An enthalpy-based algorithm for the analysis of phase change in nonhomogeneous media
O. Saro, C. Nonino, G. Comini
Dipartimento di Energetica e Macchine, Università di Udine, via delle Scienze 208, 33100 Udine, Italy

Abstract

An enthalpy based finite element procedure for the solution of phase change problems in nonhomogeneous media is described with reference to two-dimensional plane and axisymmetric geometries. The Euler explicit time integration scheme, the lumping of the capacity matrix and the use of the Kirchoff transformation in the conduction term of the governing equation represent the main features of the proposed procedure.

1 Introduction

Over the past twenty years, much interest has been directed towards the numerical modeling of phase change, with special emphasis on the solidification processes involved in metal casting. According to the apparent heat capacity method, the latent heat effect is simulated by means of an equivalent heat capacity defined over a small temperature range. However, when isothermal or nearly isothermal phase change is considered, much care has to be taken to account for the heat capacity peak [1,2]. Alternatively, enthalpy can be used as an integral part of the solution methodology [1-3]. This formulation is most conveniently implemented using explicit time integration schemes and lumped capacity matrices to deal, in a simple and natural manner, with nonhomogeneous media [4]. Apparently, enthalpy formulations for domains including more than one material are of great interest also in the context of control-volume unstructured-mesh methods where they have been recently applied, with success, to the analysis of solidification processes [5].

In this paper a further improvement of the enthalpy based algorithm presented by the authors in Reference 4 is proposed. In the new procedure,
the Kirchoff transformation is used in the conduction term of the governing equation to allow the solution of phase change problems by means of linearized equations, since all nonlinearities are included in the unknown variables. In fact, temperature dependent heat capacities and temperature dependent thermal conductivities do not appear anymore in the definition of the coefficients of the system matrices, which, thus, are constant and need to be calculated only once, at the beginning of each simulation. The proposed procedure is first validated by comparison of computed results with available analytical solutions; then its applicability to a practical casting problem is demonstrated.

2 Statement of the problem and solution method

With reference to a two-dimensional plane or axisymmetric domain \( \Omega \), the nonlinear heat conduction equation governing a phase change problem with no internal heat generation can be written in the form [2,4]

\[
x^\alpha \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( x^\alpha k \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( x^\alpha k \frac{\partial T}{\partial y} \right)
\]

(1)

where \( H \) is the enthalpy per unit volume, \( t \) is the time, \( T \) is the temperature, and \( k \) is the thermal conductivity. In plane problems, \( x \) and \( y \) are the Cartesian coordinates, and the exponent \( \alpha \) is equal to zero. In axisymmetric problems, \( x \) and \( y \) coincide with the radial and axial coordinates, respectively, while the exponent \( \alpha \) is equal to unity.

Appropriate boundary conditions for eqn (1) are represented by the Dirichlet

\[
T = T_p
\]

(2)

and the Neumann and Robin boundary conditions

\[
x^\alpha k \left( \frac{\partial T}{\partial x} \ell_x + \frac{\partial T}{\partial y} \ell_y \right) + x^\alpha q'' + x^\alpha h(T - T_a) = 0
\]

(3)

which are applied to parts of the boundary \( \Gamma_1 \) and \( \Gamma_2 \), respectively. In eqns (2) and (3), \( T_p \) is the prescribed temperature, while \( \ell_x \) and \( \ell_y \) are the direction cosines of the outward normal to the boundary, \( q'' \) is the prescribed specific heat flow rate, \( h \) is the convection coefficient, and \( T_a \) is the temperature of the surrounding environment. Parts of the boundaries on which no boundary conditions are specified (\( q'' = h = 0 \)) are assumed adiabatic.
A change of variables can be performed on the right-hand-side of eqn (1) by introducing the thermal conductivity integral $K$ obtained by means of the Kirchoff transformation [6]

$$K = \int_{T_0}^{T} k(T) \, dT$$

(5)

Therefore, eqns (1) and (3) can be rewritten as

$$x^\alpha \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( x^\alpha \frac{\partial K}{\partial x} \right) + \frac{\partial}{\partial y} \left( x^\alpha \frac{\partial K}{\partial y} \right)$$

$$x^\alpha \left( \frac{\partial K}{\partial x} \ell_x + \frac{\partial K}{\partial y} \ell_y \right) + x^\alpha q_p'' + x^\alpha h(T - T_a) = 0$$

(7)

which, as will be seen later, allows one to obtain discretized equations where all the nonlinearities are removed from the coefficients of the resulting matrices. In fact, according to a standard procedure, after discretizing the integration domain by means of a finite element mesh, functions $H(x, y, t)$ and $K(x, y, t)$ can be approximated as

$$H \approx \sum_{i=1}^{n} N_i(x, y) \, H_i(t)$$

(8)

$$K \approx \sum_{i=1}^{n} N_i(x, y) \, K_i(t)$$

(9)

where $N_i(x, y)$ are the shape functions, $H_i$ and $K_i$ are the nodal values of enthalpy and of the Kirchoff integral, and $n$ is the number of nodes of the discretization. By applying the Galerkin method to eqn (6) and then Green’s formula to the diffusion term a system of $n$ ordinary differential equations can be obtained. In matrix form this system can be written as

$$\mathbf{C} \, \dot{\mathbf{h}} + \mathbf{S} \, \mathbf{k} + \mathbf{f} = 0$$

(10)

where $\mathbf{h}$ and $\mathbf{k}$ are vectors containing the nodal values of enthalpy and of the Kirchoff integral, $\mathbf{C}$ is the capacity matrix, $\mathbf{S}$ is the diffusion matrix, and $\mathbf{f}$ is the vector originating from the application of boundary conditions (7). The system of ordinary differential equations (10) can be integrated in time using the Euler explicit algorithm. In such a case, it is common practice to approximate the capacity matrix $\mathbf{C}$ with the diagonal matrix $\overline{\mathbf{C}}$, obtained by “lumping” the coefficients of the original matrix. The time discretized system of equations can thus be written as

$$\overline{\mathbf{C}} \frac{h_{i+\Delta t} - h_i}{\Delta t} + \mathbf{S} \, \mathbf{k}_i + \mathbf{f} = 0$$

(11)
where the subscripts indicate the appropriate time levels. Typical matrix elements and vector components are

\[ \bar{C}_{ij} = \sum \int_{\Omega_e} x^\alpha N_i \delta_{ij} \, d\Omega \]  
(12)

\[ S_{ij} = \sum \int_{\Omega_e} x^\alpha \left( \frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} \right) \, d\Omega \]  
(13)

\[ f_i = \sum \int_{\Gamma^e_2} x^\alpha N_i \left[ q'_p + h (T - T_a) \right] \, d\Gamma \]  
(14)

where summations are made over all the elements, \( \delta_{ij} \) is the Kronecker delta, and \( T \) is evaluated at time \( t \). The symbol \( \Omega_e \) identifies the part of the domain which coincides with the element \( e \), while \( \Gamma^e_2 \) indicates the parts of the element boundaries coincident with the external boundary \( \Gamma_2 \).

Many authors agree that lumping the capacity matrix, that is, considering the capacity concentrated in the nodes instead of being distributed over the elements, can lead to good results in the solution of heat conduction problems [1,7], especially when liquid-solid phase change is involved [8]. It is also well known that, since \( \bar{C} \) is a diagonal matrix, its inversion is trivial, and, consequently, the solution of system (11) at each time step is very fast. Moreover, it is worth noting that because of the choice of enthalpy as the primary variable and the application of the Kirchoff transformation to the conduction term of the governing equation, all nonlinearities have been removed from the coefficients of both matrices \( \bar{C} \) and \( S \). Since they do not depend on the thermophysical properties, they are calculated only once, at the beginning of the simulation, and this makes the solution procedure very efficient. In this paper reference is made to four-node bilinear elements only, and, as it appears from eqn (12), the usual row summing technique is used to evaluate the coefficients of the lumped capacity matrix.

Lumping the capacity matrix also represents a key feature of the proposed method for another reason: it allows to overcome a difficulty arising when using an enthalpy method for the solution of a problem involving non-homogeneous media. In fact, for any given temperature, enthalpy has, in general, different values for different materials and, thus, is undefined at the nodes located along the interfaces between two or more materials. However, if the capacity, represented in this case by a volume, is assumed to be concentrated at the nodes, it is reasonable to compute the enthalpy content of an interface node as the sum of the enthalpy contents of the volumes of each material associated with that node. Therefore, at a given temperature, the
enthalpy per unit volume of the \( i \)-th interface node including \( m \) materials is

\[
H_i = \frac{1}{V_i} \sum_{k=1}^{m} H_i^{(k)} V_i^{(k)}
\]  

(15)

where \( V_i = \overline{C}_{ii} \) is the total volume associated with the node \( i \), while \( V_i^{(k)} \) is the volume of the \( k \)-th material associated with that node and \( H_i^{(k)} \) is its enthalpy per unit volume at the nodal temperature. Also the variable \( K \) is not defined at nodes on the interface between two or more materials, but this is not a problem since the matrix product \( S \kappa \) appearing in eqn (11) can be evaluated at element level, using the appropriate nodal values of \( K \), that is, those referring to the material in the element and corresponding to the nodal temperatures. Then, all element contributions are assembled.

To apply the procedure described above, the functions \( H^{(k)} = H^{(k)}(T) \) and \( K^{(k)} = K^{(k)}(T) \) must be available for each material, possibly in table form. From these data, the table of the function \( H^{(k)} = H^{(k)}(K^{(k)}) \) can be obtained without difficulty. If the volume pertaining to a node is occupied by only one material, the above relations can be directly used to calculate the nodal values of \( K \) or of the temperature \( T \) from the nodal values of enthalpy and vice versa. If two or more materials are present in the volume pertaining to a node, it is necessary to repeatedly apply eqn (15) to generate at least part of the temperature-enthalpy table for that node, and calculate the temperature corresponding to the nodal value of \( H \). With the nodal temperatures thus obtained it is then possible to evaluate the contributions to the matrix product \( S \kappa \) element by element, as explained above. It must be pointed out that since, in general, only a small number of nodes lies on the interface between different materials, the increment in computer time due to the multiple table construction required by the method is limited.

### 3 Numerical tests

The procedure has been validated by comparing the computed results with analytical and literature data. The first test problem considered demonstrates the applicability of eqn (15) to the evaluation of the nodal values of enthalpy in nonhomogeneous material. It concerns transient linear heat conduction in a two layered plane wall. No phase change is involved, but an analytical solution is available [9]. The two layers have the same thickness \((0.1 \, \text{m})\), thermal conductivities \(k_1 = 1 \, \text{W/(m K)}\) and \(k_2 = 2 \, \text{W/(m K)}\), and heat capacities \(c_1 = 2 \times 10^6 \, \text{J/(m}^3\text{K)}\) and \(c_2 = 1 \times 10^6 \, \text{J/(m}^3\text{K)}\), respectively. The initial temperature is equal to \(0^\circ\text{C}\), while for \( t > 0 \) the temperatures of the two surfaces of the wall are kept at \(T_1 = 0^\circ\text{C}\) and \(T_2 = 1^\circ\text{C}\). The one-dimensional domain is discretized using 20 equal size elements, while the time step is equal to 10 s. Computed and analytical
results are satisfactorily compared in Figure 1, which proves the reliability of the method.

The second test problem concerns the solidification of a superalloy in a ceramic mould. This problem is one of those proposed by Chandra [10] as benchmarks to test the reliability of computer procedures in the simulation of solidification in commercial investment casting. A liquid superalloy at the initial temperature of 1805 K is poured into a cylindrical ceramic mould having a temperature of 1383 K. The thermal properties of both the superalloy and the ceramic are reported in Table 1. The internal and external diameters of the mould are 12.7 mm and 22.9 mm, respectively, while the height is 127 mm. The surrounding air temperature is 300 K, and the convection coefficient on the outer surface of the mould is assumed equal to 125 W/(m²K). The top of the mould can be considered insulated, while its base is kept at a constant temperature of 300 K by a chill. The finite element mesh is reported in Figure 2(a) and consists of 135 bilinear elements and 160 nodes (mesh A). In Figure 2(b), instead, the temperature-time history for a node located on the axis, at a distance of 25.4 mm from the base of the mould (dashed line), is compared with the corresponding data obtained numerically by Chandra [10]. The time step is 0.1 s. In the same figure the curve obtained using a finer mesh (mesh B: 228 elements and 260 nodes) and a time step of 0.02 s is also reported (solid line). Again, the excellent agreement obtained with both meshes proves the reliability of the proposed procedure.
Table 1. Thermophysical properties of the superalloy (subscript \( s \)) and of the ceramic of the mould (subscript \( c \)) [10].

<table>
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<tr>
<th>( T ) [K]</th>
<th>( \varrho_s c_s ) [MJ/(m(^3)K)]</th>
<th>( k_s ) [W/(m K)]</th>
<th>( \varrho_c c_c ) [MJ/(m(^3)K)]</th>
<th>( k_c ) [W/(m K)]</th>
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<td>48.47</td>
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Figure 2: Solidification of a superalloy in a cylindrical mould: (a) finite element mesh A; (b) temperature-time history at a node on the axis at 25.4 mm from the base (— — — proposed method with mesh A; — — — proposed method with mesh B; o data from Reference 10).
4 Conclusions

An enthalpy based finite element method has been described for the solution of two-dimensional plane or axisymmetric phase change problems involving nonhomogeneous media. The lumping of the capacity matrix, the use of the Kirchoff transformation in the conduction term of the governing equation and the Euler explicit time integration scheme are the key features of the method. The algorithm, which has proved to be very efficient in terms of memory and computer time requirements, has been validated by comparing computed results with available analytical and numerical literature data.

References