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A fast, unconditionally stable finite-difference scheme for heat conduction with phase change

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Abstract – In the numerical solution of heat conduction problems with phase change by finite differences, enthalpy methods or temperature methods can be used. The former require either an explicit procedure with consequent convergence problems, or iteration at each time step if implicit procedures are used. The latter are subject to the problem of jumping the latent heat peak, necessitating the use of small time steps to avoid underprediction of phase-change times. This paper suggests a simple method that eliminates both problems and results in a fast, robust procedure that uses less computation time for the same level of prediction accuracy when compared to other finite-difference schemes.

INTRODUCTION

THE NUMERICAL solution of heat transfer processes with phase change (Stefan problems) presents special difficulties. Numerous methods have been proposed for these problems, as reviewed for example by Fox [1], Furzeland [2], Crank [3] and Voller and Cross [4]. Of these methods, many can deal only with situations where a sharp phase-change boundary exists and thus do not apply to the freezing of many materials such as solutions, foodstuffs or alloys. Others are restricted to one-dimensional problems.

This paper will concentrate on methods which do not explicitly make use of the phase-change boundary, and so are free of the restrictions mentioned above. In these methods, the heat diffusion equation can be formulated in either of the following two ways:

$$c(T)\frac{\partial T}{\partial t} = \operatorname{div}[k(T)\operatorname{grad}(T)] \tag{1}$$

or

$$\frac{\partial H}{\partial t} = \operatorname{div}[k(H)\operatorname{grad}(T(H))]. \tag{2}$$

Equation (1) is the basis of temperature methods, while (2) is the basis of enthalpy methods.

In temperature methods, the latent heat is represented by a peak of small but finite width in the $c(T)$ curve. If a large time step is used in the computation, a nodal temperature may 'jump' past the freezing temperature range in one step, resulting in the latent heat being ignored [since $c(T)$ never takes the peak value]. This is termed 'jumping of the latent heat peak' and can be a major problem. To avoid it, very small time steps have to be used.

Three-time level schemes such as that of Lees [5] goes some way towards solving this problem (Bonacina and Comini [6]). In these schemes the thermal properties are evaluated at an intermediate time level. However, jumping of the latent heat peak is still likely. To overcome this Comini and Lewis [7] suggested that c should be calculated as the mean specific heat between the temperatures of adjacent nodes. This method was also followed by Succar and Hayakawa [8]. Apart from the lack of theoretical basis it leads to ambiguities when applied to multi-dimensional situations.

Morgan *et al.* [9] suggested calculating a mean value of c from the changes in nodal temperatures and enthalpies at the previous time levels, m and $m+1$. This represents a departure from the three-level scheme. Also, because the moment when a node changes phase is not anticipated, peak jumping still occurs, unless time steps are very small and the width of the latent heat peak made artificially large (Morgan *et al.* found a 1°C-width necessary).

A further modification suggested by Wood and Lewis [10] is to change the temperature as follows, when updating at each time step:

$$T_i^m = (T_i^{m+2} + T_i^{m+1} + T_i^m)/3. \tag{3}$$

In addition to this, Cleland [11] suggests 'smoothing out' the $c(T)$ function around the peak. Cleland and Earle [12] show that to guarantee that the solution is accurate, it is essential to check the heat balance. The smoothing of the $c(T)$ peak leads to predictions of lower accuracy and makes it difficult to carry out checks against known theoretical solutions.

Enthalpy methods do not suffer from the drawbacks mentioned above. However, because the heat diffusion equation involves a highly non-linear function $T(H)$ near the phase-change region, an explicit scheme is usually employed:

$$H^{n+1} - H^n = f(H^n). \tag{4}$$

Explicit schemes are unstable for $k\Delta t/c(\Delta x)^2 > 0.5$. Thus, again small time intervals must be used, with a consequent increase in computing time. Longworth [13] and Furzeland [2] propose implicit formulations of the enthalpy method, which require iteration at each time step to determine thermal properties. Crowley [14] employed both explicit and implicit methods to

NOMENCLATURE

c	volumetric heat [J m^{-3} K^{-1}]
f	a function
f_T, f_H	functions to calculate temperature from enthalpy and vice versa
H	enthalpy [J m^{-3}]
ΔH	enthalpy change [J m^{-3}]
k	thermal conductivity
n	number of nodes
Δt	time interval [s]
T	temperature [K]
Δx	distance interval [m].

Subscripts

a	cooling medium
f	freezing point
i	spatial index
+	between nodes i and $i+1$
−	between nodes i and $i-1$.

Superscripts

m	time index
*	second-order approximation.

solve the enthalpy equation and found the latter to be less efficient in terms of computing time.

This paper proposes a method that combines the features of enthalpy and temperature methods: better convergence of implicit temperature methods and robustness with regards to peak jumping of enthalpy methods, without recourse to time-consuming iteration at each step.

THEORY

To facilitate discussion most of the following will refer to one-dimensional problems, although the same principles apply to multi-dimensional problems. Lees' [5] three-level finite-difference equation can be written:

$$c_i^{m+1}(T_i^{m+2}-T_i^m)=\frac{2\Delta t}{3(\Delta x)^2}\times[k_+^{m+1}(T_{i+1}^{m+2}+T_{i+1}^{m+1}+T_{i+1}^m-T_i^{m+2}-T_i^{m+1}-T_i^m)+k_-^{m-1}(T_{i-1}^{m+2}+T_{i-1}^{m+1}+T_{i-1}^m-T_i^{m+2}-T_i^{m+1}-T_i^m)]. \quad (5)$$

This second-order scheme is unconditionally stable and convergent. The RHS gives the enthalpy gain (due to heat conduction) at node i over the time interval Δt. A second-order approximation to this enthalpy gain is:

$$\Delta H^*=\frac{2\Delta t}{(\Delta x)^2}[k_+(T_{i+1}^{m+1}-T_i^{m+1})+k_-(T_{i-1}^{m+1}-T_i^{m+1})]. \quad (6)$$

A second-order approximation to T_i^{m+2} is:

$$T^*=f_T[f_H(T_i^m)+\Delta H^*] \quad (7)$$

and a second-order approximation to c_i^{m+1} is:

$$c_i^{m+1}=\frac{\Delta H^*}{T^*-T_i^m}. \quad (8)$$

Thus, c_i^{m+1} can be calculated from explicity known quantities (at time levels m and $m+1$) and substituted into equation (5), which can then be solved in the usual manner, using a tridiagonal matrix solving procedure.

Unlike previously suggested schemes, equations (6)–(8) yield a 'true' mean specific heat at the second time level.

As a further precaution against jumping the latent heat peak, the temperatures T_i^{m+2} are recalculated (after solutions of the tridiagonal matrix) as follows:

$$T_i^{m+2}(\text{corrected})=f_T[f_H(T_i^m)+c_i^{m+1}(T_i^{m+2}-T_i^m)]. \quad (9)$$

In equations (7) and (9), the functions f_T and f_H are approximated by segmentwise functions.

The term in square bracket on the RHS represents the calculated new enthalpy at node i. Thus, if c_i^{m+1} has been underestimated, causing T_i^{m+2} (incorrectly) to 'jump' past the freezing temperature, equation (9) will reset T_i^{m+2} to the freezing temperature.

The two-step procedure described above in effect transforms the temperature method into an enthalpy method, while retaining the convergence properties of the implicit three-level scheme [since equation (8) is an approximation of the same order as equation (5)].

Extension to two and three dimensions is described by Bonacina and Comini [15] and Cleland and Earle [16]. Essentially it consists of 'sweeping' successively in two or three directions. Step 1 (calculation of specific heats) is carried out before the first sweep, and step 2 (recalculation of temperatures) after the last sweep. The increase in computing time due to the two-step modification of this paper is undetectable.

RESULTS

1. *Performance for various specific heat curves*

Three test problems were set up (Tables 1 and 2). The proposed method was compared with its 'parent methods', the explicit enthalpy method and the three-level temperature method. Two versions of the latter were tested: version II includes the modification of equation (3), while version I does not. Note that the present method does not make use of equation (3) either. Comparison was also made against Longworth's [13] and Furzeland's [2] iterative implicit enthalpy methods. The modification suggested by

Table 1. One-dimensional test problems

	Problem 1	Problem 2	Problem 3†
Slab thickness (m)	0.100	0.500	0.025
Heat transfer coefficient ($W m^{-2} K^{-1}$)	infinite	infinite	51.9
Ambient temperature (°C)	0	−20	−40
Initial slab temperature (°C)	100	10	30
Thermal conductivity ($W m^{-1} K^{-1}$)	0.48	2.22, $T < -0.005$ 0.556, $T > 0.005$	Table 2
Volumetric heat ($10^6 J m^{-3} K^{-1}$)	3.66	1.762, $T \leqslant -0.005$ 33 800, $-0.005 < T \leqslant 0.005$ 4.226, $T > 0.005$	Table 2
Number of nodes (half slab)	10	50	5
Specified final centre‡ temperature (°C)	40	−1	−10
Known solution (s) (time to given final centre‡ temperature)	8950 (theory)	11 755 (theory)	2300 ± 150 (experiment)

† Problem 3 is from Cleland and Earle's [18] Tylose freezing test No. 1.
‡ For problem 2: replace 'centre' by '0.05 m below surface'.

Morgan *et al.* [9] was also tried, but made little difference to the performance of three-level methods, and its results will not be shown separately.

The test problems can be described as a pure cooling problem, a pure-substance freezing problem with step change in enthalpy, and a food-freezing problem with gradual phase change. The theoretical solution to the first problem is given by Carslaw and Jaeger [17, p. 124]. In the second problem, the time for a 0.5-m-thick slab to freeze to a depth of 0.05 m is calculated. For the period considered, the centre temperature remains at its initial value and the half-space solution given by Voller and Cross [4] applies. The third problem has no theoretical solution but had an experimental result of 2300 ± 150 s measured by Cleland and Earle [18].

The enthalpy step-change in problem 2 was approximated by a narrow peak 0.01 K wide in the specific heat curve. Strictly speaking such an approximation is not necessary for either the enthalpy method or the present method. However, its use simplifies the programming, since the specific heat never actually goes to infinity and thus no special feature needs to be built into the program to handle this case. (The peak width can be an arbitrarily small number, as long as the numbers involved can be handled by the computer.)

The methods were compared according to the following criteria:

1. Time interval Δt at which the calculated cooling or freezing time agrees to within 1% with the true result (i.e. result obtained when very small time intervals are used).
2. Computer processing (c.p.u.) time on a Digital Vax 11/750 computer for the above interval.

Results of the comparison are shown in Table 3. For the pure cooling problem, the present method is as fast as the explicit method and previous three-level methods, and 6.5 times as fast as the iterative methods. For the sharp-freezing problem, the present method is almost twice as fast as the explicit method and 4.5 times as fast as the iterative methods, while the previous

Table 2. Thermal properties of Tylose (Cleland and Earle [12])

Temperature (°C)	k ($W m^{-1} K^{-1}$)	Temperature (°C)	c ($10^6 J m^{-3} K^{-1}$)	H ($10^6 J m^{-3}$)
−40	1.67	−40	1.89	0
−20	1.66	−16	2.01	46.8
−10	1.63	−10	3.52	63.4
−6	1.57	−7	5.94	77.6
−4	1.47	−5	10.6	94.1
−2	1.20	−3	25.3	130.0
−1	0.83	−2	44.8	165.1
−0.6	0.49	−1	101.0	238.0
+40	0.61	−0.8	178.0	265.9
		−0.7	178.0	283.7
		−0.6	10.0	293.1
		−0.4	3.71	294.4
		+40	3.71	444.3

Table 3. Comparison of finite-difference schemes

	Problem 1	Problem 2	Problem 3
Final values of time (s)			
Explicit enthalpy method	8940	11 730	2483
Three-level temperature method†	8940	‡	‡
Three-level temperature method and equation (3)	8940	‡	2485
Ref. [13]	8940	11 740	2485
Ref. [2]	8940	11 740	2485
Present method	8940	11 730	2485
Δt for convergence (s)			
Explicit enthalpy method	50	10	10
Three-level temperature method†	100	‡	‡
Three-level temperature method and equation (3)	100	‡	2
Ref. [13]	2000	300	100
Ref. [2]	2000	300	100
Present method	100	30	50
C.p.u. time (s)			
Explicit enthalpy method	1.1	39.6	1.2
Three-level temperature method†	1.0	‡	>270.0
Three-level temperature method and equation (3)	1.0	‡	10.8
Ref. [13]	6.6	>300.0	4.0
Ref. [2]	6.6	102.7	4.0
Present method	1.0	22.6	0.4

† With or without modification by Morgan *et al.* [9].
‡ These methods do not work for any reasonable value of Δt.

three-level methods do not work for any reasonable time step. For the gradual freezing problem, the present method is three times as fast as the explicit method, 27 times as fast as the best previous three-level method, and 10 times as fast as the iterative methods.

In addition, when Δt is increased above the values given in Table 3, the explicit enthalpy method diverges while the previous three-level methods jump the latent heat peak and give nonsensical results. On the other hand, the present method always gives results within about 10% of the final value, even when Δt is about 1/5 of the total freezing time. This is illustrated in Fig. 1, which shows the percentage discrepancy against Δt values used for problem 3.

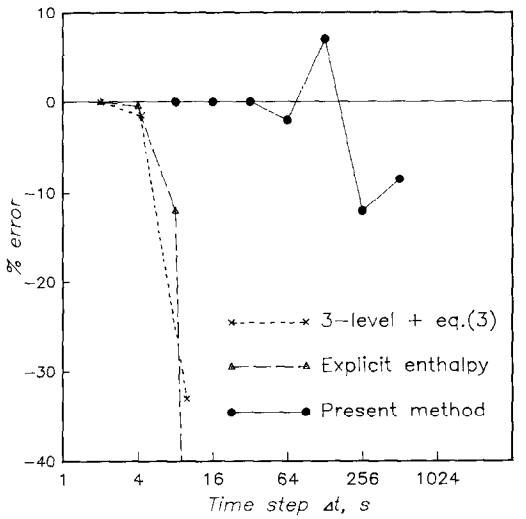

FIG. 1. Plot of discrepancy vs Δt for test problem 3.

2. *Oscillations*

Oscillations in the calculated temperature values always occur if sufficiently large time steps are used (Yalamanchili and Chu [19]; Wood and Lewis [10]). They tend to happen near the phase-change front where large temperature changes take place. As the time step is reduced, the oscillations rapidly die down. For the problems given, persistent oscillations do not occur if the Δt values of Table 3 are used, except that in problem 2, Δt has to be reduced to 50 s for the iterative methods [2, 13] and to 20 s for the present method.

3. *Complexity of programming and use*

Programming complexity can be measured by the size of the computer program. For bare-bone programs (one dimension, constant boundary conditions and no input/output statements) the present method and that of ref. [13] require 180 FORTRAN77 lines, compared with 130 lines for the explicit enthalpy and previous three-level methods, and 270 lines for the method used in ref. [2].

From the user's point of view, the iterative methods suffer from the drawback that parameters related to the iterative processes must be chosen. The wrong choice may lead either to incorrect results or to excessive computation times. Unfortunately, the optimal choice varies from problem to problem and there is no *a priori* way of determining it: a trial-and-error process must be resorted too. Thus, in ref. [13], the user must specify the relaxation parameter and the convergence criterion. In ref. [2], the convergence criteria for two different iterative processes must be specified. Non-iterative methods (including the present one) do not require the user to make these choices.

CONCLUSIONS

The method of this paper, which can be called a three-level enthalpy scheme, combines the best features of enthalpy methods and implicit temperature methods. It is simple to implement, requires no iteration and negligible extra computation per time step, and results in a robust and fast program, resistant to jumping of the latent heat peak. It works equally well for pure cooling, for phase change with abrupt enthalpy change, or for phase change with gradual release of latent heat. For phase-change problems it is two to three times as fast as the best previous method.

Although for simplicity of argument the method has been presented in the context of one-dimensional problems and the Lees [5] three-level scheme, extension to two and three dimensions and to other implicit three-level procedures (Dupont *et al.* [20]) is straightforward. Combination with automatic time step adjustment (Comini *et al.* [21]) could result in further improvement in speed.

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UN SCHEMA RAPIDE AUX DIFFERENCES FINIES INCONDITIONNELLEMENT STABLE POUR LA CONDUCTION THERMIQUE AVEC CHANGEMENT DE PHASE

Résumé—Dans la résolution numérique par différences finies des problèmes de conduction thermique avec changement de phase, on peut utiliser des méthodes enthalpiques ou des méthodes de température. Les premières demandent soit une procédure explicite avec des problèmes associés de convergence, soit une itération à chaque pas de temps si des procédures implicites sont utilisées. Les secondes sont soumises au problème du saut de chaleur latente qui nécessite l'emploi de petits pas de temps pour éviter la sous-estimation des temps de changement de phase. Cette étude suggère une méthode simple qui élimine ces problèmes et conduit à une procédure rapide et robuste qui consomme moins de temps de calcul pour le même niveau de précision par rapport aux autres schémas aux différences finies.

EIN SCHNELLES UND UNEINGESCHRÄNKT STABILES DIFFERENZENVERFAHREN FÜR WÄRMELEITUNG MIT PHASENÄNDERUNG

Zusammenfassung—Bei der numerischen Berechnung von Wärmeleitproblemen mit Phasenübergang mit Hilfe von Differenzenverfahren können Enthalpie- oder Temperaturverfahren angewandt werden. Die ersteren benötigen entweder ein explizites Verfahren mit daraus folgenden Konvergenzproblemen oder Iteration in jedem Zeitschritt, wenn implizite Verfahren angewandt werden. Aus den letzteren resultiert das Problem, daß das Maximum der latenten Wärme übersprungen wird, wodurch notwendigerweise kleine Zeitschritte erforderlich sind, um keine zu kurzen Phasenänderungszeiten zu berechnen. Dieser Bericht schlägt ein einfaches Verfahren vor, das beide Probleme eliminiert und auf eine schnelle, robuste Prozedur hinausläuft, die weniger Rechenzeit für dasselbe Genauigkeitsniveau im Vergleich zu anderen Differenzenverfahren benötigt.

БЫСТРАЯ БЕЗУСЛОВНО УСТОЙЧИВАЯ КОНЕЧНО-РАЗНОСТНАЯ СХЕМА ДЛЯ РЕШЕНИЯ ЗАДАЧ ТЕПЛОПРОВОДНОСТИ С ФАЗОВЫМ ПЕРЕХОДОМ

Аннотация—При численном решении задач теплопроводности с фазовыми переходами методом конечных разностей могут использоваться как энтальпийные, так и температурные методы. Первые из них требуют либо применения явных схем с последующим решением вопросов сходимости, либо итераций на каждом временном шаге при использовании неявных методов. Трудностью последних является скачек, связанный со скрытой теплотой фазового перехода, что приводит к необходимости использования малых временных шагов для избежания непредсказуемых времен фазового перехода. В работе предложен простой метод, устраняющий обе трудности и дающий быструю надежную процедуру, которая требует меньше расчетного времени, чем другие конечно-разностные схемы при том же уровне точности.