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AN EXPLICIT NUMERICAL METHOD TO TRACK A MOVING PHASE CHANGE FRONT

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NOMENCLATURE

C,	specific heat;
$G(T_i)$	function of nodal temperatures;
H,	enthalpy;
K,	thermal conductivity;
L,	latent heat;
P,	numerically predicted position of the phase change front;
P_u,	numerically predicted position of the phase change front uniform grid;
P_n,	numerically predicted position of the phase change front, non-uniform grid;
S,	fraction of sub-region in which change has occurred;
T,	temperature;
Tm,	phase change temperature;
t,	time;
t_1,	time at which sub-region (i) starts phase change;
t_2,	time at which sub-region (i) completes phase change;
$X(t)$,	position of phase change boundary;
x,	position.

Greek symbols

θ,	weight in finite difference scheme;
ρ,	density.

INTRODUCTION

THE MOVEMENT of the phase change front in a freezing or melting region is described by the Stefan equations [1–3]. A numerical solution of the Stefan equations involves the tracking of the continuously moving phase change boundary throughout a region approximated by a finite number of points. This renders many numerical methods complex in their implementation [2].

A popular way of generating numerical solutions of phase change problems is to reformulate the Stefan equations into a single equation in terms of enthalpy [4–15]. This step removes the need to trace the phase change boundary and thus simplifies any numerical solution method. Use of numerical solution schemes based on an enthalpy formulation, however, often lead to oscillations in both the predictions of the temperature histories and the position for the phase change front [13–15].

Recently, Voller and Cross [11, 12] have presented and implemented techniques for interpreting the results of enthalpy solutions so that oscillations may be 'by-passed'. One drawback of these methods is that the position of the phase change front is only predicted at specified points in time, i.e. when the phase change front coincides with a node point of the solution grid.

In the present paper the interpretation of the enthalpy in a discretized region [11] is extended. This extension leads to a numerical algorithm in which a single temperature point phase change front is continuously tracked in a 1-dim. region which is freezing.

INTERPRETATION OF ENTHALPY

A mathematical description of freezing in a 1-dim. semi-infinite region (i.e. $x \geqslant 0$) may be formulated in terms of the enthalpy as

$$\rho \frac{\partial H}{\partial t} = \frac{\partial}{\partial x}\left(K \frac{\partial T}{\partial x}\right), \quad x \geqslant 0 \tag{1}$$

where the conductivity K and density ρ are functions of temperature, T. The temperature and enthalpy, H, are related via

$$T = \begin{cases} H/C, & H < CTm, \\ Tm, & CTm \leqslant H \leqslant CTm + L, \\ (H - L)/C, & H > CTm + L \end{cases} \tag{2}$$

where Tm is the melting temperature, L is the associated latent heat and C is the specific heat.

Using a weighted average approximation, for generalization, the enthalpy formulation, equation (1), can be approximated in time by

$$\rho \left.\frac{\partial H}{\partial t}\right|_{(j+\theta)\delta t} = \theta \frac{\partial}{\partial x}\left(K \frac{\partial T}{\partial x}\right)_{(j+1)\delta t} + (1-\theta)\frac{\partial}{\partial x}\left(K \frac{\partial T}{\partial x}\right)_{j\delta t} \quad 0 \leqslant \theta \leqslant 1 \tag{3}$$

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Then, with a discretization in the x-direction and taking standard approximations for the derivatives on the RHS of equation (3), the rate of change of the enthalpy at node (i) on the solution grid may be written as,

$$\rho \frac{dH_i}{dt}\bigg|_{(j+\theta)\delta t} = [\theta G(T_i^{j+1}) + (1-\theta)G(T_i^j)]/\delta x \quad (4)$$

where, at time $t = k\,\delta t$, the function

$$G(T_i^k) = [K_{i-1}(T_{i-1}^k - T_i^k) - K_{i+1}(T_i^k - T_{i+1}^k)]/\delta x. \quad (5)$$

The rate of change of the phase change boundary, $X(t)$, is given by the so-called Stefan condition [1, 2]

$$\rho L \frac{dX(t)}{dt} = K\frac{\partial T}{\partial x}\bigg|_{x-} - K\frac{\partial T}{\partial x}\bigg|_{x+} \quad (6)$$

If at time $t = (j + \theta)\,\delta t$ a nodal enthalpy is such that,

$$CTm + L > H_i > CTm \quad (7)$$

a finite difference representation of equation (2) will give $T_i = Tm$ and the phase change boundary is approximated to be on node (i) of the solution grid. Therefore, using a backward difference representation for the first derivative on the RHS of equation (6), a forward difference representation for the second derivative and a weighted average approximation in time the Stefan condition may be written, on use of equation (5), as

$$\rho L \frac{dX}{dt}\bigg|_{(j+\theta)\delta t} = [\theta G(T_i^{j+1}) + (1-\theta)G(T_i^j)]. \quad (8)$$

Equations (4) and (8) imply that when $t = (j + \theta)\,\delta t$

$$\frac{L}{\delta x}\frac{dX}{dt} = \frac{dH_i}{dt}. \quad (9)$$

Experience [11, 14, 15] in using enthalpy numerical methods indicate that the ith nodal enthalpy remains in the phase change range, equation (7), for a finite time. Voller and Cross [11] interpret this time taken for the sub-region about node (i), i.e. the region bounded by $x = (i - 1/2)\,\delta x$ and $x = (i + 1/2)\,\delta x$, to complete the phase change. Therefore, equation (9) is valid over a range of time $t_1 < t < t_2$, as opposed to a single point in time, where, for freezing, $H_i^{t_1} = CTm + L$ and $H_i^{t_2} = CTm$. Now, defining $S = X/\delta x - (i - 1/2)$ so that $0 < S < 1$ while $t_1 < t < t_2$, equation (9) may be written as

$$L\frac{dS}{dt} = \frac{dH_i}{dt}, \quad t_1 < t < t_2. \quad (10)$$

Hence, while the phase change is occurring in the sub-region about node (i), the rate of change in the nodal enthalpy H_i is proportional to the velocity of the phase change front across the sub-region, with the latent heat of the phase change the constant of proportionality.

AN ALGORITHM TO TRACK A PHASE CHANGE FRONT

In a freezing problem the interpretation of the enthalpy in a discretized region, given by equation (10), implies that if at time $t = k\,\delta t$ the ith sub-region is freezing an approximation for the frozen portion is

$$S = (L + CTm - H_i^k)/L. \quad (11)$$

Therefore the true position of the freezing front can be approximated as

$$X(t) = [S + (i - 1/2)]\,\delta x. \quad (12)$$

Note, that when $H_i^j = L/2 + CTm$, equations (11) and (12) imply that $S = 1/2$ and $X(t) = i\,\delta x$, which is in agreement with the earlier interpretation of the enthalpy [11].

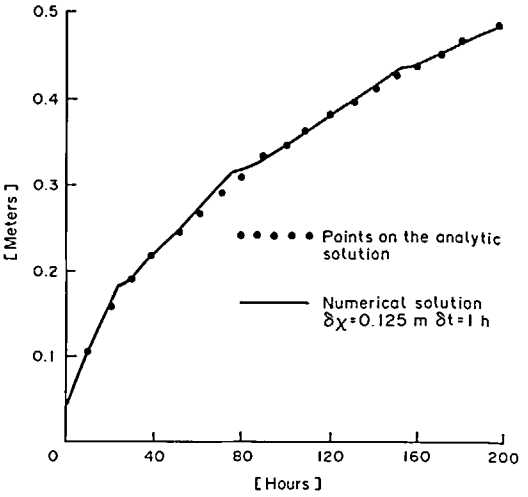

FIG. 1. Comparison of analytic and numerical solution.

In combining equations (11) and (12) with the explicit finite difference scheme

$$H_i^{j+1} = H_i^j + \frac{K}{\rho}\frac{\delta t}{(\delta x)^2}(T_{i+1}^j - 2T_i^j + T_{i-1}^j) \quad (13)$$

for the enthalpy formulation, equation (1), a simple algorithm for determining the movement of a freezing front, is obtained. To test this algorithm the following 1-dim. freezing problem [16] with known analytic solution [1, 2] will be used:

$$Tm = 0;\ T(\infty, t) = 2;\ T(x, 0) = 2\ (x \geqslant 0):$$
$$T(0, t) = -10\ (t > 0);\ K = 2;\ C = 2.5 \times 10^6;$$
$$L = 10^8;\ \rho = 1; \quad (14)$$

where all data is in S.I. units.

For the majority of time step predictions, using the proposed algorithm with $\delta x = 0.125$ m and $\delta t = 1$ h, for the position of the freezing front in the test problem [equation (14)] the results remain within $\pm$ 1% of the known solution. When the freezing front crosses over a sub-region divide, i.e. points $(i \pm 1/2)\,\delta x$, however, the accuracy of the algorithm decreases dramatically. A comparison of the plots for the movement of the freezing front obtained from the known and numerical solutions (Fig. 1) reveals that the numerical solution is oscillatory and contains plateaux, i.e. periods of time where the position of the freezing front is fixed. This behavior is due to the discretization, in particular, the approximation that the ith nodal temperature is fixed at Tm when the ith sub-region is undergoing the phase change. This approximation leads to a time lag between the nodal enthalpy H_i becoming less than CTm and the nodal enthalpy H_{i+1} becoming less than $CTm + L$. Therefore, the movement of the freezing front through the discretized region is not continuous. Hence plateaux and oscillations appear in the numerically predicted results.

There may be a number of ways of overcoming the difficulties associated with the above numerical algorithm in the vicinity of sub-region divides. A direct method is to use a dual solution grid in the x dimension, solving the test problem simultaneously on each of the grids. If the step size in each of the grids is δx but the initial step in the first grid is $\delta x/2$ every sub-region divide in the first grid will correspond to a grid node point in the second and vice versa. In this way, an area where the algorithm solution is accurate in one grid, viz. the node point [11] will coincide with the area of solution inaccuracy in the other, viz. the subregion divide. If a criterion can be found for choosing the 'better' of the two predictions

Table 1. Predictions for position of freezing front in the second sub-region

Time (h)	Analytic $X(t)$ (m)	Uniform grid	Error	Non-uniform grid	Error	Dual grid + equation (15)	Error
20	0.155	0.162	4.6	0.155	−0.01	0.155	−0.01
24	0.169	0.184	7.84	0.168	−0.58	0.168	−0.58
25	0.173	0.184	5.94	0.172	−0.57	0.172	−0.57
26	0.176	0.184	4.08	0.175	−0.52	0.175	−0.52
27	0.180	0.184	2.26	0.179	−0.44	0.179	−0.44
		sub-region divide → |					
28	0.183	0.189	2.96	0.183	−0.31	0.183	−0.31
29	0.186	0.190	2.12	0.186	−0.16	0.186	−0.16
30	0.189	0.192	1.49	0.189	0.02	0.189	0.02
40	0.219	0.217	−0.86	0.225	2.79	0.217	−0.86
50	0.245	0.243	−0.67	0.250	2.26	0.243	−0.67
51	0.247	0.246	−0.58	0.251	1.68	0.246	−0.58
52	0.249	0.248	−0.48	0.253	1.23	0.248	−0.48
		center of sub-region → |					
53	0.252	0.251	−0.38	0.254	0.87	0.251	−0.38
54	0.254	0.254	−0.27	0.256	0.57	0.254	−0.27
55	0.256	0.256	−0.15	0.257	0.33	0.256	−0.15
60	0.268	0.269	0.55	0.267	−0.38	0.267	−0.38
70	0.289	0.296	2.26	0.287	−0.71	0.287	−0.71
75	0.300	0.309	3.22	0.298	−0.61	0.298	−0.61
76	0.302	0.312	−3.41	0.300	−0.57	0.300	−0.57
77	0.304	0.312	2.78	0.302	−0.53	0.302	−0.53
78	0.306	0.312	2.15	0.304	−0.48	0.304	−0.48
79	0.308	0.312	1.61	0.306	−0.43	0.306	−0.43
		sub-region divide → |					
80	0.309	0.313	1.20	0.308	−0.38	0.308	−0.38
90	0.328	0.327	−0.51	0.329	0.35	0.327	−0.51

Error = [numerical-analytical]/numerical × 100.

from the dual grid system the problems associated with the proposed algorithm may be overcome. Such a criterion may be found on study of the accuracy of the algorithm on a single grid. Table 1 shows predictions for the position of the freezing front of the test problem as it moves across the sub-region centered on $x = 0.25$ m. Note that the behavior illustrated in this table is typical of all the sub-regions in the solution grid. The results in Table 1, columns 1–4, show that in the region of the sub-region divides the errors in the numerical results are large and positive, i.e. the numerically predicted position of the freezing front is greater then the analytic position. On the other hand, at the center of the sub-region the errors are smaller and negative. With these observations the following criterion is proposed for choosing the best solution, P, from the dual grid system,

$$P = \begin{cases} P_n, \text{ when } P_n < P_u \\ P_u, \text{otherwise} \end{cases} \quad (15)$$

where P_n is the solution obtained from the non-uniform grid with a first step of $\delta x/2$ and P_u is the solution from the uniform grid. This criterion insures that:

(1) Predictions when the phase change boundary is in the vicinity of a sub-region divide are ignored.

(2) The solution is smooth because movement in choice between the solution grids occurs when the predictions from each grid are at their closest point.

Note that before the proposed algorithm can be applied to the dual grid system the explicit finite difference scheme, equation (13) has to be modified to

$$H_1^{j+1} = H_1^j + \frac{K}{\rho}\frac{\delta t}{(\delta x)^2}\left[\frac{8}{3}T_0^j - 4T_1^j + \frac{4}{3}T_2^j\right] \quad (16)$$

at the first node point on the non-uniform grid.

Predictions, using the proposed algorithm in conjunction with the dual grid system, for the test problem, equation (14), with $\delta x = 0.125$ m and $\delta t = 1$ hr are considerably improved, cf. Table 1. After the freezing front has moved 0.1 m from the plane $x = 0$ the relative errors between the numerically predicted and analytic results are always within 1%. Furthermore, the plot for the freezing front is non-oscillatory and extremely close to the analytic plot (Fig. 2). Finally, comparison of results obtained for each of the grids, Table 1, indicates that the criterion, equation (15) for switching between the solutions will nearly always choose the best possible solution.

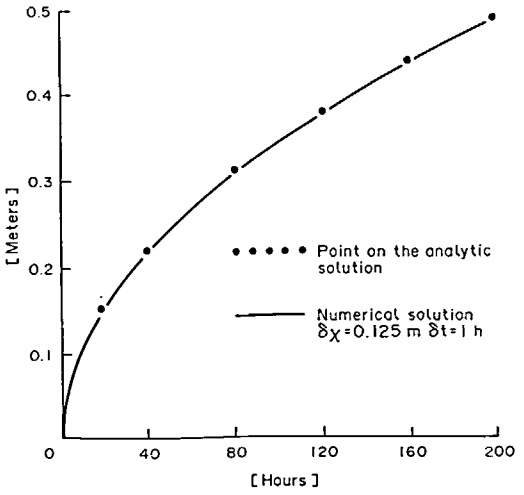

FIG. 2. Numerical solution using proposed algorithm in conjunction with a dual grid system.

CONCLUSIONS

The enthalpy in a discretized region has been interpreted in such a way that in a numerical solution of a phase change problem the value of a nodal enthalpy can be used to approximate the position of the phase change boundary. A numerical algorithm has been devised, based on this interpretation, which continuously tracks a phase change front. Implementation on a test freezing problem indicates that in some applications the accuracy in the predictions would be inadequate. Accuracy in the results is dramatically improved when simultaneous applications of the algorithm, on a dual solution grid, are used in conjunction with a criterion for choosing between the two solutions. The explicit nature of the proposed algorithm makes the computer coding and implementation straightforward.

Finally, it should be made clear that the 'dual solution grid' algorithm is *ad hoc*. However, although there is no proof that the algorithm will work in all situations, the procedure is a reasonable one and certainly performs well on the standard form of the two-phase moving boundary problem [11, 14, 16].

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