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A GENERALIZED VARIATIONAL FORMULATION FOR CONVECTIVE HEAT TRANSFER

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SUMMARY

The scope of this paper is to develop the basic equations for a variational formulation which can be used to solve problems related to convection and/or diffusion dominated flows. The formulation is based on the introduction of a generalized quantity defined as the heat displacement. The governing equation is expressed in terms of this quantity and a variational formulation is developed which leads to a system of equations similar in form to Lagrange's equations of mechanics. These equations can be used for obtaining approximate solutions, though they are of particular interest for application of the finite element method.

As an example of the formulation two finite element models are derived for solving convection–diffusion boundary value problems. The performance of the two models is investigated and numerical results are given for different cases of convection and diffusion with two types of boundary conditions. The applications of the developed formulations are not limited to convection–diffusion problems but can also be applied to other types of problems such as mass transfer, hydrodynamics and wave propagation.

KEY WORDS Diffusion Convection Heat Transfer

INTRODUCTION

Analytical and numerical solutions of the energy equation have attracted considerable attention in a variety of engineering fields due to the wide applicability of this equation. The theory for convection or diffusion dominated flows has been well-established and a variety of classical approaches exist in the literature for the solution of problems involving convective heat transfer. One such solution is given by Price *et al.*[1] Analytical solutions are valid primarily for linear equations in one dimension and their application to problems of practical interest presents difficulties due to the limitations of such solutions. It is because of the restrictive nature of the analytical solutions that research efforts have been focused on approximate or numerical solutions of the convection–diffusion equation.

A review and comparison of available numerical methods can be found in References 2, 3 and 4. Numerical methods discussed in these papers include both finite differences and finite element approximations. Finite difference schemes are the least attractive ones due to their instability and to the presence of numerical diffusion. It has been shown, by a Fourier series solution to the convection–diffusion equation,[5] that many finite difference schemes fail to propagate sharp wave fronts at the true flow velocity and due to their inherent artificial diffusion a damping of the high frequency harmonics occurs. On the other hand finite element schemes have produced more reliable numerical solutions but some of them share the same oscillatory and diffusive characteristics with finite difference methods. Another disadvantage of some finite element schemes is that they are derived through formulations

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restricted by the conditions of a particular problem. As a result such schemes are limited in application. Some of the papers found in the literature formulate finite element solutions based on a variational functional.[6] This approach is found to be of limited application since the functional is problem-dependent. A variational approach (Rayleigh–Ritz) was also considered by Smith *et al.*[7] to generate finite element solutions of the convection–diffusion equation. In the same paper the authors also considered solutions based on the Galerkin method. The latter approach is found to have wider applicability to practical problems whether advection or diffusion is dominant in the physical problem to be modelled.

In view of the limitations of certain schemes and the lack of uniformity of existing approaches, it is desirable to develop a unified formulation, based on physical consideration, which can be used to derive different approximate solutions. Such generalized formulations should be derived from the governing equations describing the physical phenomena and they should be independent of the conditions of a particular problem. In order to achieve this, certain concepts from classical mechanics can be used to derive a variational formulation for the convection–diffusion equation. Such a formulation is not restricted to this particular equation but it can be applied to other equations governing physical processes as well.

In the first part of this paper, the basic definitions are introduced and the convection–diffusion equation is expressed in terms of a generalized quantity, defined as heat displacement,[8,9] which is similar to a mechanical displacement. With this definition, changes in temperature are treated as thermal deformations which are similar to mechanical strains. A variational formulation is then derived, based on the principle of virtual work in mechanics, and by using generalized co-ordinates the variational equation is written in a form equivalent to that of the Lagrange's equations in mechanics. The generalized form of the derived variational equation is applicable to a wide variety of physical problems and it is the appropriate equation for obtaining approximate solutions to heat transfer problems.

In order to demonstrate the applicability of the variational formulations in obtaining numerical solutions, the finite element method is used, as an example, in the second part of this paper to derive two finite element models for solving initial or boundary value problems. The first model is based on a linear approximation of the displacement and the second on a third-order approximation. The matrix equation for the linear model is expressed in terms of nodal displacements and for the higher order model in terms of nodal displacements and nodal temperatures. The matrix coefficients of both models are the same as the ones derived by the conventional finite element method (Galerkin) but in the present formulation the unknown field is the displacement in contrast to temperature of the conventional method. One advantage of such presentation is that discontinuities in the temperature field can be resolved more accurately. In addition the resulting boundary forces of the present formulations contribute to the better accuracy of the approximate solutions.

Numerical results are given in the third part of this paper where a third-order, backward finite difference scheme is employed for the solution of the system of ordinary differential equations with two types of boundary conditions.[10] The present results are compared to existing analytical solutions and the accuracies and convergence of the two finite models are discussed.

BASIC EQUATIONS

Consider an incompressible medium in a flow field subjected to external heating. Initially the medium is at a uniform temperature T_0, which will be referred to as the reference temperature, and the state at this temperature will be referred to as the reference state.

The instantaneous absolute temperature is denoted by T, and the difference $T - T_0$ defines the instantaneous relative temperature $\Delta\theta$, which is a function of the space co-ordinates and time. Let

$$\theta = \frac{T - T_0}{T_0} = \frac{\Delta\theta}{T_0} \tag{1}$$

be defined as the temperature change per unit temperature T_0, or the instantaneous relative temperature per unit temperature. In the following it will be referred to as the temperature θ or the dimensionless temperature.

Assuming a co-ordinate system (x_i, $i = 1, 2, 3$) the temperature field θ satisfies the equation

$$\frac{\partial\theta(x_k, t)}{\partial t} + \frac{\partial}{\partial x_i}(V_i\theta(x_k, t)) = \frac{\partial}{\partial x_i}\left(k_{ij}\frac{\partial\theta(x_k, t)}{\partial x_j}\right) \tag{2}$$

where V_i is the velocity vector and k_{ij} is the thermal diffusivity with the property

$$k_{ij} = k_{ji}$$

so that k_{ij} is a symmetric tensor with six independent components.

We now define a vector field $H_i(x_j, t)$ as the heat displacement vector such that

$$\theta = \frac{\partial H_i(x_j, t)}{\partial x_i} = H_{i,i}(x_j, t) \tag{3}$$

The summation convention is assumed for repeated indices throughout this paper. Furthermore, the time derivative of the heat displacement vector is defined by

$$\dot{H}_i = \frac{\partial H_i}{\partial t}$$

where H_i are the components of the displacement vector and they are interpreted as being proportional to the local rate of heat flow per unit area.

In the above definition, equation (3), θ represents a thermal strain analogous to mechanical strain and $H_i(x_j t)$, with dimension of a displacement, is similar to a mechanical displacement. Thus there is a one-to-one correspondence between heat displacement–mechanical displacement and temperature–strain. Hence equation (3) can be considered as an holonomic constraint in the sense of classical mechanics and must be verified by the physical solution. Using the definition from equation (3), equation (2) is written as follows

$$\frac{\partial H_i}{\partial t} + V_i\theta - k_{ij}\frac{\partial\theta}{\partial x_j} = 0 \tag{4}$$

or

$$\lambda_{ij}\frac{\partial H_i}{\partial t} + \lambda_{ij}V_i\frac{\partial H_k}{\partial x_k} - \frac{\partial\theta}{\partial x_j} = 0 \tag{5}$$

The components of the tensor λ_{ij} in the last equation are defined as the elements of the inverse of the matrix $[k_{ij}]$ and λ_{ij} is also a symmetric tensor. Equations (4) and (5) are valid either for isotropic or anisotropic thermal diffusivity.

In the above analysis the thermal flow field is governed by the two equations (3) and (4) which, together with the appropriate boundary conditions, provide a complete formulation for convective heat transfer. They are analogous to the kinematic relations and the momentum equations in mechanics. By eliminating H_i between equations (3) and (4) one obtains equation (2) which describes conservation of energy and heat transfer. In many cases it is preferable to use the two separate equations, (3) and (4). One example is the case of thermo-mechanical coupling where the use of equations (3) and (4) provides a unified derivation of the governing equations.[9]

The advantages of introducing the heat displacement vector are more apparent when the concept of virtual work is introduced to derive the fundamental form of the variational formulation.

VARIATIONAL FORMULATION

Following the usual procedures of the principle of virtual work in mechanics, consider that the medium is subjected to an arbitrary virtual displacement δH_i from the equilibrium configuration. The corresponding variations $\delta\theta$ are given by

$$\delta\theta = \frac{\partial}{\partial x_i}(\delta H_i)$$

and equation (3) is verified by the variations δH_i and $\delta\theta$. Multiplication of equation (5) by δH_j and integration over the volume v of the medium yields

$$\int_v \left[\lambda_{ij}\frac{\partial H_i}{\partial t} + \lambda_{ij}V_i\frac{\partial H_k}{\partial x_k} - \frac{\partial\theta}{\partial x_j}\right]\delta H_j \, dv = 0$$

Integrating by parts and applying the divergence theorem, one obtains

$$\int_v \lambda_{ij}\frac{\partial H_i}{\partial t}\delta H_j \, dv + \int_v \lambda_{ij}V_i\theta\delta H_j \, dv + \int_v \theta\frac{\partial}{\partial x_j}(\delta H_j)\, dv = \int_S \theta\delta H_j\eta_j \, dS \tag{6}$$

where η_j is the unit normal vector pointing outward at the boundary surface S. From equation (3) one derives

$$\int_v \frac{\partial}{\partial x_j}(\delta H_i)\, dv = \int \theta\delta\theta \, dv = \delta E \tag{7}$$

The scalar E is defined as

$$E = \frac{1}{2}\int_v \theta^2 \, dv \tag{8}$$

and plays the role of a potential function. Equation (6) is now written as follows

$$\delta E + \int_v \lambda_{ij}\frac{\partial H_i}{\partial t}\delta H_j \, dv + \int_v \lambda_{ij}V_i\theta\delta H_j \, dv = \int_S \theta\delta H_j\eta_j \, dS \tag{9}$$

Equation (9) is considered as a variational principle in a broad sense and it represents a fundamental form in contrast to a complementary form. These two forms of variational principles are found in classical mechanics where in a fundamental form the variational principle is expressed in terms of displacements and in a complementary form is expressed in terms of forces (stresses). A significant advantage of the fundamental form of the variational principle, equation (9), is the absence of any space derivative of the temperature in its formulation. As a result better accuracy is obtained in the application of approximate solutions, especially when discontinuities may be introduced in the temperature field.

The variational equation, equation (9), can be translated to a Lagrangian type of equation by introducing generalized co-ordinates defined as

$$H_i(x_j, t) = H_i(q_n, x_j, t) \tag{10}$$

where the generalized co-ordinates q_n are functions of time. The advantage of using generalized co-ordinates is that H_i may be expresed in different functional forms. Furthermore, it is always possible to choose the generalized co-ordinates in such a way that from the physical standpoint the system is completely described by these co-ordinates. Care should be taken when the time derivative of H_i is considered, and it should be expressed as

$$\dot{H}_i = \frac{\partial H_i}{\partial q_j}\dot{q}_j + \frac{\partial H_i}{\partial t} \tag{11}$$

In terms of arbitrary variations δq_j of the generalized co-ordinates, the corresponding displacement field variations are due entirely to the variation δq_i as follows

$$\delta H_i = \frac{\partial H_i}{\partial q_j}\delta q_i \tag{12}$$

and the variation of the potential E is then given by

$$\delta E = \frac{\partial E}{\partial q_j}\delta q_j \tag{13}$$

In view of equations (12) and (13), equation (9) may be written for each arbitrary variation δq_k as follows

$$\frac{\partial E}{\partial q_k} + \int_v \lambda_{ij}\frac{\partial H_i}{\partial t}\frac{\partial H_j}{\partial q_k}\,dv + \int_v \lambda_{ij}V_i\theta\frac{\partial H_j}{\partial q_k}\,dv = \int_S \theta\frac{\partial H_j}{\partial q_k}\eta_j\,dS \tag{14}$$

From equation (11) one derives

$$\frac{\partial \dot{H}_i}{\partial \dot{q}_k} = \frac{\partial H_i}{\partial q_k}$$

and the second term in equation (14) can be expressed in a simpler form that brings out its physical significance as follows

$$\int_v \lambda_{ij}\frac{\partial H_i}{\partial t}\frac{\partial H_j}{\partial q_k}\,dv = \int_v \lambda_{ij}\frac{\partial H_i}{\partial t}\frac{\partial H_j}{\partial \dot{q}_k}\,dv = \frac{\partial}{\partial \dot{q}_k}\left[\frac{1}{2}\int_v \lambda_{ij}\dot{H}_i\dot{H}_j\,dv\right] \tag{15}$$

In view of the symmetric property of the tensor λ_{ij} the last relation is valid for both isotropic and anisotropic thermal diffusivity. In the latter case λ_{ij} is a function of the x_i-co-ordinates. The volume integral of the right-hand side, in the last equation, has an important physical meaning associated with the concept of dissipation. Combining the result from the last equation with the third term of equation (14), one obtains

$$\frac{\partial}{\partial \dot{q}_k}\left[\frac{1}{2}\int_v \lambda_{ij}(\dot{H}_i + V_i\theta)(\dot{H}_j + V_j\theta)\,dv\right] = \frac{\partial D}{\partial \dot{q}_k} \tag{16}$$

where

$$D = \frac{1}{2}\int_v \lambda_{ij}\dot{H}_i^*\dot{H}_j^*\,dv \tag{17}$$

and

$$\dot{H}_i^* = \dot{H}_i + V_i\theta \tag{18}$$

The vector $\dot{H}_i^*$ represents the total convective and diffusive local rate of heat flow and for the case of a solid medium ($V_i = 0$) it reduces to the vector $\dot{H}_i$ which corresponds to the conductive rate of heat flow. Furthermore, the heat flux vector h_i is proportional to the vector $\dot{H}_i^*$ and from equation (4) one can derive

$$\dot{H}_i^* = k_{ij}\frac{\partial\theta}{\partial x_j} = -h_i \tag{19}$$

Equation (14) takes the form

$$\frac{\partial D}{\partial \dot{q}_k} + \frac{\partial E}{\partial q_k} = Q_k \tag{20}$$

where

$$Q_k = \int_S \theta\eta_j \frac{\partial H_j}{\partial q_k} \mathrm{d}S \tag{21}$$

The quantity Q_k represents generalized thermal forces applied on the boundary S of the medium of volume v. The quantity D represents the total dissipation function and equations (20) have the same form as those of Lagrangian mechanics for the slow motion of a dissipative system with negligible inertia forces. Equations (20) as they were derived are quite general in the sense that they can be applied to different types of media with different material properties and they are independent of a co-ordinate system.

Equation (20) in its derived form is most suitable for obtaining approximate solutions to convective heat transfer problems. The representation of the unknown field H_i by generalized co-ordinates depends on the type of problem to be solved and the accuracy required in the approximate solution. In one particular case one may choose a linear representation in the form of a finite or infinite series. For such a case the representation may be given as a Fourier series or as an expansion in orthogonal functions. As an example of a special case the displacement field is considered to be approximated by a linear combination of the generalized co-ordinates as follows

$$H_i(x_j, t) = q_k(t) f_{ki}(x_j) \qquad k = 1, n, \quad j = 1, 2, 3 \tag{22}$$

In equation (22) the coefficients $q_k(t)$ represent degrees of freedom and the function $f_{ki}(x_j)$ specifies the extent to which $q_k(t)$ participates in the function $H_i(x_j, t)$. This is a restrictive application to the developed formulation but it is often used in approximate solutions. For example, in the finite element analysis equation (22) may be considered as the distribution function of the displacement field, where q_k can then be taken as the nodal displacements or nodal deformations depending on the type of approximation selected.

Differentiating equation (22) with respect to time and space we obtain

$$\begin{aligned} \dot{H}_i &= \dot{q}_k f_{ki} \\ \theta &= \frac{\partial H_i}{\partial x_i} = q_k f_{ki,i} \end{aligned} \tag{23}$$

The scalar E and the invariant D from equations (8) and (17) are expressed in terms of equations (23) as follows

$$E = \tfrac{1}{2}e_{mn}q_m q_n \qquad D = \tfrac{1}{2}d_{mn}\dot{q}_m\dot{q}_n + g_{mn}q_{mn}\dot{q}_n \tag{24}$$

$$e_{mn} = \int_v f_{mi,i}f_{nj,j}\,\mathrm{d}v \qquad d_{mn} = \int_v \lambda_{ij}f_{mi}f_{nj}\,\mathrm{d}v \qquad g_{km} = \int_v \lambda_{ij}V_i f_{kj}f_{mn,n}\,\mathrm{d}v \tag{25}$$

Substituting the specific forms of E and D from equations (24) into equation (20) one obtains

$$d_{ij}\dot{q}_j + (q_{ij} + e_{ij})q_j = Q_i \tag{26}$$

with

$$Q_i = \int_S \theta n_j f_{ij}\,\mathrm{d}S \tag{27}$$

Equations (26) constitute a system of n ordinary differential equations for the unknown field parameters q_k ($k = 1, n$), which may represent the heat displacement field H_i. This system of n equations can be solved together with the appropriate boundary condition by any numerical method. Thus the foregoing analysis is not restricted to applications of the finite element method but is appropriate for applying other numerical schemes as well. Another advantage of the derived equations is that they are not restricted to solving convective heat transfer problems. By appropriate choice of the variables q_k to represent other physical quantities, the derived equations can be used to solve problems involving such quantities as concentration or velocity fields. Furthermore this formulation can be extended to problems governed by equations such as the coupled diffusion momentum equations.[9]

The variational analysis and the Lagrangian equations were derived in a way that is independent not only of the frame of reference but also of any particular representation of the unknowns. In addition the derivations are independent of any particular boundary conditions and the volume and surface integrals are extended to instantaneous geometric configurations. As a result the derived formulation is quite general and can be applied to problems with different configurations, moving boundaries and isotropic or anisotropic properties.

FINITE ELEMENT ANALYSIS

In order to demonstrate the application of the finite element method to the previously derived variational formulation, two one-dimensional element models are chosen to approximate the heat displacement. The first model is a linear element with minimum degrees of freedom (LE) and the second is a higher order element with four degrees of freedom (CE), known as third order cubic Hermitian. Although both elements are one-dimensional approximations, they provide good test cases for the performance of the numerical scheme. An extension into the two-dimensional space is easily obtained since the previously derived equations are of general form. If the heat displacement is approximated by a third-order polynomial

$$H(x, t) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 \tag{28}$$

then the temperature θ is given by

$$\theta(x, t) = a_1 + 2a_2 x + 3a_3 x^2 \tag{29}$$

where a_i are time-dependent coefficients to be determined for each of the element models.

Linear element (LE)

For the linear element of length l the coefficients a_i are given by

$$a_0 = H_1(t), \qquad a_1 = \frac{1}{l}(H_2 - H_1), \qquad a_2 = a_3 = 0 \tag{30}$$

and the generalized co-ordinates are identified as follows

$$q_1 = H_1, \qquad q_2 = H_2$$

where H_1 and H_2 are the nodal values of the heat displacement. Thus the linear dependence of H on the generalized co-ordinates is expressed as

$$H(x, t) = H_i(t) f_i(x)$$

where f_i are the basic functions. Substituting the coefficient equations (28) and (29) yield

$$H(x, t) = \left(1 - \frac{x}{l}\right) H_1(t) + \frac{x}{l} H_2(t) \tag{31}$$

and

$$\theta(x, t) = \frac{1}{l}(H_2(t) - H_1(t)) \tag{32}$$

Note that within each element θ varies only with time for the (LE) approximations.

The matrix coefficients of equation (26) are evaluated in terms of equations (31) and (32) as follows:

$$\begin{aligned} &\text{diffusion matrix } e_{mn}: && e_{mn} = \frac{A}{l}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \\ &\text{mass matrix } d_{mn}: && d_{mn} = \frac{Al}{6k}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \\ &\text{convective matrix } g_{mn}: && g_{mn} = \frac{AV}{2k}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} \end{aligned} \tag{33}$$

and the thermal forces Q_i:

$$Q_i|_{x=0} = Q_1 = -A\theta, \qquad Q_i|_{x=1} = Q_2 = A\theta$$

Where A is the cross-sectional area of the element, k is the diffusivity and V is the fluid velocity.

In terms of equations (33), equation (26) yields

$$\frac{l}{6k}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{Bmatrix} \dot{H}_1 \\ \dot{H}_2 \end{Bmatrix} + \left[\frac{V}{2k}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{1}{l}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\right]\begin{Bmatrix} H_1 \\ H_2 \end{Bmatrix} = \begin{Bmatrix} Q_1 \\ Q_2 \end{Bmatrix} \tag{34}$$

Cubic element (CE)

For the cubic Hermitian element the coefficients a_i are evaluated from the nodal values of $H_3(x, t)$ and their spatial derivatives at the nodes, which are the nodal values of the temperature $\theta(x, t)$ as follows

$$
\begin{aligned}
a_0 &= H_1, \qquad \alpha_1 = \theta_1 \\
a_2 &= -\frac{1}{l^2}[(\theta_2+2\theta_1)l-3(H_2-H_1)] \\
a_3 &= \frac{1}{l^3}[(\theta_2+\theta_1)l-2(H_2-H_1)]
\end{aligned} \tag{35}
$$

where (H_1, H_2) and (θ_1, θ_2) are the nodal values of the heat displacement and temperature respectively, and the expressions for $H(x, t)$ and $\theta(x, t)$ are given by

$$
\begin{aligned}
H(x, t) &= f_{11}q_1+f_{12}q_2+f_{13}q_3+f_{14}q_4 \\
\theta(x, t) &= h_{11}q_1+h_{12}q_2+h_{13}q_3+h_{14}q_4.
\end{aligned} \tag{36}
$$

The shape functions f_{1i} and h_{1i} $(i=1, 2, 3)$ are given by

$$
\begin{aligned}
f_{11} &= 1-\frac{3x^2}{l^2}+\frac{2x^3}{l^3}, \qquad f_{13} = \frac{3x^2}{l^2}-\frac{2x^3}{l^3} \\
f_{12} &= x-\frac{2x^2}{l}+\frac{x^3}{l^3}, \qquad f_{14} = -\frac{x^2}{l}+\frac{x^3}{l^2}
\end{aligned} \tag{37}
$$

and

$$
h_{1i} = f_{1i,x} = \frac{\partial}{\partial x}(f_{1i}), \tag{38}
$$

The generalized co-ordinates q_i are identified as follows

$$
q_1 = H_1, \quad q_2 = \theta_1, \quad q_3 = H_2, \quad q_4 = \theta_2
$$

The corresponding e_{ij}, d_{ij} and g_{ij} are given by

$$
e_{ij} = \frac{A}{30l}\begin{vmatrix} 36 & 3l & -36 & 3l \\ 3l & 4l^2 & -3l & -l^2 \\ -36 & -3l & 36 & -3l \\ 3l & -l^2 & -3l & 4l^2 \end{vmatrix} \tag{39}
$$

$$
d_{ij} = \frac{Alk}{420}\begin{vmatrix} 156 & 22l & 54 & -13l \\ 22l & 4l^2 & 13l & -3l^2 \\ 54 & 13l & 156 & -22l \\ -13l & -3l^2 & -22l & 4l^2 \end{vmatrix} \tag{40}
$$

$$
g_{ij} = \frac{AV}{210}\begin{vmatrix} -210 & 42l & 210 & -42l \\ -42l & 0 & 42l & -7l^2 \\ -210 & -42l & 210 & 42l \\ 42l & 7l^2 & -42l & 0 \end{vmatrix} \tag{41}
$$

In terms of equations (27)–(30), equation (22) yields

$$
[d]\{\dot{q}\}+[[g]+[e]]\{q\} = \{Q\} \tag{42}
$$

The matrix coefficients for both element models, equations (34) and (42), are the same as the ones obtained through the conventional (Galerkin) finite element method, but the unknown nodal quantities of the above equations are different. For the (LE) model the solution will yield nodal displacements instead of nodal temperatures which is important for many problems. For example, in the case that discontinuities exist in the temperature field, as is the case in many practical problems, the displacement model will be more accurate since the displacement field in this case is continuous. For the (CE) model the conventional finite element method will produce nodal temperatures and their nodal derivatives, which is acceptable unless, due to discontinuities in the temperature field the derivatives do not exist. In contrast this is not the case for the displacement (CE) model, which will produce nodal displacements and temperatures. There is a tradeoff in accuracy when the displacement finite element models are used instead of the conventional ones but one should consider the advantage of the displacement model in simulating discontinuous temperature fields.

Although the displacement model has certain advantages over the conventional ones, both are very compatible in accuracy and either one of them can be obtained from the previously derived variational formulation, since this formulation is given in terms of generalized co-ordinates.

For the solution of a particular problem, the finite element models derived above are assembled according to the direct stiffness method to obtain global equations. The formulation of the overall problem is not complete unless boundary conditions are taken into consideration. The system of n equations together with the appropriate boundary and initial conditions can be solved by any numerical technique used for solving ordinary differential equations. In the following section, the system of equations is solved for two types of boundary conditions by using a backward differences in time integration technique.

NUMERICAL SOLUTION

Boundary value problem

The one-dimensional case of convective heat transfer is considered here to evaluate the two finite element models introduced previously. In applying the derived finite element formulation, the semi-infinite space is approximated by the characteristic length L with a time-dependent temperature applied on its boundary. Two different cases of the boundary conditions are considered and results are obtained for both element models.

The governing equation is

$$\frac{\partial \theta}{\partial t}+V\frac{\partial \theta}{\partial x}-k\frac{\partial^2 \theta}{\partial x^2}=0 \tag{43}$$

where k is the diffusion coefficient and V is the flow velocity of constant value.

The initial conditions are

$$\theta(x, 0)=0, \qquad 0\leq x\leq L \tag{44}$$

and the boundary conditions are

$$\text{a. } \theta(0, t)=\frac{T_1-T_0}{T_0}, \qquad t>0$$
$$\theta(L, t)=0, \qquad t>0 \tag{45}$$

$$b.\ \theta(0, t)=\begin{cases}\dfrac{T_i-T_0}{T_0}\sin(nt), & 0<t\leq t_0\\ 0, & t_0<t\end{cases}$$
$$\theta(L, t)=0, \qquad t>0 \tag{46}$$

The above boundary conditions are just two typical examples that one might encounter in physical problems. Other types of boundary conditions can be applied as well. In many practical problems it is the case that boundary conditions of the type

$$C_1 + C_2 \frac{\partial \theta}{\partial x} + C_3 \theta = 0$$

are often encountered. The constants C_1, C_2 and C_3 are usually related to the physical parameters of the particular problems. Such boundary conditions can be implemented in the present formulation by expressing the above relation in terms of the heat displacement. For example for the linear element approximation the displacement of the boundary nodal point will be given as a function of the displacement of the nodal point just inside the boundary.

At this stage it is expedient to relate the dimensionless variables to the physical variables as follows:

$$\begin{aligned} \bar{x} &= \frac{x}{L}, \qquad \bar{t} = \frac{k}{L^2} t, \\ \bar{\theta} &= \frac{T - T_0}{T_1 - T_0}, \qquad \bar{H} = \frac{T_0}{T_1 - T_0} \frac{1}{L} H, \\ V_0 &= \frac{L}{k} V, \qquad \bar{t}_0 = \frac{k}{L^2} t_0 \end{aligned} \tag{47}$$

Here L is the characteristic length, T_1 is a constant temperature at the boundary and $\bar{t}_0$ is the length of time during which T_1 is applied at the boundary. The equations for the two finite element models are written in terms of the above defined dimensionless quantities for obtaining numerical solutions.

Numerical results

The one-dimensional convective heat transfer problem has been formulated by the displacement finite element method and its solution can be obtained from the system of ordinary differential equations in matrix form presented in the previous section. For the boundary value problem, with given boundary conditions, numerical solutions are obtained by using a third-order backward finite difference approximation. The choice of this scheme for solving the system of ordinary differential equations is based on the fact that the scheme is unconditionally stable.

The boundary conditions and the governing equation are transformed due to the dimensionless quantities as follows:

Boundary conditions:

$$\text{Case I} \qquad \theta(0, t) = 1, \qquad t > 0; \tag{48}$$

$$\text{Case II} \qquad \theta(0, t) = \begin{cases} \sin(nt) & 0 \leq t \leq t_0, \\ 0 & t > t_0 \end{cases} \tag{49}$$

The boundary condition at infinity $(x = L)$ is the same for all cases

$$\theta(L, t) = 0 \tag{50}$$

and the initial condition for all cases is

$$\theta(x, 0) = 0 \tag{51}$$

Table I. Time step sizes for the numerical solution

	TNE	Δx	Δt	$\Delta t/\Delta x$	$\Delta t/\Delta x$
LE	30	1/6	0·0075	0·045	0·27
CE	20	1/4	0·0125	0·05	0·2

Numerical solutions of the governing equation

$$\frac{\partial\theta}{\partial t}+V_0\frac{\partial\theta}{\partial x}-K_0\frac{\partial^2\theta}{\partial x^2}=0 \tag{52}$$

are obtained by solving the system of n equations represented by

$$A_{ij}\dot{q}_i+B_{ij}q_i=Q_j, \tag{53}$$

where A_{ij} and B_{ij} are the global matrices, given in the terms of equation (33) for the (LE) model and equations (39)–(41) for the (CE) model in dimensionless form. After solving for the displacements for the (LE) model, the temperature for the ith element can be obtained through the relation

$$\theta_i=W_0(H_{i+1}-H_i)\quad i=1,n \tag{54}$$

which is also used to implement the initial and boundary conditions in terms of nodal displacements. For the (CE) model, the solution of the system of equations will directly give nodal displacements as well as nodal temperatures.

Numerical results for the above boundary value problems were obtained for the characteristic length $L=5$, divided into TNE = 30 for the (LE) model and TNE = 20 for the (CE) one. The corresponding element lengths and the time step sizes used in the numerical solutions are given in Table I, and the rate of convergence for both element models is shown in Figure 1. The error is evaluated as the absolute error for the particular point $x=1{\cdot}0$ at time $t=1{\cdot}0$.

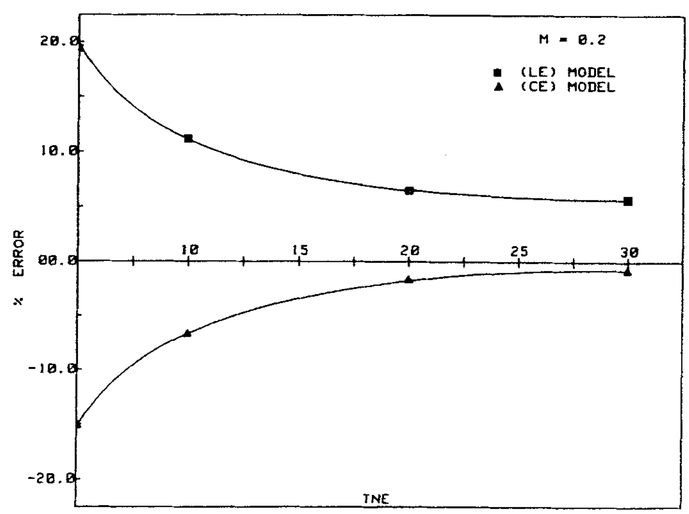

Figure 1. Convergence for the numerical solution for $M=0.2$, temperature errors at $x=1.0$ and $t=1.0$

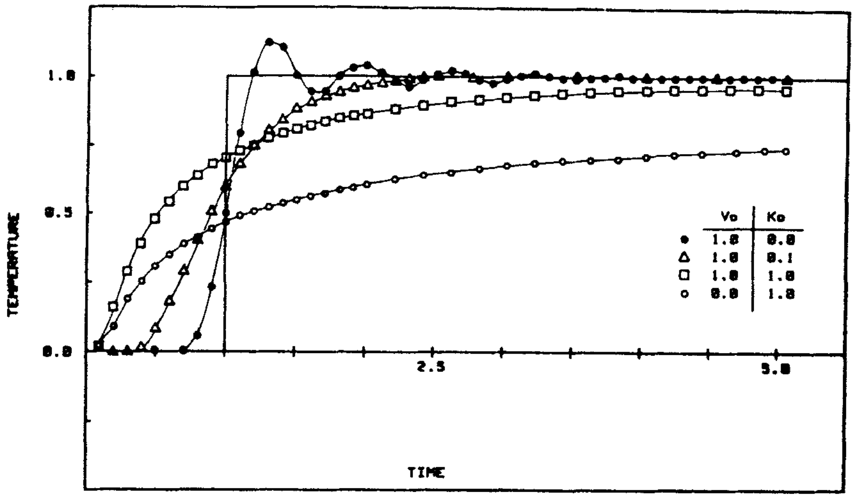

Figure 2. Temperature time history of $x = 1.0$, (LE) model, TNE = 30

Temperature time histories are given in Figures 2–5 for the point at $x = 1{\cdot}0$ and the temperature distributions as a function of x are given in Figures 6–9 at time $t = 2{\cdot}0$. Temperature time histories presented in Figures 2 and 3 are for the (LE) model and in Figures 4 and 5 for the (CE) model. Similarly, temperature distributions for the (LE) model are given in Figures 6 and 7 and in Figures 8 and 9 for the (CE) model. In each figure results are given for pure convection ($K_0 = 0{\cdot}0$, $V_0 = 1{\cdot}0$), pure diffusion ($K_0 = 1{\cdot}0$, $V_0 = 0{\cdot}0$) and for two cases of diffusion–convection ($K_0 = 0{\cdot}1$, $V_0 = 1{\cdot}0$) and ($K_0 = 1{\cdot}0$, $V_0 = 1{\cdot}0$). The analytical solution for all cases is presented by a solid line in Figures 2, 4, 6 and 8 and only for pure convection in Figures 3, 5, 7 and 9.

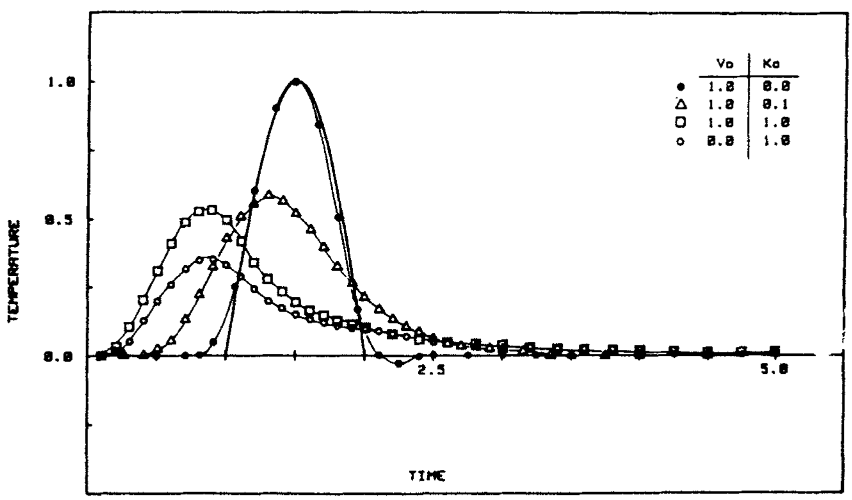

Figure 3. Temperature time history at $x = 1.0$, (LE) model, TNE = 30, $t_o = 1.0$

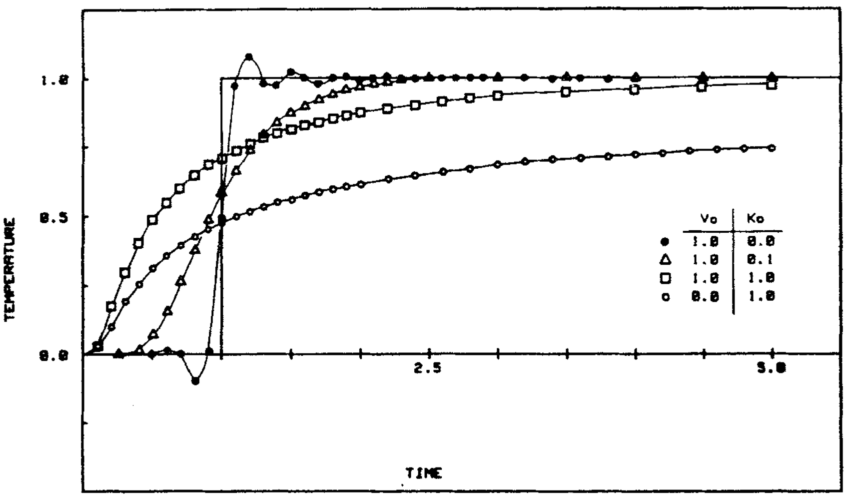

Figure 4. Temperature time history at $x = 1.0$, (CE) model, TNE = 20

For the first case of boundary conditions, Figures 2, 4, 6 and 8, the numerical solution shows good agreement with the analytical one. The oscillations around the discontinuity, typical of numerical schemes, damp out as the wave front progresses. The error can be controlled by the TNE used. A finer discretization will reduce the error of the numerical solution around the discontinuity. This finer discretization can be either uniform or localized around the discontinuity. Although the TNE used for both models is rather small, the results obtained depict only small errors.

For the second case of boundary conditions, Figures 3, 5, 7 and 9, $t_0 = 1{\cdot}0$ was used which corresponds to a half-sine wave propagating through the half-space. For pure convection, the

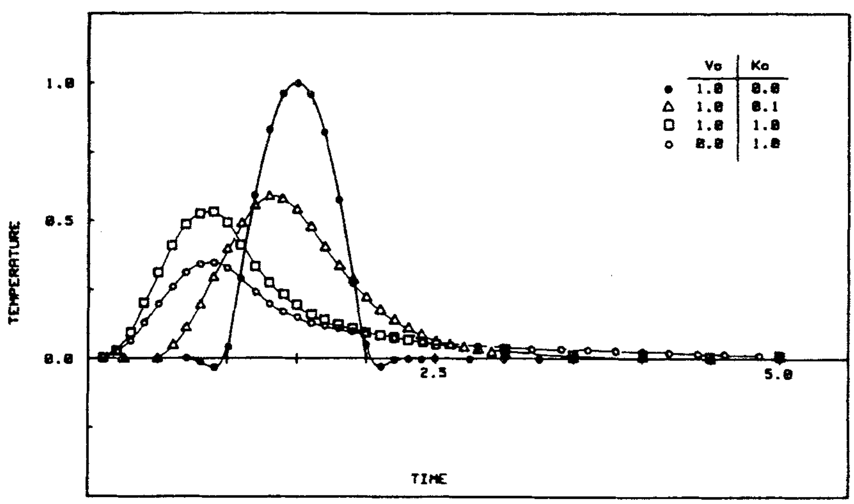

Figure 5. Temperature time history at $x = 1.0$, (CE) model, TNE = 20, $t_o = 1.0$

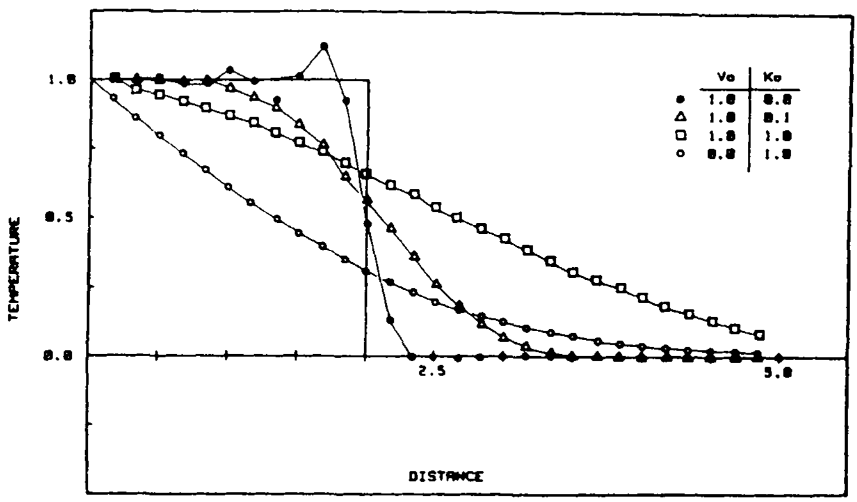

Figure 6. Temperature distribution at $t = 2.0$ for the (LE) model, TNE = 30

(LE) model propagates the wave with only a small distortion of its shape which is due to small numerical dispersion. On the other hand, the (CE) model gives a much better approximation of the wave but small oscillations of the numerical solution around the discontinuity are still present. These oscillations are inherent in any numerical solution, as can be shown by a Fourier analysis, when a discontinuity exists. From the obtained results one can observe that there is no error growth followed by unacceptable oscillations. Hence both models exhibit good stability characteristics. The oscillations and the error can be minimized by a finer discretization or by introducing some artificial diffusion into the numerical solution. However, such an artifically introduced diffusion will not allow a realistic

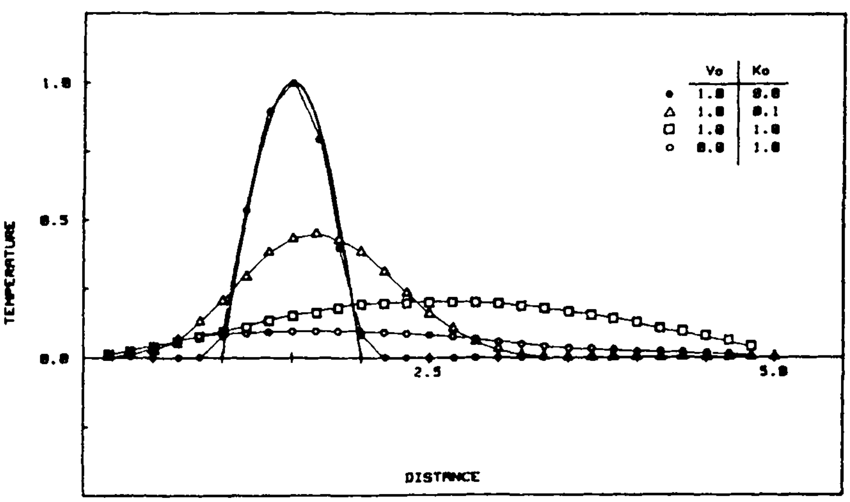

Figure 7. Temperature distribution at $t = 2.0$ for the (CE) model, TNE = 30, $t_o = 1.0$

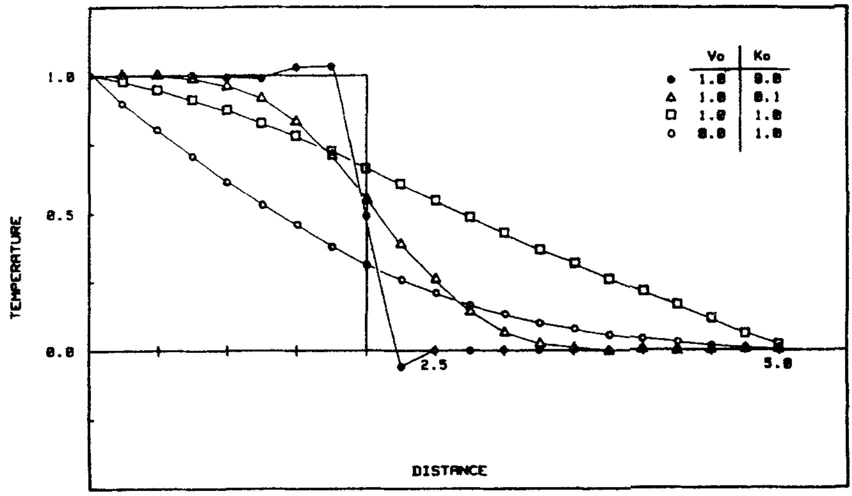

Figure 8. Temperature distribution at $t = 2.0$ for the (CE) model, TNE = 20

evaluation of the developed finite element models, and will introduce artificial errors when true diffusion is present. Many authors have introduced optimization techniques for solving a particular problem of interest. The numerical solutions presented here are not optimized in any way since a true evaluation is sought and the intent is to show the adaptibility of the developed method to different problems.

From the results obtained it can be seen that there is no phase lag between the exact and numerical wave forms, and, even for the rather coarse discretization used the shape is well approximated. This is due to the non-dispersive character of the models and also due to the fact that the two models do not exhibit any dissipation due to numerical diffusion.

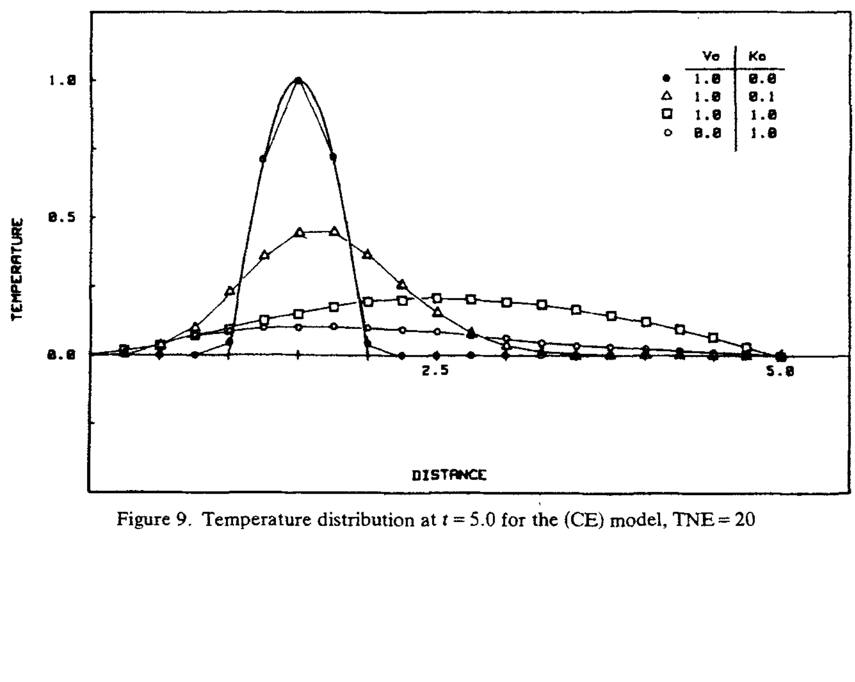

Figure 9. Temperature distribution at $t = 5.0$ for the (CE) model, TNE = 20

An increase in the TNE will improve the results for the (LE) model but it will have a very small effect to the already very accurate results of the (CE) model. For both cases of boundary conditions and all choices of the constants K_0 and V_0, the numerical models produced accurate results and the induced waves propagate through the half-space in a very satisfactory manner.

Extensive numerical experiments for the linear model were undertaken by this writer and results dealing with the error behaviour will be reported in the near future.

SUMMARY AND CONCLUSIONS

A variational formulation for convective heat transfer has been presented in this paper, and based on this formulation, two finite models have been developed for the purpose of solving problems concerned with the propagation of thermally-induced waves.

The introduction of a new quantity, defined as heat displacement, is the basis for developing a generalized variational formulation. One advantage of such a formulation is that it can be used to develop the finite element method as a special application. Furthermore, due to the generalized nature of the heat displacement and the presentation in terms of generalized co-ordinates this formulation can be extended to other types of equations. This is a strong point of the derived formulation which is based on concepts of classical mechanics and can be considered as a generalized formulation for obtaining approximate solutions. Another advantage of the formulation is the thermal force introduced, for which one should point out its significance as a boundary force.

The physical conditions for the semi-infinite space require that $\theta \to 0$ as $x \to \infty$. Since the last nodal point of the finite element approximation of the half-space represents infinity one should impose the above condition at this point. The thermal force is then zero due to zero temperature. This assumption is not the correct one since the temperature at the last nodal point changes as the thermal wave propagates. If one considers the last nodal point as a boundary point and the thermal force as a boundary force, which is proportional to the temperature at that point, then the conditions at the boundary point are properly adjusted. The presence of this boundary force into the formulation produces a much more accurate temperature distribution close to the boundary, since it represents the effect of the neglected portion of the medium.

The two finite element models developed in this study were used successfully to solve problems involving both convection and diffusion with prescribed boundary conditions for the temperature. The ability of the displacement finite element models to simulate accurately wave fronts with sharp discontinuities is due to the fact that the discontinuity exists in the temperature θ and not in the displacement H. The basic difference between the conventional and the displacement finite element models results in the reduction of the oscillations around the discontinuity, particularly for small values of the diffusivity coefficient. Comparison of present results with analytical solutions shows the performance of the cubic element model to be superior to the linear one. However, the performance of the (LE) model should not be underestimated, especially when one considers the crude approximation and the coarse space discretization involved. The choice between the two models for specific applications should depend on the particular needs of the problem under consideration.

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