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A Fixed Grid Finite Control Volume Model for the Phase Change Heat Conduction Problems with a Single-Point Predictor-Corrector Algorithm

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Abstract—A numerical scheme based on the enthalpy method is applied to one-dimensional Stefan problems. The discretization equation is derived based on the finite control volume method. To improve the convergence rate, a simple and cost-effective single-point predictor-corrector algorithm is proposed. Usefulness of the present approach is discussed by means of various solidification problems.

Key words: One-Dimensional Stefan Problem, Fixed Grid Method, Enthalpy Formulation, Source Update Method

INTRODUCTION

Phase change problems occur in many engineering applications, *e.g.* solar energy storage, single crystal growth, chemical reactions, freezing and thawing of food, solidification of alloys, and nuclear safety [Choi et al., 1995; Voller, 1997]. Phase change process is related to a moving boundary for which a heat flux condition should satisfy the conservation of heat and release of latent heat during phase change [Crank, 1984]. Although many useful analytical solutions have been derived since the first publication of Stefan in a study of the thickness of polar ice [Carslaw and Jaeger, 1959], they are quite limited to a short range of idealized cases.

There are two main approaches to the solution of the phase change problem. One is the front tracking method, which explicitly tracks the position of the phase change front and the heat flux condition including latent heat is imposed across the moving boundary. Another approach is the method known as a fixed grid method. The former is usually restricted to one-dimensional problems and to the systems which have simple topology without mushy zone [Kruz and Fisher, 1989] while the latter implicitly accounts for the phase change front determined a posteriori from the temperature field. In general, the fixed grid method is thought to be more versatile, and we adopt this method due to its inherent versatility.

The fixed grid method is basically relying on the enthalpy formulation, which uses the enthalpy as a dependent variable of conduction equation instead of the temperature. The obvious merit of the enthalpy formulation is to eliminate the effort to implement the heat flux condition at the interface between two phases. In this, the heat flux condition is automatically satisfied across the phase change front and the front can be tracked on the specification of a nodal liquid fraction. There are several numerical schemes in enthalpy formulation. The source update method, enthalpy linearization method (LINH), and apparent heat capacity method (AHC) are most common and the general description for the methods can be found in Voller [1997].

In this work, we apply the enthalpy formulation with a new effective numerical scheme to one-dimensional phase change problems. The proposed numerical algorithm is based on the fixed grid concept. The discretized heat conduction equation is obtained in the context of finite control volume. It is regarded as a variant of the source update method. Although the source update method is known to be inefficient, we adopt it due to its well-known robustness and seek to improve the calculation efficiency with simple modification. In order to verify the effectiveness of the proposed algorithm, we test various phase change problems. Examples include a critical circumstance: low Stefan number (sensible to latent heat ratio) with small dimensionless temperature (ratio of initial to boundary temperature deviation from saturation temperature). This problem usually deteriorates the numerical performance and sometimes fail to converge. Even though the proposed method is applied to one-dimensional cases, it is readily extendable to multidimension and multicomponent system without serious modification.

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MATHEMATICAL MODEL

1. Heat Conduction Equation

Let us consider the heat conduction equation in one-dimensional domain

$$\frac{\partial}{\partial t}(\rho h)=\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+S \tag{1}$$

written in terms of specific enthalpy h and temperature T, ρ being the density, k the thermal conductivity, and S the internal heat source, all of them actually depending on temperature and position. Eq. (1) is subjected to the initial condition

$$T(x, t=0)=T_i(x) \tag{2}$$

and the boundary conditions

$$\begin{aligned} &T=T_o && \text{at } \partial\Omega_T \\ &k\frac{\partial T}{\partial x}\cdot\vec{n}=q && \text{at } \partial\Omega_q \\ &-k\frac{\partial T}{\partial x}\cdot\vec{n}=h_{conv}(T-T_\infty) && \text{at } \partial\Omega_c \end{aligned} \tag{3}$$

where $\partial\Omega_T$, $\partial\Omega_q$, and $\partial\Omega_c$ are non-overlapping portion of the bound-

ary of problem domain. T_o and q are the specified temperature and incoming heat flux at $\partial\Omega_T$ and $\partial\Omega_q$, respectively. h_{conv} is the heat transfer coefficient and T_∞ is the ambient temperature.

2. Enthalpy Formulation

Specific enthalpy can be expressed as

$$h=h_s+fL+c(T-T_{sat}) \tag{4}$$

where h_s is the saturated enthalpy of solid, T_{sat} the saturated temperature, L the latent heat, c the specific heat, and f the mass fraction of liquid phase. Of course, the heat capacity can be a function of temperature, while h_s, T_{sat}, and L are assumed to be constant. The mass fraction f can be obtained from the enthalpy:

$$f=\begin{cases} 0 & \text{if } h<h_s \\ \dfrac{h-h_s}{L} & \text{if } h_s\le h\le h_s+L \\ 1 & \text{if } h_s+L<h. \end{cases} \tag{5}$$

Substituting Eq. (4) into (1), we can obtain the equation governing enthalpy-based model for phase change heat conduction problems

$$\frac{\partial}{\partial t}(\rho cT)=\frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right)+S-\frac{\partial H}{\partial t} \tag{6}$$

where

$$H\equiv\rho(h_s+fL-cT_{sat}). \tag{7}$$

The latent heat due to phase change is treated as a kind of heat source and this formulation allows us to avoid the difficulties arising from moving phase change front. It is a basic idea of the source updated method, which is known to be extremely robust and has been used to solve a various phase change problems. The price of robustness, however, is lack of computational efficiency.

NUMERICAL MODEL

1. Source Update Method

Based on fully implicit (backward Euler) time integration, the discretized equation of Eq. (6) in the context of finite control volume [Patankar, 1980] can be expressed as

$$[(\rho c)_P a_P^0+a_P]T_P=\sum_{nb}a_{nb}T_{nb}+(\rho c)_P^* a_P^{0*}T_P^*+S_P-a_P^0(H_P-H_P^*) \tag{8}$$

where subscripts 'P' and 'nb' mean the value of the present and neighboring cell, respectively. The superscript '*' denotes the value at the previous time step. The detailed expressions of the influence coefficients a_p, a_{nb}, and a_p^0 can be found in Patankar [1980]. This equation isolates the non-linear behavior associated with the phase change into a source term. A commonly used general iteration scheme is as follows.

(1) Prediction: With the known temperature and liquid mass fraction at (n−1)th iteration step, the system of equations is solved for the temperature field at iteration step 'n':

$$[(\rho c)_P a_P^0+a_P]T_P^n=\sum_{nb}a_{nb}T_{nb}^n+(\rho c)_P^* a_P^{0*}T_P^*+S_P^n-a_P^0(H_P^{n-1}-H_P^*). \tag{9}$$

(2) Correction: If we can set $T_{sat}=0$ and the phase change is occurring at cell 'P', it is recognized that the cell temperature will be given by $T_P=T_{sat}=0$. Hence Eq. (9) will be

$$0=\sum_{nb}a_{nb}T_{nb}^n+(\rho c)_P^* a_P^{0*}T_P^*+S_P^n-a_P^0(H_P^n-H_P^*). \tag{10}$$

From Eqs. (9) and (10), the update formula

$$H_P^n=H_P^{n-1}+\frac{[(\rho c)_P a_P^0+a_P]}{a_P^0}T_P^n \tag{11}$$

is obtained. The new mass fraction of liquid f_P^n can be easily calculated from Eq. (7). Steps (1) and (2) are repeated until convergence.

For the computational efficiency, Voller [1990] proposed a modification of the above procedure:

(1) Prediction: If the phase change is occurring at cell 'P' the coefficient $[(\rho c)_P a_P^0+a_P]$ is replaced by $[(\rho c)_P a_P^0+a_P]$+BIG (arbitrarily large value). This step ensures that $T_P=0$ is returned.

(2) Correction: An appropriate evaluation for the liquid mass fraction can then be obtained on rearranging Eq. (10).

A comparison of CPU times shows that the Voller's scheme is between 1.5 and 10 times faster than the previous scheme. It should be noted that both of above schemes can be modified to deal with cases where $T_{sat}\neq 0$. However, to avoid problems with round off, a temperature scaling such that $T_{sat}=0$ is recommended.

2. Other Methods

Other popular methods are the enthalpy linearization method (LINH) and apparent heat capacity method (AHC). There is no significant difference in the numerical performance, *i.e.* accuracy and computational efficiency. As pointed out by Voller [1997], LINH may not conserve heat at every time step. For the reduction of the error invoked by the failure to completely conserve heat, the time interval should be small enough.

The apparent heat capacity method introduces an apparent heat capacity, $c^A\equiv dh/dT$, to absorb the nonlinear behavior related to the phase change. Although this method is easily applicable to usual heat conduction programs and conceptually non-iterative, it has a critical drawback, that is the singularity of the apparent heat capacity. In order to circumvent the singularity, a fictitious phase change range is often introduced. But such numerical approximation is prone to producing oscillations without special treatments [Davey and Rosindale, 1999]. Also, if the incorporated thermal properties are dependent on temperature the non-iterative concept is no longer useful.

3. Single-Point Predictor-Corrector Algorithm

The most common three algorithms for phase change problems have been briefly reviewed. The major drawbacks are the computational ineffectiveness (source update method) or the robustness (LINH and AHC). Now, we will propose a simple but effective and robust algorithm.

If the discretized equation, Eq. (8), is solved properly at the n-th iteration step, the enthalpy obtained with presumed physical properties at each iteration step

$$h^{(n+1)}=h_s+f^{(n)}L+c^{(n)}(T^{(n)}-T_{sat}) \tag{12}$$

satisfies the energy conservation. The superscript denotes the itera-

tion step. Although, at this step, we do not know the exact mass fraction and the physical properties, the best choice of the mass fraction of liquid phase for the next iteration is to obtain the value from the above enthalpy with conserving the energy

$$f^{(n+1)}=\begin{cases}0 & \text{if} \quad h^{(n+1)}<h_s\\ \dfrac{h-h_s}{L} & \text{if} \quad h_s\le h^{(n+1)}\le h_s+L\\ 1 & \text{if} \quad h_s+L<h^{(n+1)}.\end{cases} \tag{13}$$

This procedure enables the energy contained in the cell to re-distribute so that the excessive (or deficient) energy can be stored into (or retrieved from) a latent heat rather than a spurious sensible heat. Also, the temperature can be re-estimated according to the new mass fraction

$$T^{(n+1)}=T_{sat}+\left(\frac{h^{(n+1)}-h_s}{L}-f^{(n+1)}\right)\frac{L}{c^{(n)}} \tag{14}$$

and it may give better estimation for the next iteration. This is quite similar to previous source update methods. However, it should be noted that we do not force the temperatures even at phase changing cells to be saturation temperature while the previous algorithms did. This may give us more versatility when the saturation temperature is not constant. If we consider a phase change between liquid and vapor we should take into account the variation of the saturation temperature according to the thermodynamic state. Then, it is suspicious whether the updated temperature, $T^{(n+1)}$, can satisfy the energy conservation equation because all physical properties are changed due to the change of mass fraction.

The most important thing in the phase change problem is to estimate accurately the mass fraction. From the enthalpy expression, the temperature can explicitly determine the updated mass fraction. The updated temperature distribution should satisfy the discretization equation at the phase changing cell. If we assume the present cell 'P' is undergoing phase change the temperature can be given by

$$T_P^{(n+1)}=\frac{\sum A_{nb}^{(n+1)}T_{nb}^{(n)}+B_P^{(n+1)}}{A_P^{(n+1)}}. \tag{15}$$

The expressions of the generalized influence coefficients A_p of cell 'P' and A_{nb} of neighboring cells and the generalized source B_P can be easily obtained from Eq. (8). These 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 be a better estimation. We can, of course, use this temperature to update the mass fraction with the enthalpy expression. This predictor-corrector procedure can be applied iteratively only to phase changing cells. We need not solve the whole set of the governing equations during the single-point predictor-corrector procedure, which can be regarded as an inner iteration. It should be noted that during the inner iteration the temperatures at neighboring cells are not changed but the updated temperature is a good estimation for the next iteration. The proposed single-point predictor corrector seems to be very effective due to its simplicity and low computational cost, which will be shown later. Furthermore, this can be readily extendable to multidimensional cases. This algorithm always ensures the energy conservation at the phase changing cell.

The proposed single-point predictor-corrector algorithm is summarized as

(1) Prediction: From the known temperature and liquid mass fraction at (n−1)th iteration step, the enthalpy and the updated mass fraction at each cell is obtained as Eqs. (12) and (13).

(2) Correction: The temperature is recalculated by Eq. (14) with updated physical properties.

(3) Single-Point Correction: For a phase changing cell, *i.e.* $f_P^{(n+1)}\neq f_P^{(n)}$, the temperature at the cell is updated by Eq. (15) with updated physical properties.

(4) Outer Iteration: Repeat (1) and (2) until convergence.

(5) Inner Iteration: Only for phase changing cells, repeat (1) and (3) during specified times or until weak convergence during every outer iteration.

EXAMPLES

1. Solidification Problems with Ste=0.2, 2.0

In order to test the accuracy and the computational efficiency of the proposed single-point predictor-corrector algorithm, let us consider two solidification problem with different Stefan numbers defined as

$$\mathrm{Ste}=\frac{c(T_{sat}-T_o)}{L}. \tag{16}$$

For the comparison with the results listed in Voller [1997], two Stefan numbers 0.2 and 2.0 are chosen. Using a fixed grid with 50 volumes ($\Delta x=0.1$) the proposed scheme is used to predict the time taken for the phase change front to reach the position x=1.0. A range of time steps, starting with $\Delta t=0.005$ (the explicit stability limit assuring the stability in Euler forward time integration and defined as $\Delta t_{crit}=\rho c\Delta x^2/2k$ [Voller, 1997] and terminating with $\Delta t=0.1$ (20 times the explicit limit), are tested. When the Euclidean norm of the residue vector of discretized equations falls below 10^{-4}, convergence in each outer iteration is declared.

The performance of LINH and AHC tested by Voller shows that there is little difference between the methods although the former is more accurate at large time steps and small Stefan numbers. The number of iterations is nearly same as the number of time steps and the relative error of LINH to the analytic solution is up to more than 2% and 10%, for Ste=0.2 and Ste=2.0, respectively. At small time steps (1-3 times the explicit limits), about 1-2% relative errors are found. However, the present method generates only about 1% for Ste=0.2 and about 6% for Ste=2.0 through the whole cases with very similar accuracy at small time steps (Fig. 1). Figs. 2 and 3 show the total number of iterations according to the number of single-point predictor-corrector (i.e. number of inner iteration) imposed on during an outer iteration. It should be noted that the single-point predictor-corrector scheme does hardly affect the numerical result, which is essentially same regardless of the activation of the scheme. The number of inner iteration of zero means the conventional source update method, which requires large number of iterations. If we, however, activate the single-point predictor-corrector algorithm, the number of iterations can be significantly reduced. Even with

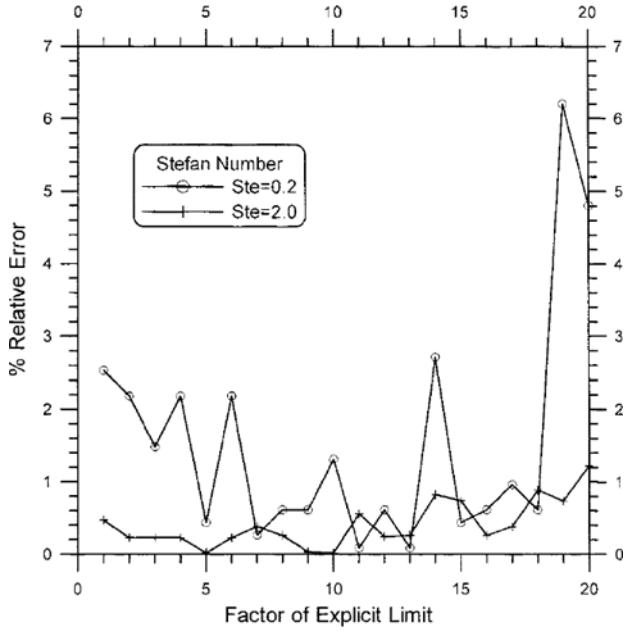

Fig. 1. % Relative error (Example 1).

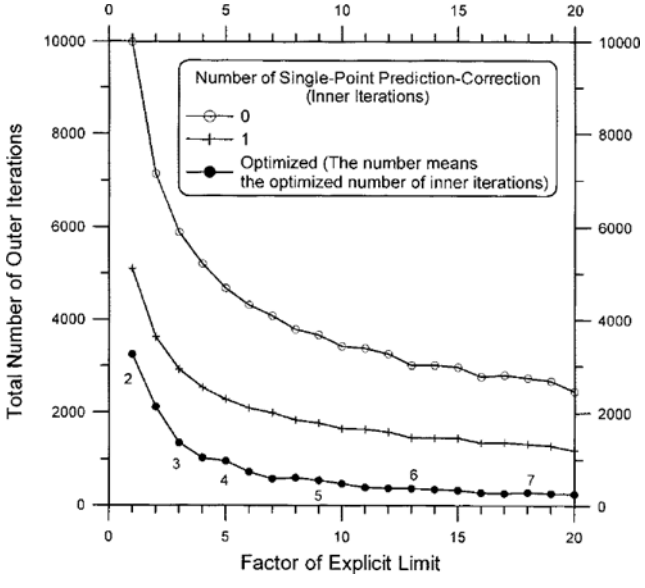

Fig. 2. Number of iterations for Ste=0.2 (Example 1).

only 1 inner iteration, the calculation speed is nearly doubled. Then, there may be an optimized number of inner iterations because during the inner iteration the neighboring temperatures are fixed. Further inner iteration over a certain number of times can not improve the speed and may worsen the performance. The optimized numbers of inner iterations for each case are obtained after the tests conducted with increasing the number of inner iterations and they are listed in the Figs. 2 and 3. As can be seen in the figure, the optimized number tends to slightly increase as the size of time step.

Comparing with LINH, for larger time steps, the present algorithm shows better accuracy than LINH. However, for smallest time steps, the accuracy of the proposed algorithm is very comparable to that of LINH and the number of iterations of LINH is less than that of the proposed algorithm. Nevertheless, the proposed algo-

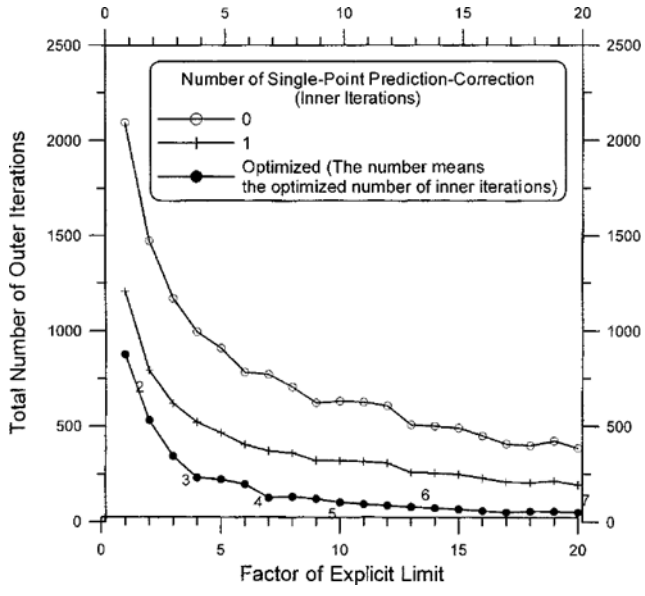

Fig. 3. Number of iterations for Ste=2.0 (Example 1).

rithm has an obvious advantage over LINH. The proposed algorithm does not require any artificial phase change range, while LINH is essentially based on the assumption that the phase change occurs over an arbitrary thin temperature range, so called the temperature window, to allow the piecewise continuous enthalpy as a function of temperature. It may be always possible to find suitable window size that can ensure the accuracy of LINH, however this process is not a straightforward and largely dependent on the problem. Sometimes, it is even a tedious job [Ding, 1995]. Also, the small window size numerically enforces the saturation temperature to be zero and it may be a serious drawback in the extension of LINH to the liquid-vapor phase change problems. However, the proposed method is free from any numerical artificial, which may deteriorate the applicability.

2. Solidification Problem under a Critical Circumstance

In Stefan problems, there are two important dimensionless numbers. The Stefan number defined by Eq. (16) is one of them and the other is the temperature ratio defined as

$$\Theta \equiv \frac{T_i - T_{sat}}{T_{sat} - T_o} \tag{17}$$

where T_i is the initial temperature and T_o the wall temperature. The Stefan number governs the temperature gradient discontinuity, while the temperature ratio is related to the magnitude of this gradient next to the wall. The solution process performance tends to deteriorate when both numbers decreases. For the purpose of the convergent numerical procedure for phase change problems, recently, Fachinotti et al. [1999] proposed a closed analytical integration procedure in the finite element formulation and they also introduced the well-known Newton-Raphson scheme for the numerical efficiency. They verified their method with a selected problem with critical values of aforementioned dimensionless numbers, *i.e.* the solidification of liquid contained in a semi-infinite slab at uniform temperature T_i=0.0 °C, just above T_{sat}=−0.1 °C, whose surface temperature suddenly falls to a constant value T_o=−45.0 °C. The physical properties are assumed to be constant: thermal conductivity k=1.08 W/

(°Cm), heat capacity ρc=1.0 J/(°Cm^3) and latent heat ρL=70.26 J/m^3. The corresponding Stefan number is Ste=1.6 and temperature ratio Θ=0.002. In this work, we adopt the same problem to test the computational ability of our proposed method. The calculation is carried out with Δx=0.125 m (32 uniform cells) and Δt=0.2 s (20 time steps).

According to Fachinotti et al. the above-mentioned dimensionless values lead to a critical circumstance wherein enthalpy models fail to converge, unless a large fictitious regularization range is introduced against the isothermal phase change character of the problem. As shown in Figs. 4 and 5 describing the calculated phase front and temperature variation with the analytical values, respectively, however, the proposed method does not exhibit any spurious behavior and the agreements are fairly good. In this, of course no regularization is introduced. Fig. 6 shows the total number of iterations required to obtain converged values as the number of inner iterations, *i.e.* the number of single-point prediction-correction, for the phase changing cell increases. Applying 10 single-point prediction-correction, we can diminish the number of iterations to about 0.1 times.

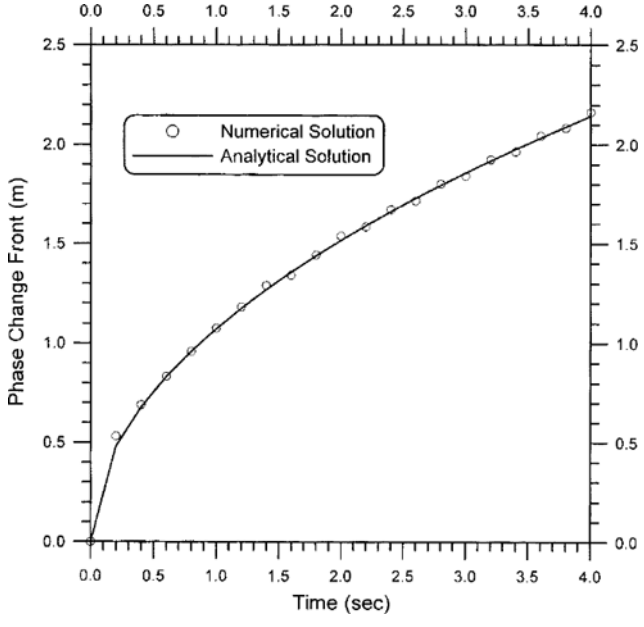

Fig. 4. Phase change front (Example 2).

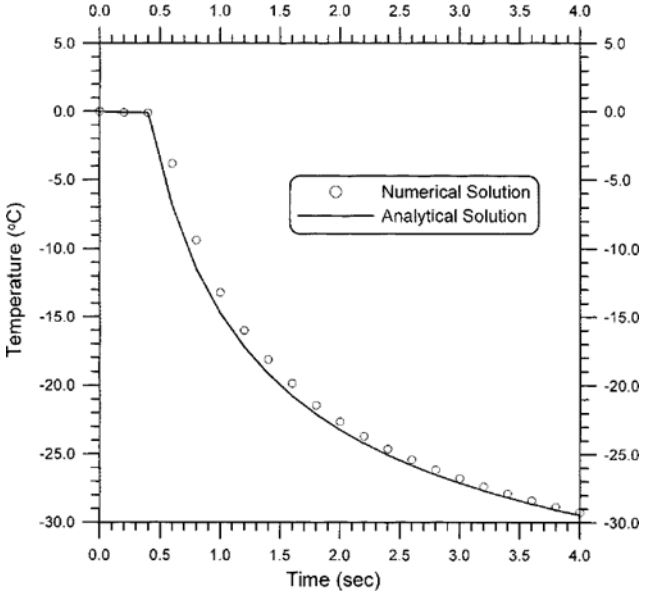

Fig. 5. Temperature at x=0.6875 m (Example 2).

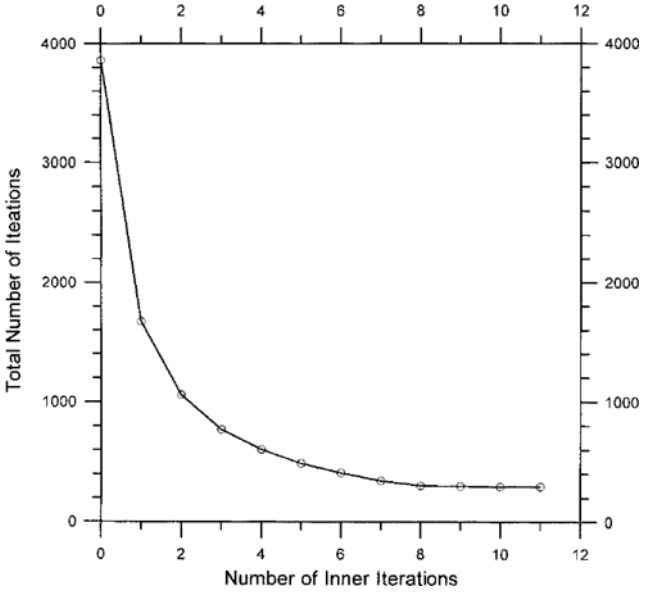

Fig. 6. Number of iterations (Example 2).

3. Solidification Problem with Two Phase Change Fronts

Now, we consider a finite slab of length 5.0 m filled with liquid at uniform temperature T_i=1.0 °C. Suddenly, a cold heat reservoir of T_o=−1.0 °C, below T_{sol}=0.0 °C, is contacted at x=0.0 m. At the

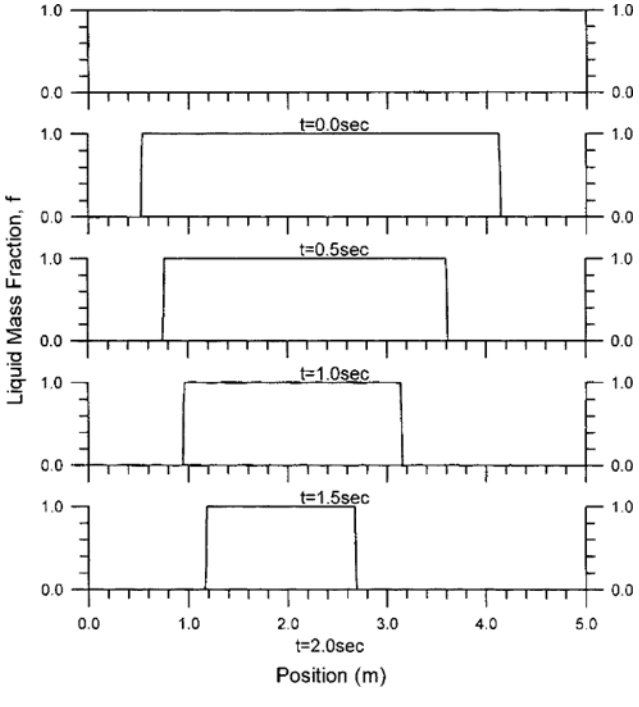

Fig. 7. Phase distributions (Example 3).

same time, the other side at x=5.0 m is exposed to a cold flow with T_∞=−10.0 °C and the slab body loses its heat through convective heat transfer (h=1.0 W/(°Cm^2) is assumed). All the physical properties are set to be constant: k=1.0 W/(°Cm), ρc=1.0 J/(°Cm^3) and ρL=1.0 J/m^3. This problem subjected to two kinds of boundary conditions is related to two different fronts of phase change. Figs. 7-9 show the results from the calculation performed with Δx=0.01 m (500 uniform cells) and Δt=0.005 s (400 time steps). Unfortunately, this problem does not have a known analytical solution to compare with. We, however, have tested with finer spatial and temporal meshes to assure the convergent solution and the above meshes are chosen for this problem.

As expected, more heat is released through the right side boundary and the right phase change front penetrates into the body faster (see Fig. 7). Also, as a result, the asymmetric temperature distribution is obtained (see Fig. 8). Fig. 9 shows the effectiveness of the proposed single-point predictor-corrector algorithm, especially for the case with multiple phase change cells. The algorithm reduces the total number of iterations to about 1/10 in Example 2 with single phase front (see Fig. 6), but it can reduce the number to about 1/25 in this example with 2 fronts. For multidimensional problems which essentially have multiple phase changing cells during the calculation, we can fairly expect the proposed algorithm to reduce the computational effort significantly.

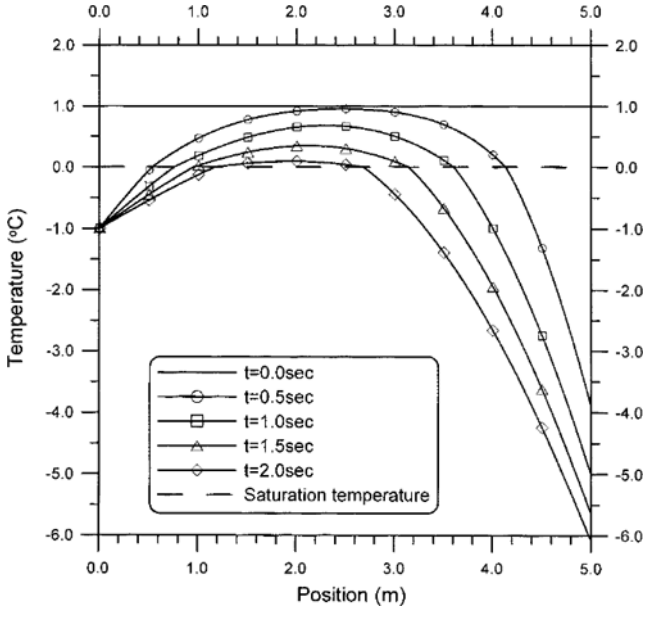

Fig. 8. Temperature distributions (Example 3).

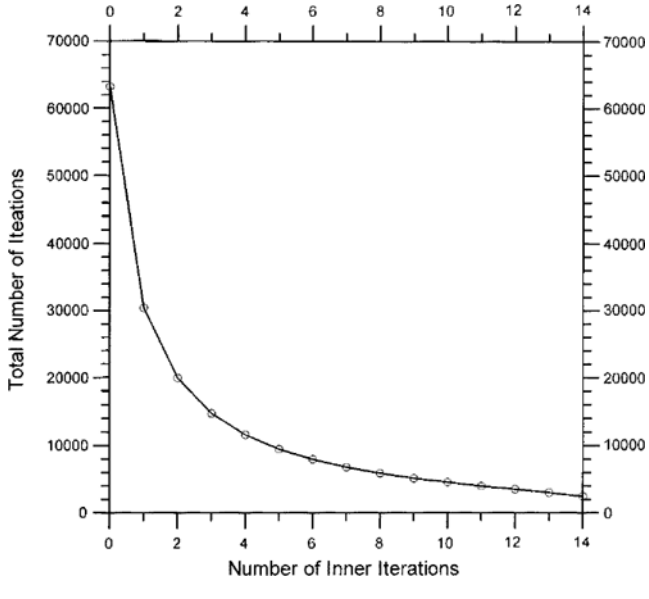

Fig. 9. Total number of iterations (Example 3).

CONCLUSIONS

A robust and cost-effective single-point predictor-corrector algorithm is proposed for phase change problems and tested with various solidification problems. The proposed algorithm can be classified into the source update method characterized by the robustness but the computational inefficiency. We can observe that the proposed algorithm can increase the calculation speed without sacrificing the accuracy. Even with just one prediction-correction, the total number of iterations is nearly halved. The results from the example under a critical circumstance, especially, show the robustness of the proposed algorithm. Also, the algorithm is so simple as to apply easily to common nonlinear heat conduction programs and it is readily expandable to multidimensional cases with only a little programming effort. It can be incorporated with other numerical schemes designed to improve the computational efficiency.

REFERENCES

Carslaw, H. S. and Jaeger, J. C., "Conduction of Heat in Solids," Chap. 11, 2nd ed., Oxford Univ. Press, Oxford (1959).

Choi, J. C., Kim, S. D. and Han, G. Y., "Heat-Transfer Characteristics in Low-Temperature Latent-Heat Storage-Systems Using Salt Hydrates," *Korean J. Chem. Eng.*, **12**, 258 (1995).

Crank, J., "Free and Moving Boundary Problems," Oxford Univ. Press, Oxford (1984).

Davey, K. and Rosindale, I., "Control Volume Capacitance Method for Solidification Modelling," *Int. J. Numer. Meth. Engrg.*, **46**, 315 (1999).

Ding, Z., "Modeling of Bulk Evaporation and Condensation with Internal Heating at Various Gravity Level," Ph.D. Dissertation, Dept. of Mech. Eng., Univ. of Florida (1995).

Fachinotti, V. D., Cardona, A. and Huespe, A. E., "A Fast Convergent and Accurate Temperature Model for Phase-Change Heat Conduction," *Int. J. Numer. Meth. Engrg.*, **44**, 1863 (1999).

Kruz, W. and Fisher, D. J., "Fundamentals of Solidification," 2nd ed., Trans Tech Pub., Switzerland (1989).

Patankar, S. V., "Numerical Heat Transfer and Fluid Flow," Hemisphere, Washington, D.C. (1980).

Voller, V. R., "An Overview of Numerical Methods for Solving Phase Change Problems," *Advances in Numerical Heat Transfer* (edited by W. J. Minkowycz and E. M. Sparrow), Taylor and Francis, Washington, D.C., **1**, 341 (1997).

Voller, V. R., "Fast Implicit Finite-Difference Method for the Analysis of Phase Change Problems," *Numer. Heat Transfer-Part B*, **17**, 155 (1990).