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Prediction of Melting Process Driven by Conduction-Convection in a Cavity Heated from the Side

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Abstract–A fixed-grid finite volume numerical approach is developed to simulate the melting during the solid-liquid phase-change driven by convection as well as by conduction. This approach adopts the enthalpy-porosity method augmented with the front-layer predictor-corrector and the pseudo Newton-Raphson algorithms that were devised to track the phase front efficiently in the conduction-driven phase-change problems. The computational results compare well with experimental data and transformed-grid results in the literature. Also, the effect of the delayed heat-up at a heated wall on the melting process is investigated.

Key words: Melting Phase Change, Fixed-Grid Method, Melt Flow, Delayed Heat-Up

INTRODUCTION

Solid-liquid phase-change processes have been receiving much interest from many engineering fields such as thermal energy storage systems using latent heat and material processes [Choi et al., 1995; Voller, 1997]. Convection as well as conduction drives the solid-liquid phase-change processes. The temperature difference in the melt can give rise to natural convection, and the flow structure initiated by the convection can significantly affect the phase-change process. The convection has a great influence on the morphology of the solid-liquid interface, which can alter the flow structure in the melt. Hence, the effect of natural convection in the melt on the phase change has been paid considerable attention for the past several decades.

In general, the usual numerical methods for phase-change problems are the fixed-grid [Brent et al., 1988; Desai and Vafai, 1993; Viswanath and Jaluria, 1993; Rady and Mohanty, 1996; Kim et al., 2001] and the transformed-grid methods [Beckermann and Viskanta, 1989; Desai and Vafai, 1993; Viswanath and Jaluria, 1993]. In the fixed-grid method, a single set of conservation equations and boundary conditions is used for the whole domain comprising the solid and liquid phases, while the transformed-grid method considers the governing equations on the basis of the classical Stefan formulation. In the transformed-grid method, the interface conditions are easily and explicitly imposed on the governing equations; however, in the fixed-grid method, they are absorbed into the governing equations as suitable source terms.

The fixed-grid method requires velocity suppression because the zero-velocity condition should be satisfied as a liquid region turns to solid. Velocity suppression can be accomplished by the large viscosity of the solid phase or by the suitable source term in the momentum equation driven to model the two-phase domain as a porous medium. The fixed-grid method combined with the porous medium method is usually referred to as the enthalpy-porosity method.

In this study, an enthalpy-porosity model for the convection-dominated melting is developed. The related numerical model is incorporated with the front-layer predictor-corrector algorithm, a multi-dimensional version of the single-point predictor-corrector algorithm that was proposed to solve heat conduction-driven phase-change problems effectively [Kim et al., 2001]. The computational results are compared with experimental and numerical data available in the literatures. The effect of the delayed heat-up at the heated wall on the prediction of the phase-change process is also investigated. In most cases, the phase change problems have been solved under the assumption of constant wall temperatures that should be suddenly reached to the desired temperatures; however, the reality in the experiments could be a time delay in the heat-up [Gau and Viskanta, 1986]. Such a delayed heat-up will affect the natural convection in the melt during the phase-change process considerably and may be a cause of the mismatch between the analytic and the experimental results.

The spatial and temporal discretizations are achieved in the context of the finite volume scheme and the fully implicit (backward) Euler scheme, respectively. The flow field is expressed in terms of primitive variables and solved by adopting the SIMPLE algorithm [Patankar, 1980].

MATHEMATICAL MODEL

Two-dimensional melting in a rectangular cavity can be summarized, as shown in Fig. 1. The melting will be driven by natural convection as well as by conduction in a rectangular cavity. The phase changing material is contained in a cavity, whose horizontal walls are insulated. Initially, the phase changing material in the cavity is kept at uniform temperature T_i below or at T_m. The temperature at the right wall, T_C, is maintained at T_i. Most of the previous numerical simulations assumed that the sudden elevation of the heated wall (the left wall) temperature above the T_m initiates the melting. Then, the temperature difference between the hot wall and the

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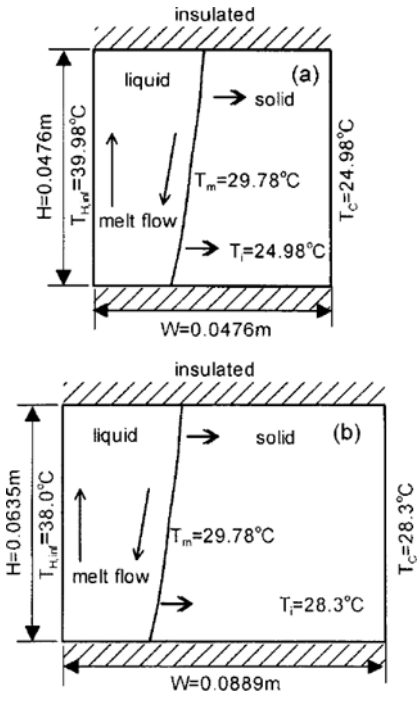

Fig. 1. Schematics of gallium melting problems: (a) Beckermann and Viskanta [1989]: Ra=3.166×10^5, Ste=0.04854; (b) Gau and Viskanta [1986]: Ra=6.057×10^5, Ste=0.03912.

melting temperatures causes natural convection in the melt. In fact, the sudden temperature rise cannot be carried out in real experiment, however, it is possible in the imaginary experiment. The time delayed heat-up occurs in a real experiment and it delays the initiation of natural convection and affects the melting process. Now, we derive a simplified model to account for the delayed heat-up. In many experiments, the constant wall temperature condition is attained by flowing liquid coming from a constant temperature reservoir. Hence, consider the heat transfer from the hot water reservoir to the hot wall and assume that the temperature of the hot reservoir is kept at a constant, T_{H0}. Then, the hot wall, which is initially cool at T_i, will be heated by the liquid flow from the reservoir. The water temperature, which is T_{H0} at the inlet of the flow path, decreases due to the heat transfer to the wall. The rate of change of the wall temperature is proportional to the temperature difference between the outlet and the inlet flow temperatures, and also to the temperature difference between the average flow temperature and the wall temperature. The proportional constants are dependent on many variables: specific heats of the wall and the liquid, mass of the wall, heat transfer area, mass flow rate of the liquid and heat transfer coefficient between the liquid flow and the wall. Hence, one can easily show that the wall temperature can be expressed as an exponential function of time. In other words, simplifying the heat exchange process between the hot reservoir and the wall, it is reasonable to take account of a time constant in T_H:

$$T_H=T_{H0}-(T_{H0}-T_i)e^{-t/\tau} \tag{1}$$

where T_H, T_{H0} ($>T_m$) and τ represent hot wall temperature, predetermined temperature to be reached and time constant, respectively. Neglecting the time delay in heating implies $\tau=0$.

The momentum field is subjected to no-slip boundary conditions at the walls. The flow is assumed to be two-dimensional, laminar, and incompressible. The thermophysical properties of the materials are constant but those of the liquid and the solid phases are different. But here the density difference between the solid and the liquid phases is neglected except when the Boussinesq approximation is invoked.

In the fixed-grid method, the absorption and evolution of the latent heat during the phase change leads to the modification of the energy equation because the interface is not tracked, and then the interface conditions are not imposed explicitly. The fixed-grid method is basically relying on the enthalpy formulation, which introduces f (the ratio of the liquid mass to the total mass in a given computational cell). If h_s and T_m are set to the reference enthalpy and temperature, respectively, the specific enthalpy will simply be

$$h=fL+cT, \tag{2}$$

where L and c represent latent heat and specific heat capacity, respectively. The liquid mass fraction can be obtained from the enthalpy:

$$f=\begin{cases} 0 & \text{if } h<0 \\ h/L & \text{if } 0\le h\le L \\ 1 & \text{if } L<h \end{cases}. \tag{3}$$

In isothermal phase change, finally, we can obtain the enthalpy-based governing equations [Viswanath and Jaluria, 1993; Rady and Mohanty, 1996]:

$$\nabla\cdot\vec{u}=0, \tag{4}$$

$$\rho\left(\frac{\partial\vec{u}}{\partial t}+\vec{u}\cdot\nabla\vec{u}\right)=-\nabla p+\mu\nabla^2\vec{u}-\rho\vec{g}\beta(T-T_m)+\vec{S}, \tag{5}$$

$$\rho\left[\frac{\partial}{\partial t}(cT)+\vec{u}\cdot\nabla(cT)\right]=k\nabla^2T-\rho L\frac{\partial f}{\partial t}, \tag{6}$$

where $\vec{u}$, ρ, $\vec{g}$, β and k are the velocity vector, density, gravitational acceleration, thermal expansion coefficient and thermal conductivity, respectively. During the solution process of the momentum field, the velocity at the computational cell located in the solid phase should be suppressed while the velocity in the liquid phase remains unaffected. One of the popular models for the velocity switch-off is to introduce a Darcy-like term [Viswanath and Jaluria, 1993; Rady and Mohanty, 1996]:

$$\vec{S}=-C\frac{(1-f)^2}{(f^3+b)}\vec{u} \tag{7}$$

which are easily incorporated into the momentum equation as shown in Eq. (5). The constant C has a big value to suppress the velocity as a cell becomes solid and b is a small number used to prevent the division-by-zero when a cell is fully located in the solid region, namely f=0. The choice of the constants is arbitrary. However, the constants should ensure sufficient suppression of the velocity in the solid region and also they do not influence the numerical results significantly. In this work, C=1×10^9 kg/m^{3}s and b=0.005 are used [Viswanath and Jaluria, 1993].

NUMERICAL MODEL

For effective calculation, the numerical procedure adopts the front-layer predictor-corrector algorithm, which was devised for, and successfully applied to, the heat conduction phase change problems by Kim et al. [2001]. The detailed numerical procedure is well described in their work, where several illustrative examples can also be found. This study introduces the pseudo Newton-Raphson algorithm in addition to the front-layer predictor-corrector algorithm. The idea of the pseudo Newton-Raphson algorithm is straightforward. The discretized energy equation in the finite volume formulation [Patankar, 1980] can be expressed as

$$a_P T_P = \sum_{nb} a_{nb} T_{nb} + S_P - a_P^0 (f_P - f_P^*) \tag{8}$$

where subscripts 'P' and 'nb' mean the value of present and neighboring cell, respectively. Superscript '*' denotes the value at previous time step. The detailed expressions of the influence coefficients a_P, a_{nb}, a_P^0 and source term S_P can be found without difficulty (refer to Patankar [1980]). The terms relating to the liquid fraction separate the non-linear behavior associated with the phase change into a source term. During the iterative predictor-corrector procedure, in order to expedite the temperature convergence from the non-linear relations, we could resort to the Newton-Raphson method. The problem is to find the temperature minimizing the objective function Φ:

$$\Phi = a_P T_P - \left[\sum_{nb} a_{nb} T_{nb} + S_P - a_P^0 (f_P - f_P^*) \right]. \tag{9}$$

The updated temperature could be written as

$$T_P^{(n+1)} = T_P^{(n)} - \Phi^{(n)} \left[\frac{\partial \Phi^{(n)}}{\partial T_P} \right]^{-1}. \tag{10}$$

If the Jacobian $\partial\Phi/\partial T_P$ is known, the Newton-Raphson method surely guarantees faster convergence. However, the Jacobian cannot be given without any cost. Now, we assume that the neighboring temperatures are constant during the predictor-corrector procedure and f does not have terms explicitly related to T_P. Also if thermophysical properties are not to be strongly dependent on temperature, the Jacobian could be fairly approximated as $\partial\Phi^{(n)}/\partial T_P \cong a_P^{(n)}$. Now, the updated temperature can be readily obtained:

$$T_P^{(n+1)} = T_P^{(n)} - \frac{\Phi^{(n)}}{a_P^{(n)}}. \tag{11}$$

We call this algorithm the pseudo Newton-Raphson since we do not strictly calculate the Jacobian.

The SIMPLE algorithm [Patankar, 1980] is employed to find the velocity and pressure field. The interpolation scheme for the convection term is known to be very important in the prediction of convection-dominated processes. In the context of the spatial discretization, introducing the central difference scheme as a second order scheme is quite natural but it is often baffling due to its well-known oscillatory behavior. As a simple way to detour such oscillatory behavior, the upwind difference scheme is referred to. It is, however, prone to false diffusion especially in the multi-dimensional problem. The power law scheme based on the exact solution of the one-dimensional convection problem is preferred in many engineering purposes. Of course, numerous interpolation schemes have been devised and used. Some of them are as simple as the interpolation schemes stated above, but most of them are more complicated, harder to implement, and even more time-consuming. These adverse features make the aforementioned classical interpolation schemes viable.

One of the simple but effective schemes is the deferred correction method [Ferziger and Peric, 1999]. The lower-order flux approximation (the upwind difference scheme is often used) is implicitly imposed while the higher-order approximation is explicitly obtained from the previous iteration. For example, the flux through the east control surface F_e is given as

$$F_e = F_e^L + \gamma (F_e^H - F_e^L)^{old}, \tag{12}$$

where γ is the blending factor, and the superscripts H and L represent higher- and lower-order approximation of the convection term, respectively. Normally, the explicit part is so small that it may not affect the convergence significantly. In this study, as the lower- and the higher-order scheme, the upwind difference scheme (UDS) and the central difference scheme (CDS) are chosen, respectively. The case with γ=0.5 is called the mixed difference scheme (MDS).

NUMERICAL RESULTS AND DISCUSSION

The proposed algorithm is applied to simulate the convection-dominated melting of a pure gallium. The numerical predictions are compared with the experimental data and numerical results determined by the transformed-grid method in the previous works. The gallium melting experiments of Viskanta and his coworkers [Gau and Viskanta, 1986; Beckermann and Viskanta, 1989] are selected as references because they have been widely cited for the verification of recently developed numerical models [Brent et al., 1988; Desai and Vafai, 1993; Viswanath and Jaluria, 1993; Rady and Mohanty, 1996]. The experimental configurations are sketched in Fig. 1. The thermophysical properties used in the calculation are adopted from Brent et al. [1988].

1. Example 1

Experiment 1 of Beckermann and Viskanta [1989] is simulated with the proposed method. Rady and Mohanty [1996] used a non-uniform 35×35 grid for the fixed-grid calculation after a grid refinement test. Hence, this study simply adopts a non-uniform 40×40 grid for Example 1. As the interpolation scheme for the convective transport term, the mixed difference scheme is adopted because it gives satisfactory results for the prediction of the flow structure in the melt and the evolution of the front location. The effect of the interpolation model for the convection term on the numerical results will be discussed later.

The predicted temperature profiles at 3, 10, and 50 min are shown in Fig. 2, where the experimental data and the transformed-grid results obtained by Beckermann and Viskanta [1989] are also given for the comparison. The calculated temperature distributions show a better agreement with the experimental data than those by the transformed-grid.

In this melting experiment, Beckermann and Viskanta reported that it took about 20 sec for the hot wall to reach the desired temperature, and the time delay in heating is small enough. Because the calculation also shows its effect to be negligible, the computational results with the delayed heat-up are not presented in Fig. 2.

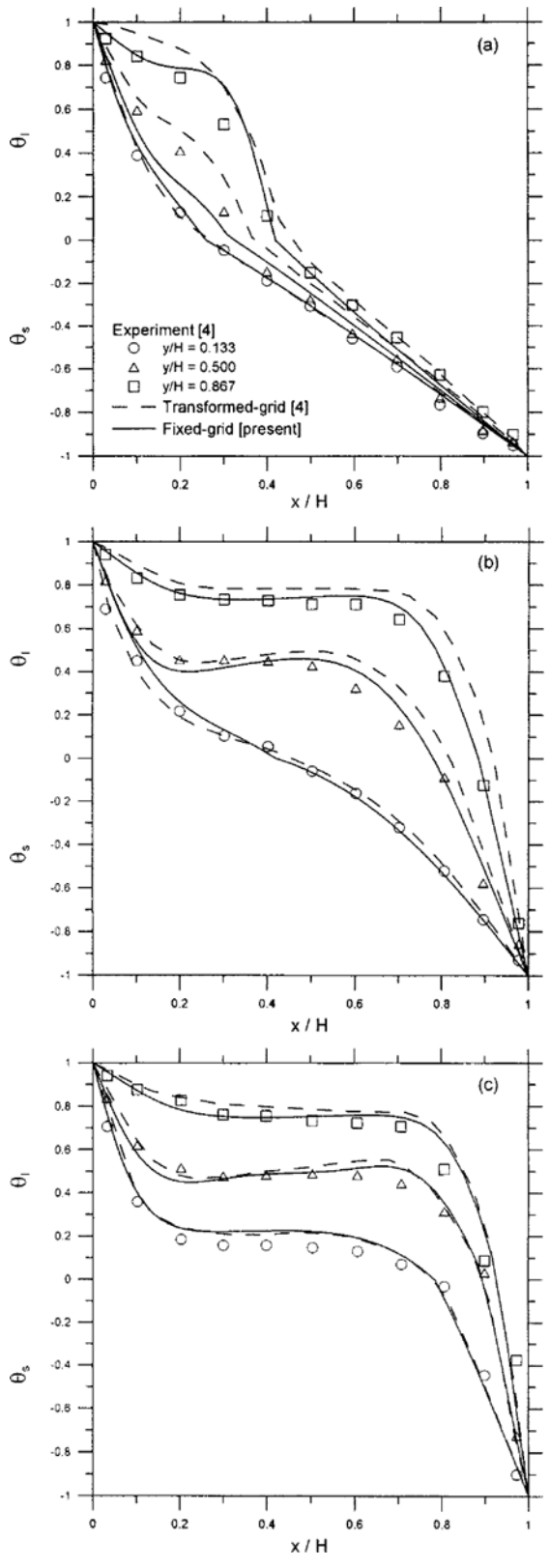

Fig. 2. Temperature profile for Example 1, where θ_l and θ_s represent dimensionless temperatures of liquid and solid phase, respectively: (a) at 3 min; (b) at 10 min; (c) at 50 min.

2. Example 2

In order to verify the predictability of the evolution of the phase front, Gau and Viskanta's [1986] melting experiment conducted in a rectangular cavity with H/W=0.714 is chosen. A uniformly spaced 50×36 grid is used for our calculations, while Viswanath and Jaluria [1993] used a uniform 50×30 grid for the fixed-grid calculation after a grid refinement test.

As for the interpolation schemes of the convection term, we tested four schemes preliminarily; UDS (γ=0.0), CDS (γ=1.0) and MDS (γ=0.5) and a power law scheme (PLS). During preliminary calculations, the delayed heat-up at the heated wall is not considered. The front locations predicted by the UDS, the MDS and the PLS are similar to each other, but the phase change front by the CDS is somewhat distorted. An interesting point to note is that the flow structures obtained in many researches [Brent et al., 1988; Viswanath and Jaluria, 1993; Voller, 1997] show only a single cell in the melt region. Viswanath and Jaluria [1993] observed a secondary recirculation cell in the lower part of the melt region with the transformed grid. However, they also were not able to capture the secondary eddies with the fixed-grid based on the enthalpy method, even with a finer resolution (60×50) than the transformed-grid calculation (40×40). Our calculations show that the CDS and the MDS predict the streamlines that are obviously distorted due to the secondary flow structure, as shown in Fig. 3 while the UDS and the PLS generate only a single cell. The results support that the upwinding algorithm tends to be overly diffusive and suppresses the secondary structure as Ferziger and Peric [1999] criticized. The tested results show that the MDS has good predictability of the front location and the flow structure in the melt. The MDS, hence, is adopted as an interpolation scheme of the convection term throughout the calculation.

As shown in Fig. 4, the measured phase fronts are plotted to verify the proposed model with the transformed-grid solutions based on the finite element method [Desai and Vafai, 1993] and the finite volume method [Viswanath and Jaluria, 1993]. Of course, in both studies, the heated wall condition was treated as ideal sudden temperature elevation and the time delay in heating up the heated wall was not considered.

When comparing solid-liquid interfaces of two methods at 6 and 10 min, the transformed-grid method gives good agreement with the experimental data. But the predicted solid-liquid interfaces by the proposed method without taking the delayed heat-up into account show some discrepancy with the experimental data. Such discrepancy is, in fact, more reasonable because the impulsive temperature rise is very difficult in the experiment and the heated wall should be heated up with time delay. The actual amount of energy transferred to the gallium through the hot wall should be less than the energy imposed in the idealized simulation, so that the retardation of the front evolution in the experiments is probable. The measurement of the reliance of the actual temperature at the heated wall is required to account for the delayed heat-up. However, a detailed history of the temperatures at the hot wall is not available in this problem. Therefore, we introduce the time constant as shown in Eq. (1) because we may approximate the temperature at the hot wall to be exponentially growing with a suitable time constant. We assume τ=67.89 sec, which corresponds to T_H (4 min)=37.71 °C and T_H (8 min)=37.99 °C. This temperature history is close to the measured data in a similar experimental condition (See Fig. 5 in Gau and Viskanta [1986]). As can be seen in Fig. 4, the inclusion of the delayed heat-up improves the numerical prediction considerably.

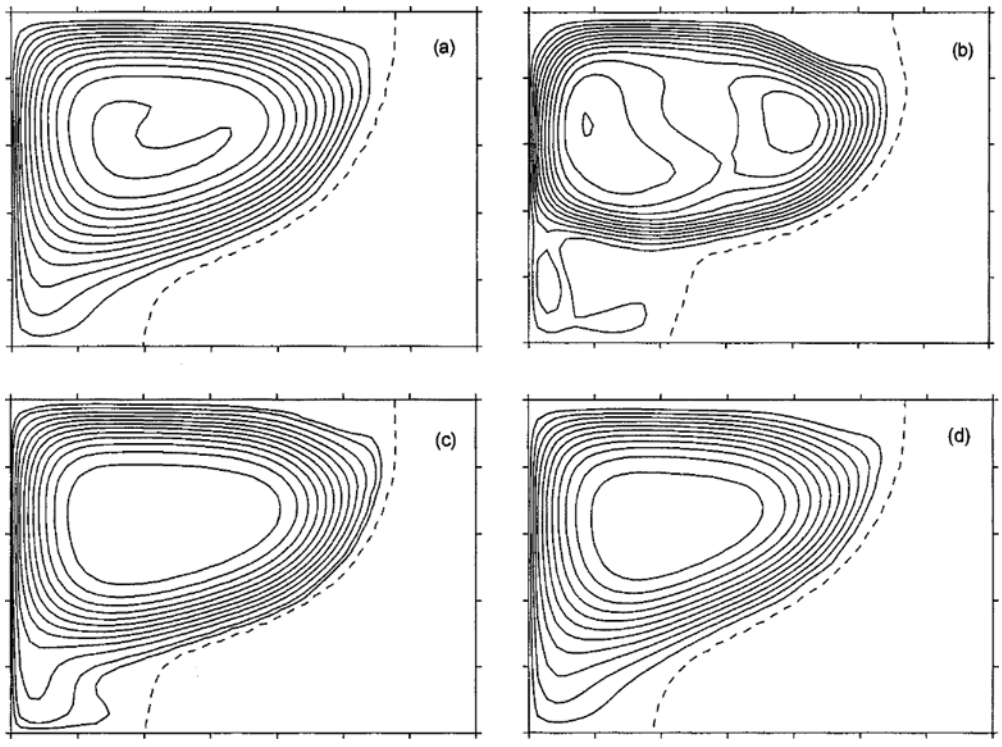

Fig. 3. Streamlines for Example 2 at 19 min: (a) UDS; (b) CDS; (c) MDS; (d) PLS.

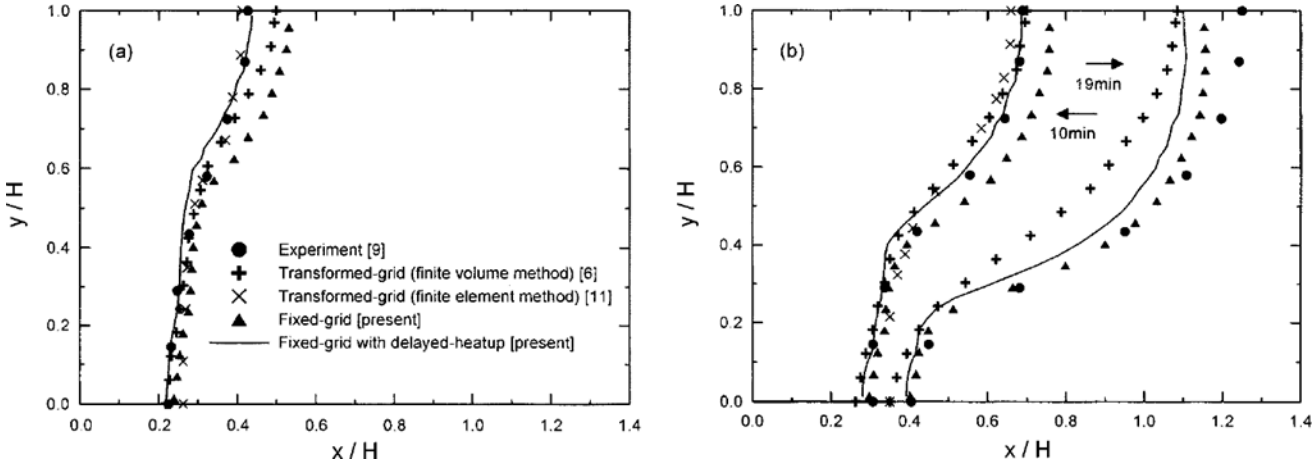

Fig. 4. Evolution of phase front for Example 2: (a) at 6 min; (b) at 10 and 19 min.

The predicted phase fronts with the consideration of time delay are retarded due to less heat transfer from the heated wall, and they are in excellent agreement with the experimental results.

The effect of delayed heat-up at the hot wall is less significant at 19 min; on the contrary, the interfaces obtained by Viswanath and Jaluria [1993] with the transformed-grid deviate much more from the experimental data than those with the proposed model. The finite element results by Desai and Vafai [1993] do not present the front location at 19 min, so that these are not compared in Fig. 4. It should be noted that all numerical results at 19 min presented in Fig. 4 show much discrepancy with the experimental data than those at 6 or 10 min. Even though the proposed model gives better prediction than the previous models, our results still have an obvious discrepancy with the experiment. Some part of the discrepancy can be explained by considering the experimental condition at the cooled wall. According to Fig. 5 in Gau and Viskanta [1986], the cold wall temperature was gradually increased from the initial temperature to the fusion temperature. Hence, as time proceeded, less heat was removed through the cold wall. The inaccurate modeling of the thermophysical properties such as the anisotropic nature of the thermal conductivity as well as the numerical modeling error, of course, can be another reason for the discrepancy.

CONCLUSIONS

The melting driven by conduction as well as convection in a rec-

tangular enclosure is investigated numerically. The mathematical model based on the enthalpy-porosity method is developed to describe the phase change accompanied with natural convection. This study adopts the front-layer predictor-corrector and the pseudo Newton-Raphson algorithms, whose effectiveness is verified through solving the conduction-driven phase-change problems. Results of the proposed model show excellent agreement with experimental data and transformed-grid results available in the literature.

The effect of the time delay in heating a hot wall on the melting is studied. The computational results indicate that the delayed heat-up will affect the phase-change process if the time constant of the heat-up at the heated wall is not small enough. They also imply the delayed heat-up causes the discrepancy between the numerical and the experimental results.

NOMENCLATURE

c : specific heat capacity
CDS : central difference scheme
f : liquid mass fraction
F_e : flux through the east face
h_s : saturation enthalpy of solid
L : latent heat
MDS : mixed difference scheme
PLS : power law scheme
$\vec{S}$: source vector to account for velocity suppression
T_i : initial temperature
T_m : fusion temperature
T_C : temperature at the right wall (cold wall)
T_H : temperature at the left wall (hot wall)
T_{H0} : predetermined temperature to be reached
UDS : upwind difference scheme

Greek Letters

α : thermal diffusivity
β : thermal expansion coefficient of liquid
γ : blending factor used in deferred correction method
ΔT : temperature difference ($T_{H0} - T_m$)
ρ : density
τ : time constant
Pr : Prandtl number ($=\nu_l/\alpha$)
Ra : Rayleigh number ($=g\beta\Delta TH^3/\alpha\nu_l$)
Ste : Stefan number ($=c\Delta T/L$)

Superscript

H, L : higher- and lower-order approximation of the convection term

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