T_{i0} = 0$ [°C].

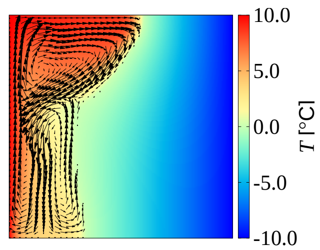
Figure 3 (b) shows the calculated distribution of f_s at t = 120 [min]. The dashed line in Fig 3 (b) is the initial water-ice interface. This result demonstrates that freezing of water and the melting of ice are simultaneously predicted by the proposed method. Figure 3 (c) shows the calculated velocity vectors and temperature distribution. The complex circulating flows due to the density inversion can be seen in the water, and which may enhance the deformation of the water-ice interface.



(a) Computational domain



(b) Distribution of f_s (t = 120 [min])



(c) Velocity vectors and temperature distribution (t = 120 [min])

Figure 3: Computational conditions and results of freezing and melting problem with natural convection including density inversion region

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