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The use of lumped capacitance in the finite-element solution of heat conduction problems with phase change

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Abstract—In the finite-element solution of heat conduction problems with phase change, the singular behaviour of the specific heat near the phase-change point causes special problems. These problems can be overcome by lumping the thermal capacitance of the material at the nodes, to obtain a diagonal capacitance matrix. In this way the specific heat can be unambiguously calculated. The lumped-capacitance principle was combined with the explicit enthalpy method and Pham's three-level enthalpy method. Tests against freezing problems show that for Stefan problems both resulting methods are more accurate than previous three-level distributed capacitance methods.

INTRODUCTION

NUMEROUS methods have been proposed for the numerical solution of heat conduction processes with phase change, as reviewed for example by Fox [1], Furzeland [2] and Crank [3]. 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 of interest such as solutions, foodstuffs or alloys. Others are restricted to one-dimensional problems.

This paper will concentrate on the so-called 'weak solution' [4] methods, which do not explicitly make use of the phase-change boundary and so are free of the restrictions mentioned above. A single partial differential equation is used to describe the heat transfer process throughout the material (rather than one equation for each phase). The differential equation can be written in one of two ways:

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

or

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

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

Temperature methods

Temperature methods have been used in conjunction with both finite-difference [5–7] and finite-element schemes [8, 9]. Their major drawback is that the specific heat c appears in the partial differential equation. Near the phase-change temperature, c changes extremely rapidly and may tend towards infinity, and the equation becomes highly non-linear. Pham [10] reviews various ways proposed to overcome this problem. Of these, the most convenient (because of its avoidance of iteration and unconditional stability) is Lees' [11] three-level scheme in which equation (1) is approximated by:

$$c(T^{m+2}-T^m)/2\Delta t = \{\text{div}\,[k\ \text{grad}\,(T^{m+2})] + \text{div}\,[k\ \text{grad}\,(T^{m+1})] + \text{div}\,[k\ \text{grad}\,(T^m)]\}/3 \tag{3}$$

and thermal properties are evaluated at the middle time level. Oscillations are often observed with non-linear problems and so the following 'damping equation' [12] is usually applied when updating at each time step:

$$T^m = (T^{m+2}+T^{m+1}+T^m)/3. \tag{4}$$

The singular behaviour of c still causes problems, and various other approximations have been resorted to. Comini *et al.* [8] assume that the enthalpy H follows the same distribution function as the temperature T, and calculate the specific heat from:

$$c = \left(\frac{\partial H}{\partial x}\Big/\frac{\partial T}{\partial x} + \frac{\partial H}{\partial y}\Big/\frac{\partial T}{\partial y} + \frac{\partial H}{\partial z}\Big/\frac{\partial T}{\partial z}\right)\Big/3. \tag{5}$$

This equation was subsequently modified by Comini and Del Giudice [9] for the two-dimensional situation to:

$$c = \left(\frac{\partial H}{\partial x}\cdot\frac{\partial T}{\partial x} + \frac{\partial H}{\partial y}\cdot\frac{\partial T}{\partial y}\right)\Big/\left[\left(\frac{\partial T}{\partial x}\right)^2+\left(\frac{\partial T}{\partial y}\right)^2\right]. \tag{6}$$

These modifications prevent jumping of the latent heat peak, but it cannot be said that they have a clear physical basis. Morgan *et al.* [13] suggest that c should, instead, be calculated from the temperature and enthalpy changes at the previous time levels, m and $m+1$. This constitutes a deviation from the three-level scheme (in which properties should be evaluated at the mid-level), and thus reasonably small time steps must still be used. Cleland *et al.* [14] use direct numerical integration over each element to calculate the specific heat. This method works only if latent heat release is gradual rather than sharp.

NOMENCLATURE

c	volumetric heat [J m^{-3} K^{-1}]
$\mathbf{C}$	global capacitance matrix
f_H, f_T	functions relating temperature to enthalpy and vice-versa
$\mathbf{F}$	global forcing vector
H	enthalpy [J m^{-3}]
k	thermal conductivity [W m^{-1} K^{-1}]
$\mathbf{K}$	global conductance matrix
L	latent heat [J m^{-3}]
N_i	element shape function related to node i
q	heat flow into a node
t	time [s]
Δt	length of time step [s]
T	temperature [°C]
$\mathbf{T}$	nodal temperature vector
T_f	freezing point [°C]
T_0	initial temperature
V	volume [m^3]
x, y, z	space co-ordinates [m]
α	thermal diffusivity.

Superscripts

(e)	relating to element
m	time level
*	estimated value.

Subscript

i	at or associated with node i
l	unfrozen phase
s	frozen phase.

Enthalpy methods

Enthalpy methods [15, 16] do not suffer from the drawbacks mentioned above, and furthermore are very simple to implement [3]. The major disadvantage is that because a highly non-linear function, $T(H)$, is involved [equation (2)], an explicit scheme must usually be employed, with consequent stability problems. Implicit schemes have been proposed such as Longworth's [17] and Furzeland's [2] but they require iteration at each time step and are less efficient in terms of computer time [10, 18].

Three-level enthalpy method

Recently, Pham [10] proposed a method that combines the advantages of three-level temperature methods and enthalpy methods, without recourse to iteration or any of the approximations listed above. Pham's method uses a finite difference, three-level temperature scheme with two modifications:

(i) At the start of each time step, the enthalpy change ΔH_i^* at each node is estimated from the local temperature profile at the intermediate time level. The estimated new temperature T_i^* is calculated from the estimated new enthalpy H_i^*. The specific heat is then defined as:

$$c_i^{m+1} = \Delta H_i^*/\Delta T_i^*. \tag{7}$$

(ii) At the end of the time step, as a precaution against jumping of the latent heat peak, the enthalpy at each node is calculated from:

$$H_i^{m+2} = f_H(T_i^m) + c_i^{m+1}(T_i^{m+2} - T_i^m) \tag{8}$$

and the new temperature corrected to:

$$T_i^{m+2}(\text{corrected}) = f_T(H_i^{m+2}). \tag{9}$$

Pham showed that this method is more efficient and robust than either previous enthalpy methods or previous temperature methods for a wide range of problems (cooling with constant properties, sharp phase change, gradual phase change).

Both the explicit enthalpy method and Pham's method rely on the ability to calculate explicitly the heat gain by each node. However, in conventional finite-element schemes, the heat gain by each node is not explicitly defined: increases in temperature at one node also affect enthalpy changes at other nodes. This paper proposes to enable enthalpy methods and Pham's method to be applied to finite-element schemes by lumping capacitances at the nodes.

THEORY

Both the finite-element and finite-difference solutions of transient field problems involve solving at each time step a matrix equation of the form:

$$\mathbf{C}\frac{\mathrm{d}\mathbf{T}}{\mathrm{d}t} + \mathbf{K}\mathbf{T} + \mathbf{F} = 0. \tag{10}$$

The major difference is that the global capacitance matrix $\mathbf{C}$ is diagonal in the finite-difference formulation and non-diagonal in the finite-element formulation. When $\mathbf{C}$ is diagonal, the rate of heat gain at each individual node, $q_i = C_{ii}(\mathrm{d}T_i/\mathrm{d}t)$, can be explicitly calculated from the rest of equation (10) if the temperatures T_is are known:

$$q_i = C_{ii}\frac{\mathrm{d}T_i}{\mathrm{d}t} = -\sum_j K_{ij}T_j - F_j. \tag{11}$$

It is well-known that the capacitance matrix $\mathbf{C}$ can be diagonalized by assuming the capacitance, or thermal mass, to be lumped at the nodes [19, 20]. For phase-change situations, this diagonalization is a major advantage: the variation of c in space ceases to be a problem. We shall therefore lump the 'thermal volume' of each element at the nodes, for example according to:

$$V_i^{(e)} = \int_{V^{(e)}} N_i \, dV. \tag{12}$$

Other lumping methods, which may differ from equation (12) in the case of higher-order elements, are discussed by Zienkiewicz [19]. If simplex elements are used, each element's thermal mass is equally divided between its vertices. By summing over all the elements in the usual manner, each node i will have associated with it a thermal volume:

$$V_i = \sum_e V_i^{(e)}. \tag{13}$$

Explicit enthalpy method

Using Euler's forward-difference scheme, the heat flow to each node can be calculated by using equation (11) at the previous time level, m:

$$q_i = -\sum_j K_{ij}^m T_j^m - F_i^m. \tag{14}$$

The new nodal enthalpy is then calculated from:

$$H_i^{m+1} = H_i^m + q_i \Delta t / V_i \tag{15}$$

where V_i is given by equation (13). The nodal temperatures T_i^{m+1} are then calculated from H_i^{m+1} using the enthalpy–temperature function.

In practice, the global capacitance matrices **C**, **K** and **F** do not have to be calculated and stored when an explicit method is used. The nodal heat gain $q_i^{(e)}$ can be calculated element-by-element, and accumulated into the nodal enthalpy array as one goes from one element to another. This is a very simple procedure to implement and avoids many of the problems associated with conventional (distributed mass) finite elements: computer memory requirements, matrix inversion, banded matrix handling. The manner in which nodes are numbered is also immaterial. It is therefore ideal for users whose requirements are occasional or limited, or who want to handle reasonably large problems on small computer installations.

Three-level enthalpy method

Pham's [10] three-level enthalpy method consists of a specific-heat-estimating step and a temperature-correction step. The first step uses equation (11) at the middle time level $m+1$ to estimate the rate of heat gain:

$$q_i = -\sum_j K_{ij}^{(m+1)} T_j^{(m+1)} - F_i^{(m+1)}. \tag{16}$$

The enthalpy change between levels m and $m+2$ at node i is then:

$$\Delta H_i^* = 2 q_i \Delta t / V_i. \tag{17}$$

Hence the estimated new nodal enthalpy is:

$$H_i^* = H_i^m + \Delta H_i^* \tag{18}$$

the estimated new temperature is:

$$T_i^* = f_T(H_i^*) \tag{19}$$

and the specific heat at the middle time level is:

$$c_i^{m+1} = \Delta H_i^* / (T_i^* - T_i^m). \tag{20}$$

The values of c_i^{m+1} from equation (20) can then be used to calculate the lumped **C**-matrix.

After the finite-element equation (10) has been solved, the following temperature correction step is applied:

$$T_i^{m+2}(\text{corrected}) = f_T[f_H(T_i^m) + c_i^{m+1}(T_i^{m+2} - T_i^m)]. \tag{21}$$

The computer is unable to handle equation (20) when $T_i^* = T_i^m$; i.e. when the step change in the enthalpy-temperature is encountered. Several methods may be used to overcome this problem:

(i) Set $T_i^{m+2} = T_i^m$ and eliminate T_i^{m+2} from the set of equations, in a manner similar to the handling of boundary conditions of type 1 (prescribed temperature) [21].
(ii) Give the step change in enthalpy (or latent heat peak) a finite but arbitrarily small width, to prevent c_i^{m+1} in equation (20) from becoming infinite.
(iii) Give c_i^{m+1} an arbitrary large value.

The second approach is the most convenient and will be used in this paper: the latent heat is assumed to be released over a range of 0.01°C. However, it must be realized that this finite step change is only a device for computational convenience, and is not essential to the methods of this paper (in contrast to some previous methods where a finite and reasonably large latent peak width is essential).

TEST PROBLEMS

1. *Freezing of a slab of infinite area*

A slab of infinite area and 148 mm thick is initially at 0°C. At time 0, the surface temperature is suddenly brought to −30°C (boundary condition of type 1). The properties of the material are: $T_f = 0$°C, $c = 2 \times 10^6$ J m^{-3} K^{-1}, $L = 2 \times 10^8$ J m^{-3}, $k = 1$ W m^{-1} K^{-1}. Calculate the time for the freezing front to reach the centre.

The test problem is one-dimensional, but two-dimensional elements will be used to solve it, since in one dimension the lumping of capacitances makes the simplex version of finite elements identical with finite differences. A strip of material 74 mm long × 7.5 mm wide was considered (Fig. 1).

Both distributed-capacitance and lumped-capacitance methods were tested. In the former, direct specific calculation, Comini *et al.*'s [8] formula [equation (5)], Comini and Del Guidice's [9] formula, and Morgan *et al.*'s [13] formula were tried.

Table 1 shows that Morgan *et al.*'s formula [13] does not handle this problem very well, because the phase-change boundary is very sharp. In their paper, phase change is assumed to take place over a range of about 1°C and the time step must be appropriately selected.

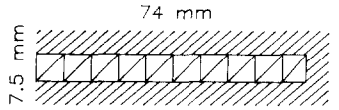

FIG. 1. Finite-element grid for freezing of a slab.

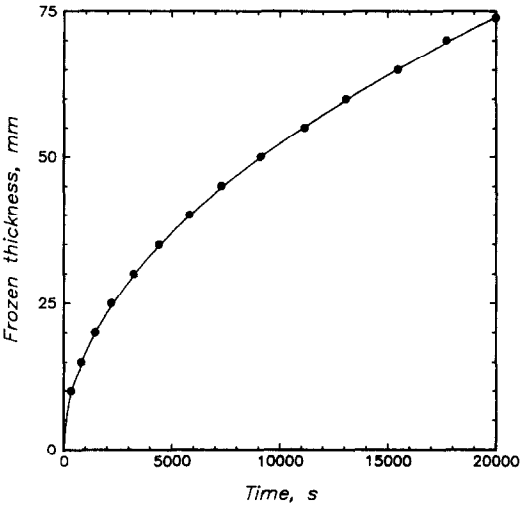

FIG. 2. Frozen thickness, problem 1 : ● finite-element solution (lumped capacitance); —— analytical solution.

Direct specific heat calculation has the same problem. Comini *et al.*'s method [8] does not yet converge at time steps as low as 2 s, and appears to overshoot the true solution by at least 70%. Comini and Del Giudice's method [9] is also slow to converge, and appears to tend to a solution 13% larger than the analytical one. On the other hand, the lumped-capacitance methods tend to a solution only 0.5% outside the analytical one. The explicit enthalpy method has satisfactorily converged at $\Delta t = 20$ s and Pham's three-level method at $\Delta t = 100$ s when damping is not used and 200 s when damping is used. (Convergence is assumed to be obtained when the solution is within 0.5% of the final solution.)

The position of the freezing front can be found by assuming that when it reaches a node, the enthalpy at that node is half-way between start-of-freezing and end-of-freezing enthalpies (since on average half the thermal mass of the node belongs to elements nearer the surface and half to elements further from the surface.) Figure 2 shows that the movement of the freezing front with time as calculated by the present method and the analytical solution [22, p. 283] are in good agreement.

2. *Freezing with step change in thermal conductivity*

A semi-infinite body of water ($c_l = 4.186 \times 10^6$ J m^{-3} K^{-1}, $c_s = 2.06 \times 10^6$ J m^{-3} K^{-1}, $k_l = 0.56$ W m^{-1} K^{-1}, $k_s = 2.3$ W m^{-1} K^{-1}, $L = 3.33 \times 10^8$ J m^{-3}) is frozen by suddenly bringing the surface temperature to -30°C. Calculate the position of the freezing front at various times, for initial water temperatures of 0° and 40°C.

The analytical solution is given in Carslaw and Jaeger [22, p. 283]. The finite-element solution is obtained by a grid similar to that in Fig. 1 but with 10-mm node spacing and extending 1 m into the body. For the duration considered, there is no perceptible cooling of the innermost nodes, so the grid adequately represents a semi-infinite body.

A strict solution would require integration of the thermal conductivity k over each element. k has a step change at the freezing point and cannot be represented by a polynomial; therefore, an exact numerical integration is not feasible. However, past experience with both finite-difference [10, 23] and finite-element [14] methods suggests that a single-point sample is sufficient; i.e. in each element k is calculated at the

Table 1. Results of finite-element calculations for freezing problem (theoretical solution 20020 s)

Time step (s)	Methods A1	A2	A3	A4	B1	B2	C
2	9630	10544	33994	22651	20117	20127	20121
5	9261	7682	30402	22530	20117	20122	20115
10	10396	1955	24273	22440	20117	20123	20110
20	3861	9812	26500	20860	20118	20126	20101
50	3901	4250	24950	19500	20128	20140	18700
100	9200	7897	22400	19500	20060	20163	Diverge
200	3791	3197	12000	8200	6691	20062	—
500	14	756	499	499	5095	7281	—
Final % error	?	?	?	13.1	0.5		0.5

Methods: A, finite-element method with distributed capacitance, three-level scheme with damping [equation (4)]. A1, Direct specific heat calculation with seven-point numerical integration. A2, Morgan *et al.*'s [13] specific heat formula. A3, Comini *et al.*'s [8] specific heat formulae. A4, Comini and Del Giudice's [9] specific heat formula.

B, Finite-element method with lumped capacitance, three-level enthalpy scheme (this paper). B1, Without damping. B2, With damping [equation (4)].

C, Finite-element method with lumped capacitance, explicit enthalpy scheme (this paper).

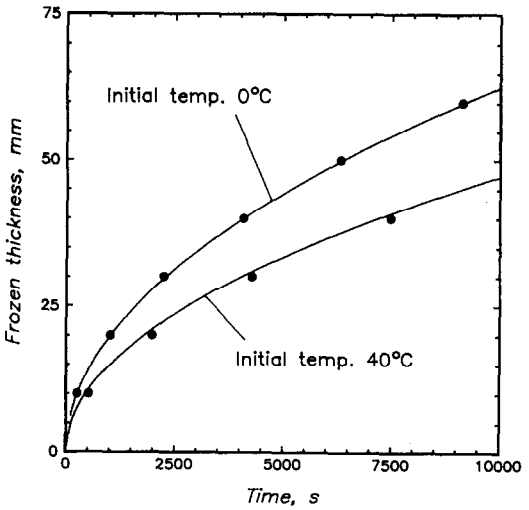

FIG. 3. Frozen thickness, problem 2: ● finite-element solution (lumped capacitance); —— analytical solution.

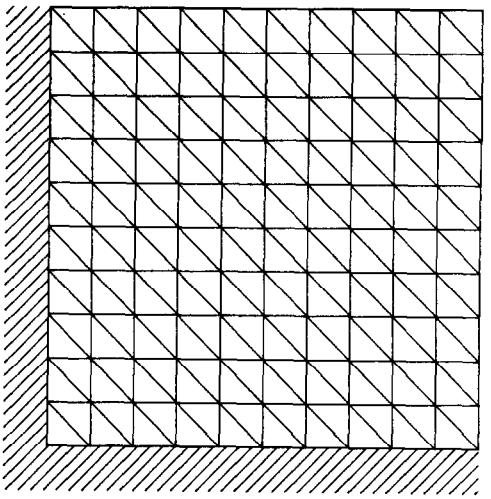

FIG. 4. Finite-element grid for corner freezing problem.

average temperature $(T_1 + T_2 + T_3)/3$, where T_i are the vertex temperatures.

Results from the present method are shown in Fig. 3 for the two different starting temperatures. Errors (if any) due to the variation in k would be present only for the 40°C case, since no heat is conducted through unfrozen material when the initial temperature is 0°C. For the latter case, the frozen thickness prediction is accurate to 0.5 mm or better, while for the former, this thickness is underpredicted by about 1 mm (1/10 the mesh size). Thus, there is only a very slight decrease in accuracy due to the approximation used for k, despite the high initial temperature of 40°C and the relatively coarse grid (the range of frozen thickness in Fig. 3 covers only 4–6 meshes).

3. *Freezing of a corner region*

The corner region of a liquid body extending infinitely in the positive x and y-directions is frozen by bringing the surface temperature to -1.0 at time $t = 0$. Thermal properties are: $k_l = k_s = 1$, $c_l = c_s = 1$, $L = 1.5613$ in one case, 0.25 in the other.

The grid of Fig. 4 was used to represent the body. The position of the front is invariant with respect to $x/\sqrt{4\alpha t}$ and $y/\sqrt{4\alpha t}$, and plotted in Fig. 5, together with the analytical solutions [24]. Very good agreement is obtained.

DISCUSSION AND CONCLUSIONS

Basically the main difficulty in the finite-element solution of heat conduction problems with phase change is that the changes in specific heat must be tracked in both time and space. This paper proposes to eliminate the space variation by lumping capacitances at the nodes. In a way, the proposed method is similar to that of Zienkiewicz *et al.* [25]. These authors lumped the latent heat at the nodes, but not the sensible heat. Apart from programming complications, this approach limits the use of their method to cases where latent heat can be clearly defined, while the present method can readily be used to solve gradual phase-change problems (such as the freezing/melting of foodstuffs and alloys).

Compared to previous methods, the advantages of the proposed lumped-capacitance methods are:

1. Accuracy, as shown in the test problems. As long as the grid is sufficiently fine, any degree of accuracy can be obtained. Although there are reservations in the literature about the use of lumped capacitances in some other types of problems, their use in heat transfer is well proven [19]. In fact, the one-dimensional simplex formulation of finite elements with lumped capacitance is identical with the finite-difference formulation. It can be expected that accuracy will be even better in phase-change

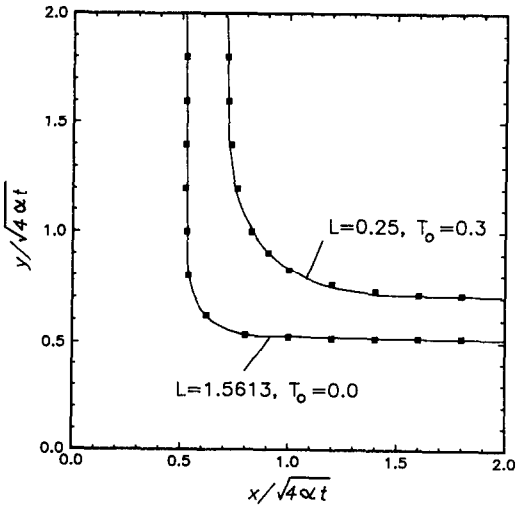

FIG. 5. Freezing front position, problem 3 (corner region): ● finite-element solution (lumped capacitance); —— analytical solution.

problems than in non-phase change problems, since for pure phase change (i.e. with zero sensible heat) the exact analytical solution has a lumped-capacitance form; i.e. a slab, infinite cylinder or sphere with all its thermal mass lumped half-way between surface and centre freezes in exactly the same time as an equivalent body with distributed mass [26].

2. Simplicity and consistency in visualization. For example, the problem of enthalpy and temperature distributions in an element does not have to be considered.
3. Ease of implementation, for the explicit enthalpy method. For the occasional user, the basic concepts and equations are easy to grasp, and computer implementation does not involve special matrix handling techniques. Memory storage requirements are reduced, enabling reasonably large problems to be solved without difficulty.
4. Computational speed (for Pham's three-level method). Convergence is reached at relatively large time steps for Stefan-type problems.

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USAGE DE LA CAPACITANCE LOCALISEE DANS LA RESOLUTION PAR ELEMENTS FINIS DES PROBLEMES DE CONDUCTION THERMIQUE AVEC CHANGEMENT DE PHASE

Résumé—Dans les problèmes de conduction thermique avec changement de phase et leur résolution par éléments finis, le comportement singulier de la chaleur massique près du changement de phase cause des difficultés spéciales. Celles-ci peuvent être surmontées en localisant la capacitance thermique du matériau aux noeuds pour obtenir une matrice capacitance diagonale. De cette manière la chaleur massique peut être calculée sans ambiguité. Le principe de capacitance localisée est combiné avec la méthode enthalpique explicite et la méthode enthalpique à trois niveaux de Pham. Des tests de problème de gel montrent que pour les problèmes de Stefan, les méthodes résultantes sont plus précises que les méthodes antérieures de capacitance à trois niveaux.

DIE ANWENDUNG KONZENTRIERTER KAPAZITÄTEN BEI DER FINITE- ELEMENT-LÖSUNG VON PROBLEMEN DER WÄRMELEITUNG MIT PHASENÄNDERUNG

Zusammenfassung—Für die Lösung von Problemen der Wärmeleitung mit Phasenänderung mit Hilfe finiter Elemente verursacht das abnorme Verhalten der spezifischen Wärmekapazität im Bereich der Phasenänderung besondere Probleme. Diese Probleme können durch Konzentration der Wärmekapazität auf Knotenpunkte überwunden werden, um eine diagonale Kapazitäts-Matrix zu erhalten. Auf diese Weise kann die spezifische Wärmekapazität eindeutig berechnet werden. Das Prinzip der konzentrierten Kapazitäten wurde mit der expliziten Enthalpie-Methode und Pham's "three-level"-Methode kombiniert. Tests für Erstarrungsprobleme zeigen, daß bei Stefan-Problemen diese beiden weiterentwickelten Methoden genauer sind als die bisher verwendete "three-level"-Methode.

ИСПОЛЬЗОВАНИЕ СОСРЕДОТОЧЕННОЙ ТЕПЛОЕМКОСТИ ПРИ РЕШЕНИИ ЗАДАЧ ТЕПЛОПРОВОДНОСТИ С ФАЗОВЫМ ПЕРЕХОДОМ МЕТОДОМ КОНЕЧНЫХ ЭЛЕМЕНТОВ

Аннотация—При решении задач теплопроводности с фазовым переходом методом конечных элементов вызывает затруднение сингулярное поведение теплоемкости вблизи точки фазового перехода. Эти трудности можно обойти, введя сосредоточенную теплоемкость материала в узлах сетки и получая таким образом диагональную матрицу теплоемкостей. В этом случае теплоемкость определяется однозначно. Принцип сосредоточенной теплоемкости использовался совместно с методом явной энтальпии и методом трехуровневой энтальпии Фама. Тестовые расчеты по замерзанию показали, что такой подход при решении задач Стефана является более точным, чем использовавшиеся ранее методы трехуровневого распределения теплоемкости.