Fixed-Grid Simulation of Convection-Dominated Melting in a Rectangular Cavity

Sin Kim, Wongee Chun*
Department of Nuclear and Energy Engineering, Cheju National University
Min-Chan Kim
Department of Chemical Engineering, Cheju National University

Numerical solutions for the convection-dominated melting in a rectangular cavity are presented. The enthalpy-porosity model is employed as the mathematical model. This model is applied in conjunction with the EIT method to detect boundary movement in a phase changing environment. The absorption and evolution of latent heat during the phase change is dealt with by the enthalpy-based energy equation. This seems to be more efficient than resolving the temperature-based energy equation. The velocity switch-off, which is required when solid changes into liquid, is modeled by the porous medium assumption. For efficiency and simplicity of the solution procedure, this paper proposes a simple algorithm, which iterates the temperature and the liquid fraction of the cells comprising the front layer. The numerical results agree reasonably well with the experimental data and other previous works using the transformed-grid system.

Key Words : Melting, Natural Convection, Enthalpy-Porosity Method, Fixed-Grid Method

Nomenclature

c : Specific heat capacity
f : Ratio of the liquid mass to the total mass
g : Gravitational constant
H : Cavity height
h : Specific enthalpy
h_s : Saturation enthalpy of solid state
k : Thermal conductivity
L : Latent heat
p : Pressure
Pr : Prandtl number, $Pr=\frac{v_l}{\alpha_l}$
Ra : Rayleigh umber, $Ra=\frac{g\beta\Delta TH^3}{\alpha_l v_l}$
Ste : Stefan number, $Ste=\frac{c_l(T_H-Tm)}{L}$

* Corresponding Author,
E-mail : wgchun@chju.ac.kr
TEL : +82-64-754-3646; **FAX** : +82-64-757-9276
Department of Nuclear and Energy Engineering, Cheju National University, #1, Ara 1-dong Cheju-do 690-756, Korea.(Manuscript **Received** November 2, 2000; **Revised** March 14, 2001)

S_u, S_v : Momentum source terms determined according to the model for velocity suppression in the solid phase
T : Temperature
T_C : Cold wall temperature (right wall)
T_H : Hot wall temperature (left wall)
T_i : Initial temperature
T_m : Melting temperature
u, v : Directional velocity for x-and y-coordinates
W : Cavity width

Greek symbol

β : Volumetric compressibility referred to the reference temperature
θ_l : Dimensionless temperature in the liquid region, $\theta_l=\frac{T-T_m}{T_H-T_m}$
θ_s : Dimensionless temperature in the solid region, $\theta_s=\frac{T-T_m}{T_m-T_C}$
μ : Viscosity
ρ : Density

1. Introduction

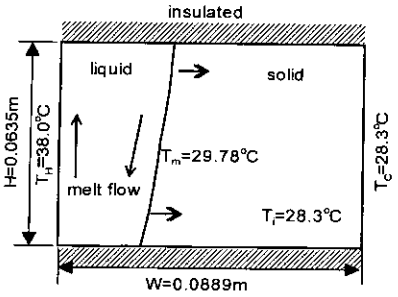
In many engineering fields such as thermal energy storage systems using latent heat and materials processing, melting is an important process to be considered for the optimal design and operation. The temperature difference in melt can give rise to natural convection and the resulting flow structure can significantly affect the phase change process. The convection gives a great influence on the morphology of solid-liquid interface, which may change the flow structure in the melt. Hence, the effect of natural convection in the melt on the phase change has drawn considerable attention for the past several decades (Voller, 1997)

In general, numerical simulations commonly used for phase change problems can be classified into two different approaches; the fixed-grid and the transformed-grid methods. In the fixed-grid method, a single set of conservation equations and boundary conditions is used for the whole domain comprising solid and liquid phases, while the transformed-grid method considers the governing equations based on the classical Stefan formulation. The interface conditions, therefore, are treated differently according to the method for solving the phase change problem. In the transformed-grid method, they are easily implemented because the interface is explicitly solved. However, in the fixed-grid method, the interface conditions are described as source terms in the governing equations. A nodal latent heat value is assigned to each computational cell according to its temperature or enthalpy. Upon phase change, the latent heat absorption, or evolution, is reflected as a source or sink term in the energy equation.

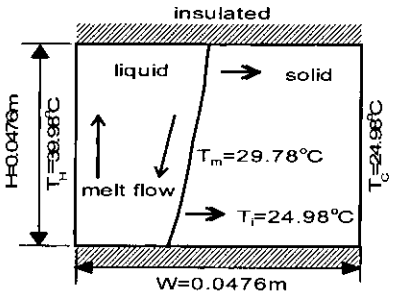
The fixed-grid method requires velocity switch-off because it is necessary to impose the zero-velocity condition whenever phase change takes place from liquid to solid. The velocity switch-off is readily accomplished either by imposing a large value of viscosity for the solid phase or by a suitable source term in the momentum equation 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.

Brent et al. (1988) introduced the enthalpy-porosity technique to model convection-diffusion melting. Lacroix and Voller (1990) applied the fixed-grid and transformed-grid methods to the solidification phase change problem. Emphasis was placed on prediction of the front location and CPU requirement. Viswanath and Jaluria (1993) compared for the fixed-grid and transformed-grid schemes. for convection-dominated melting, They focused on the relative performances regarding interface movement, heat transfer rates, and the nature of convective motion established in the melt. Rady and Mohanty (1996) presented the numerical prediction of melting and solidification of pure metal with the enthalpy-porosity fixed-grid method. They improved the solution procedure by using a dual iteration loop in which the energy equation is solved iteratively in the inner loop. The calculation then proceeded for the outer loop to resolve the rest of the unknown variables. Recently, Rady et al. (1997) employed the algorithm of Rady and Mohanty (1996) to investigate the effects of liquid superheating during solidification.

To simulate the phase change process, this paper proposes a simple numerical scheme based on the enthalpy-porosity method. The scheme facilitates the application of existing computer codes for heat and fluid flow to resolve a phase change problem. This, of course, requires some modifications to the codes which could be readily done. The proposed algorithm has been tested for the heat-conduction phase change problems, in which there is no natural convection in the liquid zone (Kim et al., 2000). The efficiency and reliability of the algorithm were proved in some extreme cases without undue difficulties: low Stefan number (sensible to latent heat ratio) with small dimensionless temperature (ratio of initial to boundary temperature deviation from saturation temperature) and large discrepancy between thermal conductivity of each phase. These problems are known to deteriorate the numerical performance and sometimes fail to



(a) Gau and Viskanta(1986)



(b) Beckermann and Viskanta(1988)

Fig. 1 Definition of gallium melting problem

converge (Fachinotti et al., 1999). This study extends the algorithm to the convection-dominated melting problem. The spatial and temporal discretizations are carried out on the basis 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 the SIMPLE algorithm.

2. Mathematical Models for Convection-Dominated Phase Change Problems

Two-dimensional melting in a rectangular cavity is schematically described in Fig. 1. Melting is driven by the combined effect of natural convection and conduction in a rectangular cavity. The phase change material is contained in a cavity, whose vertical sides are maintained at constant temperatures, while the connecting horizontal walls are adiabatic. Initially, the phase change material in the cavity is kept at uniform temperature below or at the fusion temperature, $T_i \leq T_m$, where T_i is the initial temperature and T_m is the melting temperature. The melting is initiated by raising the temperature of the left wall abruptly to a predetermined temperature, T_H, above the fusion temperature, $T_H > T_m$. The temperature at the right wall, T_C, is maintained at the initial temperature, $T_C = T_i$. As time elapses, the buoyancy force becomes large enough to overcome viscous resistance and triggers natural convection in the melt zone.

The momentum field is subject to no-slip boundary condition on the walls. The flow is assumed to be two-dimensional, laminar, and incompressible. The thermophysical properties of materials are constant, but may be different for the liquid and solid phase. The density difference between solid and liquid is neglected except when invoking the Boussinesq approximation.

In the fixed-grid method, the absorption and evolution of latent heat during phase change leads to modification of the energy equation. This is because the method doesn't track the movement of interface with phase change and no explicit conditions are given at the interface. The fixed-grid method is basically relying on the enthalpy formulation, which employs enthalpy as a dependent variable in the energy equation instead of temperature. The enthalpy formulation also introduces the liquid mass fraction f defined as the ratio of the liquid mass to the total mass in a given computational cell. If h_s and T_m are given as the reference enthalpy and temperature, respectively, the specific enthalpy will simply be

$$h = fL + cT \tag{1}$$

The heat capacity c may vary with phase. The liquid mass fraction can be obtained from the enthalpy:

$$f = \begin{pmatrix} 0 & \text{if} & h < 0 \\ \dfrac{h}{L} & \text{if} & 0 \leq h \leq L \\ 1 & \text{if} & L < h \end{pmatrix} \tag{2}$$

In the isothermal phase change with stationary solid phase, finally, we can obtain the enthalpy-based governing equations (Viswanath and Jaluria, 1993):

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0, \tag{3}$$

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)+S_u, \tag{4a}$$

$$\rho\left(\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right)=-\frac{\partial p}{\partial y}+\mu\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+\rho g\beta(T-T_{ref})+S_v, \tag{4b}$$

$$\rho\left[\frac{\partial}{\partial t}(cT)+u\frac{\partial}{\partial x}(cT)+v\frac{\partial v}{\partial y}(cT)\right]=k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right)-\rho L\frac{\partial f}{\partial t} \tag{5}$$

Here, S_u and S_v are the source terms to account for velocity switch-off.

During the solution procedure of the momentum field, the velocity at the computational cells in the solid phase should be suppressed while the velocities in the liquid phase remains unaffected. Introduction of a Darcy-like term (Viswanath and Jaluria, 1993) is popular in modeling velocity switch-off in many cases;

$$S_u=-C\frac{(1-f)^2}{(f^3+b)}u \text{ and } S_v=-C\frac{(1-f)^2}{(f^3+b)}v \tag{6}$$

This is easily incorporated into the momentum equation as shown in Eq. (4). The constant C is a large value to suppress the velocity if 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 these constants is arbitrary. However, the constants should ensure sufficient suppression of the velocity in the solid region and should not interfere with the numerical results. In this work, $C=1\times10^9$kg/m^{3}s and $b=0.005$ are used (Viswanath and Jaluria, 1993).

3. Numerical Methods for Phase Change

3.1 Front-layer predictor-corrector algorithm

The discretized energy equation in the finite volume formulation (Patankar, 1980) can be expressed as

$$a_P T_P=\sum_{nb}a_{nb}T_{nb}-a_P^0(f_P-f_P^*) \tag{7}$$

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 the source term, S_P, can be found in Patankar, 1980. The terms related with the liquid fraction separate the non-linear behavior associated with phase change into a source term.

If the discretized equation in the above is solved properly at the n-th iteration step, the enthalpy obtained with physical properties assumed at the n-th iteration step satisfies the energy conservation equation. Then, the enthalpy and the liquid fraction can be obtained from Eqs. (1) and (2), respectively. This procedure redistributes the energy contained in the cell so that the excessive (or deficient) energy can be stored into (or retrieved from) latent heat rather than spurious sensible heat. Also, the temperature can be re-estimated according to the new mass fraction

$$T^{(n+1)}=\left(\frac{h^{(n+1)}}{L}-f^{(n+1)}\right)\frac{L}{c^{(n+1)}} \tag{8}$$

which gives a better estimation for the next iteration.

At the cell with phase change, the updated temperature distribution should satisfy the discretization equation. If we assume the present cell 'P' is undergoing phase change, the temperature is given by

$$T_P^{(n+1)}=\frac{\sum a_{nb}^{(n+1)}T_{nb}^{(n)}+GS_P^{(n+1)}}{a_P^{(n+1)}} \tag{9}$$

The generalized source, GS_P, can be easily obtained from Eq. (7). The influence coefficients and the generalized source are calculated with the updated mass fraction, $f^{(n+1)}$. Although the temperatures of neighboring cells T_{nb} are obtained at the previous iteration step and may be comparatively less correct than the other updated values, the new temperature $T_P^{(n+1)}$ based on the updated mass fraction will yield a better estimation. We could use this temperature to update the mass fraction with the enthalpy expression. The foregoing predictor-corrector procedure will be

applied iteratively only to those phase changing cells existing in the phase change front. Hereafter this algorithm will be referred to as the front-layer predictor-corrector (FLPC) algorithm. Kim et al. (2000) called this algorithm the single-point predictor-corrector because they applied it to the one-dimensional heat conduction phase change problem where the phase front is limited to a single node. We don't need to solve the whole set of the governing equations during the FLPC procedure. It should be noted that during the FLPC procedure the temperatures at neighboring cells are not changed, but the updated temperature is a good estimation for the next iteration. The proposed algorithm seems to be effective due to its simplicity and a low computational cost. Furthermore, this can be readily adapted to any numerical schemes designed for computational efficiency. This algorithm always ensures energy conservation for phase changing cells.

3.2 Pseudo Newton-Rapson algorithm

In this study, another simple algorithm is introduced to further improve the convergence. Let's consider the discretized energy equation, Eq. (7), again. During the FLPC procedure, we could resort to the Newton-Rapson method in order to expedite the temperature convergence from the non-linear relations. The problem is to find the temperature minimizing the objective function Φ:

$$\Phi = a_p T_p - \left[\sum_{nb} a_{nb} + S_p - a_p^0 (f_p - f_p^*)\right] \quad (10)$$

The updated temperature could be written as

$$T_p^{(n+1)} = T_p^{(n)} - \Phi^{(n)} \left[\frac{\partial \Phi^{(n)}}{\partial T_p}\right]^{-1} \quad (11)$$

If the Jacobian $\partial \Phi / \partial T_P$ is known, the Newton-Rapson method surely guarantees faster convergence. However, the Jacobian can not be procured without any cost.

Recall that the neighboring temperatures are assumed to be constant during the predictor-corrector procedure and f does not have any terms explicitly related to T_p. Also the thermophysical properties are assumed not to be strongly dependent on temperature. From these, the Jacobian could be reasonally approximated as $\partial \Phi^{(n)} / \partial T_P \cong a_p^{(n)}$. The updated temperature can be readily obtained as,

$$T_p^{(n+1)} = T_p^{(n)} - \frac{\Phi^{(n)}}{a_p^{(n)}} \quad (12)$$

We call this algorithm pseudo Newton-Rapson (pNR), since we do not strictly calculate the Jacobian. The extra cost of the pNR is negligible. The preliminary studies on the heat conduction phase change examples demonstrate the efficiency of the pNR scheme. It is capable of reducing the total number of inner iterations required for the converged solution to about 2/3 of the original one.

4. Numerical Results and Discussions

The convection-dominated melting of pure gallium is simulated against the proposed algorithm. The numerical predictions are verified and discussed against the experimental and numerical results in literature. The experiment of Viskanta and his coworkers (Gau and Viskanta, 1986; Beckermann and Viskanta, 1988) is chosen as a reference case because they have been widely cited for verification of numerical models (Brent et al., 1988; Lacroix and Voller, 1990; Viswanath and Jaluria, 1993; Rady and Mohanty, 1996). Also, the transformed-grid results of Viswanath and Jaluria (1993) are compared.

The experimental configurations are sketched in Fig. 1. Initially, a solid gallium block is kept at a constant temperature, T_i. The temperature at the left wall is increased instantly to T_H, while the right wall is maintained at $T_C = T_i$. The thermophysical properties used in the calculation are adopted from Brent et al. (1988): density $\rho = 6095 \text{kg/m}^3$, latent heat $L = 8.017 \times 10^4 \text{J/kg}$, specific heat capacity $c = 381.5 \text{J/kg}^\circ\text{C}$, thermal diffusivity $\alpha = 1.376 \times 10^{-5} \text{m}^2/\text{sec}$ and kinematic viscosity of liquid phase $v_l = 2.970 \times 10^{-7} \text{m}^2/\text{sec}$. Hence, the Prandtl number is $Pr = 0.0216$. The Rayleigh number and the Stefan number used in the Gau and Viskanta's experiment (1986) are $Ra = 6.057 \times 10^5$, $Ste = 0.03912$; whereas $Ra = 3.166 \times 10^5$, $Ste = 0.04854$ are those of Beckermann and Viskanta's experiment (1988). The

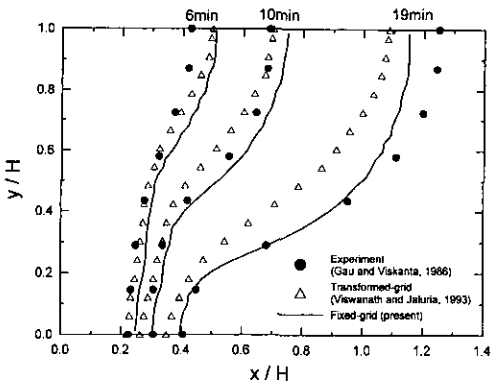


Fig. 2 Solid-liquid interface location during the melting of gallium

foregoing dimensionless numbers are defined as the following:

$$Pr=\frac{\nu_l}{\alpha_l},\ Ra=\frac{g\beta\Delta TH^3}{\nu_l\alpha_l} \text{ and}$$

$$Ste=\frac{c_l(T_H-T_m)}{L} \tag{13}$$

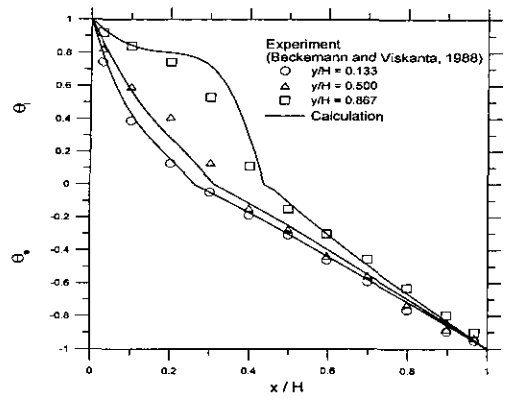
According to the experiment of Gau and Viskanta(1986), the interface continuously changes its shape as melting of gallium proceeds from its flank. At the very early stage, its shape is flat and parallel to the heating wall because the buoyancy-driven flow is still weak. However, the effect of heating propagates with time, which triggers the convective motion of melt. This is driven by buoyancy and as it develops, the distortion of interface becomes more obvious. The melt layer grows faster in the upper region since its temperature is higher than the rest. This is schematically illustrated in Fig. 1.

In the present analysis, the experiment of Gau and Viskanta is first simulated to establish reliability of the proposed model. The predicted phase change fronts are shown with the results from the experiment and the transformed-grid simulation of Viswanath and Jaluria (1993) in Fig. 2. The latter used a uniform grid system of 50x30 for their simulation following rigorous investigation on grid refinement. They tested up to a grid system of 60×50, which resulted in little improvement. Based on these results, the present work has employed a uniform grid system of 50x36, which is appropriate concerning accuracy and computational efficiency. The numerical results obtained reassure our intuitive conclusion about the outcome of the physical phenomena involved. That is, the interface evolves with time and the upper part of the phase front penetrates into the solid region effectively due to buoyancy-driven melt convection. When comparing solid-liquid interfaces at 6 and 10 min, the transformed-grid results show slightly better agreement with the experiment than the present model, but the difference is not significant. The front location at 19 min is successfully predicted with the proposed method, while the transformed-grid results show somewhat large discrepancy. It should be noted that the retardation of the front movement at 6 min is observed in both the transformed-and the fixed-grid simulations. It is quite probable that this indicates what could happen in reality. The hot wall temperature, even though it is assumed here for the sake of simulation, could not reach the desired temperature in reality. It is likely that less heat is transferred to gallium than what's been predicted in both numerical analyses. The proposed algorithm based on the fixed-grid approach shows better prediction of the interface movement than the transformed-grid approach.

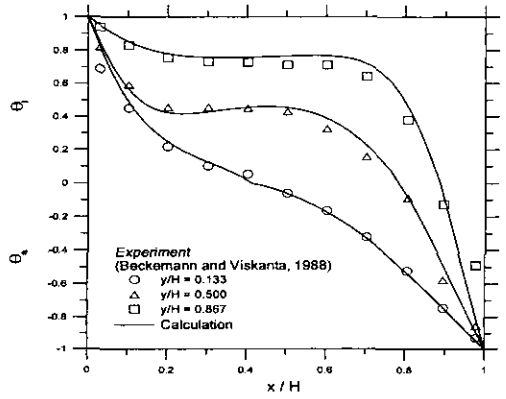
The heat transfer during melting is also well predicted by the proposed algorithm with the 40×40 uniform grid system. The calculated temperature profiles agree quite well with the measurements of Beckermann and Viskanta (1988), as seen in Figs. 3(a)-(c). The measured and calculated results confirm occurrence of distortion in the phase interface and its evolution with time as the wall heating continues. In these figures, the temperature is non-dimensionalized to comply with the notations of Beckermann and Viskanta. The dimensionless temperatures in the solid region, θ_s, and in the liquid region, θ_l, are

$$\theta_s=\frac{T-T_m}{T_m-T_C} \text{ and } \theta_{sl}=\frac{T-T_m}{T_H-T_m} \tag{14}$$

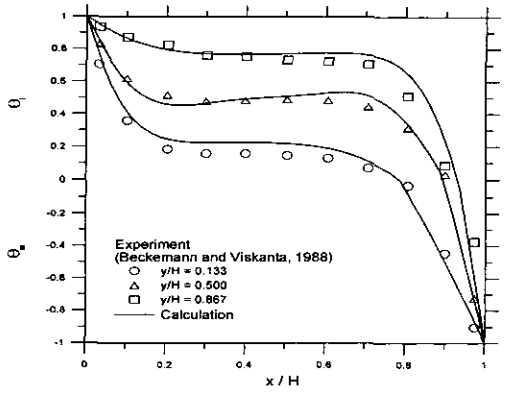
respectively. Hence, θ_s has a negative value while θ_l has a positive value. Except for the temperature distribution in the upper region at 3 mins, the agreement between experiment and calculation seems excellent. The temperatures in the upper



(a) At 3 min



(b) At 10 min



(c) At 50 min

Fig. 3 Temperature profile during the melting of gallium

melt zone at 3 mins are somewhat overestimated. This overestimation seems to be natural because, as mentioned in the above, the amount of heat transferred to gallium in the calculation should be more than in the experiment. Hence, the calculated flow, especially in the upper melt region, tends to be more developed than the real flow.

5. Conclusions

The convection-dominated melting in a rectangular cavity is investigated numerically with the fixed-grid formulation. Especially, this work proposes a simple numerical scheme that predicts and corrects the temperature and liquid fraction for a phase changing cell during the computation. It also introduces the pseudo Newton-Raphson algorithm.

The location of the phase front and the temperature distribution during the melting of gallium are simulated for verification of the numerical model. Except for the earlier stage of melting, the agreement between experiment and calculation seems excellent. The discrepancy between experiment and calculation at the earlier stage of melting can be explained quite reasonably if one considers the fact that an abrupt change in temperature for one of the boundaries (i. e. the hot wall in this case) is almost impossible to implement in reality. Hence, the actual amount of the heat transferred to the gallium is less than what's been given by the simulation. Also, comparisons are made between the fixed- and transformed-grid schemes with regard to prediction of the front location. Results show that both schemes are comparable in this regard.

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