An Explicit Method for Convection Problems Involving a Change of Phase

K. Morgan
Department of Civil Engineering, University of Wales, Swansea SA2 8PP, United Kingdom

The numerical analysis of problems of heat transfer in materials which undergo a liquid/solid change of phase has attracted much interest as such problems are of practical importance in the steel and nuclear industries. It is normally assumed that transfer of heat by conduction is the dominant mechanism whereas it is known from experimental evidence that convection plays a dominant role in many phase change problems of practical interest.

In this paper an attempt has been made to include the effect of convection in two-dimensional heat transfer problems involving a change of phase. The finite element method is used to solve the heat conduction equation in the solid and to solve the full Navier-Stokes equations and the convective-diffusion in the fluid. The explicit fractional step method is used to solve the momentum and continuity equations and the phase change is modelled by means of the enthalpy method. The velocity and temperature fields are re-resented by the use of four noded bilinear elements with a discontinuous, elementwise constant, representation for the pressure field. With the explicit time stepping scheme, the representation adopted for the temperature field is shown to be capable of modelling accurately the phase change process by comparing numerical results with the analytical solution for a one-dimensional problem involving conduction only.

Results are presented for the problem of freezing in a plane thermal cavity when the temperature of one of the vertical walls is suddenly reduced and the effect of convection on the freezing process is illustrated.

1. Introduction

Much attention has been given to the development of numerical methods capable of analysing the heat transfer problems involving a solid/liquid change of phase which occur in the nuclear, steel and other industries. However, in most of this work, the variation of the temperature field is determined by the solution of the heat conduction equation whereas it is known that convection plays a dominant role in many situations of practical interest. This has been confirmed by a recent series of experiments [1,2] which show the importance of natural convection in the processes of melting and freezing.

Gartling [3] has proposed a numerical model in which the effects of convection on the phase change process are included. In this model the velocity and pressure distributions in the fluid are obtained by the finite element solution of the incompressible Navier-Stokes equations and the temperature is given by the solution of the convection-diffusion equation. The phase boundary was not maintained as a sharp front but was spread into a transition zone by using rapid variations in the heat capacity over a narrow temperature range to model the latent heat effect. With this method, and the implicit time-stepping scheme which was adopted, it was found that quadratic finite elements, were necessary if accurate solutions for temperature were to be produced.

In the present paper the computer code CONDIF [4] developed at J.R.C. Ispra for the transient analysis of convective-conductive heat transfer is modified to allow consideration of phase change problems in the same manner. This code is, however, based on 4-noded linear elements for the representation of temperature and velocity and an explicit method of time integration is used. With this explicit time-stepping method the linear elements are shown to be capable of producing accurate results when their performance is compared against the exact solution to a conduction problem involving a change of phase. Excessive recomputation of the heat capacitance matrix is best avoided with an explicit method and this has been overcome by assuming the liquid and solid specific heats to be separately constant. Then in any time step, only the heat capacitance matrix for those elements currently undergoing a change of phase has to be recalculated and the resulting efficiency of the scheme is very good.

Results are presented for the problem of freezing in a cavity when the temperature of one of the walls is suddenly reduced and the effect of convection on the freezing process is illustrated.

2. Governing Equations

The equations governing natural convection in two dimensions, where the fluid motion is produced by buoyancy forces, can be written relative to cartesian axes (x,y) as

Momentum

$$\rho \frac{\partial u}{\partial t} = - u \frac{\partial u}{\partial x} - v \frac{\partial u}{\partial y} + \frac{\partial}{\partial x}\left|-p + 2\mu \frac{\partial u}{\partial x}\right| + \frac{\partial}{\partial y}\left|\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right| \qquad (1)$$

$$\rho \frac{\partial v}{\partial t} = - u \frac{\partial v}{\partial x} - v \frac{\partial v}{\partial y} + \frac{\partial}{\partial x}\left|\mu\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right)\right| + \frac{\partial}{\partial y}\left|-p + 2\mu \frac{\partial v}{\partial y}\right| + \rho g \beta \, (T - T_{ref}) \qquad (2)$$

Continuity

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \qquad (3)$$

Energy

$$\rho c \frac{\partial T}{\partial t} = - \rho c u \frac{\partial T}{\partial x} - \rho c v \frac{\partial T}{\partial y} + \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(k \frac{\partial T}{\partial y}\right) \quad (4)$$

Here ρ denotes the density, u and v the fluid velocities in the x and y directions respectively, p the pressure, μ the viscosity, g the acceleration due to gravity, β the coefficient of volume expansion, T the temperature, k the thermal conductivity, c the specific heat and T_{ref} is a reference temperature at which the buoyancy forces are zero. On the boundary curve Γ of the region Ω of interest these equations are subject to the no-slip condition u=v=0 and to conditions of specified temperature or heat flux.

When a change of phase from liquid to solid occurs it is assumed that associated changes in density may be neglected. At the same time the velocity is reduced to zero and the temperature distribution through the solid phase is then governed by equation (4) with u=v=0. To account for the associated latent heat effect a form of the standard enthalpy method [5] is adopted in which it is assumed that the phase change occurs over an interval

$$\Delta T = T_\ell - T_s \quad (5)$$

where T_ℓ is a liquidus and T_s is a solidus. Over this interval the specific heat is evaluated as

$$c_\Delta = c + L/\Delta T \quad (6)$$

where L is the latent heat. Integration of equation (6) then shows that the change in enthalpy H in moving from T_s to T_ℓ is, as required,

$$\Delta H = \int_{T_s}^{T_\ell} c \, dT + L \quad (7)$$

Of course, for pure materials, this representation of the latent heat effect accompanying a change of phase can only be an approximation to the true behaviour where the phase change occurs at a fixed temperature. Other materials exhibit a true solidus and liquidus and in this case the use of equation (6) will be more accurate.

3. Finite Element Formulation

The governing partial differential equations (1) - (4) are solved by the finite element method using the computer code CONDIF which was written by Donea and Giuliani [4] at J.R.C., Ispra. In this code the solution is achieved by means of the fractional step method which was originally introduced in the context of the finite difference method by Chorin [6]. The code has been well documented [7] and consequently only a brief description of the method is required here.

Using the standard weighted residual method [8] with equations (1) - (4) produces the set of matrix equations

$$\underline{M} \frac{d\underline{u}}{dt} = - (\underline{A} + \underline{K}) \underline{u} + \underline{C} \underline{p} + \underline{f} \quad (8)$$

$$\underline{C}^T \underline{u} = \underline{0} \quad (9)$$

$$\underline{M}_T \frac{d\underline{T}}{dt} = - (\underline{A}_T + \underline{K}_T) \underline{T} + \underline{g} \quad (10)$$

where $\underline{M}$ is the mass matrix, $\underline{C}$ the pressure matrix, $\underline{M}_T$ the capacitance matrix, $\underline{A}$ and $\underline{K}$ are the matrices arising from the convection and diffusion terms in the momentum equations, $\underline{A}_T$ and $\underline{K}_T$ arise from the convection and diffusion terms in the energy equation and $\underline{f}$ and $\underline{g}$ are produced by the buoyancy forces and the temperature boundary conditions. Four noded linear elements are used for velocity and temperature interpolation and a discontinuous pressure interpolation is adopted.

The method of solution of this set of equations is an explicit fractional step method in which, in each step, an auxiliary velocity field is first computed and which accounts for all contributions to equation (8) except those arising from the pressure. The step is completed by adding, to these auxiliary velocities, pressure contributions which are computed so as to satisfy equation (9). The final stage is explicit calculation of the temperature field. Lumped mass and capacitance matrices are used throughout. A detailed flow chart for this process has been given in [7].

4. Implementation of the Phase Change Algorithm

With a temperature dependent specific heat, the capacitance matrix $\underline{M}_T$ should be recalculated at each time step. The need for such excessive computation can be removed by making the assumption that the specific heat in the liquid and in the solid are separately constant and defining the specific heat in the phase-change region by equation (6). Then only the element capacitance matrices for those elements currently undergoing a change of phase need be recalculated and the efficiency of the resulting scheme is very good.

As in Gartling's method [3] , no attempt is made to change with time the region over which the hydrodynamic equations are solved. The whole region is analysed at each time step with the velocity reduced to zero at points in the solid phase. Gartling was able to accomplish this reduction in velocity by the use of a large viscosity in the solid phase but this method did not appear to work in the explicit context. The method adopted here, therefore, is to sweep the field of mesh points at the end of each time step and to apply, over the next time step, the condition of zero nodal velocity if the nodal temperature is less than the liquidus value T_ℓ.

5. Applications

In order to ensure that the thermal model described above is capable of accurately representing the phase change process it was firstly used to analyse a problem of pure conduction with phase change in one dimension. The problem chosen has been the study of much attention in the literature [3,9] and an exact analytical solution is available [10]. In this problem the semi-infinite region $x > 0$ is initially in a liquid state at zero temperature and the temperature at $x = 0$ is reduced to -45 instantaneously at time $t=0$. For the analytical solution the phase change is assumed to occur when the temperature reaches -0.15. The finite element simulation of this problem is shown in Figure 1 in which the region $0 \leq x \leq 4$ is covered by an equally spaced mesh of 128 4-noded linear elements. The material is taken to have thermal properties defined by

$$\rho = 1.0 \qquad k = 1.08$$
$$c = 1.0 \qquad L = 70.26 \tag{11}$$

and the calculations were performed with a time step of 1.66×10^{-4}, which ensured stability of the explicit scheme. With the phase change interval $\Delta T = 0.5$ accurate results were

produced when the surface temperature was instantaneously reduced and the accuracy improved when this temperature reduction was carried out over 100 time steps (i.e. to time 0.0166) as illustrated by Figures 2 and 3. The variation of temperature with distance at two distinct times is shown in Figure 2 while Figure 3 depicts the curve giving the time of arrival of the freezing front against distance. In the numerical model the freezing front is assumed to have reached a certain point when the temperature at that point reaches the value 0.5 ($T_s + T_\ell$). Also shown on Figure 3 are the results obtained by Gartling [3] using an implicit finite element model for the cases $\Delta T = 0.5$ and $\Delta T = 2.0$. Gartling found it necessary to use quadratic elements for accurate modelling of this problem with the larger time step allowed by his method but here it can be seen that high accuracy can be obtained by the use of linear elements in conjunction with an explicit scheme.

To illustrate the use of the model for natural convection problems involving phase change, an analysis was performed on the plane thermal cavity defined by $0 \leq x,y \leq 1$ and shown in Figure 4. Initially the cavity is filled with fluid at unit temperature and the temperature along the side $x = 0$ is instantaneously reduced to zero at time $t = 0$. The sides $y = 0$ and $y = 1$ are non-conducting while the side $x = 1$ is held at unit temperature. The initial velocity is zero and the condition of zero velocity is applied along the walls of the cavity. The material thermal properties are taken to be defined by

$$\rho = 1.0 \qquad k = 1.0 \times 10^{-3} \qquad c = 1.0$$
$$\beta = 3.0 \times 10^{-3} \qquad \mu = 1.0 \times 10^{-3} \tag{12}$$

and an equally spaced mesh of 10x10 linear elements is used. The value of the acceleration due to gravity, g, is adjusted to give a Rayleigh number of 6×10^3 as previous experience [7] had indicated that, at such a Rayleigh number, the coarse mesh used here should be capable of providing a good description of the flow. An initial calculation was performed without phase change and it was found that a steady state was reached after time 400. The distribution of the temperature and stream function at steady state in this case is shown in Figure 5. The effect of allowing a liquid/solid phase change to occur was then investigated by assuming that the solidus and liquidus temperatures were defined by

$$T_s = -.65 \qquad T_\ell = -0.6 \tag{13}$$

With the phase change assumed to occur with $L = 0$ a steady state is now attained at time 584. The distributions of temperature and stream function at this time are shown in Figure 6 and it can be seen that, in comparison with Figure 5, the effects of convection are reduced but the solution differs markedly from the pure conduction solution of a plane expansion of the freezing front. When this calculation was repeated with $L = 5$ the steady state is reached at time 1076 and the corresponding distributions of temperature and stream function are shown in Figure 7.

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References

[1] SPARROW,E.M., SCHMIDT,R.R., RAMSEY,J.W., "Experiments on the role of natural convection in the melting of solids", J. Ht. Trans. 100, pp. 11-16 (1978).

[2] SPARROW,E.M., RAMSEY,J.W., KEMINK,R.G., "Freezing controlled by natural convection", J. Ht. Trans. 101, pp. 578-584 (1979).

[3] GARTLING,D.K., "Finite element analysis of convective heat transfer problems with change of phase", Computer Methods in Fluids, Pentech Press, pp. 257-284 (1980).

[4] DONEA,J., GIULIANI,S., "The computer code CONDIF for transient convective-conductive heat transfer, Part 1: Finite element modelling", EUR 6822/I EN, J.R.C. Ispra (1980).

[5] CRANK,J., "How to deal with moving boundaries in thermal problems", Numerical Methods in Heat Transfer, John Wiley (1981).

[6] CHORIN,A.J., "Numerical solution of the Navier-Stokes equations", Math. Comp. 22, pp. 745-762 (1968).

[7] DONEA,J., GIULIANI,S., LAVAL,H., "Accurate explicit finite element schemes for convective-conductive heat transfer problems", Finite element methods for convection dominated flows, A.S.M.E. AMD-Vol.34 (1979).

[8] ZIENKIEWICZ,O.C. "The finite element method" McGraw-Hill (1977).

[9] MORGAN,K., LEWIS,R.W., ZIENKIEWICZ,O.C., "An improved algorithm for heat conduction problems with phase change", Int. J. Num. Meth. Engng. 13, pp. 1191-1195.

[10] CARSLAW,H.S., JAEGER,J.C., "Conduction of heat in solids", Oxford Univ. Press (1959).

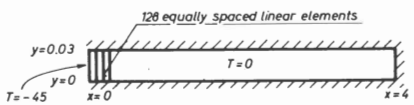

FIGURE 1

Analysis of a pure conduction problem involving a change of phase.

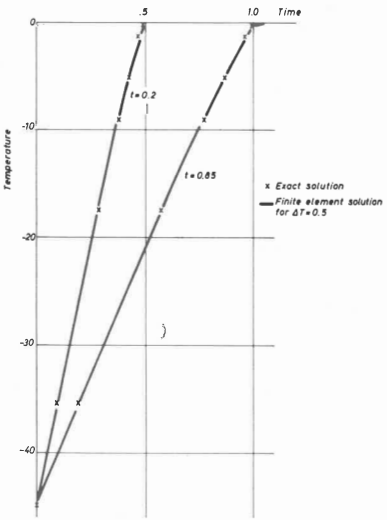

FIGURE 2

Variation of temperature with time in the pure conduction problem.

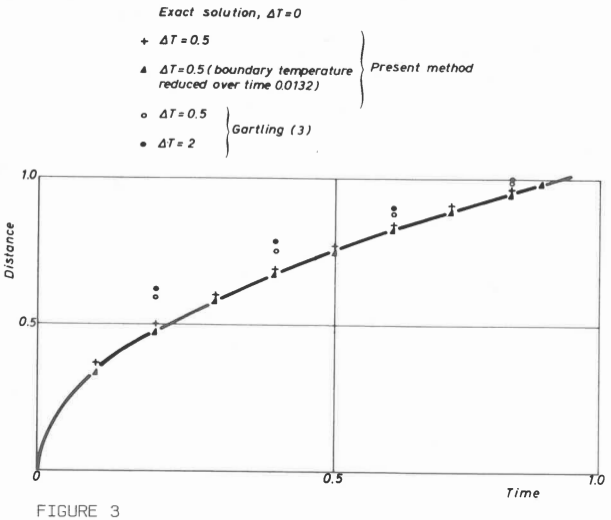

FIGURE 3

Time of arrival of the freezing front in the pure conduction problem.

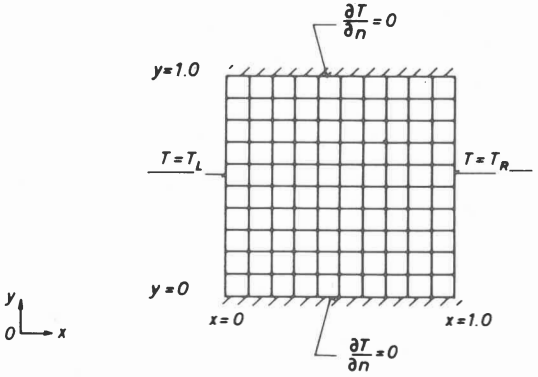

FIGURE 4

Analysis of freezing in a thermal cavity.

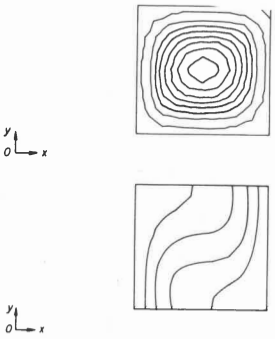

FIGURE 5

Steady state distribution of stream function and temperature when no freezing occurs.

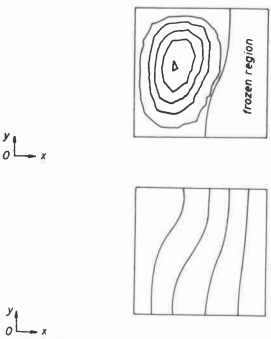

FIGURE 6

Steady state distribution of stream function and temperature when freezing occurs with L = 0.

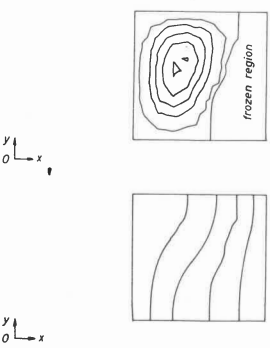

FIGURE 7

Steady state distribution of stream function and temperature when freezing occurs with L = 5.