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An Implicit Solution Procedure for Finite Difference Modeling of the Stefan Problem

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A new procedure is presented for application to energy transport problems involving solid-to-liquid phase transition. The procedure is more implicit than previous solution procedures in an equation-solving sense and results in significantly lower computational costs. The method is formulated as a modified enthalpy model and is capable of solving problems for which many phase change interfaces exist simultaneously within the computational domain. The procedure is presented in a one-dimensional format but can be readily extended to multidimensional problems. Two rules which are reflections of the physical evolution are provided, are easily implemented, and form the basis of the new procedure. The procedure is demonstrated by application to several one-dimensional problems. Computational costs are compared to conventional procedures for a variety of boundary condition specifications, Stefan numbers, and mesh discretizations. The results indicate that a highly significant computational savings is realized with the new procedure, with cost reduction factors in excess of an order of magnitude.

Nomenclature

B^w, B^p, B^e = finite difference coefficients
c = specific heat
C^w, C^p, C^e = discrete conductance coefficients
e = internal energy
f = function for time-varying boundary condition
Fo = Fourier modulus, $\equiv \alpha t/L^2$
h = enthalpy
k = thermal conductivity
L = domain length
NCV = number of control volumes
PCM = phase change material
q = specified surface flux
Q = heat-transfer rate
S = finite difference right-hand side
Ste = Stefan number, $\equiv c_\ell \Delta T_{\text{ref}}/\lambda$
t = time
T = temperature
ΔT_{ref} = reference temperature difference, $= T_b - T_f$ for Dirichlet, $= q_b L/k$ for Neumann
V = phase change interface velocity
W = computational effort, CPU seconds
x = Cartesian coordinate
α = thermal diffusivity
γ = implicit time-step factor
ϵ = parameter characterizing melt
λ = latent heat of fusion
ρ = density

Superscripts

$(\ )^*$ = nondimensional
e = east coefficient
n = time level
p = central coefficient
w = west coefficient

Subscripts

f = reference or fusion value
i = interface or discrete location
j = phase indicator
ℓ = liquid
m = melt
p = general phase
ref = reference
s = solid

Introduction

PHASE change energy storage systems involving the change of state from solid to liquid possess the capability of storing large quantities of thermal energy while experiencing relatively small temperature excursions at their exterior surfaces. As a result, phase change energy storage systems find application in the areas of solar energy storage systems, refrigerated cargo transport, spacecraft thermal control, and as a heat pipe variable conductance control mechanism. In order to assess the operational performance of such systems, however, it is necessary to determine the temperature time history of the system so that the impact of system surface temperature excursions on mating components can be evaluated.

The Stefan problem, describing energy transport within a phase change material, is intrinsically highly nonlinear. This nonlinearity is due to the compatibility constraints imposed at the solidification/melt front and involves the energy fluxes and front propagation velocity at the interface location. However, neither the fluxes, the interface propagation velocity, nor the interface location itself are known a priori. As a result of this nonlinearity, analytical solutions to the Stefan problem are difficult, at best, and available for only a few relatively simple configurations.[1-5] For more realistic problem specifications, discrete methods are required to effect the solution. In this regard, the enthalpy finite difference model by Shamsundar and Sparrow[6] is widely used.

In the application of the enthalpy model to phase change energy transport problems, the solution of the algebraic system of equations consumes a considerable amount of computing time. This is attributable to the fact that complete transient histories are generally required and, more significantly, to the fact that Gauss-Siedel iteration or an

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equivalent procedure is used to solve the equation system. The requirement for the use of an iterative solution method emerges from the highly nonlinear character of the interface compatibility constraint.[7] This nonlinear behavior is highly concentrated within the context of a simultaneous variable procedure for the equation system.[8]

Recently, Williams and Curry[9] presented a more implicit procedure for the solution of the algebraic equation system for the case of one-dimensional phase change energy transport. In their paper, they attest to the difficulties involved in solving phase change problems and provide a procedure for implementation to multiple interface problems. Williams and Curry[9] achieve this through an energy distribution technique in the vicinity of phase change interfaces which leads to a very complex solution procedure. In addition, extension of their procedure to more than one space dimension does not appear to be possible.[10]

Finite Difference Formulation

The physical problem domain and specification is illustrated in Fig. 1, with parameters shown, with the finite difference mesh used to demonstrate the new computational procedure shown in Fig. 2 with the nodes located at the center of the one-dimensional control volumes. The equation representing conservation of thermal energy on a differential control volume can be used to provide the starting point for the finite difference development. The conservation equation is used in the form

$$\frac{\partial}{\partial x^*}\left[k_p^*\frac{\partial T_p^*}{\partial x^*}\right]=\rho_p^*\frac{\partial e_p^*}{\partial Fo} \tag{1}$$

where the subscript p denotes the particular constituent under consideration. For the invariant conductivity hypothesis employed for demonstration purposes $k_p^*=1$, where the asterisk denotes normalization with respect to the liquid phase property value. Consistent with the enthalpy model, p is allowed to take on the value of m corresponding to a discrete control volume undergoing phase transition or in a state of "melt." The finite difference equations can be determined for a typical control volume either by integration of Eq. (1) over the control volume or by performing an energy balance on the ith control volume of the figure. The result of either procedure, after integration over the time interval ΔFo, is

$$-\left[k^*\frac{\partial T^*}{\partial x^*}\right]_{i-½}^{n+\gamma}\Delta Fo+\left[k^*\frac{\partial T^*}{\partial x^*}\right]_{i+½}^{n+\gamma}\Delta Fo=\rho^*\Delta x_i^*[e_i^{*n+1}-e_i^{*n}] \tag{2}$$

where the phase subscripts have been dropped for convenience and superscripts n and $n+1$ refer to time levels Fo and $Fo+\Delta Fo$, respectively. The superscript $n+\gamma$ denotes the time level at which the conductive fluxes should be evaluated so that these fluxes are typical of the average value over the time interval. The range of γ is $0\leq\gamma\leq1$.

If the evaluation of the diffusion terms at $n+\gamma$ is intended to typify the average diffusion flux over time interval ΔFo, then the evaluation can be represented in the form

$$\left[k^*\frac{\partial T^*}{\partial x^*}\right]_{i+½}^{n+\gamma}\Delta Fo=-Q_{i+½}^{*n+\gamma}\Delta Fo \tag{3}$$

where Q^* is an effective heat flow rate per unit cross-sectional area over the time interval ΔFo and the location $i+½$ is taken for illustrative purposes. To determine the representation of Q^*, the locally one-dimensional heat flow rate is employed.

This can be expressed in the form

$$Q_{i+½}^{*n+\gamma}=\left[\frac{2k_i^*k_{i+1}^*}{\Delta x_i^*k_{i+1}^*+\Delta x_{i+1}^*k_i^*}\right][T_i^{*n+\gamma}-T_{i+1}^{*n+\gamma}] \tag{4}$$

Using a similar expression for the remaining heat flow rate in Eq. (2), the finite difference equation emerges in the form

$$\rho_i^*\Delta x_i^*e_i^{*n+1}=\rho_i^*\Delta x_i^*e^{*n}+C_i^wT_{i-1}^{*n+\gamma}+C_i^eT_{i+1}^{*n+\gamma}+C_i^pT_i^{*n+\gamma} \tag{5}$$

where

$$C_i^e=\left[\frac{2k_i^*k_{i+1}^*}{\Delta x_i^*k_{i+1}^*+\Delta x_{i+1}^*k_i^*}\right]\Delta Fo \tag{6}$$

and C_i^w is determined through rearrangement of the subscripts in Eq. (6). The coefficient C_i^p is given by

$$C_i^p=-[C_i^e+C_i^w] \tag{7}$$

The final step in the formulation of the finite difference model is to introduce the equation of state relating energy to temperature for the component constituents. For most materials and environmental conditions involved in phase change energy transport, the assumption can be employed that

$$\Delta e^*\approx\Delta h^* \tag{8}$$

where h^* is a nondimensional enthalpy normalized in the same manner as that used for e^*; namely, normalization by $c_l\Delta T_{\mathrm{ref}}$. The equation of state relating enthalpy to temperature is itself modeled in a piecewise linear fashion to include, in a single equation, the phase transition region. Denoting the solid, phase transition, and liquid regions by subscripts *1, 2,* and *3*, respectively, the equation of state is given by the general equation

$$h^*=h_{f,j}^*+c_j^*(T^*-T_{f,j}^*),\qquad j=1,2,3 \tag{9}$$

where f denotes a reference value. In the above equation of state, one consistent set of reference values is given by

$$h_{f,1}^*=0,\qquad T_{f,1}^*=-\epsilon,\quad c_1^*=1 \tag{10a}$$

$$h_{f,2}^*=0,\qquad T_{f,2}^*=-\epsilon,\quad c_2^*=0.5/(Ste\cdot\epsilon) \tag{10b}$$

$$h_{f,3}^*=1/Ste,\qquad T_{f,3}^*=+\epsilon,\quad c_3^*=1 \tag{10c}$$

where for demonstration purposes it has been assumed that $c_l^*=c_s^*$. In the above, ϵ is a small value, typically of order 10^{-4} whose influence is equivalent to representation of the phase transition region by a very large specific heat over a negligibly small temperature range. The Stefan number appears in the discrete problem through its appearance in the above property relations, therefore, whereas it appears in the continuum problem in the interface compatibility constraint. Using the above format for the equation of state permits a single form of the finite difference equation to be used in the solution of phase change problems. Using the above equation of state,

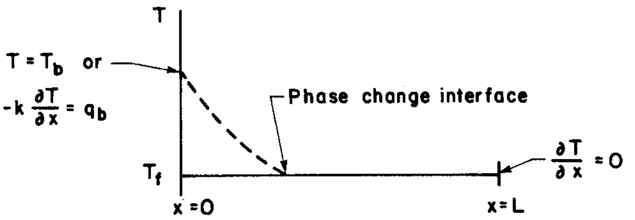

Fig. 1 One-dimensional problem geometry.

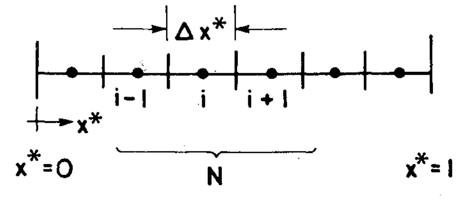

Fig. 2 One-dimensional discrete mesh.

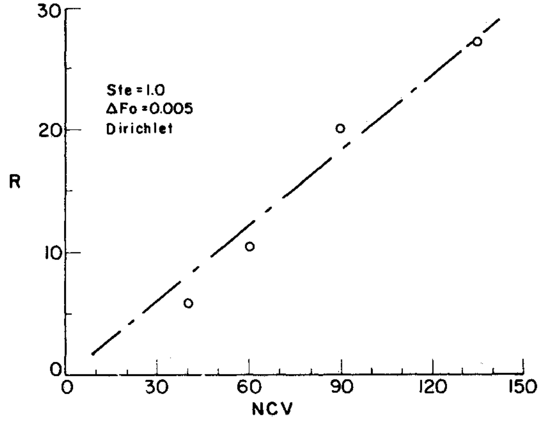

Fig. 3 Computational reduction factor for Dirichlet problem; dependence on mesh size.

and the approximation that

$$T^{*n+\gamma} = \gamma T^{*n+1} - (\gamma - 1)\, T^{*n} \tag{11}$$

in the diffusion terms, the finite difference equation becomes

$$B_i^w T_{i-1}^{*n+1} + B_i^p T_i^{*n+1} + B_i^e T_{i+1}^{*n+1} = S_i \tag{12}$$

where

$$B_i^w = \gamma C_i^w, \quad B_i^e = \gamma C_i^e \tag{13}$$

$$B_i^p = -\,[B_i^w + B_i^e] - \rho_i^* \Delta x_i^* c_j^{*n+1} \tag{14}$$

and where the right-hand side of the equation, S_i, is given by

$$S_i = (\gamma - 1)\,[C_i^w T_{i-1}^{*n} + C_i^e T_{i+1}^{*n}] + [(\gamma - 1)\, C_i^{p*} - \rho_i^* \Delta x_i^* c_j^*]^n\, T_i^{*n}$$

$$-\{\,[h_{f,j}^* - c_j^* T_{f,j}^*]\,\rho_i^* \Delta x_i^*\}^n + \{\,[h_{f,j}^* - c_j^* T_{f,j}^*]\,\rho_i^* \Delta x_i^*\}^{n+1} \tag{15}$$

where the superscripts n and $n+1$ indicate evaluation at time level Fo and $Fo + \Delta Fo$, respectively. The subscript j denotes evaluation for the appropriate phase of control volume i, where $j = 1,2,3$ corresponds to the solid, melt, and liquid phases, respectively.

It is noted that the finite difference formulation presented above, culminating with an equation system consisting of equations of the form of Eq. (12), is a fully implicit one, not in the sense of time evaluation, i.e., explicit, Crank-Nicolson, fully implicit, but rather in the equation-solving sense. Thus, the form of the finite difference equations might more appropriately be referenced as simultaneous, even though iteration methods may be employed in the solution. This will be discussed in greater detail in the following section. However, for the purpose of procedure demonstration, the fully implicit time-integration formulation has been employed; that is, $\gamma = 1$ has been used in the formulation of the equations.

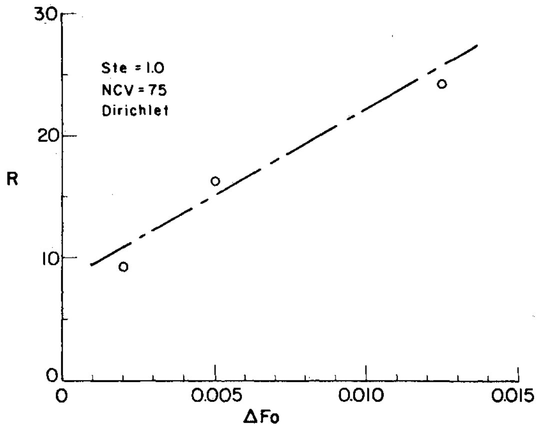

Fig. 4 Computational reduction factor for Dirichlet problem; dependence on ΔFo.

New Computational Procedure

The nonlinearity of the continuum problem emerges in the form of the interface compatibility constraint, wherein the solid and liquid interfacial heat fluxes as well as the interface propagation velocity are unknown, a priori, and, in fact, form part of the solution. In the discrete problem, the nonlinearity appears through the equation of state in which the enthalpy changes dramatically through the melt temperature range. As a result of this nonlinear behavior, it has become customary, indeed, almost essential, to employ iterative solution procedures to solve the equation system in order that changes in state of the PCM can be recognized by the solution as the solution procedure proceeds.[6,7] This leads to high computational costs since the solution must assume the state of each control volume in order to compute the new estimate for the solution and this new estimate may be in disagreement with the states of control volumes that were used in its evaluation.

In the new computational procedure presented in this paper, iteration is still required to accommodate the nonlinearity associated with the control volumes undergoing phase transition, i.e., the interface compatibility constraint. However, the iteration of the proposed procedure is of a significantly different nature and represents more closely a predictor-corrector method rather than point iteration, or line iteration in two dimensions. Each step of the iteration entails solving the discrete equation system represented by Eq. (12) wherein the phase of all control volumes is held fixed while the solution is effected. In this context, it is immaterial what solution method is employed for the system and iteration as well as direct methods are suitable candidates for this solution. On the basis of the previous solution and the new solution, as obtained above, a correction is made to the phase distribution of the control volumes and a new solution is obtained. This procedure is repeated until the phase distribution does not change between successive solutions. Experience indicates that the number of iterations required for convergence is small, typically three for initial startup if the boundary excitation experiences a step change at $Fo = 0$ and typically two during the transient evolution of the problem wherein step changes in problem specification are not present. Further, if the phase interface does not cross a control volume boundary during the time interval, a single iteration is all that is required. The computational economy which is reflected by such a low iteration requirement is a result of two very simple rules governing the transition of control volumes from one phase to a different phase. These rules are presented below.

Table 1 Summary of results

Run No.	*Ste*	Dirichlet vs Neumann	NCV	ΔFo	W_c (conv.)	W_p (present)	$R = W_c / W_p$
1	1.0	D	40	0.005	19.48	3.30	5.90
2	1.0	D	60	0.005	45.83	4.41	10.39
3	1.0	D	90	0.005	130.68	6.50	20.10
4	1.0	D	135	0.005	278.13	10.20	27.27
5	1.0	D	75	0.002	88.15	9.36	9.42
6	1.0	D	75	0.005	90.34	5.55	16.28
7	1.0	D	75	0.012	70.69	2.91	24.29
8	10.0	D	75	0.005	42.14	9.88	5.28
9	1.0	D	75	0.005	90.34	5.55	16.28
10	0.1	D	75	0.025	42.14	6.95	17.83
11	10.0	N	75	0.003	63.06	4.02	15.70
12	1.0	N	75	0.010	125.25	5.12	24.46
13	0.1	N	75	0.100	207.80	4.38	47.44

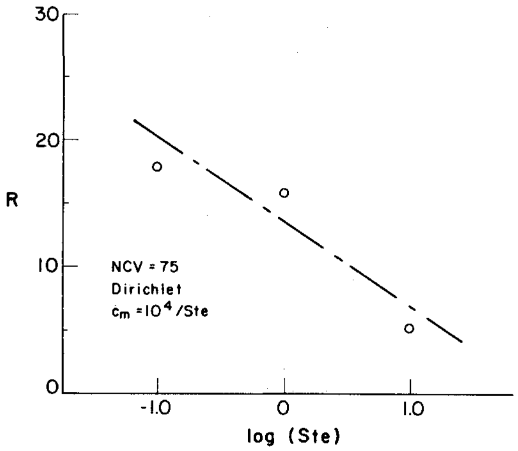

Fig. 5 Computational reduction factor for Dirichlet problem; dependence on *Ste*.

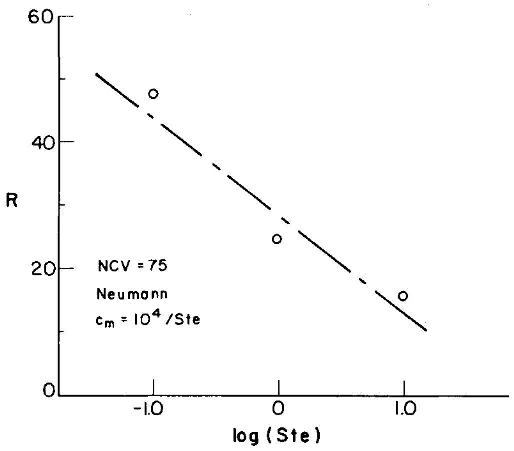

Fig. 6 Computational reduction factor for Neumann problem; dependence on *Ste*.

Rule 1:

In a single iteration, i.e., as a result of one direct (or converged iterative) solution to Eq. (12), any given control volume will be allowed to change state by only one state. That is, for example, in the heating case transition will be allowed from solid to phase transition or from phase transition to liquid in a single iteration, but not from solid to liquid.

Rule 2:

If control volumes on both sides of the one undergoing phase transition had the same phase as the one proposed for transition had at the last iteration, then this transition will not be allowed.

Both of the above rules are easy to implement and highly effective. Further, in both cases the rules represent the desire that the solution procedure, including the iteration sequence, reflect the physical situation to the maximum extent possible. In the first case, for example, the phase change is forced to pass through the phase transition, or melt state. In this way the control volumes must recognize full transition passage with the associated high effective specific heat influence of its possibly temporary duration in the melt region. Were this not the case, it is possible that transition, on the basis of temperature, would permit complete solid to liquid transition and with the lower capacity of the liquid phase be sufficiently responsive to fall back into the solid region in a subsequent iteration. This is particularly relevant if an adjacent control volume erroneously entered the melt region and if the original control volume that passed directly from solid to liquid originally was in a significant state of subcool.

In the second case, the physics is again being reflected by the statement that if control volumes on both sides of the one under consideration had the same phase as the subject control volume in the previous iteration, it is not possible for it to change phase until its neighboring control volumes have realized phase transition. Indeed, it represents a situation, realized in effecting computational runs, wherein the phase transition of a neighboring control volume has left the neighboring control volume in a state of melt and thereby, in fact, does preclude the subject control volume from embarking on its own phase transition initiation.

The two rules presented previously are directed at reflecting the physics of phase change energy transport throughout the iteration sequence. The rules were introduced in order to reduce the computational costs of phase change energy transport problems significantly by requiring an orderly progression of phase change interface progression. The results of the following comparisons indicate a highly significant reduction in the computational cost through adoption of the proposed procedure.

Results

In the preceding section a new computational procedure for application to the Stefan problem has been presented. The procedure has as its basis two simple, easily implemented, and highly effective rules, both of which reflect the physical processes involved in phase front propagation. In this section, results will be presented which compare the computational costs incurred in solving one-dimensional phase change problems using the conventional procedure with those in-

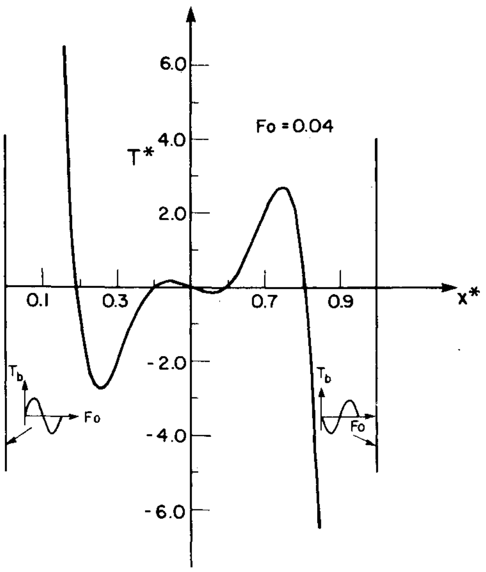

Fig. 7 Temperature distribution showing multiple fronts due to oscillatory boundary conditions.

curred when employing the proposed new computational procedure.

The comparisons will be made for several one-dimensional problem specifications in order to provide evidence of universality of the proposed procedure. These problem specifications are: 1) constant Dirichlet boundary condition at one end, 2) constant Neumann boundary condition at one end, and 3) oscillatory Dirichlet boundary condition at both ends. In the first two cases, Stefan numbers of 0.1, 1.0, and 10 are examined. In addition, for the first case, the effect of mesh discretization level on solution cost is examined as well as the impact of time step on solution cost. The last case of oscillatory boundary condition at both ends was examined to demonstrate the versatility of the new procedure in treating several phase fronts existing within the solution domain simultaneously.

The results of the computational tests are presented graphically in Figs. 3-7 and are summarized in Table 1 for the cases for which comparison with the conventional procedure was made. All tests were performed using codes compiled with the FORTVS compiler and executed on an IBM 4341 installation. All times quoted, i.e., W, are given in CPU seconds. $R \equiv W_c / W_p$ is the ratio of the conventional execution times to those of the new procedure and represents the factor by which computing costs can be reduced when the new procedure is employed. The iterative convergence criterion employed for the conventional enthalpy model for the solution of the algebraic equation system was 10^{-5}, based on enthalpy normalized with respect to the maximum enthalpy variation throughout the field at the appropriate time level. For the new procedure, a TDMA direct solution was employed for each solution of the algebraic equation system. Results comparable to those presented herein were obtained for an iterative convergence criterion of 10^{-4}. All solutions, including the oscillatory one, were executed from zero subcool solid initial conditions until a state of complete melt was achieved.

The dependence of the cost ratio R on the mesh size is illustrated in Fig. 3 for the Dirichlet problem. Mesh sizes of 40, 60, 90, and 135 control volumes were examined. It is observed that the cost ratio for the coarsest mesh is 5.9 and increases to 27.27 for the finest mesh. The character of the dependence on mesh size is approximately a linear dependence on the number of control volumes (NCV). Thus the higher resolution sought by the analyst, the higher the savings realized through the use of the new procedure. This is consistent with the significantly slower solution convergence of iteration algorithms as the problem size increases.

The dependence of the cost ratio R on the time-step interval ΔFo is presented in Fig. 4 for the NCV = 75, $Ste = 1.0$, and for the Dirichlet boundary condition. It is observed, again, that the cost savings are significant and that they increase with increasing time steps. This is attributed to the realization that as the time step increases, the interface traverses a greater number of control volume boundaries. Due to the iterative nature of the conventional procedure, the associated computational costs decrease at the largest time step only marginally. Conversely, for the new procedure, a reduction in the number of time steps at which a solution is required translates almost linearly to a reduction in the associated computational effort. Thus the net time savings grow as the time step is increased.

The dependence of the cost ratio on the problem Stefan number is presented in Fig. 5 for NCV = 75 and for the Dirichlet boundary condition. For the cases presented in this figure the melt region specific heat was determined from $c_m = 10^4/Ste$ in order to avoid having ϵ approach the truncation limits of the computations too closely. It is observed from this figure that the cost ratio decreases with increasing Stefan number from 17.83 for $Ste = 0.1$ to 5.28 for $Ste = 10.0$. This is a reflection of the fact that as the Stefan number increases, the influence of latent heat on solution evolution, and hence the influence of the problem nonlinearity, decreases. At low Stefan numbers, i.e., less than 10, the savings are highly significant. It is noteworthy that for $Ste = 0.01$, the conventional procedure was unable, without underrelaxation, to produce a solution, while the new procedure required 4.59 CPU seconds to effect complete melt. This same dependence on Stefan number is illustrated in Fig. 6 for the Neumann boundary condition problem. Trends similar to those discussed above are observed and, again, as the Stefan number increases and the nonlinearity vanishes, the cost ratio decreases. For small Stefan numbers ($Ste < 10$), however, the savings are highly significant.

The final figure, Fig. 7, is presented not in a comparative sense but rather as demonstration of the versatility of the procedure to include the prediction of several melt fronts existing simultaneously within the solution domain. In this problem, for $Ste = 5$, sinusoidal, 180-deg out-of-phase temperature excitations were applied at both ends of the domain. At $x^* = 0$, $T_b = 100 \sin(200Fo)$ was prescribed, while the negative of this value was applied at $x^* = 1$. The initial condition was one of zero subcool solid and the solution was terminated at $Fo = 0.04$ using time steps of 0.0004. Total execution time for the 100 time steps was 5.73 s. The profile shown in Fig. 7 demonstrates the multiple interface capability and exhibits five simultaneous melt fronts. It is noted that a large number of parameter combinations leading to two, three, or four simultaneous fronts were examined before the five front case was observed. On all of these test cases the solution procedure performed flawlessly.

Discussion and Conclusions

A novel, implicit solution procedure for the numerical solution of phase change energy transport problems has been presented herein. The new procedure is based on two simple but highly effective computational rules, both of which reflect the problem physical behavior as phase front propagation occurs. The computational procedure has been presented in a one-dimensional format but the underlying principles embedded in the two computational rules do not preclude their extension to multidimensional problems.

The capability of the new procedure has been demonstrated by application to a wide range of discrete problem scenarios. In all cases the new procedure proved superior to the conventional procedures with cost reductions ranging from a factor of five (minimum observed) to a factor of 47 (maximum observed). The observed trends suggest that even higher cost reductions may be experienced for higher mesh refinement, larger time steps, or smaller values of the Stefan number. The gains appear to be insensitive to boundary condition specification with respect to availability of gain although the Neumann problem appears to offer greater cost reduction than the Dirichlet problem.

Finally, the procedure has demonstrated its capability of solving problems in which multiple phase front interfaces exist simultaneously within the solution domain. While a larger number of oscillatory boundary condition cases were examined, a single example has been presented in the paper. For this example, five interfaces are present within the domain simultaneously. The new procedure experienced no difficulty whatsoever in resolving this problem.

The authors feel that the procedure presented in this paper represents a significant advance in the state-of-the-art of the numerical solution of phase change energy transport problems. Cost reductions which are typically in excess of an order of magnitude are significant whenever they can be achieved. The capability of treating multiple phase front propagation and the simplicity of method implementation are additional attributes of significance.

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