Finite Element Solution of Non-Linear Heat Conduction Problems with Special Reference to Phase Change

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FINITE ELEMENT SOLUTION OF NON-LINEAR HEAT CONDUCTION PROBLEMS WITH SPECIAL REFERENCE TO PHASE CHANGE

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SUMMARY

The paper presents a generally applicable approach to transient heat conduction problems with non-linear physical properties and boundary conditions. An unconditionally stable central algorithm is used which does not require iteration.

Several examples involving phase change (where latent heat effects are incorporated as heat capacity variations) and non-linear radiation boundary conditions are given which show very good accuracy.

Simple triangular elements are used throughout but the formulation is generally valid and not restricted to any single type of element.

INTRODUCTION

The application of the finite element method to heat conduction analysis has attracted considerable attention since the procedure was first proposed for field problems.[1] While the solution process is now well established for linear situations involving complicated multi-dimensional geometries and time dependent boundary conditions,[2,3,4] relatively little work has been reported for temperature dependent thermophysical properties and/or non-linear radiation-convection boundary conditions. Most authors discuss only one aspect of non-linearity at a time and use algorithms which involve iterations.[5,6,7] In this paper we are concerned with a unified approach permitting simultaneous temperature dependence of thermal conductivity, heat capacity, rate of internal heat generation and surface heat transfer coefficients. A three time level difference scheme is utilized for the solution of the resulting matrix differential equations as this allows a direct evaluation of thermophysical properties and heat transfer coefficients at the intermediate time level, thus eliminating the need of iterations within each time step.[8,9] Since the algorithm employed is unconditionally stable, a time step adjustment procedure is included in the numerical model in order to follow the thermal behaviour of solids up to steady state without using an unreasonable amount of computer time.

In the general formulation latent heat effects are not included separately as these can be approximated to a very high degree of accuracy by rapid variations of heat capacity within a narrow temperature range,[10] as shown in Figure 1. While for certain substances the phase change occurs within a wide band of temperatures, and thus a physically realistic approximation can be easily dealt with computationally, for other materials the phase change takes place with almost no temperature variation, and a heat capacity (ρc) versus temperature (t) curve resembling

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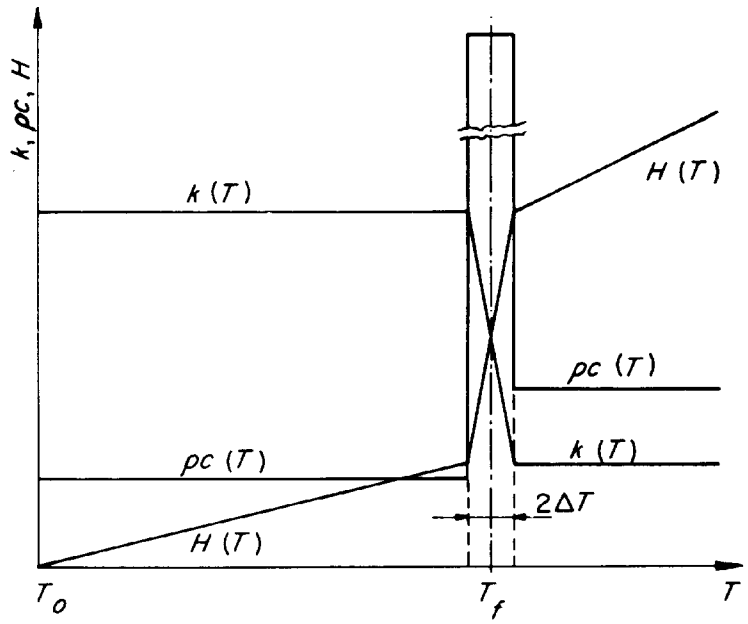


Figure 1. Estimation of thermophysical properties in phase change problems. Latent heat effect is approximated by a large heat capacity over a small temperature interval $2\Delta T$

a Dirac function must be used. In the next sections it is shown that, in this latter case, it is convenient to define a new variable H (enthalpy), as an integral of the $\rho c - t$ curve (Figure 1), and then estimate, for each element, average heat capacity values based on well known enthalpy properties. This way a critical class of non-linear problems is dealt with in subsequent examples.

FINITE ELEMENT FORMULATION

The problem considered in this paper is governed, in region Ω, by the quasilinear parabolic equation:

$$\rho c\frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k\frac{\partial T}{\partial y}\right) + \frac{\partial}{\partial z}\left(k\frac{\partial T}{\partial z}\right) + Q \tag{1}$$

subjected to boundary conditions:

$$T = T_w \text{ on } \Gamma_1 \tag{2}$$

and:

$$k\left(\frac{\partial T}{\partial x}l_x + \frac{\partial T}{\partial y}l_y + \frac{\partial T}{\partial z}l_z\right) + q + q_c + q_r = 0 \quad \text{on } \Gamma_2 \tag{3}$$

The equations refer to unsteady thermal fields in substances with thermophysical properties dependent on temperature, where ρc is the heat capacity, k is the thermal conductivity and Q is the rate of internal heat generation. The terms l_x, l_y and l_z are the direction cosines of the outward normal to the boundary surface, while q, q_c and q_r represent respectively the imposed heat flux and the rates of heat flow per unit area due to convection and radiation. The following relationships are usually written:

$$q_c = \alpha_c(T - T_{ac}) \tag{4}$$

and

$$q_r = \varepsilon\sigma(T^4 - T_{ar}^4) = \alpha_r(T - T_{ar}) \tag{5}$$

where α_c is the convective heat transfer coefficient, ε is the emissivity, σ is the Stefan constant, α_r is a parameter related to the effects of radiation by the expression

$$\alpha_r = \varepsilon\sigma(T^2 + T_{ar}^2)(T + T_{ar}) \tag{6}$$

and T_{ac} and T_{ar} are the equilibrium temperatures for which, respectively, no convection or no radiation occurs.

In general k, ρc, Q and α_r are thus temperature dependent functions, the last variation being expressed explicitly by equation (6), the others being known numerically. The spacewise discretization of equation (1), subjected to boundary conditions (2) and (3) can be accomplished using Galerkin's method as shown by Zienkiewicz *et al.*[2,3,7]

Let the unknown function T be approximated, throughout the solution domain at any time t, by the relationship:

$$T = \sum_{i=1}^{n} N_i(x, y, z)T_i(t) = \mathbf{NT} \tag{7}$$

where N_i are the usual shape functions defined piecewise element by element, T_i or $\mathbf{T}$ being the nodal parameters. The simultaneous equations, allowing the solution for n values of T_i, are obtained typically for point i by equating to zero the integral over the domain Ω of the product of the weighting function N_i and the residual resulting from substitution into equations (1) of equation (7). After making use of Green's theorem, in order to avoid second derivatives in the integrals imposing unnecessary continuity conditions between elements, the n equations can be written down in a matrix form as:

$$\mathbf{K}\ \mathbf{T} + \mathbf{C}\ \dot{\mathbf{T}} + \mathbf{F} = 0 \tag{8}$$

Typical matrix elements are:

$$K_{ij} = \sum \int_{\Omega^e} k\left(\frac{\partial N_i}{\partial x}\frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y}\frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z}\frac{\partial N_j}{\partial z}\right) \mathrm{d}\Omega + \sum \int_{\Gamma_2^e} (\alpha_c + \alpha_r)N_iN_j \,\mathrm{d}\Gamma; \tag{9}$$

$$C_{ij} = \sum \int_{\Omega^e} \rho c N_i N_j \,\mathrm{d}\Omega; \tag{10}$$

$$F_i = -\sum \int_{\Omega^e} N_i Q \,\mathrm{d}\Omega + \sum \int_{\Gamma_2^e} N_i(q - \alpha_c T_{ac} - \alpha_r T_{ar}) \,\mathrm{d}\Gamma. \tag{11}$$

In the above the summations are taken over the contributions of each element, Ω^e is the element region and Γ_2^e refers only to elements with external boundaries on which condition (3) is specified.

It must be noted that the set of equations (8) is highly non-linear since the material properties k, ρc and Q as well as the radiation parameter α_r and, therefore, the matrices $\mathbf{K}$, $\mathbf{C}$ and $\mathbf{F}$ are strongly dependent on $\mathbf{T}$.

TIME-STEPPING SCHEME

The set of ordinary differential equations (8) which define the discretized problem can be solved using one of the many recursion schemes. The most popular in this context is the mid-interval

Crank-Nicolson algorithm,[2,5,7] of unconditional stability but unfortunately requiring an iteration within each time step. To avoid this difficulty Bonacina and Comini[9] used the unconditionally stable, three level, scheme proposed by Lees[8] and this is utilised here.

If it is assumed that the temperature varies linearly in the small time interval between $t-\Delta t$ and $t+\Delta t$, equation (8) can be approximated as:

$$\mathbf{K}_t(\mathbf{T}_{t+\Delta t}+\mathbf{T}_t+\mathbf{T}_{t-\Delta t})/3+\mathbf{C}_t(\mathbf{T}_{t+\Delta t}-\mathbf{T}_{t-\Delta t})/(2\Delta t)+\mathbf{F}_t = 0. \tag{12}$$

This, after some algebra, results in the following recurrence formulae for final integration:

$$\mathbf{T}_{t+\Delta t} = -\left(\mathbf{K}_t+\frac{3}{2\Delta t}\mathbf{C}_t\right)^{-1}(\mathbf{K}_t\mathbf{T}_t+\mathbf{K}_t\mathbf{T}_{t-\Delta t}-\frac{3}{2\Delta t}\mathbf{C}_t\mathbf{T}_{t-\Delta t}+3\mathbf{F}_t) \tag{13}$$

in which only central values of the matrices **K**, **C** and **F** occur. If the vector **T** is known at two-consecutive time steps the prediction can be obtained explicitly without iteration.

The scheme is apparently not self starting but as we shall always refer to known stationary conditions, two starting values can easily be assumed.

The algorithm (13) has been shown to be unconditionally stable and convergent in the context of finite differences.[9,10] Extensive numerical experiments done by the authors have confirmed that this is the case also with the finite-element formulation.

SOME SPECIAL FEATURES OF THE NUMERICAL MODEL

The program for implementing the algorithm derived on the previous section follows the usual pattern.[3] However, the matrices **K**, **C** and **F** are now time dependent, through the variation of coefficients with temperature, and a completely new solution has to be obtained at each stage. The evaluation of temperature dependent quantities in the integrals (9), (10) and (11) require special care, particularly if a rather coarse mesh is employed and spatial variation of the quantities is abrupt. Numerical integration has obviously to be adopted here and therefore heat capacity, thermal conductivity and rate of internal heat generation must be estimated at integrating points in Ω^e. A direct evaluation, in fact, can be expected to lead to satisfactory numerical integrations only if the ρc, k and Q versus temperature curves do not present sharp peaks in the range of interest. If, instead, a 'true' melting or freezing process is considered, difficulties are likely to arise.[10]

In fact, when the temperature approaches the phase change temperature, the equivalent heat capacity tends to the Dirac δ function and, therefore, cannot be satisfactorily represented across the peak, by any smooth function. Such extreme problems can be successfully tackled by the technique proposed here, where a more appropriate averaging process is employed.

The approach is a physical one and is based on the observation that the integral of heat capacity with respect to temperature (enthalpy);

$$H = \int_{T_0}^{T} \rho c \, \mathrm{d}T \tag{14}$$

is a smooth function of temperature even in the phase change zone. Therefore, it is reasonable to interpolate the enthalpy, rather than the heat capacity directly, writing the relationship:

$$H = \sum_{i=1}^{n} N_i(x, y, z)H_i(t) = \mathbf{NH} \tag{15}$$

where again N_i are the shape functions and H_i are the enthalpy values at nodal points. Since

by definition we have:

$$\rho c = \mathrm{d}H/\mathrm{d}T \tag{16}$$

the values of heat capacity at the integrating points can be approximated by determining the gradient of enthalpy with respect to temperature, i.e.

$$\langle \rho c \rangle_{x,y,z} \cong \frac{1}{3}\left(\frac{\partial H}{\partial x}\Big/\frac{\partial T}{\partial x}+\frac{\partial H}{\partial y}\Big/\frac{\partial T}{\partial y}+\frac{\partial H}{\partial z}\Big/\frac{\partial T}{\partial z}\right) \tag{17}$$

This averaging process gives representative values of heat capacity and preserves a correct heat balance by avoiding the possibility of missing peak values of the quantity ρc. Similar techniques are used in the program for the best determination of k and Q values.

A second special feature of the calculation involves an algorithm for a correct estimate of the radiation coefficient α_r. Since α_r is a cubic function of T and the temperature is assumed to vary linearly with time, it can be easily verified that the expression:

$$\begin{aligned}
\langle \alpha_r \rangle &= \frac{1}{2\Delta t}\int_{t-\Delta t}^{t+\Delta t} \varepsilon\sigma(T^2+T_{ar}^2)(T+T_{ar})\,\mathrm{d}t \\
&\cong \varepsilon\sigma\{[T(t)^2+T_{ar}(t)^2][T(t)+T_{ar}(t)] \\
&\quad +\tfrac{1}{4}[T_{ar}(t+\Delta t)-T_{ar}(t-\Delta t)]^2[T_{ar}(t)+T(t)-\tfrac{2}{3}T(t-\Delta t)] \\
&\quad +\tfrac{1}{3}[T_{ar}(t+\Delta t)-T_{ar}(t-\Delta t)][T(t)-T(t-\Delta t)][T(t-\Delta t)+T_{ar}(t-\Delta t)] \\
&\quad +[T(t)-T(t-\Delta t)]^2[T(t)+\tfrac{1}{2}T_{ar}(t+\Delta t)-\tfrac{1}{6}T_{ar}(t-\Delta t)]\}
\end{aligned} \tag{18}$$

which still involves only known values of temperatures, is a much better approximation to the time average value of α_r, in the interval from $t-\Delta t$ to $t+\Delta t$, than the direct calculation of α_r at time t.

Finally, as the algorithm (13) is unconditionally stable, it has been possible to incorporate into the program an automatic time step adjustment feature. The norm of the difference $(\mathbf{T}_{t+\Delta t}-\mathbf{T}_t)$ is computed at each stage of the calculation process, excluding obviously those points of Γ where $\mathbf{T}$ is specified. If the norm is less than a prefixed value $\Delta T_{\min}$, Δt is doubled before going on to the next time step whereas, if the norm is greater than a prespecified value $\Delta T_{\max}$, Δt is halved and the calculation for that time step is repeated until the norm is acceptable. Over the spectrum of problems solved by this method, Δt has been changed from initial values as low as 200 sec up to 210,400 sec for slowly varying temperatures in the vicinity of an equilibrium situation.

SOME ILLUSTRATIVE EXAMPLES

The formulation given in the previous sections is general and applicable to any type of finite-element discretization. In this paper the simplest, triangular elements have been used to illustrate the principles involved.

The first three examples are of a comparative nature and deal with simple configurations for which analytical solutions exist. The last example is more general and illustrates a practical application.

Example 1. Solidification of an infinite slab of liquid

This problem has been solved exactly by several authors.[11] In the present context it is solved as a two dimensional problem with temperature dependent heat capacity and thermal conductivity.

The heat capacity is assumed to vary in a discontinuous manner (as a pulse) between the liquid and solid phases while the thermal conductivity varies linearly as shown in Figure 1. In Figure 2(b) and Figure 3 the progress of the freezing front and the spatial temperature distributions are compared with analytical results of Reference 11.

The position of the freezing front is given by the isotherm $T_f - \Delta T$. The initial temperature was taken to be above freezing (283·15°K) as previous investigations have shown that such conditions are more critical for a numerical calculation than those with the water initially at the freezing point.[10] The phase change interval $2\Delta T$ was assumed as 0·5 K but the results proved to be relatively insensitive to this value.

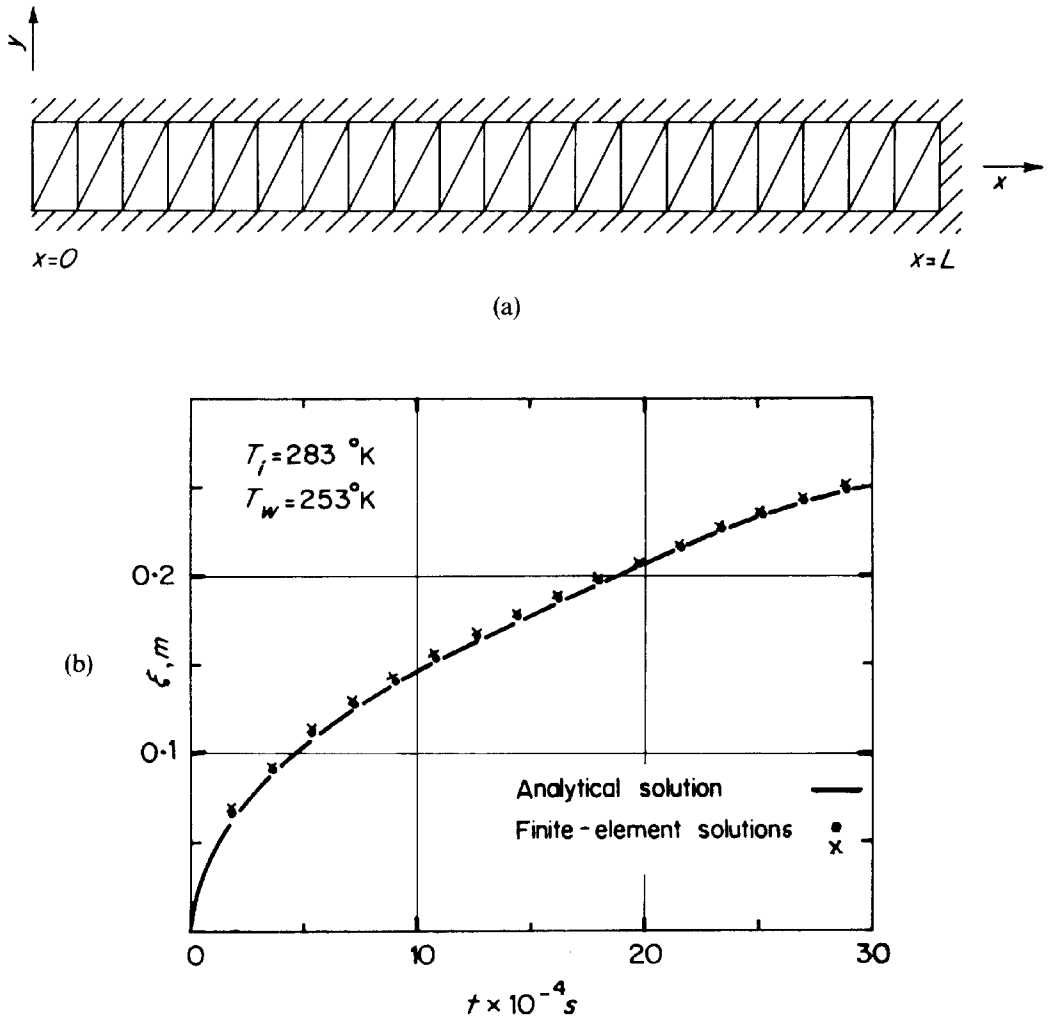


Figure 2. Solidification of a slab in liquid. (a) Finite-element mesh. Non-conductive boundaries are assumed throughout but at the face $x = 0$. Slab thickness: $L = 1$ m. (b) Progress of freezing front through slab: distance vs time. Solid curve analytical solution[11]; large dot finite-element solution for $\Delta t = 200$ s, constant; x finite-element solution using variable time steps and a total of 40 cycles of computation. Material properties: (frozen) $k = 2{\cdot}22$ W/mK $\rho c = 1{\cdot}762 \times 10^6$ J/m^{3}K; (unfrozen) $k = 0{\cdot}556$ W/mK $\rho c = 4{\cdot}226 \times 10^6$ J/m^{3}K; latent heat effect $\lambda = 338 \times 10^6$ J/m^3. Assumed width of the phase change interval: $2\Delta t = 0{\cdot}5$ K

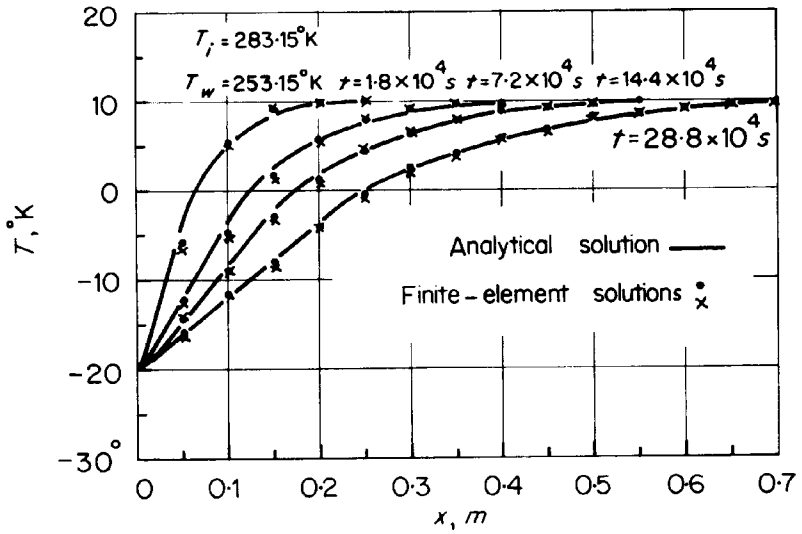


Figure 3. Temperature distributions at different time values during the freezing process referred to in Figure 2.

As the slab involved is finite, comparisons with the theoretical infinite slab solution were terminated when temperature began to change appreciably at $x = L$. Excellent agreement with theory was found, the maximum errors being less than 2 per cent.

Example 2. Solidification of a corner region

Solidification of a liquid in an internal corner with the surfaces of the wedge maintained at equal temperatures lower than the freezing temperature was next considered. In order to allow a comparison of the results obtained from the present method with exact analytical solutions, the following values of the characteristic dimensionless parameters were assumed‡

(a) Liquid initially at fusion temperature:

$$T^*_{wx} = T^*_{wy} = -1{\cdot}0; \qquad T^*_i + 0{\cdot}0; \qquad \beta = 1{\cdot}5613; \tag{19}$$

(b) Liquid initially at a temperature higher than the fusion temperature:

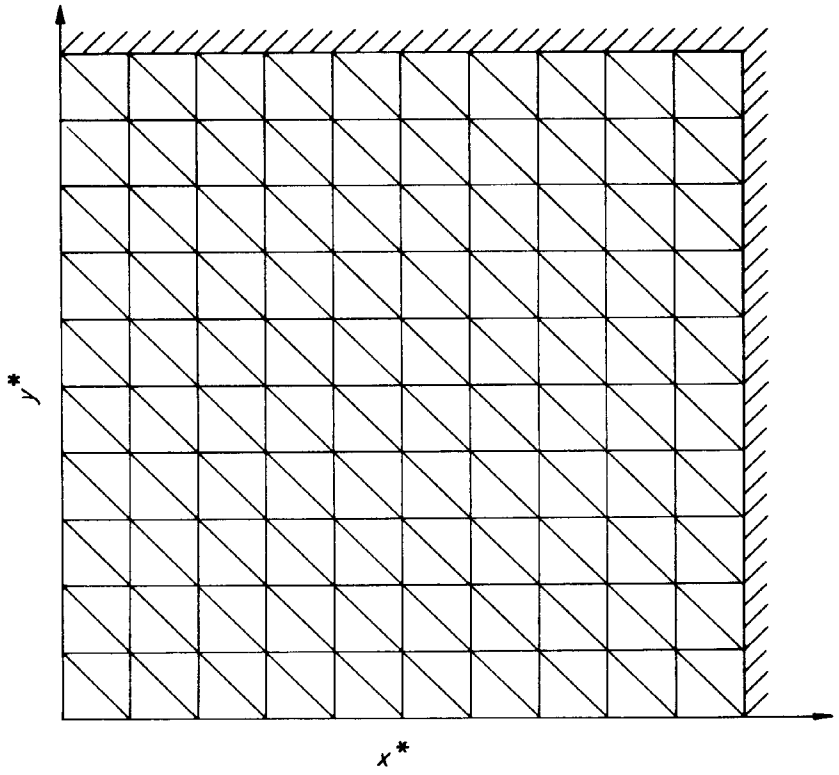
$$T^*_{wx} = T^*_{wy} = -1{\cdot}0; \qquad T^*_i = 0{\cdot}3; \qquad \beta = 0{\cdot}25; \qquad a_s/a_l = 1{\cdot}0 \tag{20}$$

Computed locations of the interface are compared in Figure 4 with the results from the analytical solutions of Budhia and Kreith[12] for case (a) and of Rathjen and Jiji[13] for case (b). With reference again to case (b), in Figure 5 the temperatures along the diagonal, as predicted by the finite-element method, and by the analytical solution are presented.

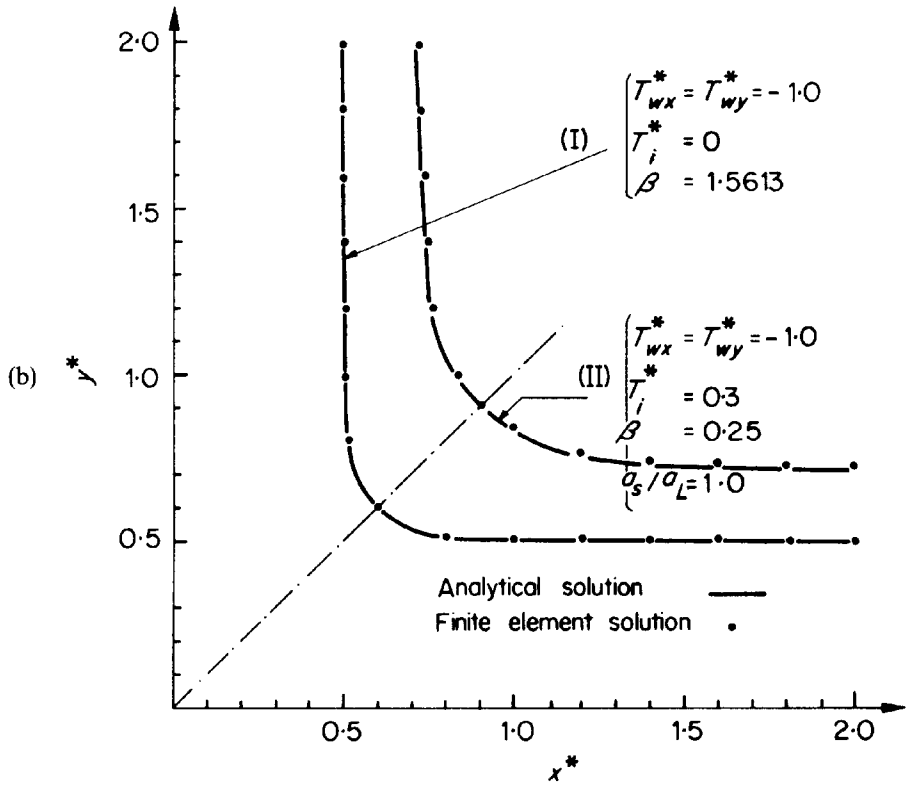
Example 3. Slab with radiation boundary conditions

A plane slab, with thermophysical properties indepedent of temperature ($k \equiv \rho c \equiv a \equiv 1{\cdot}0$), subjected to radiation and convection, was considered as an example of non-linear boundary conditions. The following assumptions were made:

‡ It must be noted that the available analytical solutions for this problem are exact only if the liquid is initially at the fusion temperature or if the ratio of the thermal diffusivity in the solid to that in the liquid phase is unity.[12,13]



(a)



(b)

Figure 4. Solidification of an internal corner with the surfaces maintained at equal temperatures. (a) Finite-element mesh. Infinite boundaries are replaced by finite ones which are assumed to be non-conductive. (b) Interfacial positions: (I) for a liquid initially at the fusion temperature; (II) for a liquid initially at a uniform temperature above the melting point. Material properties: (frozen) $k = 1$ W/mK; $\rho c = 1$ J/m^{3}K; (unfrozen) $k = 1$ W/mK; $\rho c = 1$ J/m^{3}K; latent heat effects $\lambda = 1{\cdot}5613$ J/m for case I; $\lambda = 0{\cdot}25$ J/m^3 for case (II). Assumed width of the phase change interval: $\Delta T^* = 0{\cdot}01$

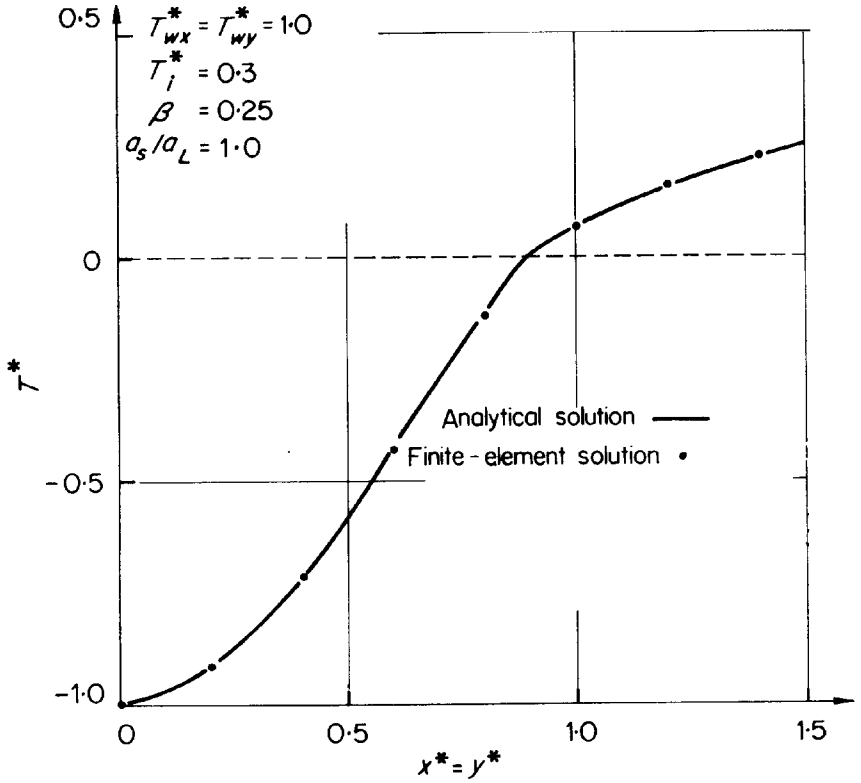


Figure 5. Temperature along the diagonal for internal corner during the freezing process referred to in Figure 4, case (II)

$$q_c + q_r = \alpha_c[T(0,t) - T_{ac}] + \alpha_r[T(0,t) - T_{ar}], \qquad t > 0; \tag{21}$$

$$\partial T(L,t)/\partial x = 0, \qquad t > 0, \tag{22}$$

$$T(x,0) = T_i; \qquad 0 < x < L \tag{23}$$

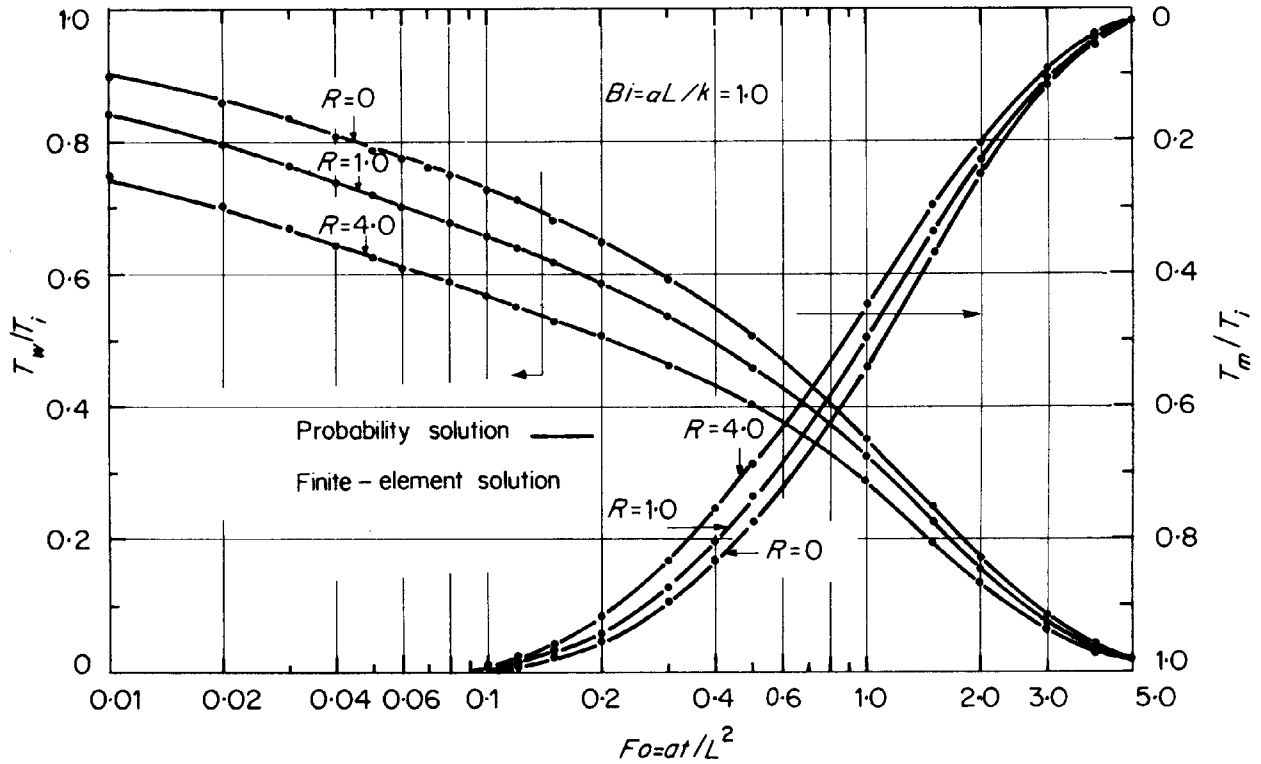


Figure 6. Transient temperature results for a slab with radiation-convection boundary conditions and uniform initial temperature. The mesh used is the same as in Figure 2(a); the face $x = 0$ is exposed to convection and radiation while the end $x = L$ is thermally insulated. The thermophysical properties of the material are independent of temperature and no phase change occurs

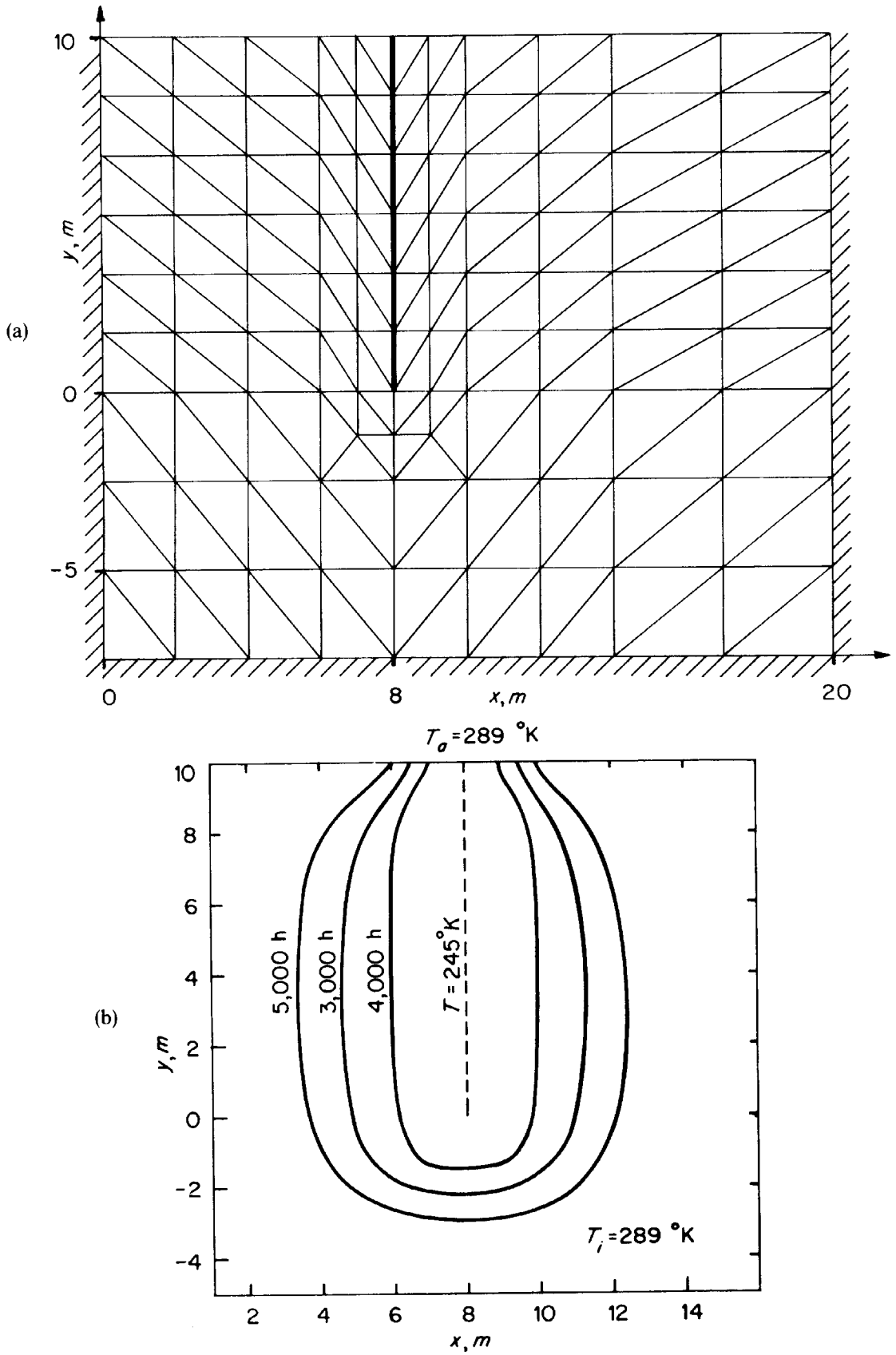


Figure 7. Freezing of a moist soil (sand) (a) Transverse section illustrating the finite-element mesh used. The thick line corresponds to the freezing sheath. The infinite boundary is replaced by a finite one which is assumed to be non-conductive. Convection heat transfer takes place at the surface. (b) Freezing front positions as computed by the finite-element method. The freezing sheath is maintained at -245°K. External temperature is 289°K and the convective heat transfer coefficient is: $\alpha = 20$ W/m^{2}K. Material properties[15]: (frozen) $k = 2{\cdot}32$ W/mK; $\rho c = 2{\cdot}04 \times 10^6$ J/m^{3}K; (unfrozen) $k = 1{\cdot}65$ W/mK; $\rho c = 2{\cdot}815 \times 10^6$ J/m^{3}K; latent heat effect $\lambda = 120 \times 10^6$. Assumed width of the phase change interval $2\Delta T = 1$ K

and it was decided to consider $T_{ac} \equiv T_{ar} \equiv 0$ and $B_i = \alpha_c L/k = 1$ while varying $R = \varepsilon\sigma T_i^3 L/k$. The results obtained by the present approach can be compared with those obtained from a Monte Carlo method by Haji-Sheikh and Sparrow.[14] The comparison is shown in Figure 6 for the surface and the centre temperatures computed employing the same mesh as in Example 1. The agreement is always within 1 per cent and of the same order as that obtained by Beckett and Chu[6] through the use of an iterative finite element procedure.

Example 4. Ground freezing

This final example concerns a practical problem, often encountered in civil engineering, for which no alternative exact solutions exist. Here we consider a situation where a ground region inside two lengths of cooling pipes is to be frozen. In Figure 7 the relevant aspects of the problem and its solution are presented, showing the time progression of the freezing front. Thermophysical properties of the ground, used in the computations, are those reported in Reference 15.

CONCLUDING REMARKS

The approach to non-linear heat conduction problems presented in this paper is very generally applicable and we feel presents one of the most efficient algorithms. Examples have demonstrated the accuracy obtainable.

The capability of dealing with phase change problems opens the door to many practical applications, such as determination of thermal stresses in castings, ground freezing, food freezing and thawing technology etc.

ACKNOWLEDGEMENT

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APPENDIX

Notation

a	thermal diffusivity [m^2/s]
$Bi = \alpha_c L/k$	Biot criterion
c	specific heat [J/kgK]
$F_o = at/L^2$	Fourier criterion
H	enthalpy per unit volume [J/m^3]
k	thermal conductivity [W/mK]
l_x, l_y, l_z	direction cosines of the outward normal to the boundary surface
L	slab thickness [m]
q	heat flux density [W/m^2]
Q	rate of internal heat generation per unit volume [W/m^3]
$R = \varepsilon\sigma T_i^3 L/k$	radiation criterion
t	time [s]
T	absolute temperature [°K]
$T^* = (t-t_f)/(t_f-t_w)$	dimensionless temperature

x, y, z	position co-ordinates [m]
$x^* = x/\sqrt{4a\tau}$, $y^* = y/\sqrt{4a\tau}$	dimensionless co-ordinates
α	heat transfer coefficient [W/m^{2}K]
$\beta = \lambda/(c_s(t_f - t_w))$	latent to sensible heat ratio
ε	emissivity
λ	latent heat per unit volume [J/m^3]
ξ	phase front position [m]
ρ	density [kg/m^3]
σ	Stefan constant [W/m^{2}K^4]

Subscripts

a = ambient
c = convection
f = phase change
i = initial
l = liquid
m = centre
r = radiation
s = solid
w = surface
O = reference

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