Application of a Variable Time-Step Finite-Difference Method for the One-Dimensional Melting Problem Including the Effect of Subcooling

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A new numerical method is proposed for the one-dimensional melting problem. Unlike many of the existing numerical techniques which either immobilize the moving interface by a suitable coordinate transformation or search for the moving interface under a fixed grid, fixed-time-step finite-difference formulation, the present method was a fixed grid, variable time-step approach. Each time step in the computation is determined iteratively by requiring that the interface be located at a mesh point, one grid space from the previous interface location.

Results of two sample calculations show that the present method is superior to the conventional finite-difference method both in its accuracy and computational efficiency. The formulation is mathematically simple and can be applied with no difficulty to problems with nonplanar geometry and initial subcooling. The present method is applied to the analysis of the melting of a finite slab subjected to a constant heat flux boundary condition. Some interesting effects of initial subcooling on the physics of melting are illustrated and discussed.

Many practical heat transfer problems involve a change in phase of the material due to either melting or freezing, for example, the solidification of castings, freezing or thawing of soil, ice formation, heat transfer in reactor fuel elements, etc. An extensive amount of literature on this subject has been written over the years. Most of these works deal only with situations in which the medium is initially at its melting temperature. As noted in a recent publication (Sparrow et al., 1978), this situation is not only unrealistic for most practical applications, but it is also difficult to attain even under controlled laboratory conditions.

The only phase change problem with initial subcooling that has been solved analytically is the melting of a one-dimensional, semi-infinite, initially subcooled plane with constant wall temperature. This is the well-known Neumann problem, and its solution can be found in many standard heat conduction texts (Carslaw and Jaeger, 1959). Most of the remaining theoretical works describe the development of approximation methods. But while techniques such as the integral method (Goodman, 1964) and the variational method (Biot, 1957) are useful for many one-dimensional melting problems with no initial subcooling, they all seem too complicated for problems with initial subcooling.

Many numerical techniques have been reported for the simple one-dimensional melting problem. The major difference between these numerical techniques is the method of handling the difficult nonlinear interface condition between the two phases. Except for some minor variations, many researchers such as Douglas and Gallie (1959), Murray and Landis (1959) and Stephens and Campbell (1967) formulate the interface condition by a finite-difference, lump parameter approach originally

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proposed by Eyres and his associates (1947). This approach uses a fixed grid, fixed time-step formulation for the general numerical solution. Solutions of the two phases are coupled by the condition $T_i = T_m$. The movement of the interface occurs when the heat gained by the i^{th} node equals the latent heat capacity. Despite its mathematical simplicity, this approach has two obvious difficulties. It fails to describe the travel of the interface continuously and it fails to give a reliable estimate of the material's temperature near the interface. Another popular approach is to introduce a coordinate transformation so that the moving interface becomes immobilized. But while this approach has been demonstrated to be successful by a number of investigators such as Landau (1950), Leaf et al. (1978) and Sparrow et al. (1978), it is mathematically difficult. After the coordinate transformation, the governing equation and its associated boundary conditions generally become nonlinear and can only be solved approximately or iteratively. Different computational schemes are required for problems with different boundary conditions. Applications of these coordinate transformation techniques for practical calculations are thus extremely limited.

The objective of this work is to introduce a new numerical method for the one-dimensional melting problem. Similar to Eyres' method (Eyres' method will be called the conventional method for the remainder of this paper), the present method uses a fixed grid, implicit finite-difference formulation. It has the same mathematical simplicity and numerical stability as the conventional method, but unlike the conventional method, a variable time step (VTS) is used. At each step of the computation, the moving interface is located exactly at a nodal point, one grid space from the previous interface location. The time step is determined iteratively by the false position technique, requiring that both the temperature and the energy conservation conditions at the interface be satisfied. A detailed description of the mathematical formulation of the VTS method is given later. Based on the solution of a simple one-dimensional melting problem, the accuracy of the VTS method and the conventional method are compared later. The VTS method is demonstrated to be superior in generating accurate results for the movement of the interface and the medium's temperature near the interface. The computation is also more efficient than the conventional method. The applicability of the present method to problems with nonplanar geometry will be considered. Results of the melting of a semi-infinite, initially subcooled cylindrical medium are obtained and agree very well with a recent published solution (Sparrow et al., 1978) obtained by a difficult coordinate transformation technique. Finally, the melting of a one-dimensional finite slab subjected to a constant heat flux boundary condition is analyzed by means of results obtained with the VTS method. Effects of initial subcooling on the physics of melting are considered and discussed.

MATHEMATICAL FORMULATION

The applicable differential equations for the one-dimensional heat conduction problem in a planar medium with constant properties in both the liquid and the solid regions are

$$\frac{\partial T_s}{\partial t} = \alpha_s \frac{\partial^2 T_s}{\partial x^2} \tag{1a}$$

in the solid region and

$$\frac{\partial T_l}{\partial t} = \alpha_l \frac{\partial^2 T_l}{\partial x^2} \tag{1b}$$

in the liquid region. At the interface between the two phases, the above two equations are coupled by the following temperature continuity and energy conservation boundary conditions:

$$T_s = T_l = T_m \qquad \text{at } x = H \tag{2a}$$

$$\frac{dH}{dt} = \frac{1}{\rho L}\left[k_s \frac{\partial T_s}{\partial x}\bigg|_H - k_l \frac{\partial T_l}{\partial x}\bigg|_H\right] \tag{2b}$$

Together with the necessary initial and boundary conditions, Equations (1*a*), (1*b*), (2*a*) and (2*b*) constitute a complete mathematical description of the one-dimensional melting problem.

The VTS numerical procedure expresses Equations (1*a*) and (1*b*) in the following implicit finite-difference form:

$$\frac{T_{n,p} - T_{n,p-1}}{\Delta t} = \alpha \frac{(T_{n+1,p} + T_{n-1,p} - 2T_{n,p})}{(\Delta x)^2} \tag{3}$$

Where the first subscript represents the space-grid location, the second subscript indicates the time step and α_s or α_l will be used depending on whether the point is in the solid or liquid region. At each step of the computation, the interface is assumed to be located at a nodal point i, one grid space away from the previous interface location. Instead of rewriting Equation (2*b*) directly in a finite-difference form, the VTS method expresses the energy balance at the interface as

$$Q_{i-1,i} = Q_r + Q_m - Q_{i,i+1} \tag{4a}$$

where

$$Q_{i-1,i} = k_l\left(\frac{T_{i-1,p} - T_m}{\Delta x}\right) \tag{4b}$$

$$Q_r = \rho c \frac{\Delta x}{\Delta t}(T_m - T_{i,p-1}) \tag{4c}$$

$$Q_m = \rho L \frac{\Delta x}{\Delta t} \tag{4d}$$

$$Q_{i,i+1} = k_s \frac{(T_m - T_{i+1,p})}{\Delta x} \tag{4e}$$

Physically, $Q_{i-1,i}$ stands for the heat flux from the $(i\text{-}1)^{th}$ node to the i^{th} node, Q_r the heat required to raise the temperature of the i^{th} node from $T_{i,p-1}$ to T_m, Q_m the heat of fusion of the i^{th} node and $Q_{i,i+1}$ represents the heat flux from the i^{th} node to the $(i+1)^{th}$ node. In the limit of $\Delta x \to 0$ and $\Delta t \to 0$, $Q_{i-1,i}$ Q_m and $Q_{i,i+1}$ reduce to the appropriate derivatives and $Q_r \to 0$ since $(T_m - T_{i,p-1}) \to 0$. Equation 4(*a*) then reduces to Equation (2*b*). Since $T_{i-1,p}$ and $T_{i+1,p}$ are generally functions of Δt, Equation (4*a*) is a nonlinear equation for the unknown time step Δt. Its solution at each step of the computation must be obtained by iteration.

To determine Δt, the computational procedure utilized by the VTS method is as follows. Consider that the computation has been completed up to time step $p-1$ so that the temperature profile at time $t_{p-1} = \sum_{i=1}^{p-1} \Delta t_i$ is known. A trial value of Δt_p is assumed. By requiring the interface to be one nodal point away from the previous interface location, Equations (3), (2*a*) and the specified boundary conditions at $x = 0$ are sufficient for the calculation of a new temperature profile. Since the problem is one dimensional and the formulation is implicit, this computation

can be done quite efficiently by the tridiagonal algorithm. The new temperature profile is then substituted into Equation (4*a*). If the energy balance is not satisfied, Δt_p is changed. This process is repeated until Equation (4*a*) is satisfied.

Results of this work show that for most problems, the above iteration for the time step Δt_p converges quickly because, generally, an accurate order of magnitude initial guess for the required time step is not too difficult to obtain. If the melting has started, the previous time step Δt_{p-1} clearly constitutes a reasonable initial estimate for Δt_p. At the beginning of melting, an energy balance can give a fairly accurate approximation forΔt. Once initial estimates of Δt are obtained, the subsequent approximations for Δt are determined by the false position technique. This method consists of rewriting Equation (4*a*) into the following form:

$$\theta_p(\Delta t) = k_s\left(\frac{T_{i+1,p}-T_m}{\Delta x}\right) - k_l\left(\frac{T_m-T_{i-1,p}}{\Delta x}\right) - \rho L\frac{\Delta x}{\Delta t} - \rho c\frac{\Delta x}{\Delta t}(T_m - T_{i,p-i}) \quad (4f)$$

To find Δt_p so that $\theta_p(\Delta t_p) = 0$, two initial guesses y_1 and y_2 are first selected so that $\theta_p(y_1)$ and $\theta_p(y_2)$ are of the opposite signs. The next guess for Δt_p is obtained by

$$y_{j+1} = y_j - \theta_p(y_j)\frac{y_j - y_{j-1}}{\theta_p(y_j) - \theta_p(y_{j-1})} \quad j = 3,4,.... \quad (5)$$

In all cases considered in this work, the above iteration procedure yeilds an accurate value for Δt in less than twenty iterations. An average of fifteen iterations, for example, are required to determine Δt when melting begins, and an average of only seven iterations is needed after the melting has started. It is demonstrated by direct comparisons in a later section that the VTS method with this iteration scheme represents a substantial improvement of computational efficiency over the conventional method.

Table 1. Thermal Properties, Boundary Conditions and Initial Conditions for the Sample Planar Problem

Physical properties	Solid	Liquid	Units
Specific heat, C_p	950.1854	662.7449	J/kg°K
Thermal conductivity, k	28.4512	12.5520	w/m°K
Density	7 001.1	7 001.1	kg/m³
Latent heat, L	37 145.5110		j/kg

Slab thickness: B = 0.005 mm
Surface heat flux rate: F = 854133369 s m² w/m²

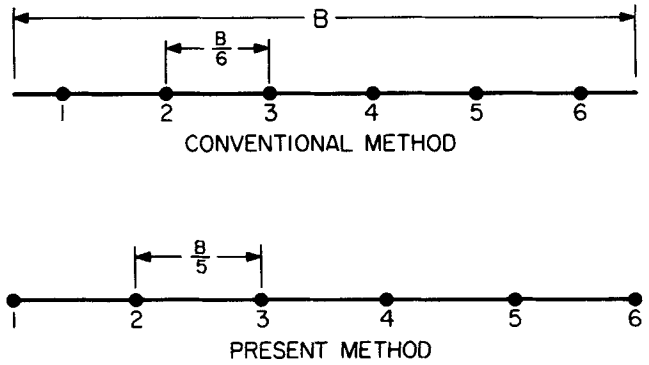

Figure 1. Illustration of the difference between the finite-difference grid used by the conventional method and that of the present method with N = 6.

SAMPLE SOLUTIONS

Planar Case

To illustrate the effectiveness of the VTS method, the melting of an initially subcooled finite slab subjected to a constant heat flux boundary condition on one face and an adiabatic condition on the other is considered. Physical properties and constants are listed in Table 1. This problem is selected because solutions obtained by two other methods are available. Results generated by a recently developed multipurpose heat conduction program (Leaf et al., 1975) utilizing the conventional method and those obtained by a method which first introduces a coordinate transformation and then solves the resulting equations by a collocation technique are presented in detail in a recent publication (Leaf et al., 1975). Advantages of the VTS method can thus be readily demonstrated by some direct comparisons.

The relative accuracy of the VTS method in the prediction of the interface location as compared to that of the conventional method is demonstrated by Table 2. Results for the time when melting starts (t_{sm}), the time when melting is finished (t_{fm}) and the position of the interface (H^*) at a time about halfway through melting (t = 14.111 s) obtained by the VTS method and the conventional method are presented with the exact result generated by the method of collocation in that table. It is seen that as the grid size decreases, results generated by the VTS method converge quickly to the exact result. When the grid size is large, the accuracy of the present method is comparable to that of the conventional method. But the present method is clearly superior as the grid size decreases.

Results for the medium's temperature at locations around the melting interface H^* are presented in Table 3. The three points chosen for the presentation are the three nodal points closest to the interface in the finite difference grid used by the conventional method. It is important to note that because of the difference in the emphasis of the computation, the present method and the conventional method use slightly different grids, as illustrated in Figure 1. Since variable time steps are used, the time t = 14.111 s also does not correspond exactly to one of the computational steps in the VTS calculation. Results in Table 3 generated by the VTS method are thus obtained by linear interpolations in both time and space from numerical data. But even with the added error from the usage of linear interpolation, Table 3 demonstrates the superiority of the VTS method in the determination of the medium's temperature near the interface.

In terms of computational efficiency, the VTS method is much superior to the conventional method. To generate the solutions as shown in Tables 2 and 3 for the four grid sizes, it was reported (Leaf et al., 1975) that the conventional method must use a time step of Δt = 0.01 s or less

Table 2. Comparison of T_{sm}, T_{fm} and H^* Obtained by the VTS Method with Values Obtained by the Conventional Method (THTB) and the Exact Results

N+	t_{sm}	t_{fm}	H^*
6	11.1864	16.5329	0.0830649 (0.0850425)++
12	11.1707	16.7120	0.0825763 (0.0820208)
24	11.1697	16.8105	0.0819650 (0.0821521)
48	11.1697	16.8628	0.0819650 (0.0823027)
Exact	11.1697	16.9130	0.081539

+N = Number of grid points used in computation.
++Values in parenthesis are results generated by the conventional method.

Table 3. Comparison of the Temperature Distribution Surrounding the Melting Interface Obtained by the Conventional Method with Values Obtained by the Conventional Method and the Exact Results

Node	Conventional method	VTS method	Exact
	$N = 6$		
2	1 737.95	1 742.25	1 739.75
3	1 703.15	1 705.95	1 703.05
4	1 697.05	1 695.35	1 697.75
	$N = 12$		
5	1 714.15	1 712.15	1 711.05
6	1 703.15	1 701.05	1 701.35
7	1 698.95	1 697.55	1 698.15
	$N = 24$		
10	1 709.45	1 707.45	1 706.75
11	1 703.15	1 702.15	1 702.15
12	1 701.45	1 700.35	1 700.55
	$N = 48$		
20	1 705.85	1 704.95	1 704.75
21	1 703.15	1 702.15	1 702.55
22	1 702.15	1 701.75	1 701.75

($\Delta t = 0.01$ for $N = 6$ *and* $N = 12$), $\Delta t < 0.01$ s for $N = 24$ and $N = 48$) after the melting has started. Since the total melting time for the slab is about 5.7 s, the conventional method must compute the medium's temperature at least 570 times during the melting period. For the VTS method, on the other hand, the required number of computations during this period is much less because the iteration scheme for the determination of Δt converges quickly. The actual number of computations performed by the VTS method during the melting period for the four cases $N = 6$, 12, 24 and 48, for example, are 39, 73, 128 and 231, respectively. In all cases, the VTS method gives at least a 60% reduction in the number of calculations.

Cylindrical Case

For problems with nonplanar geometry, the various difficulties of the conventional method appear to be more severe because of the unequal volumes of the different nodal elements. The authors have found no published results on the melting of nonplanar media using the conventional method. The VTS method, on the other hand, has no apparent difficulty in its application to such problems. As an illustration, this work considers the melting of a semi-infinite subcooled solid with constant thermal properties surrounding a heated circular cylinder of radius r_w. This initial temperature of the solid T_i is lower than the melting temperature T_m. At time equals zero, the temperature of the inner cylinder surface is raised and maintained at a value $T_w > T_m$. This problem is selected because of the availability of another numerical solution. Utilizing a difficult coordinate transformation, Sparrow et al. (1978) presented the solution to this problem in a recent publication.

This problem has two prescribable parameters: the Stefan number $St = c(T_w - T_m)/L$ and the subcooling ratio $\epsilon = (T_w - T_m)/(T_w - T_i)$. Choosing $St = 1.0$ and $\epsilon = 1.0$, results of the melting thickness δ_c as a function of the dimensionless time $\tau = (\alpha t/r_w^2)\,[c(T_w - T_m/L]$ generated by the VTS method are presented in Table 4. For comparison, the melting thickness δ_p for the corresponding planar case and the ratio δ_c/δ_p are presented in the same table. Results for δ_c/δ_p are presented graphically by Sparrow et al. (1978) and consequently do not give precise values, but within this limitation, it appears that values for δ_c and δ_p generated by the VTS method are accurate.

EFFECT OF SUBCOOLING ON MELTING

Because of its accuracy and computational efficiency, the VTS method is convenient to use for case studies of the effects of subcooling on melting. Detailed case studies under all possible physical conditions, however, are quite extensive and beyond the scope of this work. This paper will consider only the effect of subcooling on the melting of a finite slab with a uniform initial temperature subjected to a constant heat flux boundary condition on one face and an adiabatic condition on the other.

We introducing the following dimensionless variables:

$$\eta = \frac{F c_s x}{k_s L}, \quad \theta = \frac{F^2 c_s}{k_s \rho L^2} t, \quad \phi = \frac{c_s(T - T_m)}{L} \tag{6}$$

$$\eta_H = \frac{F c_s H}{k_s L}, \quad B^* = \frac{F c_s B}{k_s L}, \quad \phi_i = \frac{c_s(T_i - T_m)}{L}$$

The governing equations can be written as

$$\frac{\partial \phi}{\partial \theta} = \frac{\alpha_l}{\alpha_s} \frac{\partial^2 \phi}{\partial \eta^2} \qquad 0 \le \eta \le \eta_H \tag{7a}$$

$$\frac{\partial \phi}{\partial \theta} = \frac{\partial^2 \phi}{\partial \eta^2} \qquad \eta_H \le \eta \le B^* \tag{7b}$$

The associated boundary conditions and initial conditions become

$$-\frac{k_l}{k_s} \frac{\partial \phi}{\partial \eta}\bigg|_{\eta = 0} = 1 \tag{8a}$$

$$\frac{\partial \phi}{\partial \eta}\bigg|_{\eta = B^*} = 0 \tag{8b}$$

$$\phi(\eta_H) = 0 \tag{8c}$$

$$-\frac{k_l}{k_s} \frac{\partial \phi}{\partial \eta}\bigg|_{\eta_H^-} + \frac{\partial \phi}{\partial \eta}\bigg|_{\eta_H^+} = \frac{d\eta_H}{d\theta} \tag{8d}$$

and

$$\phi = \phi_i \text{ at } \theta = 0 \tag{8e}$$

If we assume that $k_l/k_s = 1.0$ and $\alpha_l/\alpha_s = 1.0$, exact solutions for problems with $B^* = 1.0$ and $B^* = 5.0$ with various degrees of subcooling ($\phi_i = 0, -1.0, -5.0, -10.0$) are generated utilizing the VTS method. Physically, the interesting quantities are θ_{sm}, θ_{fm} and $\Delta\theta_m = \theta_{sm} - \theta_{fm}$, which stands for the dimensionless values for the time when melting begins, the time when melting finishes and the total melting time, respectively.

Table 4. Melting Thickness of the Sample Cylindrical Problems and the Corresponding Planar Care Obtained by the Present Method. [Values in parenthesis for δ_p are tabulated from exact analytical solutions (1)]

τ	0.007465	0.02862	0.06347	0.1120	0.1743	0.2503	0.3402
δ_c	0.0599	0.1177	0.1721	0.2242	0.2741	0.3222	0.3687
δ_p	0.0625	0.1250	0.1875	0.2500	0.3125	0.3750	0.4375
	(0.0653)	(0.1278)	(0.1903)	(0.2538)	(0.3154)	(0.3780)	(0.4406)
δ_c/δ_p	0.9584	0.9416	0.9179	0.8968	0.8771	0.8524	0.8427

TABLE 5. EFFECT OF INITIAL SUBCOOLING ON θ_{sm}, θ_{fm} AND $\Delta\theta_m$ FOR THE MELTING OF A FINITE SLAB

B^*	ϕ_i	θ_{sm}	θ_{fm}	$\Delta\theta_m$
1.0	0	0	1.36	1.36
	−1.0	0.67	2.36	1.69
	−5.0	4.67	6.36	1.69
	−10.0	9.67	11.36	1.69
5.0	0	0	11.29	11.29
	−1.0	0.78	16.44	15.66
	−5.0	16.67	36.49	19.81
	−10.0	41.67	61.49	19.82

As expected, both θ_{sm} and $\Delta\theta_m$ increase as B^* increases and ϕ_i decreases. A thicker, cooler slab must be heated for a longer period of time before its surface reaches the melting temperature. It also has a longer melting time. But it is interesting to note that $\Delta\theta_m$ does not increase indefinitely as ϕ_i decreases. For a fixed B^*, $\Delta\theta_m$ approaches a constant limiting value as $\phi_i \to -\infty$. Physically, this phenomenon can be explained by considering the slab's temperature profile when melting begins. For small $|\phi_i|$, the surface of the slab remembers its initial temperature, since parts of the slab are still at that initial temperature. $\Delta\theta_m$ thus increases with increasing subcooling. For large $|\phi_i|$, on the other hand, a longer heating time is required before the slab's surface reaches the melting temperature. The slab forgets more of its initial temperature since the temperature at everywhere of the slab will be larger than ϕ_i when melting begins. Small differences in ϕ_i have little effect on the total melting time, and $\Delta\theta_m$ approaches a constant as $\phi_i \to -\infty$. The behavior of $\Delta\theta_m$ and its dependence on other physical parameters is clearly an interesting phenomenon which requires more detailed consideration. This work is currently under way, and results will be presented in future publications.

NOTATION

B = thickness of slab, m
B^* = dimensionless thickness defined by Equation (6)
c = specific heat, J/kg - °K
F = surface heat flux, W/m²
H = location of interface, m
k = thermal conductivity, W/m-K
L = latent heat of fusion, J/kg
Q = heat fluxes defined in Equation (4c)
r_w = radius of inner cylinder in the sample cylindrical problem
t = time coordinate, s
T = temperature, °K
x = space coordinate, m
y = iterative solution to Equation (4f) defined by Equation (5)

Greek Letters

α = thermal diffusivity, m²/s
δ = dimensionless melting thickness in the sample cylindrical problem
η = dimensionless space coordinate defined by Equation (6)
η_H = dimensionless location of interface defined by Equation (6)
θ = dimensionless time defined by Equation (6)
Θ = function defined by Equation (4f)
ρ = density, Kg/m³
ϕ = dimensionless temperature defined by Equation (6)
τ = dimensionless time

Subscripts

c = cylindrical
i = interface
m = melting
l = liquid
s = solid
p = planar

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Gas Absorption with Consecutive Second-Order Reactions

For gas absorption accompanied by two consecutive second-order reactions, the reaction factors of the film and penetration theories were solved by the orthogonal collocation method. For equivalent definition of the other physico-chemical parameters, the reaction factors from the two theories differ only slightly. In film theory, it is shown that the film-bulk boundary condition is of importance only for small values of M. It is also shown that the difference between the point yields of the film and penetration theories is generally small, although it is larger than the difference in reaction factors for the two theories.

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SCOPE

The reaction (enhancement) factor, which shows the effect of chemical reaction on the rate of gas absorption, is of importance in the design of gas-liquid reactors (Hoffman et al., 1975; Sharma et al., 1976; Raghuram and Shah, 1977; Charpentier, 1978). In modeling gas-liquid reactors, it is usually preferable to use the reaction factor rather

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