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Finite Element Modeling for Convection-Diffusion Problems

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The scope of this study is to develop the basic equations for deriving a finite element formulation which can be used to solve problems related to convection and diffusion dominated flows.

The formulation is based on the introduction of a generalized quantity defined as heat displacement. The governing equation is expressed in terms of this quantity and a variational formulation is developed which leads to an equation similar in form to Lagrange's equation of mechanics. This equation may be solved by any numerical method, though it is of particular

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20. ABSTRACT (Continued)

mechanics. This equation may be solved by any numerical method, though it is of particular interest for application of the finite element method.

The developed formulation is used to derive two finite element models for solving convection-diffusion boundary value problems. The performance of the two element models is investigated and numerical results are given for different cases of convection and diffusion with three types of boundary conditions.

The numerical results obtained show not only the efficiency of the numerical models to handle pure convection, pure diffusion and mixed convection-diffusion problems but also good stability and accuracy. The applications of the developed numerical models is not limited to diffusion-convection problems but can also be applied to other types of problems such as mass transfer, hydrodynamics and wave propagation.

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CONTENTS

LIST OF SYMBOLS

x_i	Cartesian coordinates	E	Thermal potential
t	Time	q_i	Generalized coordinates
T_o	Reference temperature	Q_i	Generalized thermal forces
T	Absolute temperature	f_{ij}	Generalized basis functions
θ	Temperature change per unit temperature	d_{ij}	Mass matrix
H_i	Heat displacement	e_{ij}	Diffusivity matrix
V_i	Velocity components	g_{ij}	Convective matrix
σ	Heat stress	l	Element length
k_{ij}	Thermal diffusivity	A	Cross-sectional element area
λ_{ij}	Thermal resistivity	L	Characteristic length
v	volume	CE	Cubic element model
S	Surface of volume v	LE	Linear element model
n_i	Unit vector	TNE	Total number of elements

FINITE ELEMENT MODELING FOR
CONVECTION-DIFFUSION PROBLEMS

INTRODUCTION

The simulation of thermally induced waves requires the solution of the convection-diffusion equation. Analytical and numerical solutions of this equation have attracted considerable attention in a variety of engineering fields due to its wide applicability.

The theory for convective or diffusive dominated flows has been well-established and a variety of classical approaches exist in the literature for the solution of problems in this area. One such solution is given by Price, Cavendish and Varga [1]. Analytical solutions are valid primarily for linear equations 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 Lee et al (1976), Ehlig (1977), and Genuchten (1977). Numerical methods discussed in these papers include finite differences and some finite element approximations [5]. Most of the numerical schemes produce results of acceptable accuracy either for convection dominated flows, or for diffusion dominated flows, but they lack uniformity in performance. Finite difference schemes are the least attractive ones due to their instability, large oscillations, and, for some of them inherent artificial diffusion. On the other hand finite element schemes have produced more reliable numerical solutions but their application is limited to certain types of dispersion while performing poorly for other types. Another disadvantage of

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existing finite element solutions is that they are based on formulations restricted by the condi-tions of a particular problem and they are limited in applications to other types of problems.

In view of the limitations and lack of uniformity of existing approaches, it is desirable to develop a unified formulation which is capable of treating not only pure convection-through-dispersion to pure diffusion problems, but also other types of problems governed by similar equations. In order to achieve this, a unified variational formulation is introduced for the convection-diffusion equation; this equation is written in terms of a generalized quantity, defined as heat displacement [6,7], which is similar to a mechanical displacement and has units of length. As of this definition, changes in temperature are treated as thermal deformations which are similar to mechanical strains.

In the first part of this study, the basic definitions are introduced and the convection-diffusion equation is expressed in terms of the heat displacement. A variational formulation is then derived, based on the principle of virtual work in mechanics, and by using generalized coordinates the variational equation is written in a form equivalent to that of the Lagrangian equation in mechanics. Since the derived equation is expressed in terms of generalized coordi-nates, it is applicable to a wide variety of physical problems and can be solved by any numerical method.

The variational form of the derived equation is most suitable for applying the finite ele-ment method for its numerical solution. This is done in the second part of this study, where the basic finite element method is used to derive two finite element models for solving initial or boundary value problems. The first model is based on a linear approximation of the displace-ment 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.

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Each element model can be used for: a) pure convection, b) pure diffusion, and c) mixed convection-diffusion problems with the appropriate boundary conditions. Also, dynamic or quasi-static solutions can be obtained respectively by retaining or neglecting the inertia term.

Numerical results are given in the third part of this study where a third-order, backward finite difference scheme is employed for the solution of the system of differential equations [8,9]. For the combined finite element-finite difference scheme the stability, convergence, and accuracy are investigated and some uniform convergence criteria are discussed. Numerical results are also given for a number of convection through diffusion cases and for three types of boundary conditions. The present results are compared to existing analyical solutions and the accuracies of the two finite element models are discussed.

1. BASIC EQUATIONS

Consider an incompressible medium in a flow field subjected to external heating. Intially the medium is at a uniform temperature T_o, 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 $T-T_o$ defines the instantaneous relative temperature $\Delta\theta$, which is a function of the space coordinates and time. Let

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

be defined as the temperature change per unit temperatue T_o, 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 cartesian coordinates $(x_i, \ i = 1, 2, 3)$, the temperature field θ satisfies the convection-diffusion equation

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

where V_i is the velocity vector and k_{ij} the thermal diffusivity ($k_{ij} = k_{ji}$).

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

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

The summation convention is assumed for repeated indices throughout this study.

In the above definition, Eq. (3), θ represents a thermal strain analogous to mechanical strain. Note that $H_i(x_j,t)$ has the dimension of displacement, which makes it analogous to a mechanical displacement. Thus there is a one-to-one correspondence between heat displacement-mechanical displacement and temperature strain.

Using the definition from Eq. (3), we now write Eq. (2) as follows

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

or

$$\lambda_{ij}\frac{\partial H_i}{\partial t} + \lambda_{ij}\,V_k\,\frac{\partial H_i}{\partial x_k} - \frac{1}{cT_o}\,\frac{\partial \sigma}{\partial x_j} = 0 \qquad (5)$$

where the thermal stress σ is defined by

$$\sigma = c\,T_o\,\theta \qquad (6)$$

with c the heat capacity per unit volume, and $\lambda_{ij} = (k_{ij})^{-1}$.

In the above analysis the thermal flow field is governed by the three Eqs. (3), (5) and (6) which, together with the appropriate boundary conditions, provide a complete formulation for convective heat transfer. They are analogous to the kinematic relations, stress-strain relations and momentum equations in mechanics.

The advantage of introducing the heat displacement vector are more apparent when the concept of virtual work is used to derive the variational formulation. Furthermore, the above

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analysis is more suitable for applying the finite element method which is based on displacement approximations.

2. VARIATIONAL FORMULATION

Following the usual procedures of the principle of virtual work in mechanics, we consider that the medium is subjected to an arbitrary infinitesimal virtual displacement δH_i from the equilibrium configuration. The corresponding variations $\delta\theta$ are given by Eq. (3). Multiplication of Eq. (4) by δH_i and integation over a volume ν of the medium yields

$$\int_v \left[\frac{\partial H_i}{\partial t} + V_i\theta - k_{ij} \frac{\partial \theta}{\partial x_j} \right] \delta H_i dv = 0$$

Integrating by parts and applying the divergence theorem, one obtains

$$\int_v \frac{\partial H_i}{\partial t} \delta H_i dv + \int_v V_i\theta\delta H_i dv + \int_v k_{ij}\theta \frac{\partial}{\partial x_j} (\delta H_i) dv = \int_S k_{ij}\theta\delta H_i \eta_j dS$$

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

$$\int_v k_{ij}\theta \frac{\partial}{\partial x_j} (\delta H_i) dv = \int \delta_{ij} k_{ij}\theta\delta\theta dv = k_{ii}\delta E \tag{7}$$

where δ_{ij} is the Kronecker's delta and 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

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

Eq. (9) may be considered as a variational principle in a broad sense and a more compact form of this equation can be derived by introducing generalized coordinates defined as

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

where the generalized coordinates q_n are functions of time. The advantage of using generalized coordinated is that H_i may be expressed in different functional forms. Care should be taken when the time derivative of H_i is considered, and it should be expressed as

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$$\dot{H}_i = \frac{\partial H_i}{\partial q_j} \dot{q}_i + \frac{\partial H_i}{\partial t}.$$ (11)

In terms of arbitary variations of the generalized coordinates, the corresponding displacement field variations are

$$\delta H_i = \frac{\partial H_i}{\partial q_j} \delta q_j$$ (12)

and the variation of the potential E becomes

$$\delta E = \frac{\partial E}{\partial q_j} \delta q_j$$ (13)

In view of Eqs. (12) and (13), Eq. (9) may be written for each arbitrary variation δ_{J_k} as follows

$$\frac{\partial E}{\partial q_k} + \int_v \lambda_{ij} \frac{\partial H_i}{\partial t} \frac{\partial H_j}{\partial q_k} dv + \int_v \lambda_{ij} V_i \theta \frac{\partial H_j}{\partial q_k} dv = \int_s \theta \frac{\partial H_j}{\partial q_k} \eta_j dS.$$ (14)

From Eq. (11) one derives

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

and the second term in Eq. (14) is then expressed

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

where

$$D = \frac{1}{2} \int_v \lambda_{ij} \dot{H}_i \dot{H}_j dv$$ (15)

Eq. (14) then takes the form

$$\frac{\partial D}{\partial \dot{q}_k} + \frac{\partial E}{\partial q_k} + L_k = Q_k$$ (16)

where

$$L_k = \int_v \lambda_{ij} V_i \theta \frac{\partial H_j}{\partial q_k} dv$$ (17)

and

$$Q_k = \int_s \theta \eta_j \frac{\partial H_j}{\partial q_k} dS$$

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The quantity Q_k can be regarded as the thermal force applied on the boundary S of the medium of volume ν. The quantity L_k represents the convection term and for the case of a solid medium ($V_i = 0$) it is equal zero and Eq. (16) reduces to a form similar to Lagrange's equation in mechanics. Eq. (16) as it was derived is quite general in the sense that it can be applied to different types of media with different material properties.

Consider now a special case where the displacement field can be approximated by a linear combination of the generalized coordinates as follows

$$H_i(x_j,t) = q_k(t)f_{ki}(x_j) \qquad k = 1, \ n, \ j = 1,2,3. \tag{18}$$

In Eq. (18) the coefficients $q_k(t)$ represent a degree of freedom and the function $f_{ki}(x_j)$ specifies the extent to which $q_k(t)$ participates in the function $H_i(x_j,t)$. In finite element analysis, for example, Eq. (18) may be considered as the distribution function of the displacement field, where q_k can then be taken as nodal displacement or nodal deformations depending on the type of element selected.

Differentiating Eq. (18) with respect to time and space we obtain

$$\dot{H}_i = \dot{q}_k f_{ki} \tag{19}$$

$$\theta = \frac{\partial H_i}{\partial x_i} = q_k f_{ki,i}.$$

The scalar E, the vector L_k and the invariant D from Eqs. (8), (15), and (17) are expressed in terms of Eqs. (19) as follows

$$E = \frac{1}{2} e_{mn} q_m q_n$$

$$D = \frac{1}{2} d_{mn} \dot{q}_m \dot{q}_n$$

$$L_k = g_{km} q_m \tag{20}$$

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where

$$e_{mn} = \int_v f_{m\iota,\iota} f_{n\jmath,\jmath} \, dv$$

$$d_{mn} = \int_v \lambda_{\iota\jmath} f_{m\iota} f_{n\jmath} \, dv$$

$$g_{km} = \int_v \lambda_{\iota\jmath} V_\iota f_{k\jmath} f_{mn,n} \, dv \tag{21}$$

Substituting the specific forms of E, D, and L_k from Eqs. (20) into Eq. (16) one obtains

$$d_{\iota\jmath} \dot{q}_\jmath + (q_{\iota\jmath} + e_{\iota\jmath}) q_\jmath = Q_\iota \tag{22}$$

with

$$Q_\iota = \int_s \theta n_\jmath f_{\iota\jmath} \, dS \tag{23}$$

Equations (22) constitute a system of n ordinary differential equations for the unknown field parameters q_k $(k = 1, n)$, and it may represent the heat displacement field H_ι. This system of n equations can be solved together with the appropriate boundary condition by any numerical technique. Thus this variational formulation 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 convection-diffusion 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.

3. FINITE ELEMENT ANALYSIS

In order to demonstrate the application of the finite element method to the previously derived variational formulation, two 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 first order cubic Hermitian. Although both elements are one dimensional approximations, they provide a good test case for the performance of any variational formulations. An extension into the two

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dimensional space is easily obtained since the derived equations are of general form. If the heat displacement is approximated by a third order polynomial

$$H(x,t) = a_o + a_1 x + a_2 x^2 + a_3 x^3, \tag{24}$$

then the temperature θ is given by

$$\theta(x,t) = a_1 + 2a_2 x + 3a_3 x^2 \tag{25}$$

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

a. Linear element (LE)

For the linear element of length l the conditions at the nodal points are:

$$\text{at } x = 0 \rightarrow H = H_1$$

and

$$\text{at } x = l \rightarrow H = H_2$$

where H_1 and H_2 are the nodal values of the heat displacement and the coefficients a_i are given by

$$a_o = H_1(t), \quad a_1 = \frac{1}{l}(H_2 - H_1), \quad a_2 = a_3 = 0. \tag{26}$$

Substituting these coefficients in Eqs. (24) and (25) yields

$$H(x,t) = \left[1 - \frac{x}{l}\right] H_1(t) + \frac{x}{l} H_2(t) \tag{27}$$

and

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

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

The matrix coefficients of Eq. (22) are evaluated in terms of Eqs. (27) as follows

$$e_{mn} = \frac{A}{l} \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$d_{mn} = \frac{Al}{6k} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \tag{28}$$

$$g_{mn} = \frac{AV}{2k} \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

and

$$Q_i\big|_{x=0} = Q_1 = -A\theta, \quad Q_i\big|_{x=l} = Q_2 = A\theta$$

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

In terms of Eqs. (28), Eq. (22) yields

$$\frac{l}{6k}\begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}\begin{Bmatrix} \dot{H}_1 \\ \dot{H}_2 \end{Bmatrix} + \left[\frac{V}{2k}\begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix} + \frac{1}{l}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}\right]\begin{Bmatrix} H_1 \\ H_2 \end{Bmatrix} = \begin{Bmatrix} Q_1 \\ Q_2 \end{Bmatrix} \tag{29}$$

b. Cubic element (CE)

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

The conditions at the nodes are

$$at\ x = 0 \rightarrow H = H_1, \ \theta = \theta_1;$$

and

$$at\ x = l \rightarrow H = H_2, \theta = \theta_2;$$

where (H_1, H_2) and (θ_1, θ_2) are the nodal values of the heat displacement and temperature respectively. Thus, the coefficients of Eq. (24) can be found as

$$a_o = H_1, \ \alpha_1 = \theta_1$$

$$a_2 = -\frac{1}{l^2}[(\theta_2 + 2\theta_1)l - 3(H_2 - H_1)]$$

$$a_3 = \frac{1}{l^3}[(\theta_2 + \theta_1)l - 2(H_2 - H_1)] \tag{30}$$

and the expressions for $H(x,t)$ and $\theta(x,t)$ are given by

$$H(x,t) = f_{11}q_1 + f_{12}q_2 + f_{13}q_3 + f_{14}q_4$$

$$\theta(x,t) = h_{11}q_1 + h_{12}q_2 + h_{13}q_3 + h_{14}q_4. \tag{31}$$

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

$$f_{11} = 1 - \frac{3x^2}{l^2} + \frac{2x^3}{l^3}, \quad f_{13} = \frac{3x^2}{l^2} - \frac{2x^3}{l^3}$$

$$f_{12} = x - \frac{2x^2}{l} + \frac{x^3}{l^3}, \quad f_{14} = -\frac{x^2}{l} + \frac{x^3}{l^2} \tag{32}$$

and

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

and the generalized coordinates q_i are

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

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

$$e_{ij} = \frac{A}{30l} \begin{vmatrix} 36 & 3l & -36 & 3l \\ 3l & 4l^2 & -3l & -l^2 \\ -36 & -3l & 36 & -3l \\ 3l & -l^2 & -3l & 4l^2 \end{vmatrix} \tag{33}$$

$$d_{ij} = \frac{Alk}{420} \begin{vmatrix} 156 & 22l & 54 & -13l \\ 22l & 4l^2 & 13l & -3l^2 \\ 54 & 13l & 156 & -22l \\ -13l & -3l^2 & -22l & 4l^2 \end{vmatrix} \tag{34}$$

$$g_{ij} = \frac{AV}{210} \begin{vmatrix} -210 & 42l & 210 & -42l \\ -42l & 0 & 42l & -7l^2 \\ -210 & -42l & 210 & 42l \\ 42l & 7l^2 & -42l & 0 \end{vmatrix} \tag{35}$$

and the components of the generalized force are

$$Q_1 = -A\theta_1, \quad Q_3 = A\theta_2, \quad Q_2 = Q_4 = 0. \tag{36}$$

In terms of Eqs. (27)-(30), Eq. (22) yields

$$[d] \begin{Bmatrix} \dot{H}_1 \\ \dot{\theta}_1 \\ \dot{H}_2 \\ \dot{\theta}_2 \end{Bmatrix} + [[g] + [e]] \begin{Bmatrix} H_1 \\ \theta_1 \\ H_2 \\ \theta_2 \end{Bmatrix} = \begin{Bmatrix} -\theta_1 \\ 0 \\ \theta_2 \\ 0 \end{Bmatrix} \tag{37}$$

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or

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

For the solution of a particular problem, the finite element models derived above are assembled according to the direct stiffness method to obtain the 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 conditions can be solved by any numerical technique used for solving ordinary differential equations. In the following section, the above system of equations is solved for two types of boundary conditions by using a backward differences in time integration technique.

4. BOUNDARY VALUE PROBLEM

The one dimensional case of the convention-diffusion equation is considered here to evaluate the two finite element models introduced previously with the following initial and boundary conditions.

a. Convection dominated flow

The equation to be solved is

$$\frac{\partial \theta}{\partial t} + V \frac{\partial \theta}{\partial x} = 0 \tag{38}$$

where V is the flow velocity of constant value.

The initial conditions are

$$\theta(x,0) = 0, \quad 0 \leqslant x \leqslant L \tag{39}$$

and the boundary conditions are

$$\text{I.} \ \theta(0,t) = \frac{T_1 - T_o}{T_o} \qquad t > 0 \tag{40}$$

$$\text{II.} \ \theta(0,t) = \begin{cases} \dfrac{T_1 - T_o}{T_o} & 0 < t \leqslant t_o \\ 0 & t_o < t \end{cases}$$

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b. Combined convection and diffusion

The equation to be solved is

$$\frac{\partial \theta}{\partial t} + V \frac{\partial \theta}{\partial x} - k \frac{\partial^2 \theta}{\partial x^2} = 0 \qquad (41)$$

where k is the diffusion coefficient.

The initial conditions are

$$\theta(x, 0) = 0, \qquad 0 \leqslant x \leqslant L \qquad (42)$$

and the boundary conditions are

$$a.\ \theta(0, t) = \frac{T_1 - T_o}{T_o}, \qquad t > 0$$

$$\theta(L, t) = 0, \qquad t > 0 \qquad (43)$$

$$b.\ \theta(0, t) = \begin{cases} \dfrac{T_1 - T_0}{T_o}, & 0 < t \leqslant t_0 \\ 0, & t_0 < t \end{cases}$$

$$\theta(L, t) = 0, \qquad t > 0$$

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

$$\bar{x} = \frac{x}{L}, \qquad \bar{t} = \frac{k}{L^2} t, \qquad (44)$$

$$\bar{\theta} = \frac{T - T_o}{T_1 - T_o}, \qquad \bar{H} = \frac{T_o}{T_1 - T_o} \frac{1}{L} H,$$

$$V_o = \frac{L}{k} V, \qquad \bar{t}_o = \frac{k}{L^2} t_o.$$

Here L is the characteristic length, T_1 is a constant temperature applied at the boundary and $\bar{t}_o$ the length of time during which T_1 is applied at the boundary.

The equations for the two finite element models are now written in terms of the above defined dimensionless quantities as follows,

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I. Linear element:

$$[d_e]\ \{\dot{H}\} + [[g_e] + [e_e]]\ \{H\} = \{Q\}$$

with

$$[d_e] = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, \quad [g_e] = 3\ V_o\ W_o \begin{bmatrix} -1 & 1 \\ -1 & 1 \end{bmatrix}$$

$$[e_e] = 6 W_o^2 K_o \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \quad \text{and} \quad \{Q\} = 6 W_o K_o \begin{Bmatrix} -\theta \\ \theta \end{Bmatrix} \quad (45)$$

II. Cubic element:

$$[d_c]\ \begin{Bmatrix} \{\dot{H}\} \\ \{\dot{\theta}\} \end{Bmatrix} + [[g_c] + [e_c]]\ \begin{Bmatrix} \{H\} \\ \{\theta\} \end{Bmatrix} = \{Q\}$$

with

$$[d_c] = \begin{vmatrix} 165 & 54 & 22/W_0 & -13/W_0 \\ 54 & 156 & 13/W_0 & -22/W_0 \\ 22/W_0 & 13/W_0 & 4/W_0^2 & -3/W_0^2 \\ -13/W_0 & 22/W_0 & -3/W_0^2 & 4/W_0^2 \end{vmatrix}$$

$$[g_c] = 2V_0 W_o \begin{vmatrix} -210 & 210 & 42/W_0 & -42/W_0 \\ -210 & 210 & -42/W_0 & 42/W_0 \\ -42/W_0 & 42/W_0 & 0 & -7/W_0^2 \\ 42/W_0 & -42/W_0 & 7/W_0^2 & 0 \end{vmatrix} \quad (46)$$

$$[e_c] = 14 W_0^2 K_o \begin{vmatrix} 36 & -36 & 3/W_0 & 3/W_0 \\ -36 & 36 & -3/W_0 & -3/W_0 \\ 3/W_0 & -3/W_0 & 4/W_0^2 & -1/W_0^2 \\ -3/W_0 & -3/W_0 & -1/W_0^2 & 4/W_0^2 \end{vmatrix}, \quad \{Q\} = 420\ W_0 K_0 \begin{Bmatrix} -\theta_1 \\ \theta_2 \\ 0 \\ 0 \end{Bmatrix}$$

where $W_o = L/l$, and V_o and K_o are the dimensionless constant velocity and diffusivity respectively. The bar over the variables has been eliminated for simplicity. The boundary conditions are transformed due to the dimensionless quantities as follows

a. Convection—dominated flow

$$\text{I. } \theta(0,t) = 1.0, \qquad t > 0$$

$$\text{II. } \theta(0,t) = \begin{cases} 1.0, & 0 < t \leqslant t_o \\ 0, & t > t_o \end{cases} \tag{47}$$

b. Convection-diffusion

$$\text{I. } \theta(0,t) = 1.0, \qquad t > 0$$

$$\theta(L,t) = 0, \qquad t \geqslant 0 \tag{48}$$

$$\text{II. } \theta(0,t) = \begin{cases} 1.0, & 0 < t \leqslant t_0 \\ 0.0, & t > t_0. \end{cases}$$

$$\theta(L,t) = 0.0, \qquad t \geqslant 0.$$

The assembly of the above equations for the overall problem and their modification due to the boundary conditions is coded in a computer program given in Appendix C. After solving for the displacements of the (LE) model, the temperture for the ith element can be obtained through the relation

$$\theta_i = W_o \, (H_{i+i} - H_i) \quad i = 1,n \tag{49}$$

For the (CE) model, the solution of the system of equations will directly give nodal displacements as well as nodal temperatures.

5. NUMERICAL SOLUTION

The one-dimensional convection-diffusion problem has been formulated by the 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 applying suitable numerical integration techniques.

In this section, the numerical errors induced by the time integration scheme and by the finite element method are evaluated as are the convergences of the solution. Furthermore, results are given for the different types of boundary conditions considered in the previous section.

a. Time integration technique

The systems of ordinary differential equations obtained for the two element models are solved by using a third-order, backward finite difference approximation. The general formula for the first derivative can be written in the following form.

$$\frac{dy(t_i)}{dt} = \frac{1}{h} \sum_{j=0}^{n} a_j y(t_{i-j}) + 0(h^{n-1}) \tag{50}$$

where h is the size of the time discretization and a_j are constant coefficients. If only third order and lower terms are retained ($n = 4$), then the coefficients are given by

$$a_0 = \frac{11.0}{6.0}, \; a_1 = -\frac{18.0}{6.0}, \; a_2 = \frac{9.0}{6.0}, \; a_3 = -\frac{2.0}{6.0}, \; a_4 = 0.0 \tag{51}$$

for the third-order approximation.

In order to evaluate the stability and convergence of the above numerical scheme, results were obtained for a number of different time-step sizes. A stability analysis given in Appendix A shows that the scheme is unconditionally stable. This stability is not related to error estimates or rate of convergence.

Consider the case of pure diffusion ($K_o = 1$, $V_o = 0$) as a test case for illustrating some numerical results. A characteristic length $L = 5$ is chosen to represent the semi-infinite space, which is divided into 10 elements (TNE = 10). Results with respect to time are given for the point $x = 1.0$ and for the following boundary conditions

$$\theta(0,t) = 1.0, \; t \geq 0$$
$$\theta(L,t) = 0.0, \; t \geq 0$$

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This choice of boundary conditions is appropriate for evaluating numerical solution errors and convergence. Numerical results for different time step sizes are presented in Figs. 1,2 and Table 1 for the two element models. The optimum time step was found to be within the range of 0.01 to 0.2. For smaller or larger time steps the error of the numerical solution increases. Referring to Fig. 1, it is apparent that as the time step becomes smaller, the solution does not converge monotonically. Comparing the results for the two models, the (CE) as expected, is much more accurate than the (LE). An optimum time step size, approximately in the range of 0.01 to 0.025, yields the most accurate results.

The non-monotonic convergence is due to the fact that the numerical solution depends not only on the time step size but also on the spatial discretization as well. This is demonstrated in the following, where numerical experiments provide a criterion for uniform convergence.

b. Convergence of the Finite Element Solution

In order to investigate the convergence of the two finite element models, the previously discussed problem is considered and with the same constants. The total number of elements by which the characteristic length L is represented is designated as TNE and the numbers of elements from $x = 0$ to $x = 1.0$ is denoted by NE. The results of this part are given for two cases, one where the time step size Δt is kept constant for different TNE, and the other case where the ratio $\Delta t/\Delta x^2$ is kept constant, where Δx is the dimensionless length of an element.

Convergence For Constant Δt

Results for this case are given for the time step size $\Delta t = 0.025$ for both element models. For the (LE) model TNE is 5, 10, 20, 30 with the NE being 1,2,4 and 6 respectively. For the
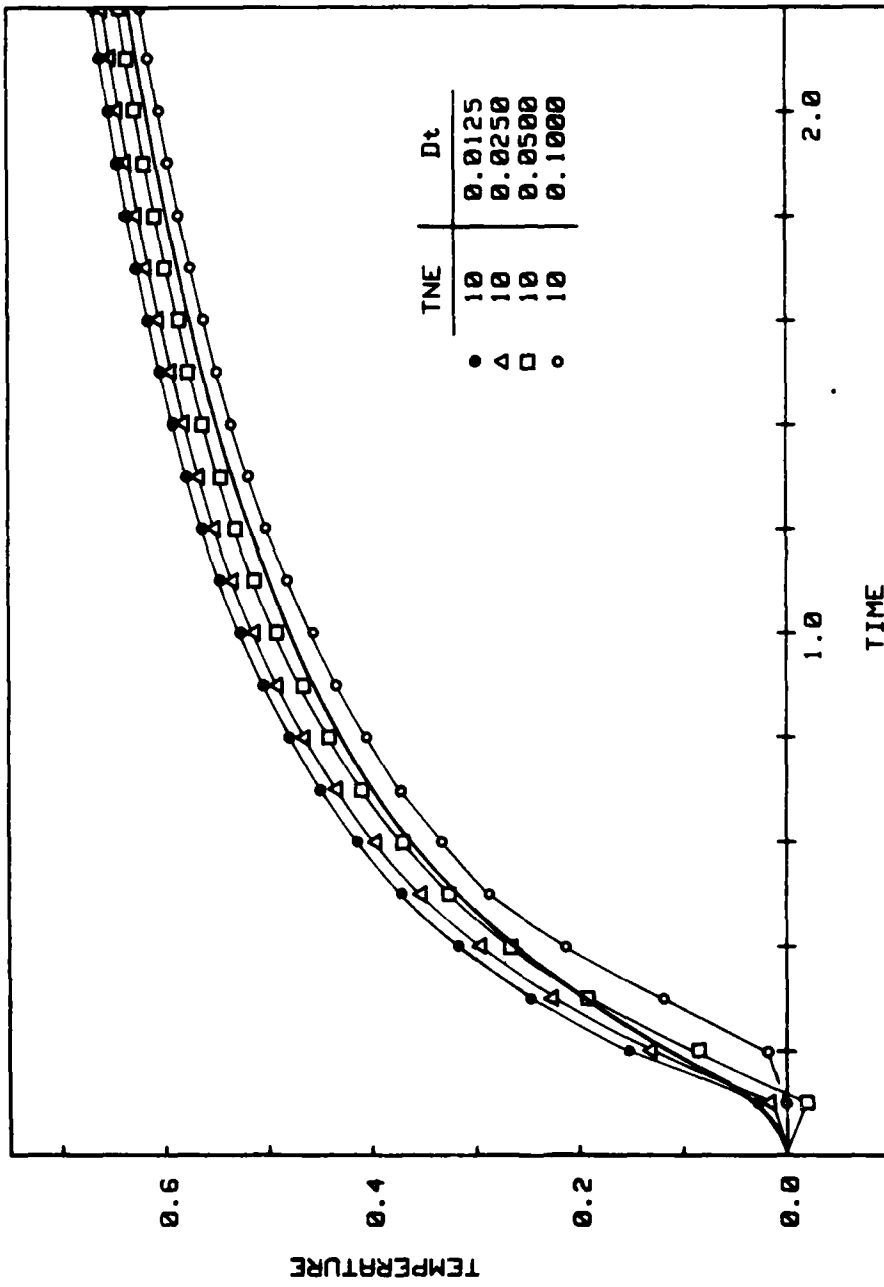
Fig. 1—Temperature distribution at $x = 1.0$ as a function of time for the (LE) model, TNE = 10.
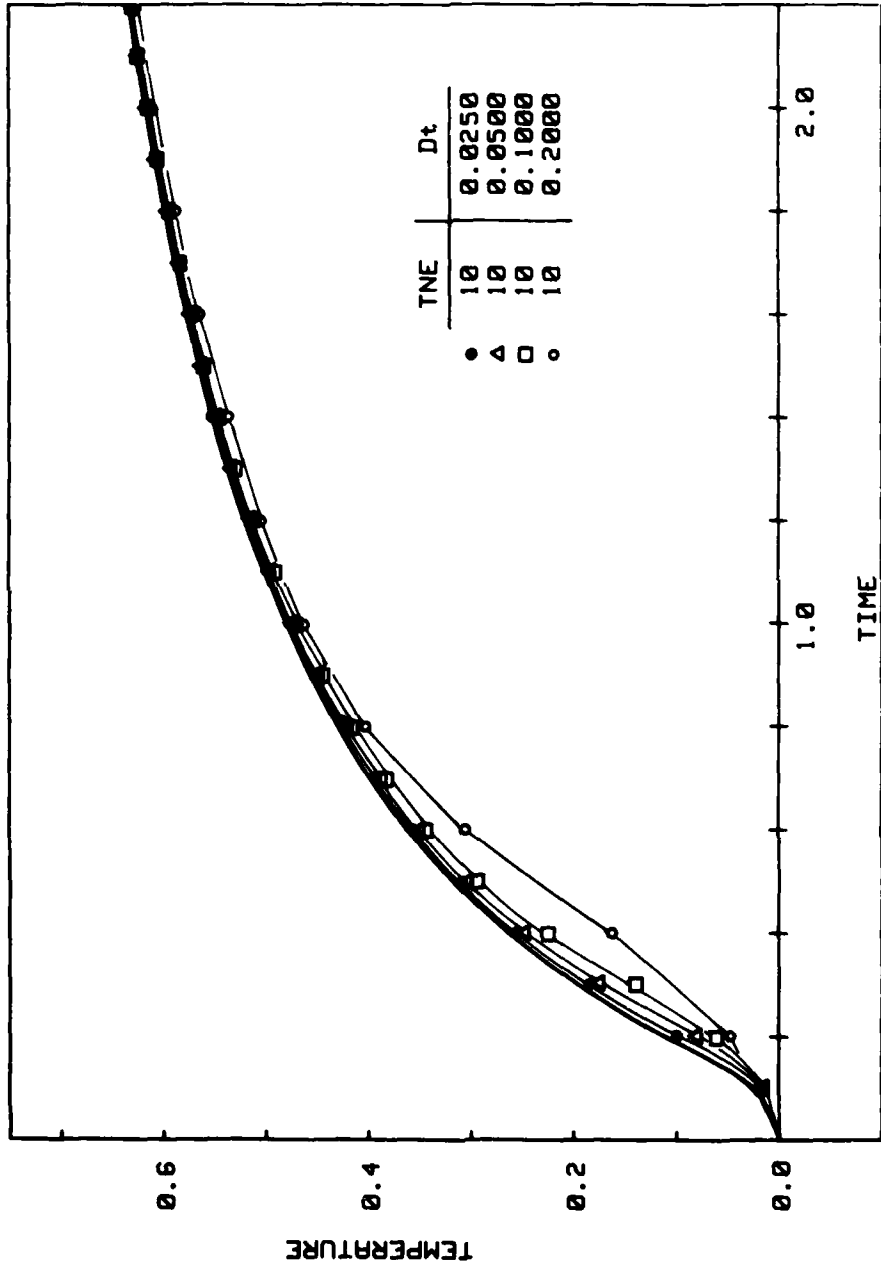
Fig. 2—Temperature distribution at $x = 1.0$ as a function of time for the (CE) model, TNE = 10.

Table 1. Numerical results for the temperature at $x = 1.0$ for
the (CE) model with constant TNE = 10.

Time	$\Delta t = 0.2$	$\Delta t = 0.1$	$\Delta t = 0.05$	$\Delta t = 0.025$	Exact
0.2	0.050761	0.061340	0.082475	0.099961	0.113846
0.4	0.167021	0.226432	0.24890	0.254928	0.263552
0.6	0.305074	0.345081	0.350841	0.355827	0.361310
0.8	0.405435	0.414393	0.421731	0.425394	0.429195
1.0	0.464985	0.468150	0.473867	0.476695	0.479500
1.2	0.503298	0.509717	0.514170	0.516448	0.518605
1.4	0.535127	0.542831	0.546491	0.548389	0.550090
1.6	0.563341	0.570084	0.573147	0.57478	0.576149
1.8	0.587542	0.592999	0.595609	0.597047	0.598161
2.0	0.608034	0.612611	0.614868	0.616085	0.617074
2.2	0.625647	0.629639	0.631614	0.632687	0.633553
2.4	0.641050	0.644596	0.646344	0.647267	0.648076

(CE) model TNE is 5, 10, 20, 25 with NE being 1,2,4,5 respectively. In Fig. 3 results for the (LE) model are presented for the temperature at $x = 1.0$ with respect to time for the four different values of TNE. As one may see from this figure, the results of the finite element solution do not converge monotonically to the exact solution as TNE increases.

For the CE, the results are given in Table 2 for the time history of the temperature of $x = 1.0$ and for different values of TNE (i.e. 5,10,20,25). By increasing the TNE the results show improvement. However, increasing the number of elements does not necessarily imply uniform convergence.

To obtain a better view of the convergence of a typical data point, Fig. 4 shows the errors for the temperature with respect to TNE for constant Δt and with respect to Δt for constant
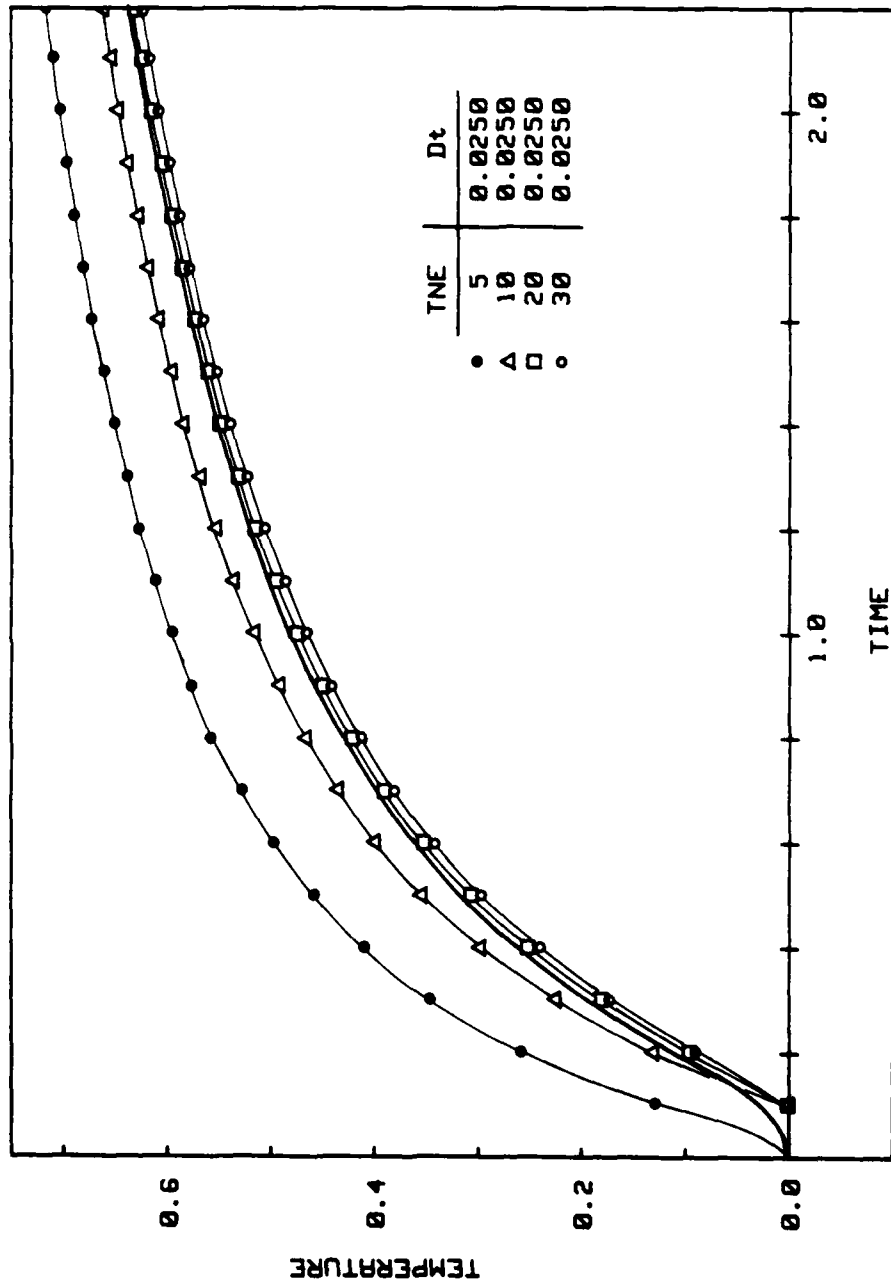
Fig. 3—Temperature distribution at $x = 1.0$ as a function of time for the (LE) model, $\Delta t = 0.025$.

Table 2. Numerical results for the temperature at $x = 1.0$ for
the (CE) model with constant $\Delta t = 0.025$.

Time	TNE = 5	TNE = 10	TNE = 20	TNE = 25	Exact
0.2	0.072260	0.099961	0.102454	0.102548	0.113846
0.4	0.242260	0.254928	0.256015	0.256053	0.263552
0.6	0.350094	0.355827	0.356245	0.356256	0.361310
0.8	0.422881	0.425394	0.425537	0.425540	0.429195
1.0	0.475747	0.476695	0.476705	0.476708	0.479500
1.2	0.516323	0.516448	0.516484	0.516389	0.518605
1.4	0.548726	0.548389	0.548282	0.548282	0.55090
1.6	0.575355	0.574780	0.574628	0.574627	0.576149
1.8	0.597759	0.597047	0.596864	0.596864	0.598161
2.0	0.616944	0.616085	0.615944	0.615948	0.617074
2.2	0.633653	0.632697	0.632549	0.632551	0.633553
2.4	0.648339	0.647267	0.647159	0.647161	0.648076

TNE, for both element models. The errors are evaluated at point $x = 1.0$ and time $t = 1.0$. Figure 4 clearly shows that convergence cannot be achieved by increasing the number of elements alone or by decreasing the step size alone.

Convergence For Constant $\Delta t/\Delta x^2$

In the previous analyses of the time integration technique and the finite element method, the results demonstrated that an increase of the time step size or the number of elements alone does not guarantee uniform convergence. This phenomenon is similar to the numerical instability of the direct finite difference analysis (e.g. [10]).

A modulus M is proposed here, defined as
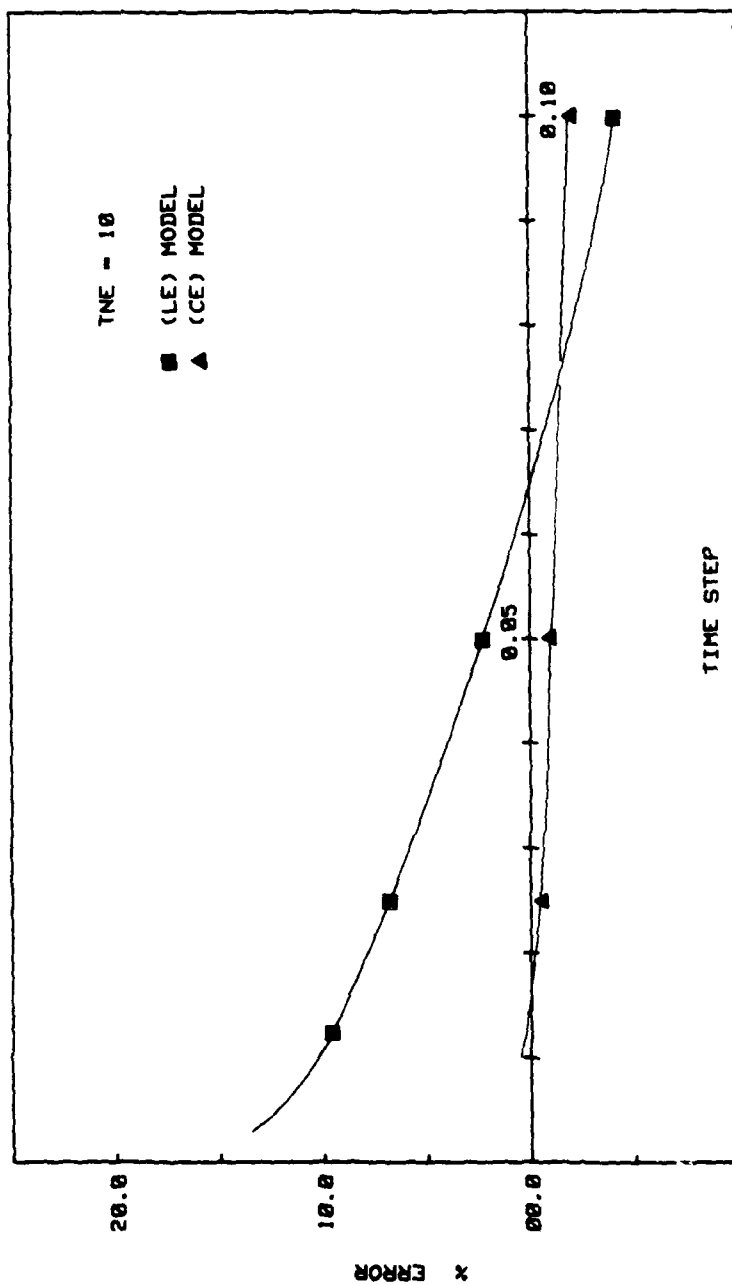
$$M = \frac{\Delta t}{\Delta x^2},$$

(52)

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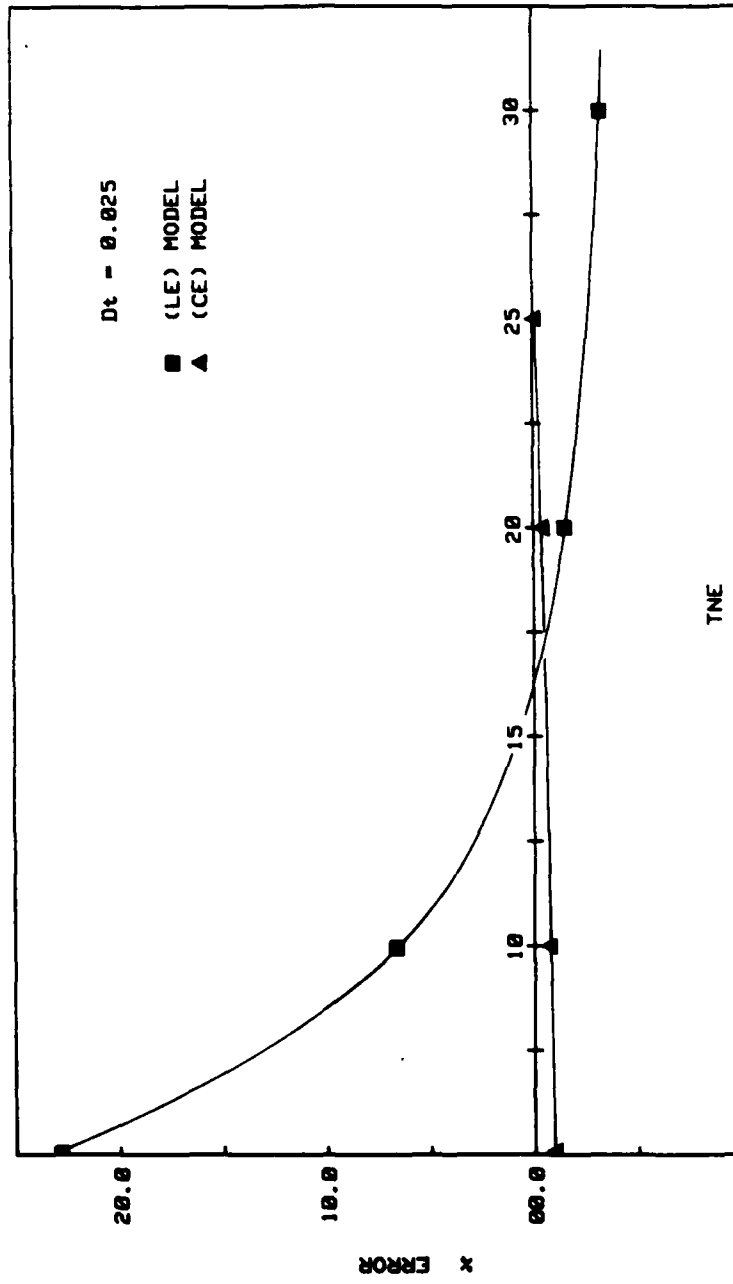Fig. 4a—Convergence of the numerical solution for constant Δx, TNE = 10.

Fig. 4b—Convergence of the numerical solution for constant $\Delta t = 0.025$.

where Δt is the dimensionless time step size and Δx the dimensionless element length. This modulus M is of similar form to the stability parameter of the finites difference method. By maintaining M constant for different values of TNE, the corresponding values of Δt are calculated from the above definition as follows

Relation between Δx and Δt for $M = 0.2$

TNE	NE	Δx^{-1}	Δx^{-2}	Δt	M
5	1	1.0	1.0	0.2	0.2
10	2	2.0	4.0	0.05	0.2
20	4	4.0	6.0	1./80.	0.2
30	6	6.0	36.0	1./180.	0.2

Results for constant M are given in Fig. 5 for the (LE) and Fig. 6 and Table 3 for the (CE).

Both sets of results represent temperture time histories for different values of TNE at $x = 1.0$. As one may see from these numerical results, the convergence of the finite element solution is uniform and approaches the exact solution as the value of TNE increases.

The error percentage is show in Fig. 7 for the particular point at $x = 1.0$ and $t = 1.0$ for both element models. This figure clearly demonstrates the uniform convergence of the numerical solution for both element models and the decrease of numerical error as TNE increases.

Comparing the results obtained for the two parts of this section it is concluded that the modulus M is an appropriate parameter for error control of the combined numerical scheme of finite element and finite difference methods.
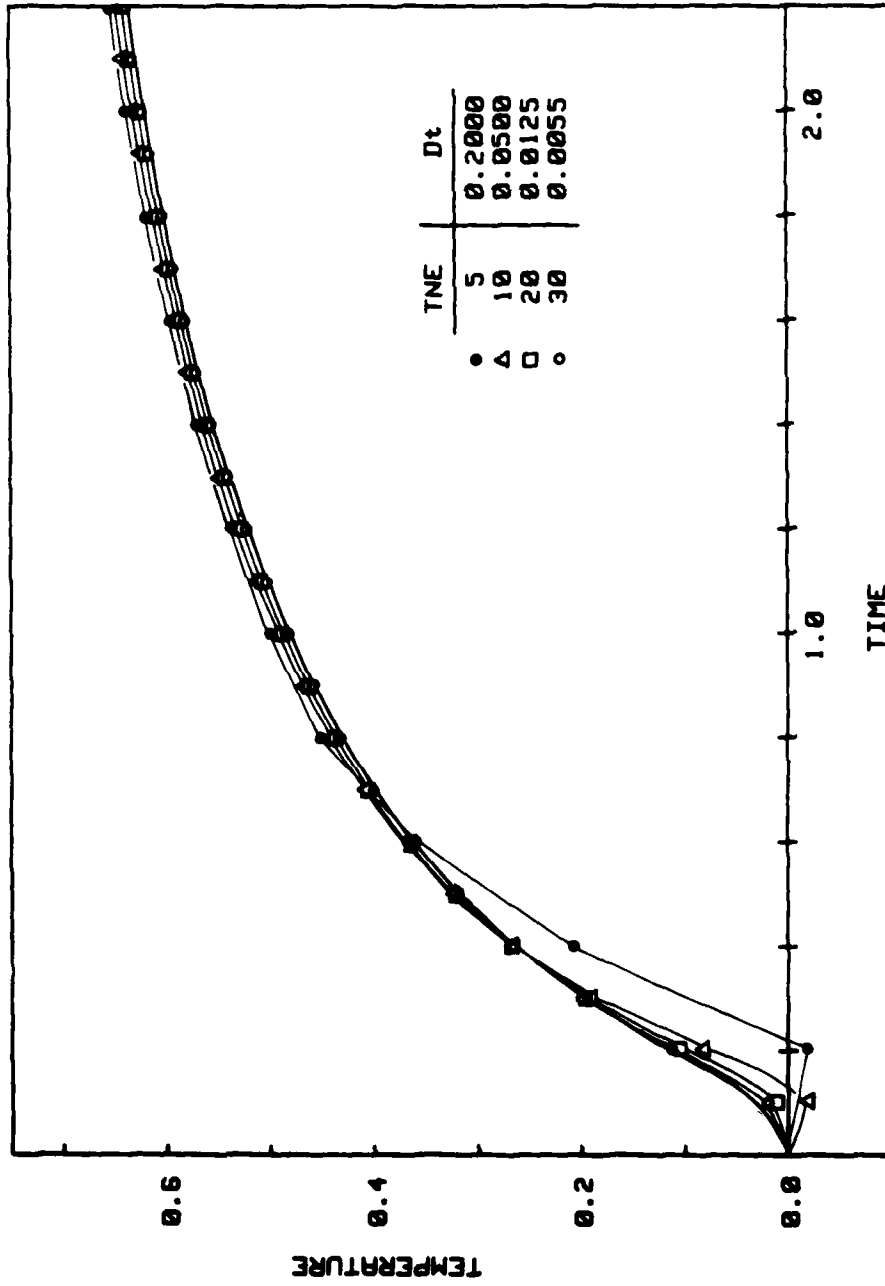
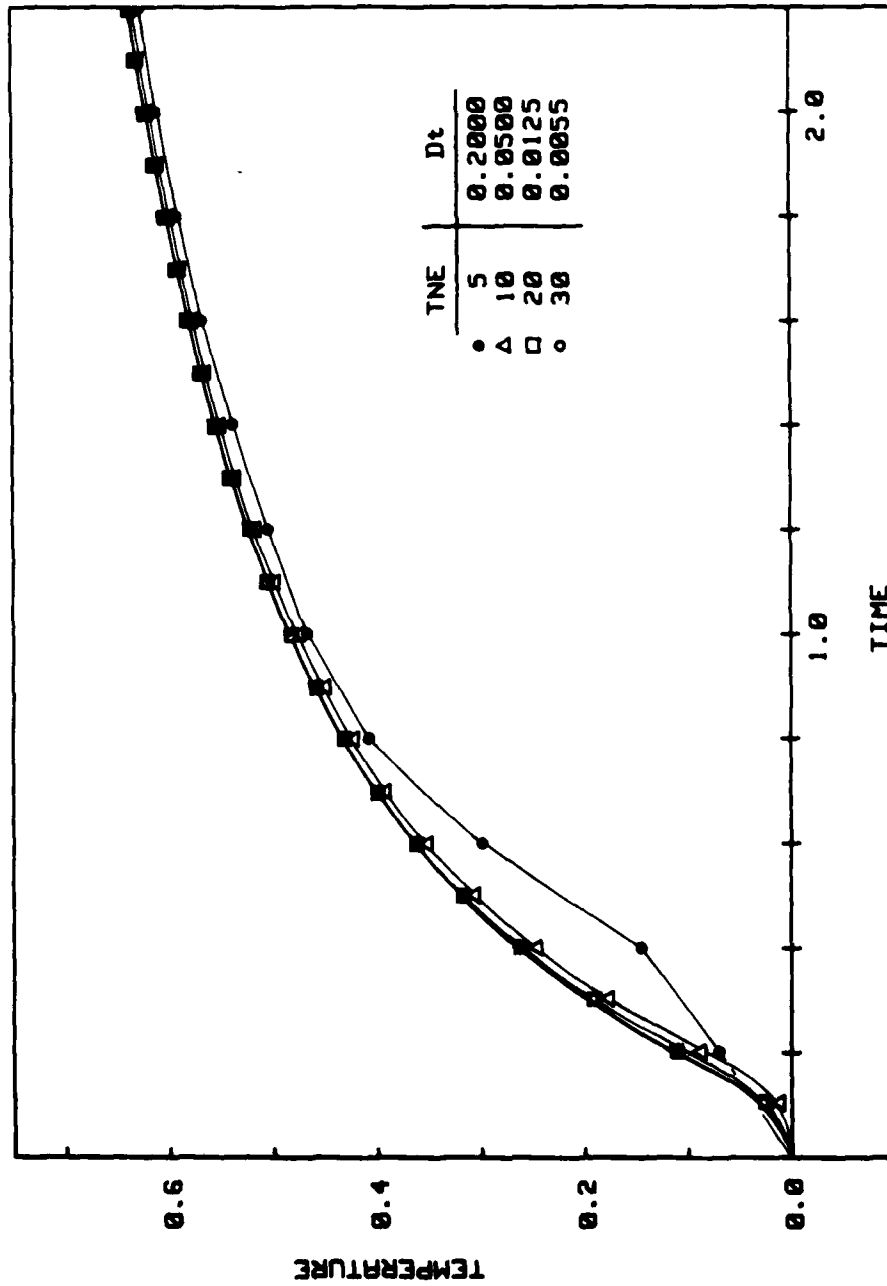Fig. 5—Temperature distribution at $x = 1.0$ as a function of time for the (LE) model, $M = 0.2$

Fig. 6—Temperature distribution at $x = 1.0$ as a function of time for the (CE) model. $M = 0.2$.

Table 3. Numerical results for the temperature at $x = 1.0$ for
the (CE) model with constant $M = 0.2$.

Time	TNE = 5 $\Delta t = 0.2$	TNE = 10 $\Delta t = 0.025$	TNE = 20 $\Delta t = 0.0025$	TNE = 30 $\Delta t = 0.0055$	Exact
0.2	0.069741	0.082475	0.107999	.111522	.113846
0.4	0.144791	0.248910	0.259719	.261983	0.263552
0.6	0.297175	0.350841	0.358799	.360226	0.361310
0.8	0.406438	0.421731	0.427436	.428403	.429195
1.0	0.464971	0.473867	0.478166	.478931	.479500
1.2	0.502502	0.514170	0.517715	.518280	.518605
1.4	0.534534	0.543491	0.549360	.549906	.550090
1.6	0.563076	0.573147	0.575505	.576005	.576144
1.8	0.587472	0.595604	0.597619	.598086	.598161
2.0	0.608067	0.614868	0.616490	.617113	.617074
2.2	0.625727	0.631614	0.632925	.633571	.633553
2.4	0.641165	0.646344	0.647125	.648091	.648076

A comparison of the two element models shows the superiority of the cubic one over the linear. This higher order element not only produces a more stable solution but also a much more accurate one than does the linear element. Even though the number of equations to be solved for (CE) is twice the number for (LE), and the computer time required for the solution is about two to one, the (CE) is preferred due to better accuracy even for small TNE. Another advantage of (CE) is that any type of boundary condition may be imposed accurately to the boundary nodal points since the generalized coordinates represent both heat displacements and temperatures.

Similar error and convergence criteria can be derived for the dimensionless ratio $\Delta t/\Delta x$ when the convection-diffusion equation is solved ($V_o, K_o \neq 0$) or when the pure convection
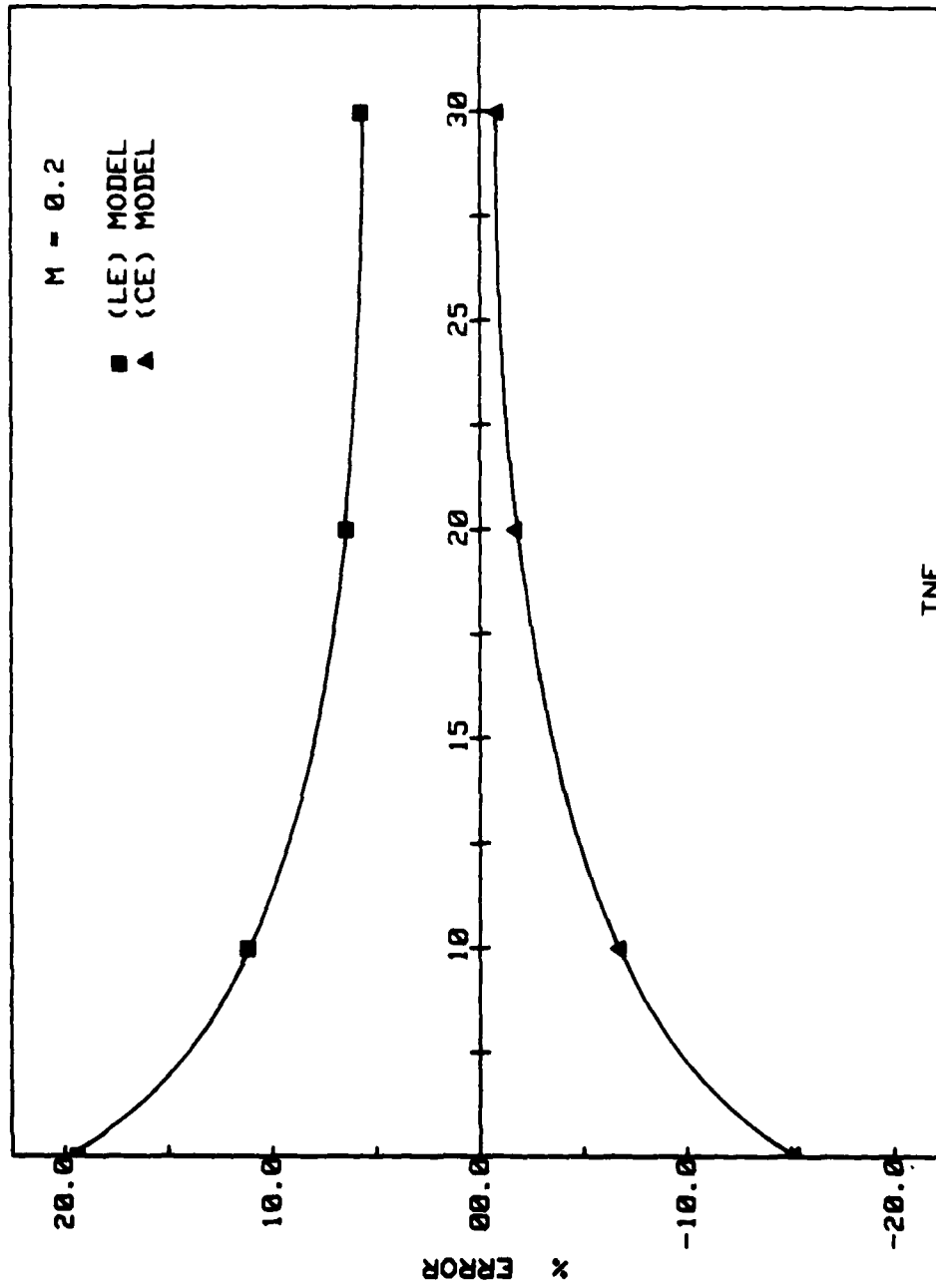
Fig. 7—Convergence for the numerical solution for $M = 0.2$, temperature errors at $x = 1.0$ and $t = 1.0$.

equation ($K_u - 0$, $V_u - 1$) is solved. Using the latter as a test case we choose the same characteristic length L as in previous examples and the same constants. The boundary condition is assumed to be a half-sine wave with period 2π and the initial conditions are zero, i e $\theta(x,0) - 0$. This type of boundary condition is suitable for investigating solution convergence since it has a continuous form. Results for the convergence of the numerical solution are presented in Figs. 8-11. The first two figures (8 and 9) show temperature time histories at $x -$ 1.0 for the two models (LE) and (CE) respectively. The time step size is kept constant and TNE is given four different values to show convergence of the solution with respect to Δx. Figure 10 shows temperature time histories for the (CE) model with a constant value for TNE and four different values for Δt. It is apparent from these figures that uniform convergence is not obtained by changing only Δt or Δx. Numerical experimentation showed that when the value of the ratio $\Delta t/\Delta x$ is maintained constant uniform convergence of the solution is obtained. Results for this case are given in Fig. 11 for the (LE) model with four values of TNE and corresponding values of Δt. Similar results were obtained for the (CE) model. The value for the ratio $\Delta t/\Delta x$ was equal to 0.05.

Comparing the above results for the case of pure convection it is apparent that the ratio $\Delta t/\Delta x$ is the appropriate parameter for error control of the numerical solution.

As a last test for the stability of the solution experimentations were performed with different values for the characteristic length L ranging from 1 to 5 and constant TNE. Since for every different value of L the values of Δx will change, the ratio $\Delta t/\Delta x$ and the modulus M were kept constant by adjusting the value of Δt accordingly. It was observed that changes in the values of L had no effect on the solution and on the propagation of the wave. For small values of TNE as L becomes smaller, for example TNE $- 5$ and $L - 1$, the numerical solution becomes more accurate. This is expected since Δx is five times smaller for $L - 1$ than for $L - 5$ (i.e. $\Delta x - 0.2$ for $L - 1$ and TNE $- 5$ while $\Delta x - 1.0$ for $L - 5$ and TNE $- 5$).

Fig. 8—Temperature distribution at $x = 1.0$ as a function of time for the (LE) model, $\Delta t = 0.025$.
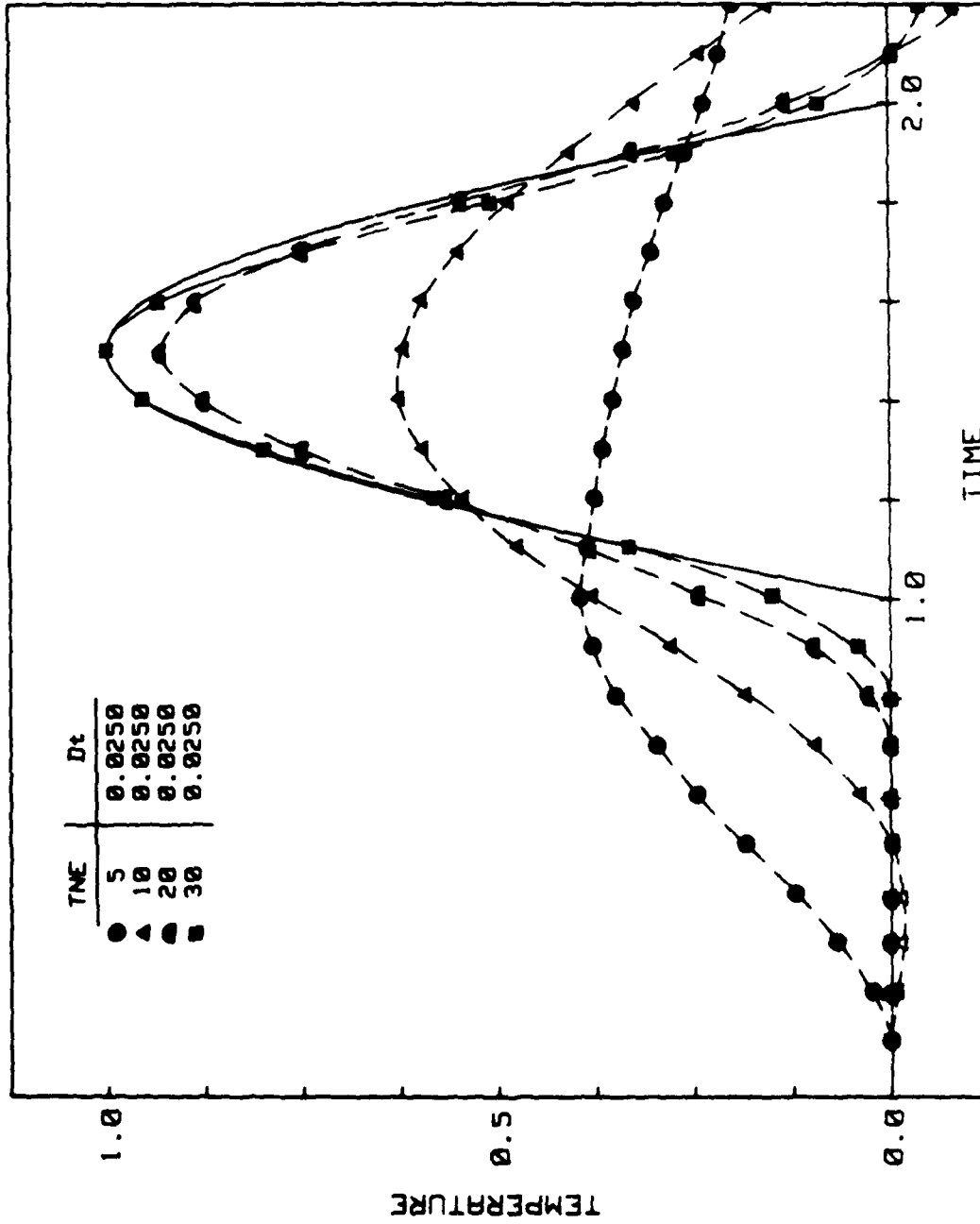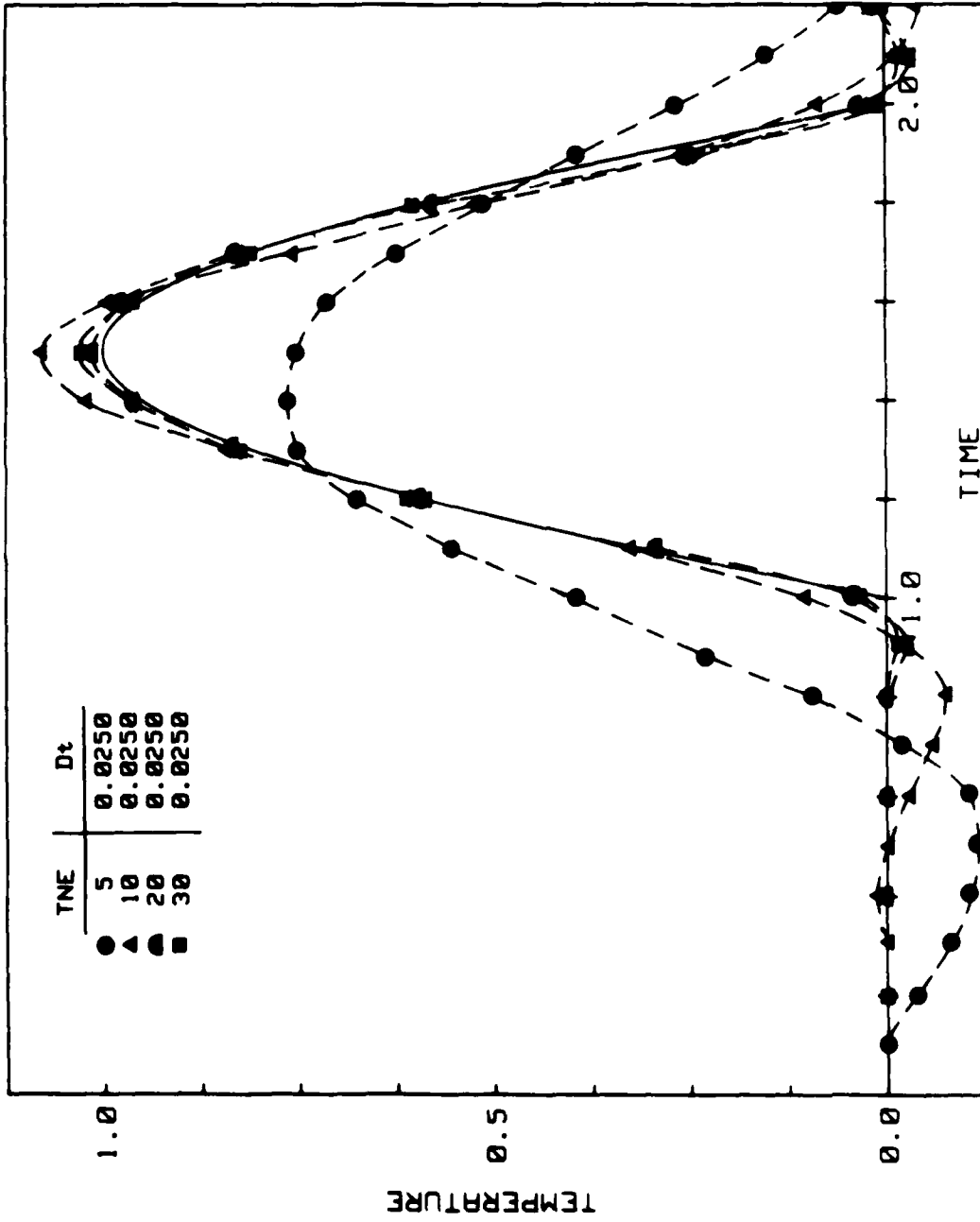
Fig. 9—Temperature distribution at $x = 1.0$ or a function of time for the (CE) model. $\Delta t = 0.025$.

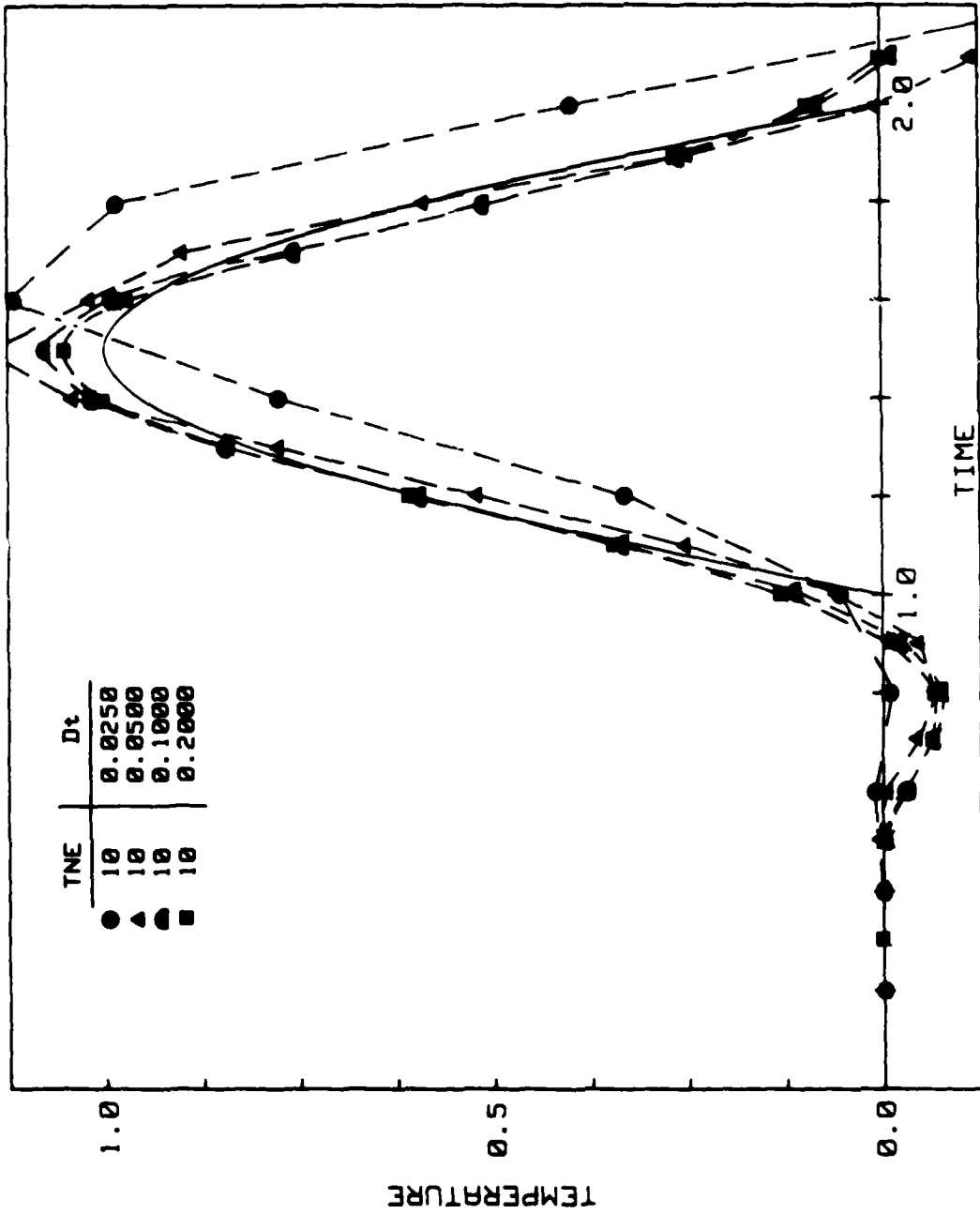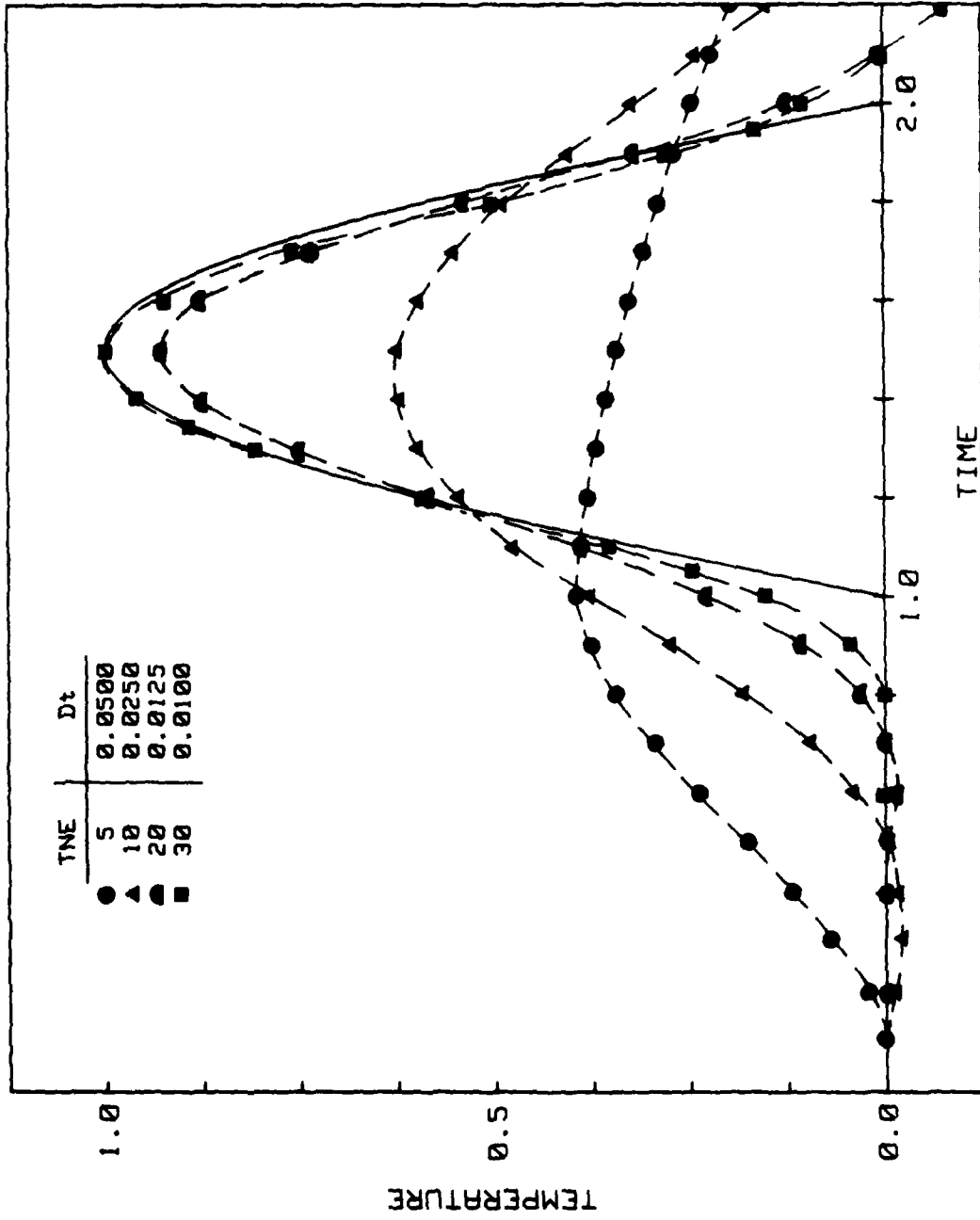Fig. 10—Temperature distribution at $x = 1.0$ or a function of time for the (CE) model, TNE = 10.

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Fig. 11.—Temperature distribution at $x = 1.0$ as a function of time for the (LE) model, $\Delta t / \Delta x = 0.05$.

c. Numerical Results For Boundary Value Problems.

In applying the derived finite element formulation to diffusion-convection problems, the semi-infinite space is approximated by the characteristic length L with a time-dependent temperature applied on its boundary. Three different cases of boundary conditions are considered and results are obtained for both element models.

Boundary conditions:

Case I $\theta(0,t) = 1, \quad t > 0;$

Case II $\theta(0,t) = \begin{cases} = 1, & 0 < t \leqslant t_o, \\ = 0, & t > t; \end{cases}$

Case III $\theta(0,t) = \begin{cases} \sin(nt) & 0 \leqslant t \leqslant t_o, \\ = 0 & t > t_o \ . \end{cases}$

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

$$\theta(L,t) = 0$$

and the initial condition for all cases is

$$\theta(x,0) = 0$$

Numerical solutions of the governing equation

$$\frac{\partial\theta}{\partial t} + V_o \frac{\partial\theta}{\partial x} - K_o \frac{\partial^2\theta}{\partial x^2} = 0 \tag{53}$$

are obtained by solving the system of n equations represented by

$$A_{ij}\dot{Q}_j + B_{ij}Q_i = Q_j, \tag{54}$$

where A_{ij} and B_{ij} are the global matrices, given in terms of Eq. (45) for the (LE) model and Eq. (46) for the (CE) model.

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)

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one. The corresponding element lengths and time step sizes used in the numerical solution are given in Table 4.

Table 4. Time step sizes for the numerical solution.

	TNE	Δx	Δt	$\Delta t/\Delta x$	$\Delta t/\Delta x^2$
LE	30	1/6	0.0075	0.045	0.27
CE	20	1/4	0.0125	0.05	0.2

Temperature time histories are given in Figs. (12-19) for the point at $x = 1.0$ and temperature distributions as a function of x are given in Figs. (20-27) at time $t = 2.0$. Temperature time histories presented in Figs. (12-15) are for the (LE) model and in Figs. (16-19) for the (CE) model. Similarly, temperature distributions for the (LE) model are given in Figs. (20-23) and in Figs. (24-28) for the (CE) model. In each figure results are given for pure convection ($K_o = 0.0$, $V_o = 1.0$), pure diffusion ($K_o = 1.0$, $V_o = 0.0$) and for two cases of diffusion-convection, ($K_o = 0.1$, $V_o = 1.0$) and ($K_o = 1.0$, $V_o = 1.0$). The analytical solution for pure convection is presented by a solid line in all figures.

For the first case of boundary conditions, Figs. (12), (16), (20) and (24), the numerical solution shows good agreement with the analytical one. The oscillations around the discontinuity damp out as the wave front progresses. The error can be controlled by the TNE used. A finer discretization reduces the error of the numerical solution around the discontinuity. This finer discretization can be either uniform or localized around the dicontinuity. Although the TNE used for both models is rather small, the results obtained depict only small errors.

For the second case of boundary conditions, Figs. (13), (17), (21) and (25), $t_o = 1.0$ was used which corresponds to a square wave propagating through the half-space. For pure convection, the (LE) model propagates the square wave but its shape is distorted due to numerical
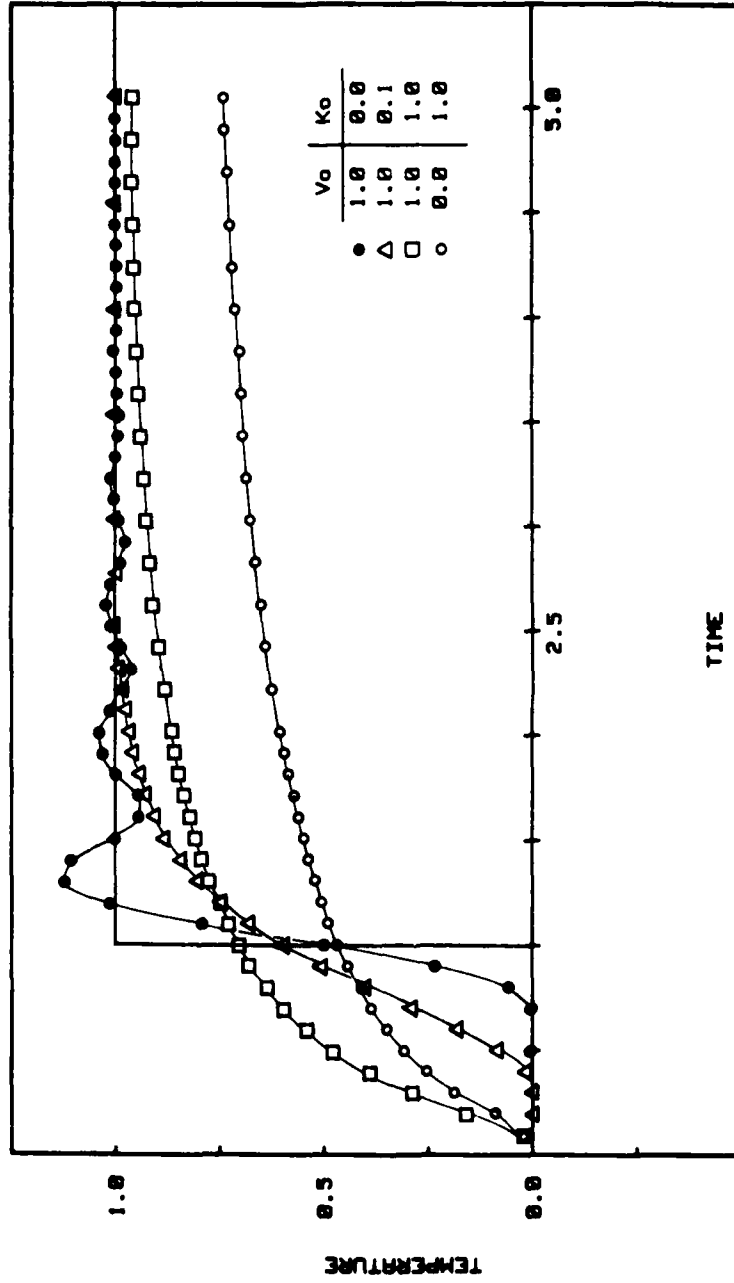
Fig. 12 — Temperature time history at $x = 1.0$, (LE) model, TNE $= 30$.
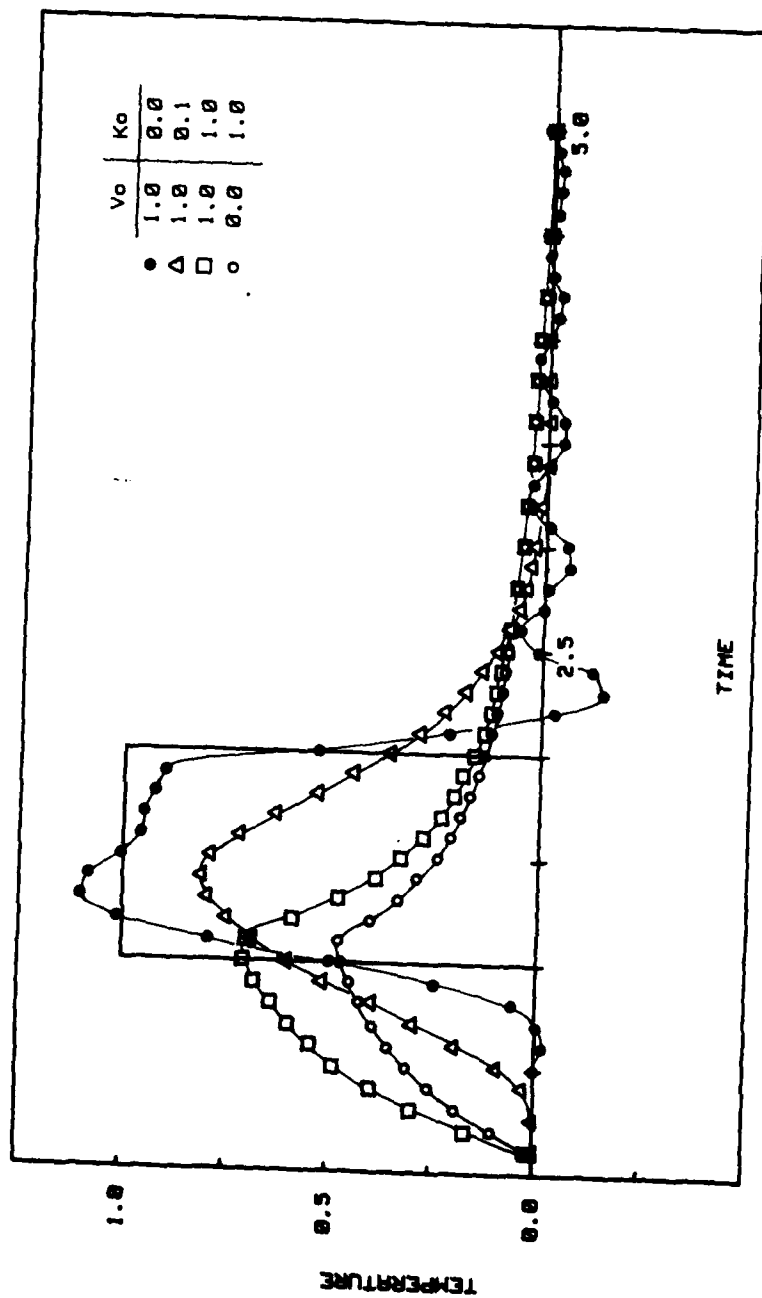
Fig. 13—Temperature time history at $x = 1.0$, (LE) model, TNE $= 30$, $t_o = 1.0$.
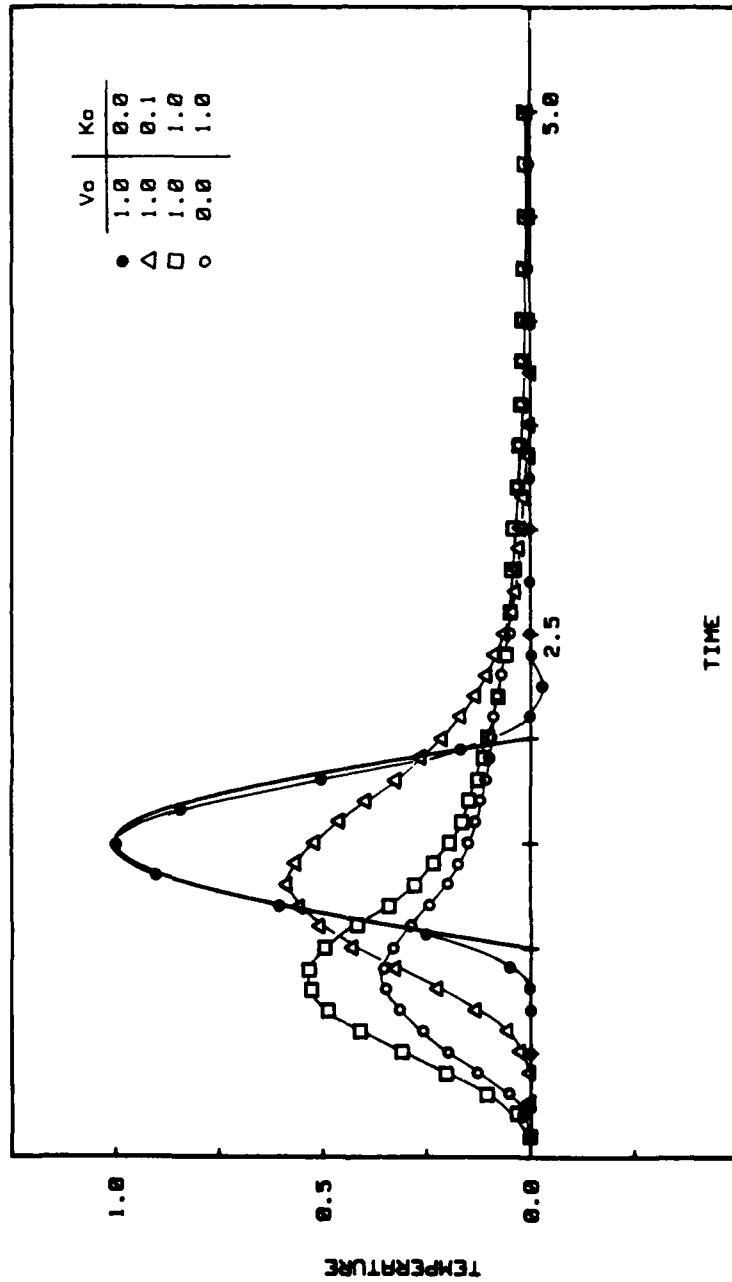
Fig. 14—Temperature time history at $x = 1.0$, (LE) model, TNE $= 30$, $t_o = 1.0$.

Fig. 15—Temperature time history at $x = 1.0$, (LE) model, TNE = 30.

Vo	Ko	
1.0	0.0	●
1.0	0.1	◁
1.0	1.0	□
0.0	1.0	○
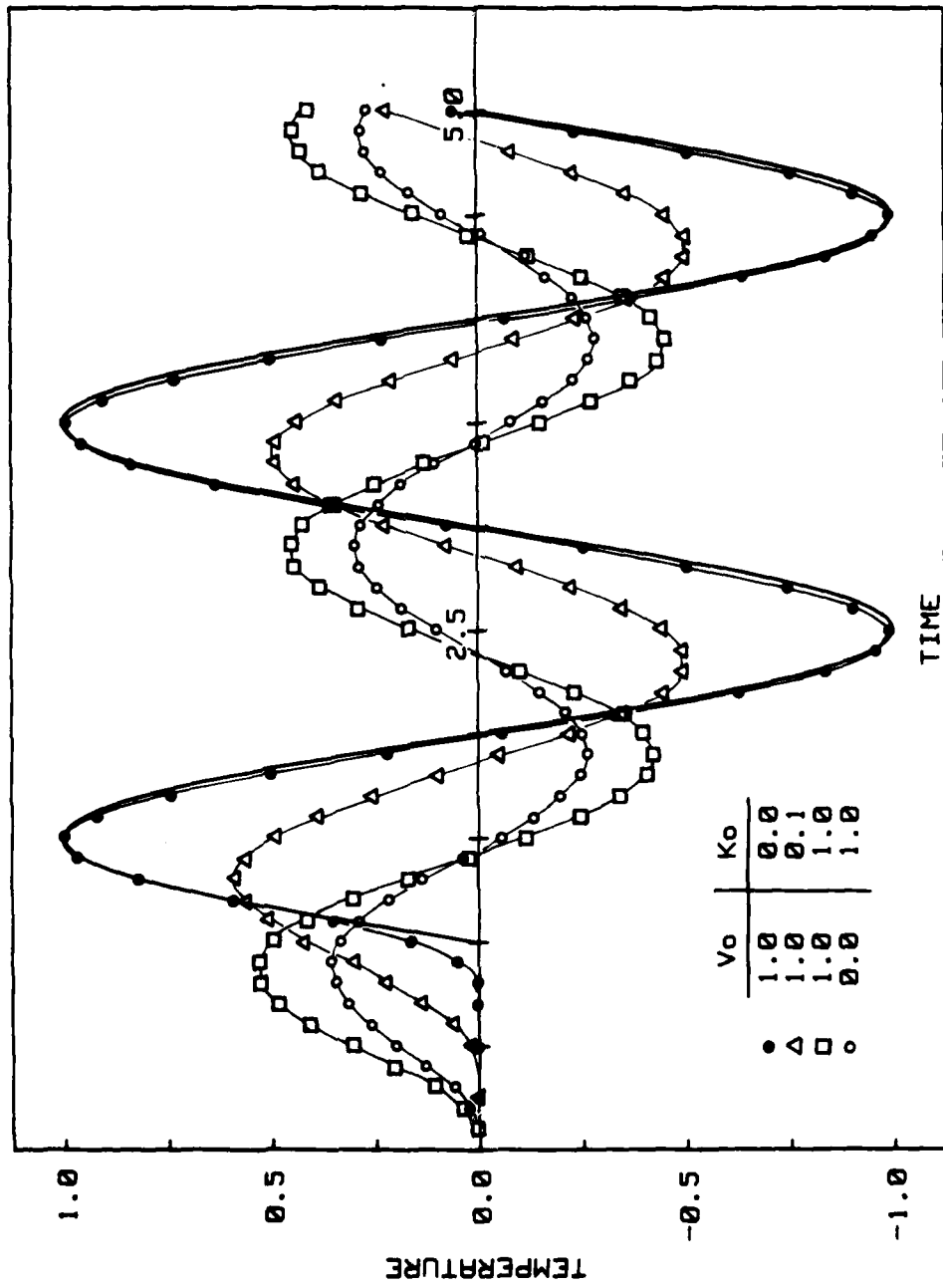
Va	Ko
1.0	0.0
1.0	0.1
1.0	1.0
0.0	1.0

● △ □ ○
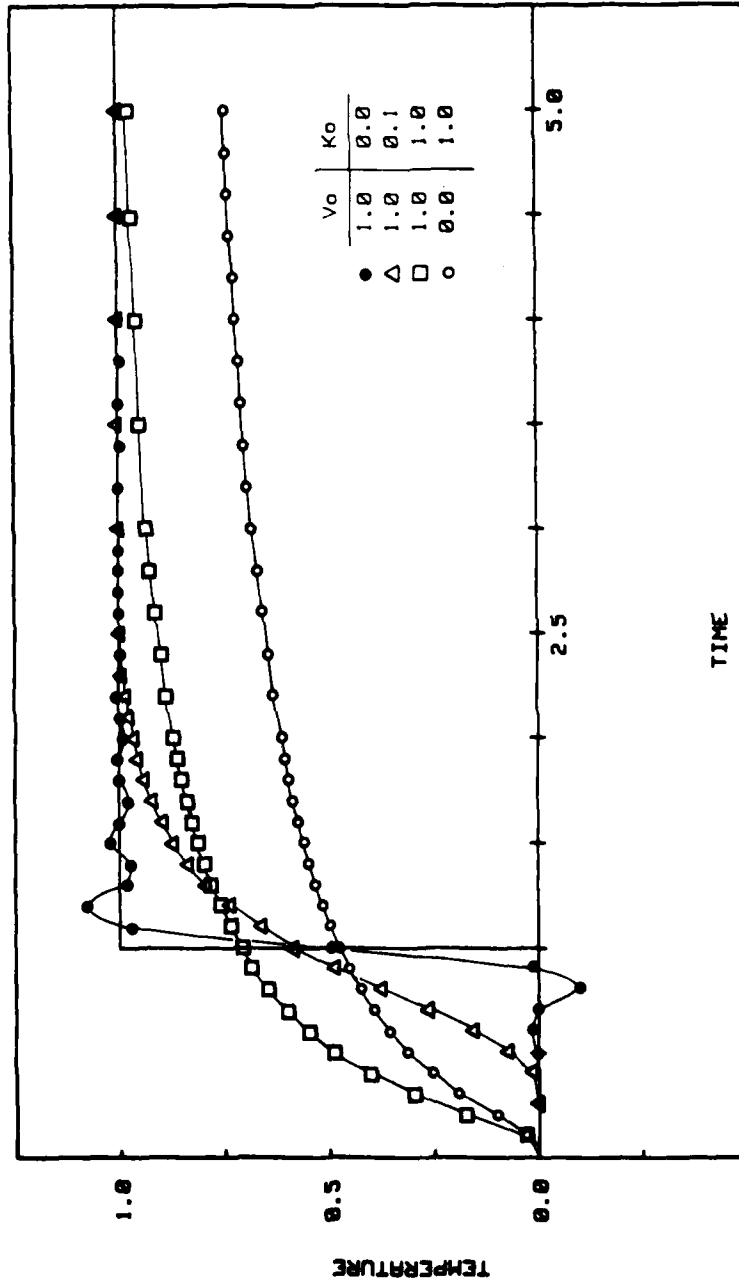
Fig. 16—Temperature time history at $x = 1.0$, (CE) model, TNE = 20.
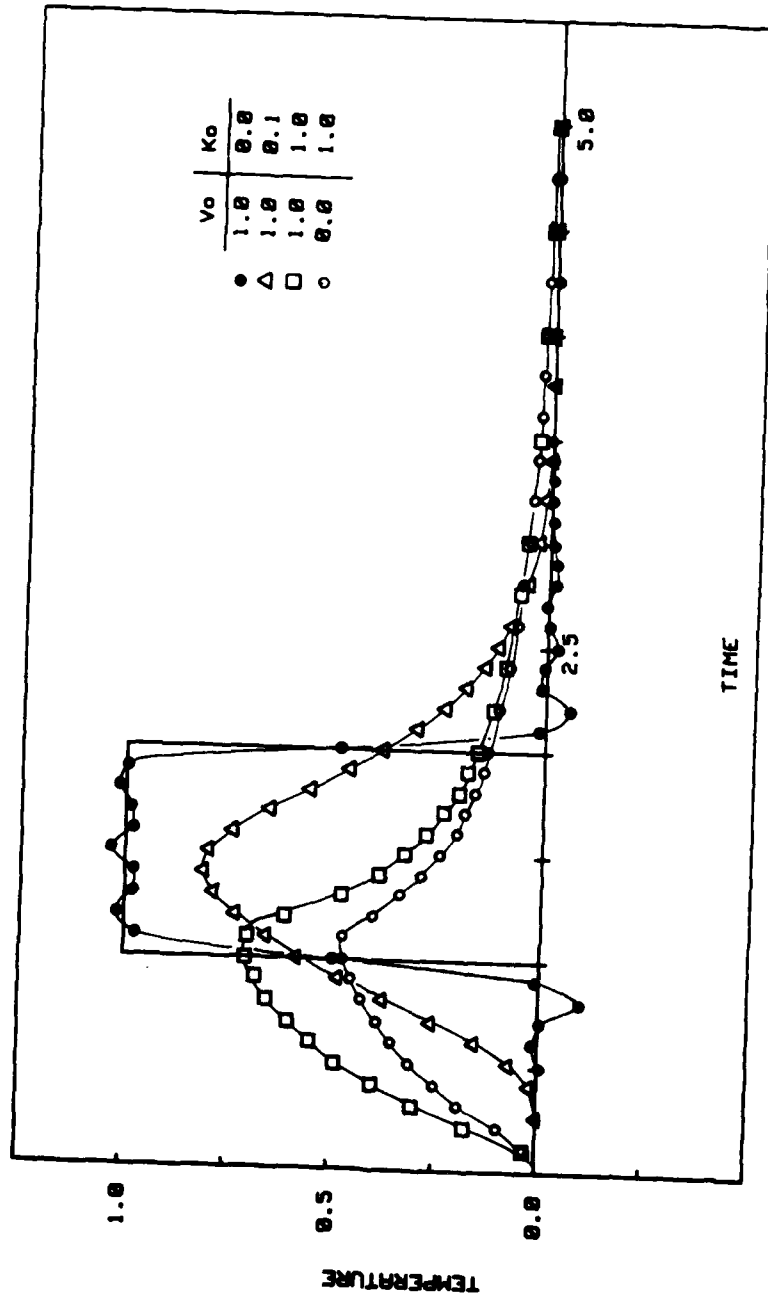
Fig. 17 — Temperature time history at $x = 1.0$ (CE) model, TNE $= 20$, $t_o = 1.0$.
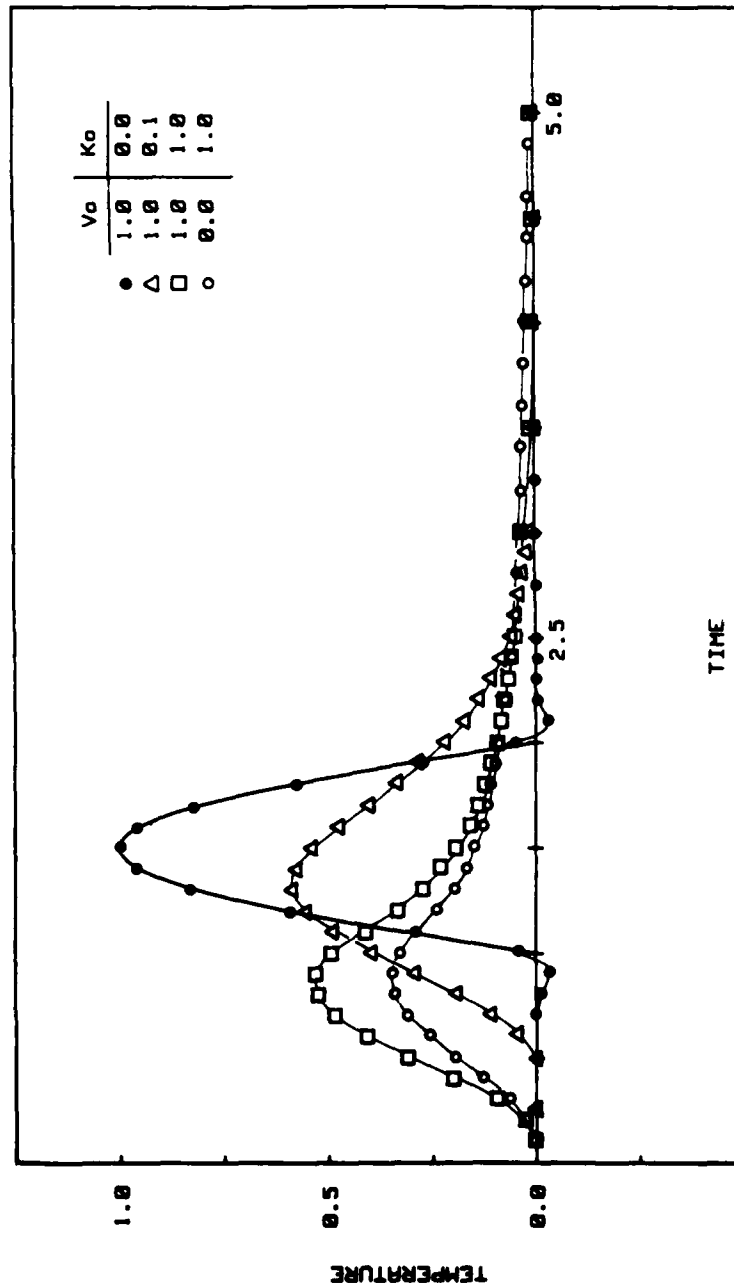
Fig. 18—Temperature time history at $x = 1.0$, (CE) model, TNE = 20, $t_o = 1.0$.
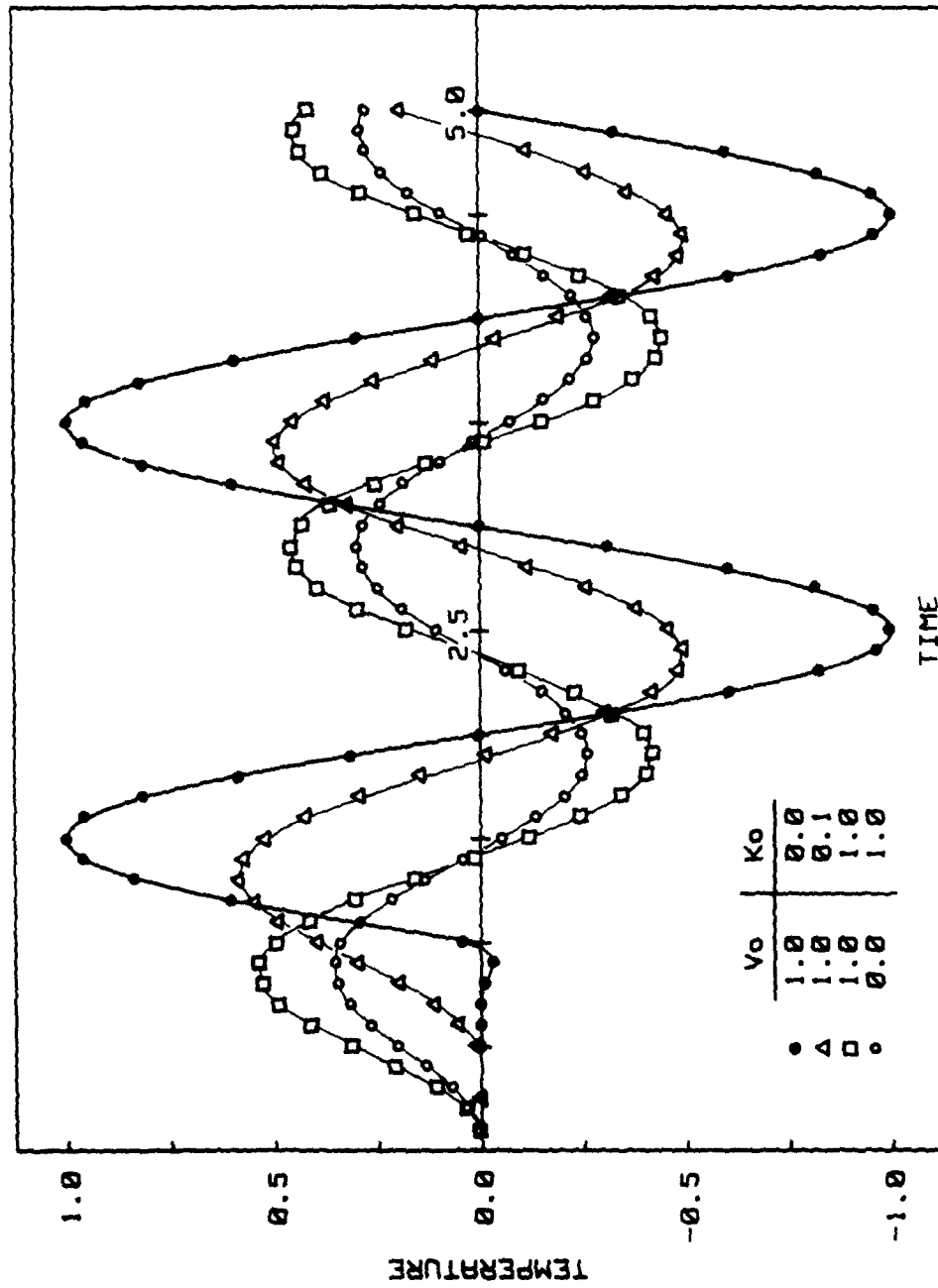
Fig. 19—Temperature time history at $x = 1.0$, (CE) model, TNE = 20.

Fig. 20 — Temperature distribution at $t = 2.0$ for the (LE) model, TNE = 30.

Fig. 21 — Temperature distribution at $t = 2.0$ for the (LE) model. TNE = 30, $t_o = 1.0$

Va	Ko
1.0	0.0
1.0	0.1
1.0	1.0
0.0	1.0
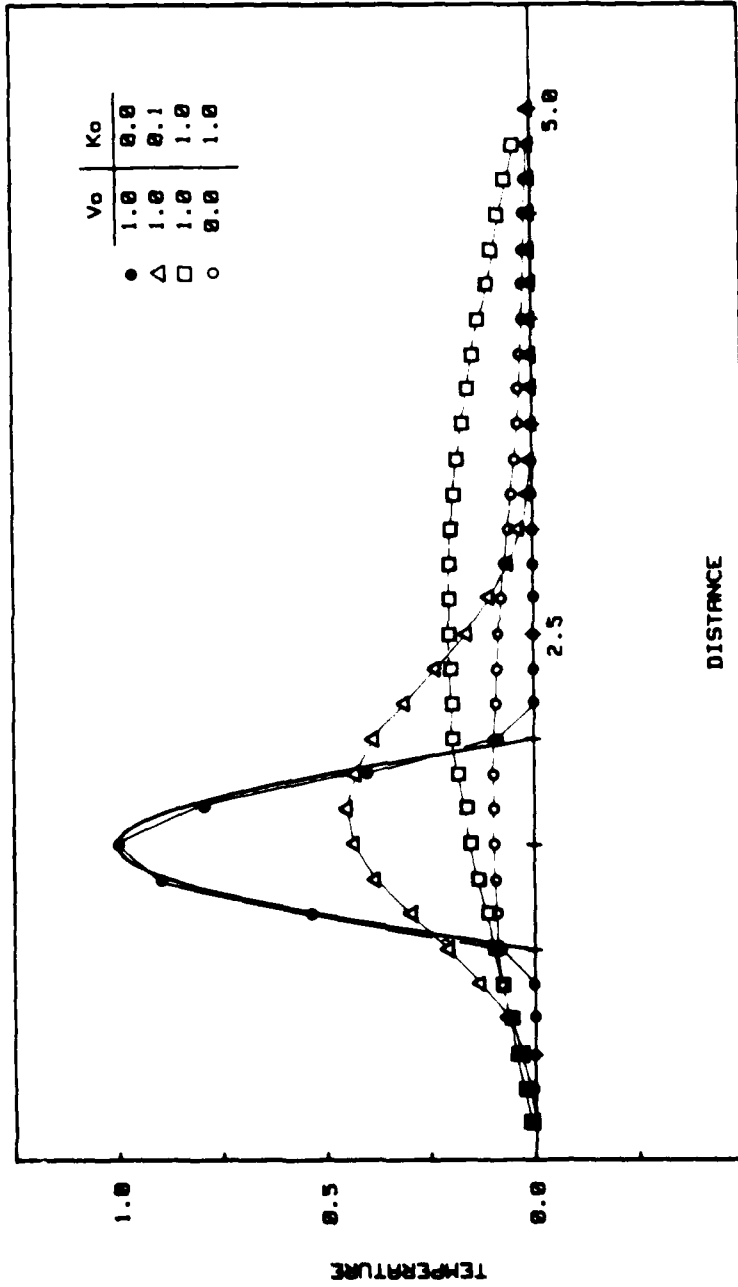
Fig. 22 — Temperature distribution at $t = 2.0$ for the (CE) model, TNE $= 30$, $t_o = 1.0$.

47
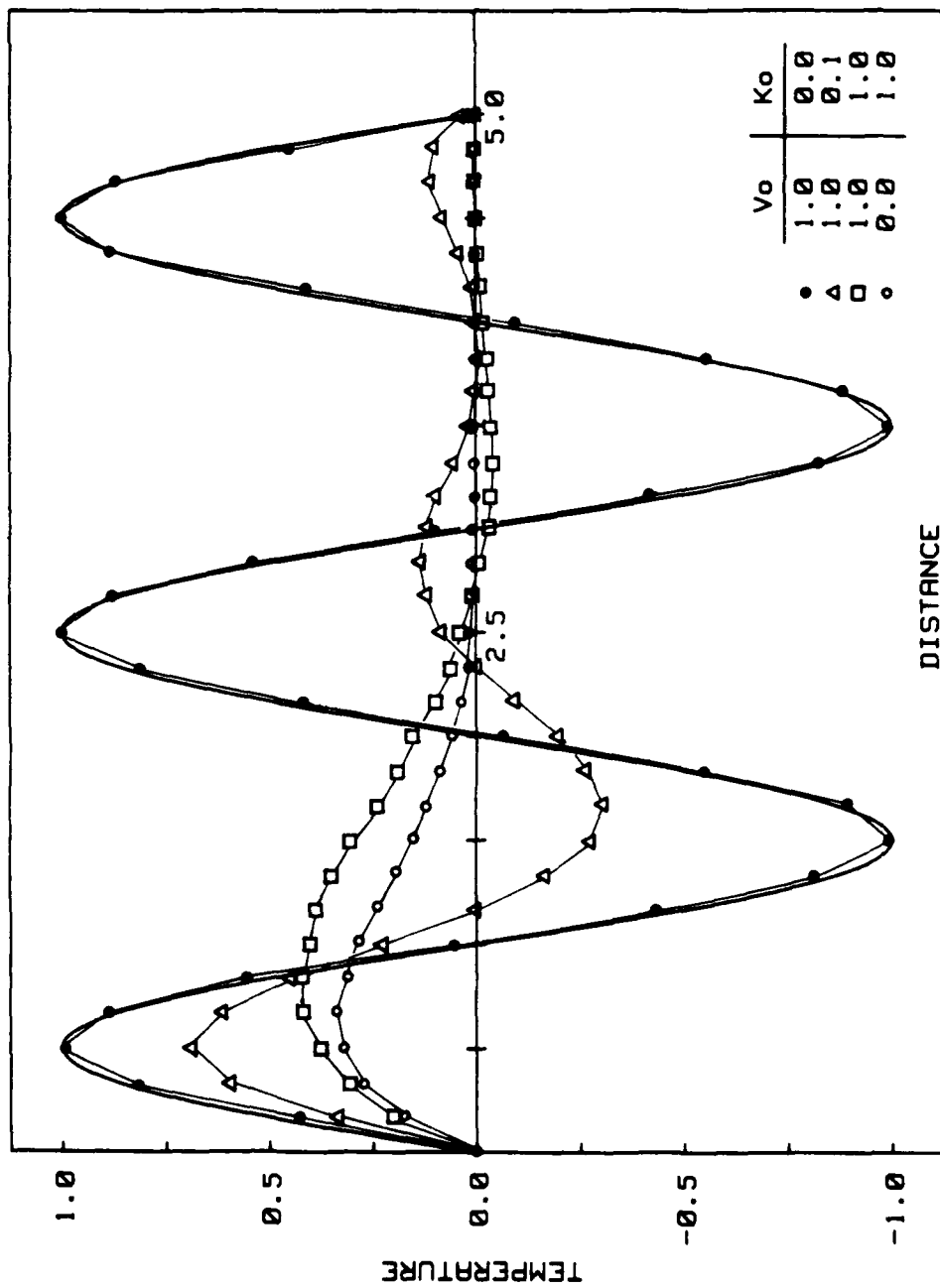
Fig. 23—Temperature distribution at $t = 5.0$ for the (LE) model, TNE $= 30$.
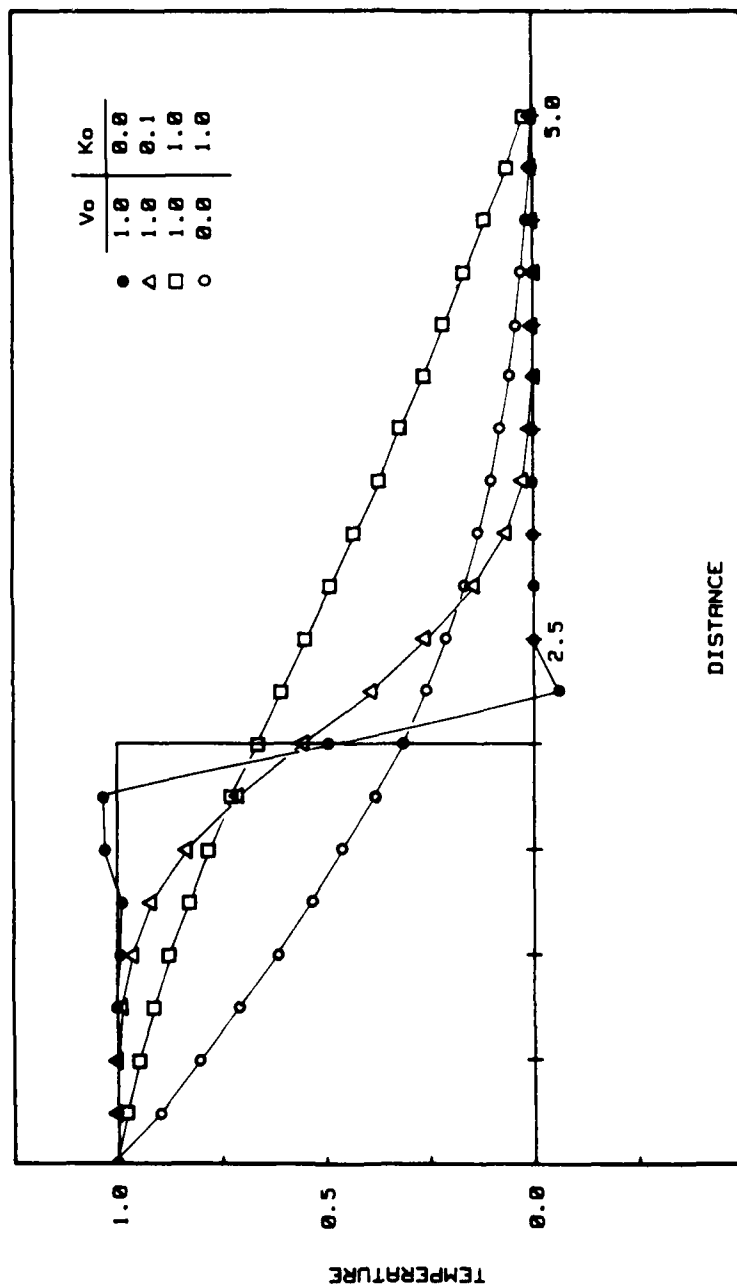
Fig. 24—Temperature distribution at $t = 2.0$ for the (CE) model, TNE = 20.
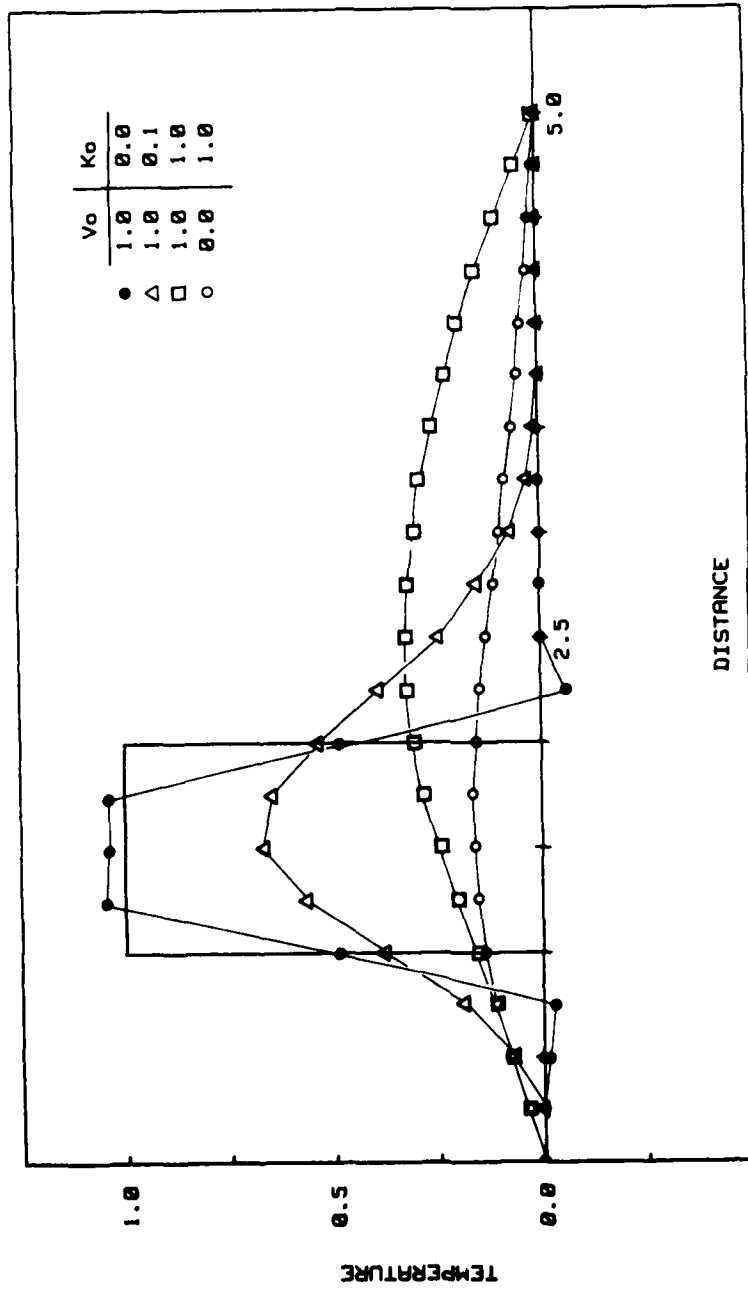
Fig. 25—Temperature distribution at $t = 2.0$ for the (CE) model, TNE $= 20$, $t_n = 1.0$.

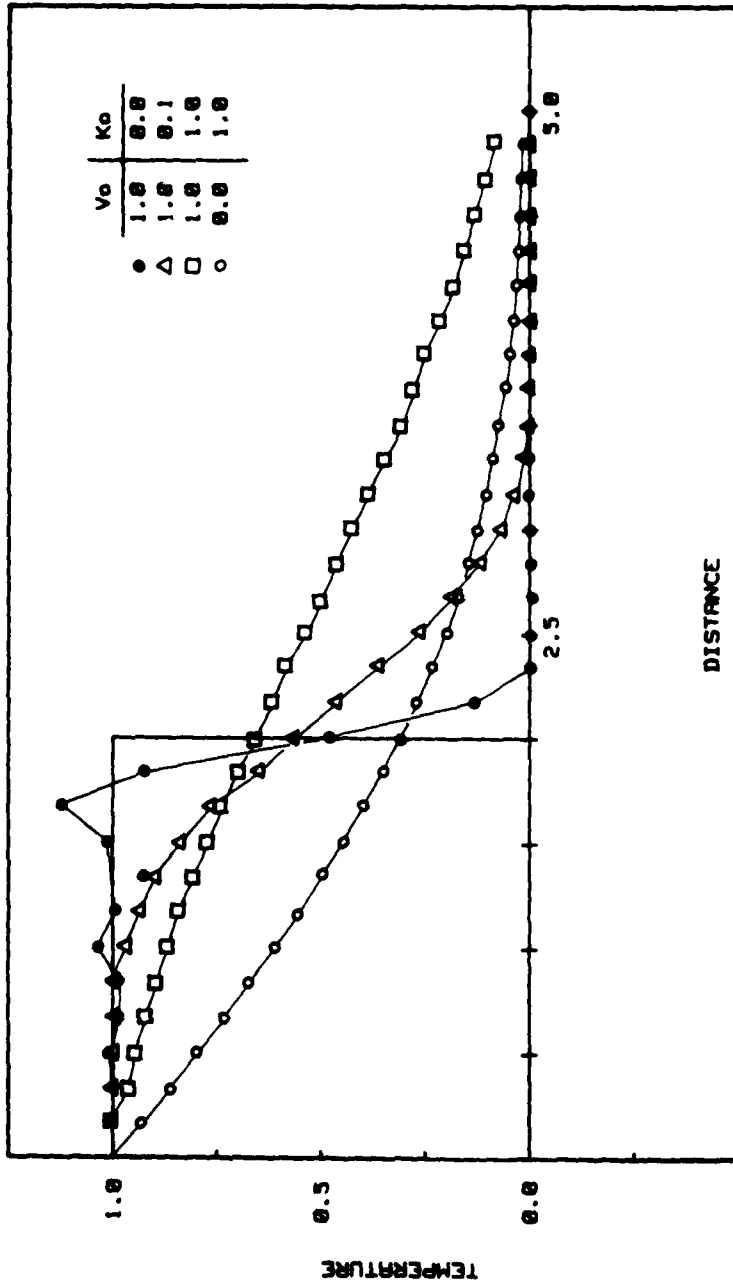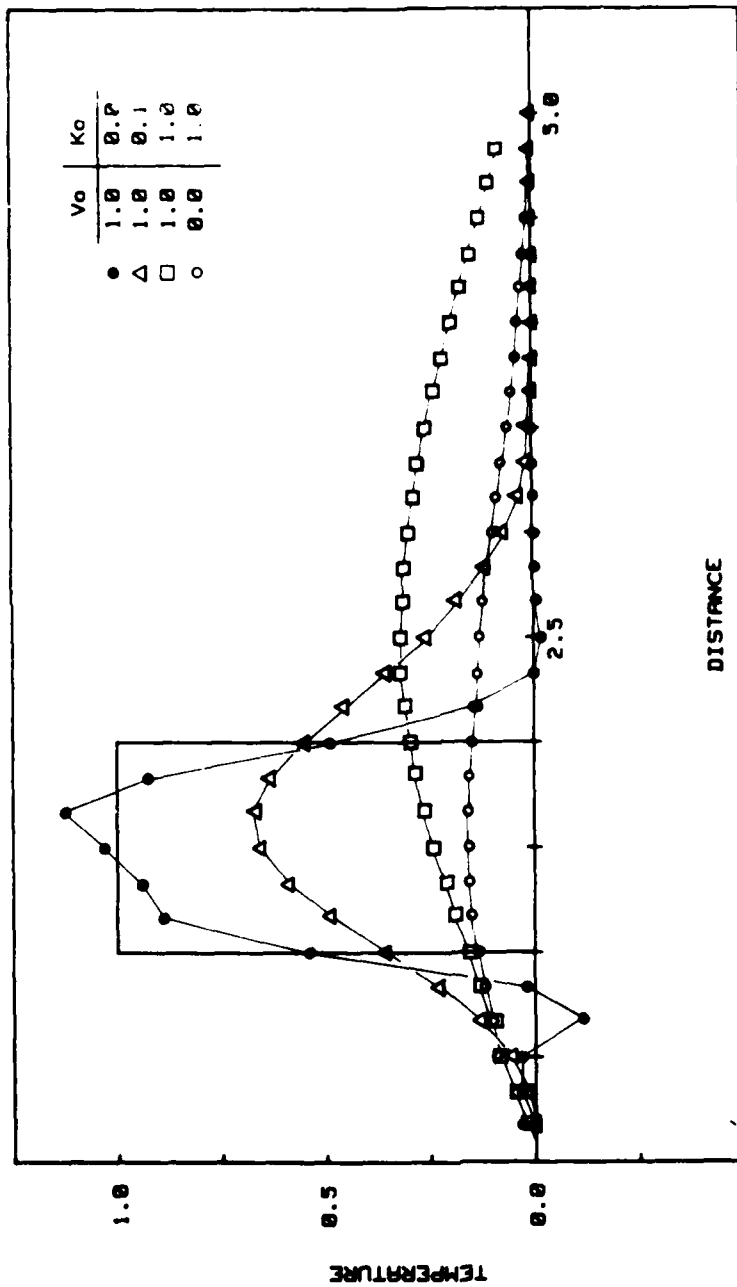Fig. 26 — Temperature distribution at $t = 2.0$ for the (CE) model, TNE = 20, $t_o = 1.0$.

Va	Ka
●	1.0	0.0
△	1.0	0.1
□	1.0	1.0
○	0.0	1.0

TEMPERATURE

DISTANCE
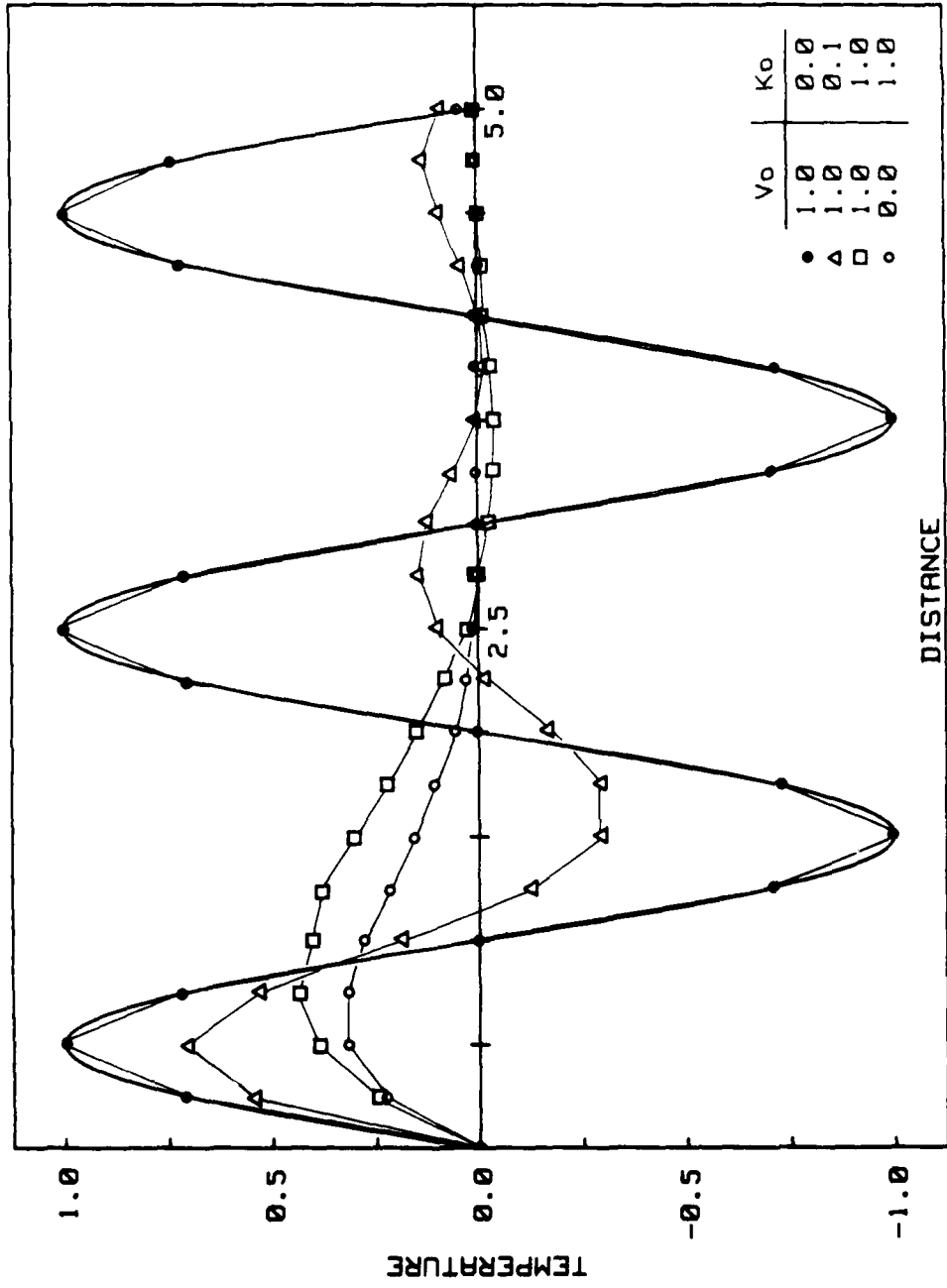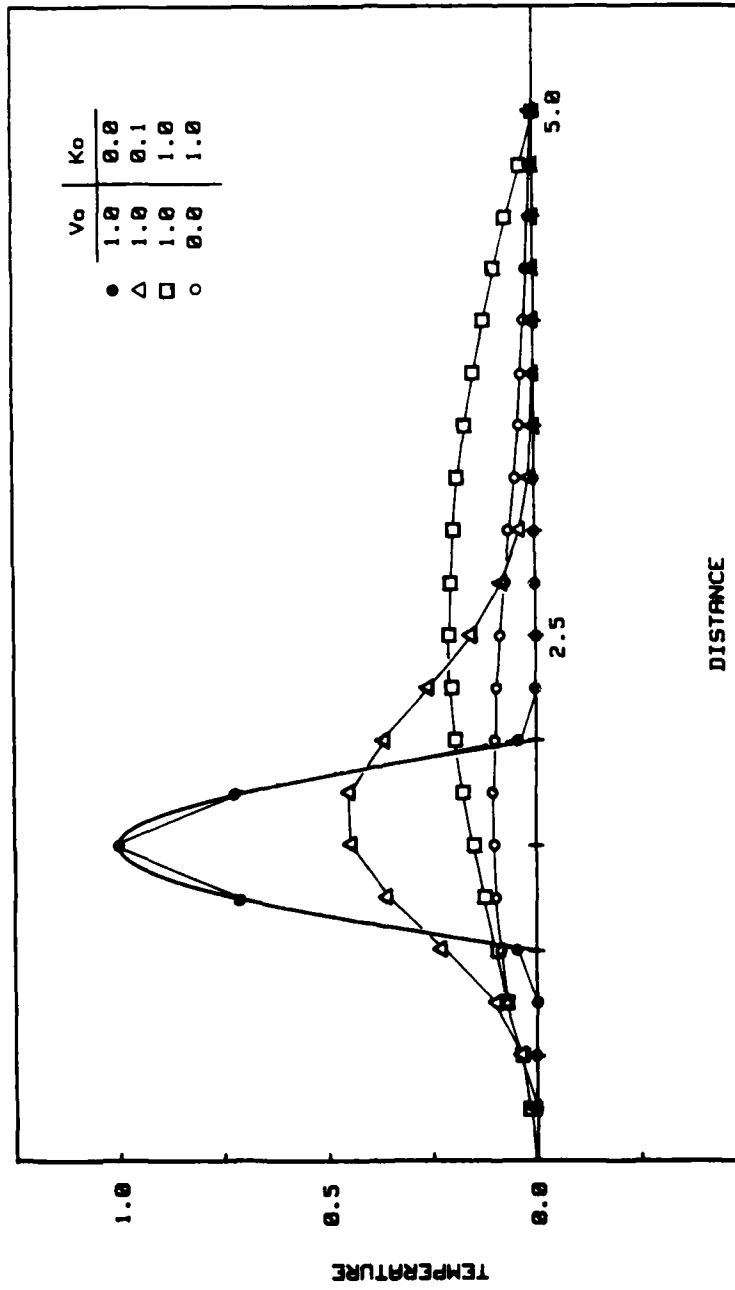
Fig. 27—Temperature distribution at $t = 5.0$ for the (CE) model, TNE = 20.

dispersion. On the other hand, the (CE) model gives a much better approximation of the wave but the oscillations of the numerical solution around the discontinuity are still present. These oscillations are inherent in any numerical solutions as is shown by a Fourier analysis in Appendix B. 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 artificially introduced diffusion will not allow a realistic evaluation of the developed finite element models, and will introduce artificial errors when true diffusion is present. From the obtained results 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.

The last set of boundary conditions represents the propagation of a sine wave through the half-space. In Figs. (14), (18), (22) and (26) results are given for $t_o = 1.0$ and in Figs. (15), (19), (23) and (27) the sine wave is continuously applied at the boundary. For the (LE) model results show some small error but the shape of the wave is not distorted. The higher order element model (CE) shows an excellent agreement with the exact wave even for the small number of elements used (TNE = 20). For these boundary conditions, 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 all the cases of boundary conditions and all choices of the constants K_o and V_o, the numerical solutions produced accurate results and the thermally induced waves propagate through the half-space in a very satisfactory manner.

SUMMARY AND CONCLUSIONS

A variational formulation for the convection-diffusion equation has been presented in this report, and, based in this formulation, two finite element models have been developed for the purpose of solving problems on propagation of thermally-induced induced waves.

The introduction of a new quantity, defined as heat displacement, is the basis for a generalized development of the convection-diffusion equation. The advantage of such a formulation is that it can be used to develop a displacement formulation for the finite element method. Furthermore, due to the generalized nature of the heat displacement, the formulation may be extended to other types of equations. Another advantage of the formulation is the introduced thermal force, for which one should point out its significance as a boundary force.

The physical conditions for the semi-infinite space require that $\theta \rightarrow 0$ as $x \rightarrow \infty$; 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 we consider the last nodal point as a boundary point and the thermal force as a boundary force, which is equal 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.

For the solution of the matrix differential equation, a third order backward finite difference scheme was used which is proved to be unconditionally stable. Further, the convergence of the two element models was investigated and some convergence criteria were discussed.

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. Comparison of present results with analytical solutions show 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 approxima-

tion 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.

In conclusion, the generalized form of the derived formulation, its efficiency in handling various types of boundary conditions, and its efficiency in solving not only diffusion-dominated flows but also convection-dominated flows deserve special emphasis. The superiority of the cubic element model over the linear one, especially for simulating sharp wave fronts, is also noted. An extension of the present formulation to two dimensional problems and its application to other types of equations are planned as future work.

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APPENDIX A

The variational formulation in this study and the application of the finite element method produced a system of simultaneous ordinary differential equations which may be represented by

$$D_{ij}\dot{q}_i + C_{ij}q_i = Q_j. \tag{A.1}$$

For the solution of (A.1), the first derivative is approximated by a third-order Newton backward difference scheme and at time step n has the form

$$\dot{q}_j^{(n)} = \frac{1}{6\Delta t}(11q_j^{(n)} - 18q_j^{(n-1)} + 9q_j^{(n-2)} - 2q_j^{(n-3)}). \tag{A.2}$$

In terms of (A.2) the system (A.1) yields

$$[11D_{ij} + 6\Delta tC_{ij}]q_j^{(n)} = 6\Delta tQ_i^{(n)} - D_{ij}[-18q_j^{(n-1)} + 9q_j^{(n-2)} - 2q_j^{(n-3)}]$$

or

$$[11\delta_{ij} + 6\Delta tD_{ik}^{-1}C_{kj}]q_j^{(n)} = 6\Delta tD_{ij}^{-1}Q_j + \delta_{ij}[18q_j^{(n-1)} - 9q_j^{(n-2)} \tag{A.3}$$
$$+ 2q_j^{(n-3)}].$$

Let the errors associated with each time step be given by

$$E_j^{(n-k)}, \quad k = 0, 1, 2, 3.$$

If these errors are added to (A.3), one obtains

$$A_{ij}[q_j^{(n)} + E_j^{(n)}] = 6\Delta tD_{ij}^{-1}Q_j^{(n)} + \delta_{ij}[18(q_j^{(n-1)} + E_j^{(n-1)})$$
$$- 9(q_j^{(n-2)} + E_j^{(n-2)}) + 2(q_j^{(n-3)} + E_j^{(n-3)})] \tag{A.4}$$

where

$$A_{ij} = 11\delta_{ij} + 6\Delta tD_{ik}^{-1}C_{kj}. \tag{A.5}$$

Subtraction of (A.4) from (A.3) yields

$$A_{ij}E_j^{(n)} = \delta_{ij}[18E_j^{(n-1)} - 9E_j^{(n-2)} + E_j^{(n-3)}]$$

or

$$E_i^{(n)} = A_{ij}^{-1}[18E_j^{(n-1)} - 9E_j^{(n-2)} + 2E_j^{(n-3)}].$$

For solution stability the errors at various time steps should be related as follows

$$E_j^{(n)} \leqslant E_j^{(n-1)} \leqslant E_j^{(n-2)} \leqslant g_{jk} E_k^{(n-3)}$$

with the amplification matrix g_{ij} given by

$$g_{ij} = A_{ik}^{-1} B_{ik} \tag{A.6}$$

where

$$B_{kj} = \delta_{kj} [18 W^{(2)} - 9 W^{(1)} + 2] \tag{A.7}$$

and

$$W^{(2)} \leqslant W^{(1)} \leqslant 1.$$

If one assumes that $W^{(2)} = W^{(1)} = 1$, then (A.7) becomes

$$B_{kj} = 11 \delta_{kj}$$

and (A.6) yields

$$g_{ij} = 11 A_{ij}^{-1} \tag{A.8}$$

for stable solution $g_{ij} \leqslant \delta_{ij}$, then Eq. (A.8) yields

$$\left[\delta_{ij} + \frac{6}{11} \Delta t D_{ik}^{-1} C_{kj} \right]^{-1} \leqslant \delta_{ij}$$

For the last relation to be valid the following should hold

$$\left[\delta_{ij} + \frac{6}{11} \Delta t D_{ik}^{-1} C_{kj} \right] \delta_{ij} \geqslant 1 \tag{A.9}$$

which is true for all values of Δt as long as the product $D_{ik}^{-1} C_{kj}$ is positive definite. Thus, the numerical integration scheme is unconditionally stable.

As an example, consider the case of the linear element model to approximate the solution given by (A.1). Assuming that the characteristic length L, is divided in three equal elements, the matrices D_{ij} and C_{ij} are given by

$$D_{ij} = \frac{\Delta x}{6} \begin{vmatrix} 2 & 1 & 0 & 0 \\ 1 & 4 & 1 & 0 \\ 0 & 1 & 4 & 1 \\ 0 & 0 & 1 & 2 \end{vmatrix}$$

$$C_{ij} = \frac{K_o}{\Delta x} \begin{vmatrix} 1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{vmatrix} + \frac{V_o}{2} \begin{vmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 0 & 0 & -1 & 1 \end{vmatrix}$$

For a two-point boundary value problem with

$$q(o,t) = q(L,t) = 0$$

the above matrices reduce to

$$D_{ij} = \frac{\Delta x}{6} \begin{vmatrix} 4 & 1 \\ 1 & 4 \end{vmatrix}, \quad C_{ij} = \begin{vmatrix} \dfrac{2K_o}{\Delta x} & -\dfrac{K_o}{\Delta x} + \dfrac{V_o}{2} \\ -\dfrac{K_o}{\Delta x} - \dfrac{V_o}{2} & \dfrac{2K_o}{\Delta x} \end{vmatrix} \qquad (A.10)$$

Substituting (A.10) into (A.9) one obtains

$$D_{ij}^{-1} C_{kj} = \frac{6}{15\Delta x} \begin{vmatrix} \dfrac{9K_o}{\Delta x} + \dfrac{V_o}{2} & -\dfrac{6K_o}{\Delta x} + \dfrac{V_o}{2} \\ -\dfrac{6K_o}{\Delta x} - \dfrac{V_o}{2} & \dfrac{9K_o}{\Delta x} - \dfrac{V_o}{2} \end{vmatrix} \geqslant 0$$

or

$$\left(\frac{12}{55} \right) \left(\frac{\Delta t}{\Delta x} \right) \left(\frac{18K_o^2}{\Delta x} \right) \geqslant 0 \qquad (A.11)$$

which is true for all values of Δt and Δx. Therefore, the numerical scheme is unconditionally stable.

APPENDIX B

The presence of oscillation in a numerical solution for the propagation of discontinuities is known as Gibbs phenomenon. To better understand this pheomenon, assume that a rectangular wave $H(t)$ of perod 2π (Figure B.1) is propagating with a certain velocity.
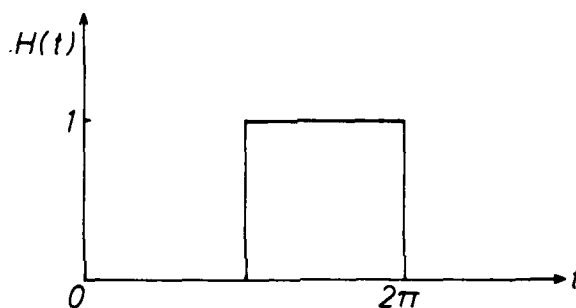
Figure B.1

An approximation of this wave can be obtained by a Fourier series for which the partial sum of the first $2n$ terms is given by

$$H_{2n}(t) = \frac{1}{2} + \frac{2}{\pi} \sum_{k=1}^{n} \frac{1}{2k-1} \sin(2k-1)t \qquad (B.1)$$

with the cosine terms all zero. This partial sum H_{2n} overshoots the function $H(t)$, as Gibbs pointed out, by the amount

$$H_{2n}\left(\frac{\pi}{2n}\right) \rightarrow 1.0895 \text{ as } n \rightarrow \infty$$

In fact, not only does this overshoot of H_{2n} exist, Figure B.2, but the sum also oscillates about $H(t)$ with these oscillations decreasing only away from the discontinuity.

60
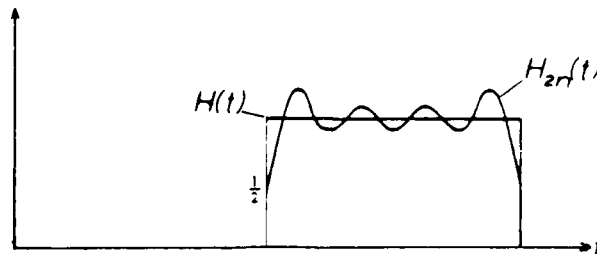
Figure B.2

The phenomenon can be explained by rewriting Eq. (B.1) as follows

$$H_{2n}(t) = \frac{1}{2} + \frac{2}{\pi} \sum_{k=1}^{n} \int_0^t \cos(2k-1)x \ dx$$

$$= \frac{1}{2} + \frac{2}{\pi} \int_0^t \sum_{k=1}^{n} \cos(2k-1)x \ dx$$

$$= \frac{1}{2} + \frac{1}{2} \int_0^t \frac{\sin 2nx}{\sin x} \ dx \qquad (B.2)$$

The maxima and minima of H_{2n} are obtained from Eq. (B.2) by requiring that

$$\frac{dH_{2n}(t)}{dt} = 0, \qquad \pi \leqslant t \leqslant 2\pi.$$

This requirement is satisfied when

$$\frac{\sin 2nt}{\sin t} = 0,$$

which is true for

$$t = \frac{m\pi}{2n} \quad m = 1, 2, \ldots, 2n-1.$$

The maxima and minima alternate and their values have been calculated by Carslow [11]. It is apparent that the oscillations of the approximation of the rectangular wave can be only reduced by including additional terms into the partial sum $H_{2n}(t)$. Damping of the oscillations and reduction of the overshoot can be achieved by introducing certain artificial factors into the terms of the summation.

61

```
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC
C                                                                         C
C                                                                         C
C      *********************************************************          C
C      *                                                       *          C
C      *              THERMAL  WAVE PROPAGATION                *          C
C      *                                                       *          C
C      *********************************************************          C
C                                                                         C
C      THIS PROGRAM SOLVES THE DIFFUSION-CONVECTION EQUATION              C
C                                                                         C
C                   DH/DT + V*DH/DX - D(K*DH/DX)/DX = 0                    C
C                                                                         C
C         FOR V=1 & K=0  : ADVECTION                                      C
C         FOR V=0 & K=1  : DIFFUSION                                      C
C                                                                         C
C                                                                         C
CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCC

C
      PROGRAM WAVE(N2,NK)
C
C*
C*************************************************************************
C*
C*             PROGRAM CONSTANTS
C*
C*      N = NUMBER OF ELEMENTS = NUMEL
C*    N+1 = NUMBER OF NODES = NNODE
C*     WO = INVERSE OF ELEMENT LENGTH
C*     VO = DIMENSIONLESS VELOCITY
C*     TK = DIMENSIONLESS DIFFUSIVITY
C*     DT = DIMENSIONLESS TIME STEP SIZE
C*     TO = DIMENSIONLESS TIME CONST. FOR BOUNDARY CONDITIONS
C*   TMAX = MAXIMUM TIME LIMIT FOR INTEGRATION
C*  IFREQ = CONSTANT FOR PRINTING RESULTS
C*  LCASE = ORDER OF F.E.M.
C*        = 1 ,FIRST ORDER ELEMENT
C*        = 2 , CUBIC HERMITIAN ELEMENT
C*     NB = NUMBER OF BOUNDARY CONDITIONS
C*    IBC = INITIAL CONDITINS CONST.
C*        = 0 , I.C. SET TO ZERO
C*        = 1 , I.C. SPECIFIED AT NODES
C*     AN = INTEGRATION CONSTANTS, N = 0,1,2,3,4,5
C*     R1 = BOUNDARY CONDITION CONST.
C*     RN = BOUNDARY CONDITION CONST.
C*         R1 = 1.0, RN = 0.0 SQARE WAVE
C*         R1 = 0.0, RN = 1.0 SINE WAVE
C*     AT = GLOBAL MASS MATRIX
C*     BT = GLOBAL STIFFNESS MATRIX
C*     TE = TEMPERATURE VECTOR
C*      H = DISPLACEMENT VECTOR
C*      C = PARTITIONED GLOBAL MATRIX
C*
C*************************************************************************
C*
```

```
        COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
        COMMON/BLOCK2/ X1(200),X2(200),X3(200),X4(200),YX(200)
        COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
        COMMON/BLOCK4/ NNTS,NNOS,NTS(100),NOS(200)
        COMMON/BLOCK5/ AO,A1,A2,A3,A4,A5,N1,R1,RN
        DIMENSION  AT(N2,N2),BT(N2,N2),C(NK,NK),IP(NK)
        DIMENSION TIME(200),TT(200)
        DIMENSION ID1(20), ID2(20)
        DATA STOP / 'STOP'/
C
        CALL R$STOP
C
C.....READ AND PRINT TITLE.....
C
100     READ(5,120,END=9999) ID1
        READ 120, ID2
        PRINT 125, ID1,ID2
C
C.....READ AND PRINT DATA.....
C
        READ 500, LCASE,R1,RN
        IF(LCASE.EQ.1)  GO TO 5
        WRITE(6,2015)
        GO TO 6
5       WRITE(6,2020)
6       CONTINUE
        READ(5,505) N,WO,VO,TK,TO,DT,TMAX,IFREQ,IBC,NB
        WRITE(6,600) N,WO,VO,TK,TO,DT,TMAX,IFREQ,IBC
C
C.....ELEMENT CONSTANTS
C
        NUMEL = N
        NNODE = N + 1
            NO = LCASE*(N - 1)
            N1 = LCASE*NUMEL + 1
            N2 = LCASE*(NUMEL + 1)
            MK = NK - 1
C
             T = 0.0
            IT = 0
C
C.....INTEGRATION CONSTANTS FOR 3RD ORDER BACKWARD DIFF....
C
            A0 = 11./6.
            A1 = 3.0
            A2 = -1.5
            A3 = 1./3.
            A4 = 0.0
C
            ICUNTE = 0
C
C.....READ INITIAL CONDITIONS
C
        CALL INCON(N2,NK,NUMEL,NNODE)
C
```

```
C.....SET BOUNDARY CONDITIONS FOR TEMPERATURE.....
C
C.....READ NODE NUMBERS AND SPECIFIED TEMPERATURES.....
C
      DO 110 I=1,NNODE
                INX = I
      READ(5,1015) WORD,NT,TNT
      IF(WORD.EQ.STOP) GO TO 115
              NTS(I) = NT
          TE(NTS(I)) = TNT
110   CONTINUE
C
C.....COUNT NODES WITH SPECIFIED TEMPERATURES.....
C
115       NNTS = INX - 1
          NNQS = N2 - NNTS
            NX = NNTS
            NY = NNQS
C
C.....SPECIFY THERMAL FORCES AT NODES.....
C
      DO 130 I=1,NY
            NQS(I) = I + 1
          TE(NQS(I)) = 0.0
130   CONTINUE
C
      WRITE(6,1060)
      DO 160 I=1,NNTS
      WRITE(6,1065) I,NTS(I),TE(NTS(I))
160   CONTINUE
      DO 15 I=1,N2
      DO 15 J=1,N2
          AT(I,J) = 0.0
15        BT(I,J) = 0.0
C
.C.....FORM THE MATRIX COEFFICIENT BT(I,J)
C
C     FROM THE MASS & STIFFNESS GLOBAL MATRICES.....
C
      CALL ELMAT(N2,NK,NUMEL,AT,BT)
C
C
C.....PARTITION THE SINGULAR MATRIX BT(I,J)
C     ACCORDING TO BOUNDARY CONDITIONS TO C(I,J)
C
      DO 50 I=1,NNQS
      DO 50 J=1,NNQS
          C(I,J) = BT(NQS(I),NQS(J))
      DO 45 K=1,NNTS
45        C(I,J) = C(I,J) -
     1            BT(NQS(I),NTS(K))/BT(NTS(K),NTS(K))*BT(NTS(K),NQS(J))
50    CONTINUE
C
      CALL DECOMP(NY,NY,C,IP,IER)
C
```

```
C.....PRINT INITIAL CONDITIONS & AFTER FIRST TIME STEP
C
C      THE RESULTS AT SPECIFIED TIME INTERVALS.....
C
10     CALL OUTPUT(N2,NK,T,NUMEL,NNODE)
C
C.....START TIME INTEGRATION
C
20        T = T + DT
C
C.....PLOT RESULTS WITH RESPECT TO TIME.....
C
          IT = IT + 1
         IWO = INT(WO)
          N4 = IWO + 1
       IF(MOD(IT,IFREQ).NE.0)  GO TO 25
                ITR = IT/IFREQ
             TT(ITR) = TE(N4)
           TIME(ITR) = T
25     CONTINUE
C
C.....FORM THE RIGHT HAND SIDE VECTOR Q(J) OF THE MATRIX EQUATION
C
C                          C(I,J)*X(I) = Q(J)
C
C      AND SOLVE FOR X(I).....
C
       CALL QVECT(N2,NX,NY,T,NUMEL,AT,BT,C,IP)
C
C.....IF T EXCEEDS TMAX, TERMINATE INDEGRATION ... .
C
       IF(T.LE.TMAX) GO TO 30
       CALL ONPLOT(TIME,TT,ITR)
       GO TO 100
30     ICUNTE = ICUNTE + 1
C
C.....PRINT RESULTS OR CONTINUE THE SOLUTION.....
C
       IF(ICUNTE.NE.IFREQ) GO TO 20
       ICUNTE = 0
       GO TO 10
C
```

```
C
C.....FORMAT STATEMENTS.....
C
120   FORMAT(20A4)
125   FORMAT(1H1,14X,44H********************************************,
     150H**********************************************,/15X,
     254H**********************************************,
     340H*******************************************,/15X,6H******.
     482X,6H******,/15X,6H******,
     520X,42H DIFFUSION-CONVECTION IN ONE DIMENSION     ,20X,
     66H******,/15X,6H******,
     76X,50H-------------------------------------------------,
     820H-------------------,6X,6H******,/15X,6H******,82X,
     96H******,/15X,6H******,1X,20A4,1X,6H******,/15X,6H******,
     11X,20A4,1X,6H******,/15X,6H******,
     282X,6H******,/15X,34H********************************,
     355H**********************************************,
     45H*****,/15X,44H*********************************************,
     550H**********************************************,/////)
500   FORMAT(I10,2F10.4)
505   FORMAT(I5,F6.2,2F8.4,3F6.4,3I5)
510   FORMAT(6F10.4)
600   FORMAT('1',2X,'N=',I2,5X,'WO=',F5.2,5X,'VO=',F8.6,5X,'TK=',F8.6,5X
     1,'TO=',F4.2,5X,'DT=',F6.4,5X,'TMAX=',F6.3,5X,'IFREQ=',I3,5X,'B.CON
     2D.=',I2,///)
2015  FORMAT(40X,'CUBIC-HERMITIAN FINITE ELEMENT APPROXIMATION',//)
2020  FORMAT(40X,'LINEAR FINITE ELEMENT APPROXIMATION',//)
1015  FORMAT(6X,A4,I10,F10.6)
1060  FORMAT(10X,'BOUNDARY CONDITIONS FOR TEMPERATUE',
     1//,8X,'I',4X,'NODE',5X,'TEMPERATURE',//)
1065  FORMAT(2X,2(4X,I3),3X,F12.3)
9999  STOP
      END
```

```
      SUBROUTINE CUBEL(N2,KL,NUMEL,AT,BT)
C**
C***********************************************************************
C**
C**      CUBEL CALCULATES THE ELEMENT MARTICES FOR THE
C**      CUBIC HERMITIAN ELEMENT MODEL
C**
C***********************************************************************
C**
      COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
      COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
      DIMENSION  A(4,4),B(4,4),AT(N2,N2),BT(N2,N2)
C
      TKO = TK
C
      DO 30 L=1,NUMEL
          KL1 = LCASE*(L-1)
C
C.....ELEMENT MASS MATRIX A(I,J).....
C
          A(1,1) =   4.*W(L)**2
          A(1,2) = 22.*W(L)
          A(1,3) =  -3.*W(L)**2
          A(1,4) = 13.*W(L)
          A(2,1) = 22.*W(L)
          A(2,2) = 156.0
          A(2,3) = -13.*W(L)
          A(2,4) = 54.0
          A(3,1) =  -3.*W(L)**2
          A(3,2) = -13.*W(L)
          A(3,3) =   4.*W(L)**2
          A(3,4) = -22.*W(L)
          A(4,1) = 13.*W(L)
          A(4,2) = 54.0
          A(4,3) = -22.*W(L)
          A(4,4) = 156.0
C
C.....ELEMENT STIFFNESS MATRIX B(I,J).....
C
C.....CONVECTIVE TERMS.....
C
          V11 =   0.0
          V12 = -42.*VO
          V13 =  -7.*VO*W(L)
          V14 = 42.*VO
          V21 = 42.*VO
          V22 = -210.*VO/W(L)
          V23 = -42.*VO
          V24 = 210.*VO/W(L)
          V31 =   7.*VO*W(L)
          V32 = 42.*VO
          V33 =   0.0
          V34 = -42.*VO
          V41 = -42.*VO
          V42 = -210.*VO/W(L)
          V43 = 42.*VO
          V44 = 210.*VO/W(L)
```

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```
C
C.....DIFFUSION TERMS.....
C
            CK11 =   56.*TKO
            CK12 =   42.*TKO/W(L)
            CK13 = -14.*TKO
            CK14 = -42.*TKO/W(L)
            CK21 =   42.*TKO/W(L)
            CK22 = 504.*TKO/W(L)**2
            CK23 =   42.*TKO/W(L)
            CK24 =-504.*TKO/W(L)**2
            CK31 = -14.*TKO
            CK32 =   42.*TKO/W(L)
            CK33 =   56.*TKO
            CK34 = -42.*TKO/W(L)
            CK41 = -42.*TKO/W(L)
            CK42 =-504.*TKO/W(L)**2
            CK43 = -42.*TKO/W(L)
            CK44 = 504.*TKO/W(L)**2
C
            B(1,1) = V11 + CK11
            B(1,2) = V12 + CK12
            B(1,3) = V13 + CK13
            B(1,4) = V14 + CK14
            B(2,1) = V21 + CK21
            B(2,2) = V22 + CK22
            B(2,3) = V23 + CK23
            B(2,4) = V24 + CK24
            B(3,1) = V31 + CK31
            B(3,2) = V32 + CK32
            B(3,3) = V33 + CK33
            B(3,4) = V34 + CK34
            B(4,1) = V41 + CK41
            B(4,2) = V42 + CK42
            B(4,3) = V43 + CK43
            B(4,4) = V44 + CK44
C
      DO 25  I=1,KL
      DO 25  J=1,KL
C
C.....FORMATION OF THE GLOBAL MASS MATRIX AT(I,J).....
C
            AT((I+KL1),(J+KL1)) = AT((I+KL1),(J+KL1)) + A(I,J)
C
C.....FORMATION OF THE GLOBAL STIFFNESS MATRIX BT(I,J).....
C
25          BT((I+KL1),(J+KL1)) = BT((I+KL1),(J+KL1)) + B(I,J)
30    CONTINUE
      RETURN
      END
```

```
      SUBROUTINE DECOMP(NN, NDIM, C, IP, IER)
C*
C*********************************************************************
C*  LINEAR SYSTEM SUBROUTINE
C*
C*  DECOMPOSE THE NN X NN MATRIX C INTO TRIANGULAR L AND U SO THAT
C*        L * U = P * C FOR SOME PERMUTATION MATRIX P.
C*  MATRIX TRIANGULARIZATION BY GAUSSIAN ELIMINATION.
C*
C*  INPUT..
C*    NN = ORDER OF MATRIX.
C*    NDIM = DECLARED DIMENSION OF ARRAY  C .
C*    C = MATRIX TO BE TRIANGULARIZED.
C*  OUTPUT..
C*    C(I,J), I.LE.J = UPPER TRIANGULAR FACTOR, U .
C*    C(I,J), I.GT.J = MULTIPLIERS = LOWER TRIANGULAR FACTOR, I - L.
C*    IP(K), K.LT. NN = INDEX OF K-TH PIVOT ROW.
C*    IP(NN) = (-1)**(NUMBER OF INTERCHANGES) OR 0 .
C*    IER = 0 IF MATRIX C IS NONSINGULAR, OR K IF FOUND TO BE
C*            SINGULAR AT STAGE K.
C*  USE  SOLVE  TO OBTAIN SOLUTION OF LINEAR SYSTEM.
C*  DETERM(C) = IP(N)*C(1,1)*C(2,2)*...*C(N,N).
C*  IF IP(NN)=0, A IS SINGULAR, SOLVE WILL DIVIDE BY ZERO.
C*********************************************************************
C*
85    FORMAT(5X,'SINGULAR MATRIX C AT STAGE K =',I3)
      DIMENSION C(NDIM,NN), IP(NN)
C
C.........INITIALIZE IER, IP(NN) .....
C
      IER = 0
      IP(NN) = 1
      IF (NN .EQ. 1) GO TO 70
      NM1 = NN - 1
      DO 60 K = 1,NM1
      KP1 = K + 1
      M = K
      DO 10 I = KP1,NN
10    IF (ABS(C(I,K)) .GT. ABS(C(M,K))) M = I
      IP(K) = M
      T = C(M,K)
      IF (M .EQ. K) GO TO 20
      IP(NN) = -IP(NN)
      C(M,K) = C(K,K)
      C(K,K) = T
20    IF (T .EQ. 0.0) GO TO 80
      T = 1.0/T
      DO 30 I = KP1,NN
30       C(I,K) = -C(I,K)*T
      DO 50 J = KP1,NN
      T = C(M,J)
      C(M,J) = C(K,J)
      C(K,J) = T
      IF (T .EQ. 0.0) GO TO 50
      DO 40 I = KP1,NN
40       C(I,J) = C(I,J) + C(I,K)*T
50    CONTINUE
```

```
60      CONTINUE
70         K = NN
        IF (C(NN,NN) .EQ. 0.0) GO TO 80
        RETURN
80         IER = K
           IP(NN) = 0
        WRITE(6,85)  IER
        RETURN
        END



C
        SUBROUTINE ELMAT(N2,NK,NUMEL,AT,BT)
C**
C**********************************************************************
C**
C**     ELMAT FORMS THE OVERALL GLOBAL MATRIX BT(I,J)
C**        IF LCASE = 1, BT(I,J) IS FOR THE LINEAR MODEL.
C**        IF LCASE = 2, BT(I,J) IS FOR THE CUBIC MODEL
C**
C**********************************************************************
C**
        COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
        COMMON/BLOCK5/ AO,A1,A2,A3,A4,A5,N1,R1,RN
        DIMENSION  AT(N2,N2),BT(N2,N2)
C
           KL = 2*LCASE
C
        IF(LCASE.EQ.1)  CALL LINEL(N2,KL,NUMEL,AT,BT)
        IF(LCASE.EQ.2)  CALL CUBEL(N2,KL,NUMEL,AT,BT)
C
        DO 10 I=1,N2
        DO 10 J=1,N2
10         BT(I,J) = AO*AT(I,J) + DT*BT(I,J)
        RETURN
        END
```

```
      SUBROUTINE INCON(N2,NK,NUMEL,NNODE)
C**
C****************************************************************************
C**
C**      INCON SETS THE INITIAL CONDITIONS FOR THE SYSTEM
C**      VARIABLES EQUAL ZERO IF NB = 0, OR TO SPECIFIED
C**      VALUES IF NB = 1.
C**
C****************************************************************************
C**
      COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
      COMMON/BLOCK2/ X1(200),X2(200),X3(200),X4(200),YX(200)
      COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
      COMMON/BLOCK5/ A0,A1,A2,A3,A4,A5,N1,R1,RN
C
      PI = 3.14159/2.0
C
      DO 10 I=1,N2
           X(I) = 0.0
          YX(I) = 0.0
          X1(I) = 0.0
          X2(I) = 0.0
          X3(I) = 0.0
10        X4(I) = 0.0
      DO 15 I=1,NNODE
          H(I) = 0.0
15    CONTINUE
C
C.....CALCULATE THE LENGTH FOR EACH ELEMENT.....
C
C
      DO 20 I=1,NUMEL
20    W(I) = 1./WO
      IF(NB.EQ.0)  GO TO 100
C
C.....IF NB = 1 SET INITIAL CONDITIONS.....
C
          L0 = N/10 + 1
          L1 = N/5 + 1
          H(L0-1) = -W(L0)
      DO 25 I=L0,L1
          TE(I) = 1.0
25        H(I) = H(I-1) + W(I)
          H(L0-1) = 0.0
      DO 30 I=L1,N
30        H(I+1) = H(L1)
C
      IF(LCASE.EQ.2)  GO TO 40
      DO 35 I=1,NNODE
35        X(I) = H(I)
      GO TO 50
40    DO 45 I=1,NNODE
        X(2*I-1) = TE(I)
45      X(2*I) =  H(I)
50    DO 55 I=1,N2
          X1(I) = X(I)
          X2(I) = X1(I)
          X3(I) = X2(I)
55        X4(I) = X3(I)
C
100   RETURN
      END
```

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```
      SUBROUTINE LINEL(N2,FL,NUMEL,AT,BT)
C**
C:*********************************************************************
C**
C**      LINEL CALCULATES THE ELEMENT MATRICES
C**      FOR THE LINEAR ELEMENT MODEL
C**
C:*********************************************************************
C**
      COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREO,LCASE,NB,IBC
      COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
      DIMENSION  A(2,2),B(2,2),AT(N2,N2),BT(N2,N2)
C
      DO 15 L=1,NUMEL
          KL1 = LCASE*(L-1)
C
C.....ELEMENT MASS MATRIX A(I,J).....
C
          A(1,1) = 2.0
          A(1,2) = 1.0
          A(2,1) = 1.0
          A(2,2) = 2.0
C
C.....ELEMENT STIFFNESS MATRIX B(I,J).....
C
          TKO = TK
          WO = 1./W(L)
C
C.....CONVECTIVE TERMS.....
C
          V11 = -3.*WO*VO
          V12 =  3.*WO*VO
          V21 = -3.*WO*VO
          V22 =  3.*WO*VO
C
C.....DIFFUSION TERMS.....
C
          CK11 =  6.*TKO*WO**2
          CK12 = -6.*TKO*WO**2
          CK21 = -6.*TKO*WO**2
          CK22 =  6.*TKO*WO**2
C
          B(1,1) = V11 + CK11
          B(1,2) = V12 + CK12
          B(2,1) = V21 + CK21
          B(2,2) = V22 + CK22
      DO 10 I=1,KL
      DO 10 J=1,KL
C
C.....FORMATION OF THE GLOBAL MASS MATRIX AT(I,J).....
C
          AT((I+KL1),(J+KL1)) = AT((I+KL1),(J+KL1)) + A(I,J)
C
C.....FORMATION OF THE GLOBAL STIFFNESS MATRIX BT(I,J).....
C
10        BT((I+KL1),(J+KL1)) = BT((I+KL1),(J+KL1)) + B(I,J)
15    CONTINUE
      RETURN
      END
```

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```
        SUBROUTINE OUTPUT(N2,NK,T,NUMEL,NNODE)
C**
C***********************************************************************
C**
C**     OUTPUT PRINTS RESULTS AT SPECIFIED TIME
C**     INTERVALS BY IFREQ.
C**     OUTPUT CALLS EXTERNAL SUBROUTINE ONPLOT(   )
C**     FOR PLOTING RESULTS.
C**
C***********************************************************************
C**
        COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
        COMMON/BLOCK2/ X1(200),X2(200),X3(200),X4(200),YX(200)
        COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
        COMMON/BLOCK5/ A0,A1,A2,A3,A4,A5,N1,R1,RN
        DIMENSION  DH(200),DX(200),RNODE(200)
C
C
C.....COMPUTE THE DISPLACEMENT & TEMPERATURE FOR THE LINEAR ELEMENT.....
C
          TKO = TK
          SUM1 = 0.0
          SUM2 = 0.0
        IF(LCASE.EQ.2)  GO TO 100
        DO  10 I= 1,NNODE
10        H(I) = X(I)
        DO  15 I=1,NUMEL
15        TE(I) = (H(I+1) - H(I))/W(I)
        DO  20 I=1,NUMEL
          DH(I) = AO*(H(I) + H(I+1)) - (YX(I) + YX(I+1))
          DX(I) =  2.*(H(I) -   H(I+1))*VO*DT/W(I)
          SUM1 = SUM1 + DH(I)
20        SUM2 = SUM2 + DX(I)
          SUM3 = ABS(SUM1) - ABS(SUM2)
C
        GO TO 150
C
C.....COMPUTE THE DISPLACEMENT & TEMPERATURE FOR THE CUBIC ELEMENT.....
C
100     DO 110 I=1,NNODE
          TE(I) = X(2*I-1)
110       H(I) = X(2*I)
        DO 115 I=1,NUMEL
          DH(I) = (TE(I+1) - TE(I))*AO - YX(2*I+1) + YX(2*I-1)
     1            - 6.*((H(I+1) + H(I))*AO - YX(2*I+2) - YX(2*I))/W(I)
          DX(I) = 12.*DT*(VO*(H(I+1)-H(I)) + TKO*(TE(I+1)-TE(I)))/W(I)**2
          SUM1 = SUM1 + DH(I)
115       SUM2 = SUM2 + DX(I)
          SUM3 = ABS(SUM1) - ABS(SUM2)
C
C.....PRINT THE RESULTS.....
C
150     WRITE(6,610) T
        WRITE(6,620)     SUM1,SUM2,SUM3
        WRITE(6,605)
          DH(NNODE) = 0.0
          DX(NNODE) = 0.0
        WRITE(6,615) (I,H(I),TE(I),DX(I),DH(I),I=1,NNODE)
```

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```
C
C.....PLOT RESULTS.....
C
      DO 30 I=1,NNODE
30        RNODE(I) = FLOAT(I)
C
      CALL ONPLOT(RNODE,TE,NNODE)
C
600   FORMAT(5X,E14.6)
605   FORMAT(////,'  NODAL POINT    H-DISPLACEMENT TE-TEMPERATURE
     1    DH/DX         DH/DT',//)
610   FORMAT(1H1,5X,'TIME =',F6.3,//)
615   FORMAT(1I10,4X,4F15.6)
620   FORMAT(20X,'DH/DT  =',F10.6,5X,'DH/DX  =',F10.6,5X,F12.6,//)
      RETURN
      END



      SUBROUTINE QVECT(N2,NX,NY,T,NUMEL,AT,BT,C,IP)
C**
C***********************************************************************
C**
C**       QVECT SETS THE RIGHT HAND SIDE VECTOR Q(J)
C**       AND FORMS THE SYSTEM OF EQUATIONS
C**                         C(I,J)*X(I) = Q(J) ,   I,J = 1,NY
C**       QVECT CALLS SUBROUTINE SOLVE FOR THE
C**       SOLUTION OF THE SYSTEM OF EQS.
C**
C***********************************************************************
C**
      COMMON/BLOCK1/ N,WO,VO,TK,TO,DT,TMAX,IFREQ,LCASE,NB,IBC
      COMMON/BLOCK2/ X1(200),X2(200),X3(200),X4(200),YX(200)
      COMMON/BLOCK3/ X(200),W(200),TE(200),H(200),FQ(200)
      COMMON/BLOCK4/ NNTS,NNQS,NTS(100),NQS(200)
      COMMON/BLOCK5/ A0,A1,A2,A3,A4,A5,N1,R1,RN
      DIMENSION AT(N2,N2),BT(N2,N2),C(NY,NY),IP(NY)
      DIMENSION  F(200),Q(200),LISTX(100),LISTY(200)
C
      PI = 3.14159
C
C.....BOUNDARY CONDITIONS.....
C
      IF(T.LE.TO) GO TO 10
          TE(1) = 0.0
      GO TO 15
10        TE(1) = R1 + RN*SIN(T*PI)
15    CONTINUE
      IF(NB.EQ.1)  TE(1) = 0.0
```

```
C
C.....FORM THE RIGHT HAND SIDE VECTOR Q(I).....
C
      DO 20 I=1,N2
         FQ(I) = 0.0
20       YX(I) = A1*X1(I) + A2*X2(I) + A3*X3(I) + A4*X4(I)
C
      IF(LCASE.EQ.2) GO TO 25
         FQ(1) = -6.*TK*DT*TE(1)/W(1)
         FQ(N1) =  6.*TK*DT*TE(N)/W(N)
      GO TO 30
25    CONTINUE
         FQ(2) = -420.*TK*DT*TE(1)/W(1)
         FQ(N2) =  420.*TK*DT*TE(N+1)/W(N)
30    CONTINUE
C
      DO 40 I=1,N2
         F(I) = FQ(I)
      DO 40 J=1,N2
40       F(I) = F(I) + AT(I,J)*YX(J)
C
      DO 50 I=1,NY
          Q(I) = F(NQS(I))
      DO 45 K=1,NX
45        Q(I) = Q(I) - BT(NQS(I),NTS(K))/BT(NTS(K),NTS(K))*F(NTS(K))
50    CONTINUE
C
C.....SOLVE THE SYSTEM OF EQUATIONS.....
C
      CALL SOLVE(NY,NY,C,Q,IP)
C
      DO 100 I=1,NY
100      X(NQS(I)) = Q(I)
      IF(LCASE.EQ.2) GO TO 120
         X(1) = X(2) - TE(1)*W(1)
      IF(IBC.NE.1)
     * X(N+1) = X(N) + TE(N)*W(N)
      GO TO 130
120   CONTINUE
      DO 125 I=1,NX
125      X(2*NTS(I)-1) = TE(NTS(I))
130   CONTINUE
      DO 150 I=1,N2
          X4(I) = X3(I)
          X3(I) = X2(I)
          X2(I) = X1(I)
          X1(I) = X(I)
150   CONTINUE
      RETURN
      END
```

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```
C
      SUBROUTINE SOLVE (NN, NDIM, C, Q, IP)
C*
C***********************************************************************
C*   SOLUTION OF LINEAR SYSTEM, C*X = Q .
C*   INPUT..
C*     NN = ORDER OF MATRIX.
C*     NDIM = DECLARED DIMENSION OF ARRAY  C .
C*     C = TRIANGULARIZED MATRIX OBTAINED FROM DECOMP.
C*     Q = RIGHT HAND SIDE VECTOR.
C*     IP = PIVOT VECTOR OBTAINED FROM DECOMP.
C*   DO NOT USE IF DECOMP HAS SET IER .NE. 0.
C*   OUTPUT..
C*     Q = SOLUTION VECTOR, X .
C***********************************************************************
C*
      DIMENSION C(NDIM,NN), Q(NN), IP(NN)
C
      IF (NN .EQ. 1) GO TO 50
         NM1 = NN - 1
      DO 20 K = 1,NM1
         KP1 = K + 1
         M = IP(K)
         T = Q(M)
         Q(M) = Q(K)
         Q(K) = T
      DO 10 I = KP1,NN
10       Q(I) = Q(I) + C(I,K)*T
20    CONTINUE
      DO 40 KB = 1,NM1
         KM1 = NN - KB
         K = KM1 + 1
         Q(K) = Q(K)/C(K,K)
         T = -Q(K)
      DO 30 I = 1,KM1
30       Q(I) = Q(I) + C(I,K)*T
40    CONTINUE
50       Q(1) = Q(1)/C(1,1)
      RETURN
      END
*
```