A FINITE ELEMENT METHOD FOR UNSTEADY HEAT CONDUCTION IN MATERIALS WITH OR WITHOUT PHASE CHANGE

by

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A thesis submitted to the Faculty of Graduate Studies and Research in partial fulfillment of the requirements for the degree of Master of Engineering

Department of Mechanical Engineering
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August, 1980
To my parents,
ABSTRACT

The formulation of a general numerical method for the solution of unsteady heat conduction in materials with or without solid-liquid phase change is presented. A fully-implicit control-volume based finite element method is merged with the so-called enthalpy model to construct the proposed method. This enables the solution of problems with irregular-shaped and multiply-connected domains. In its present form, the method is formulated to handle two-dimensional problems, but its key ideas are also applicable to three-dimensional problems. Problems that involve both subcooled solid regions and superheated liquid regions can be solved by the proposed method. In the case of the latter, however, the method is strictly applicable only when the exclusion of natural convection effects is justifiable.

In the proposed method, the calculation domain is first discretized into either three-node triangular elements or four-node rectangular elements. Then polygonal control volumes surrounding each node in the domain are constructed by joining the centroids of the elements to the midpoints of the corresponding sides. The governing equations of the enthalpy model are then nondimensionalized and applied to these control volumes. Next, suitable interpolation functions
for the dependent variables are selected and algebraic discretization equations are derived. Following this, a modified Gauss-Seidel iterative method is formulated for the solution of the discretization equations.

The proposed method has been successfully applied to numerous test problems. The results of a few illustrative examples are presented to demonstrate the validity and capabilities of the method.
Le présent ouvrage propose une méthode numérique générale pour résoudre la conduction instable de la chaleur dans des matériaux avec ou sans changement de phase solide-liquide. La présente méthode émerge de la combinaison d'un modèle d'enthalpie et d'une méthode implicite des éléments finis basée sur un élément de volume. Ceci permet de résoudre des problèmes avec des domaines de forme irrégulière et à embranchements multiples. Dans sa forme actuelle, la méthode permet la résolution de problèmes bidimensionnels, mais ses principes de base peuvent aussi s'appliquer à des problèmes tridimensionnels. La méthode ici proposée peut résoudre des problèmes impliquant des régions solides sous-réfrigérées ou des régions liquides surchauffées. Dans ce dernier cas, cependant, l'application de la méthode n'est justifiable que lorsque les effets naturels de convection sont exclus.

Dans la méthode proposée, le domaine de calcul est d'abord discrétisé en éléments triangulaires de trois noeuds ou en éléments rectangulaires de quatre noeuds. Des volumes polygonaux, entourant chaque noeud du domaine, sont alors construit en joignant les centroïdes aux points de milieu des côtés correspondants. Les équations fondamentales du modèle d'enthalpie sont alors mises sous forme non-dimensionnelle et appliquées à ces volumes. En suite, des fonctions d'interpolation
admissibles pour les variables dépendantes sont choisies et les équations de discretization sont dérivées. Finalement une méthode itérative modifiée de Gauss-Seidel est utilisée pour résoudre les équations de discretization.

La méthode ici proposée a été appliquée avec succès à plusieurs problèmes types. Les résultats de quelques uns de ces exemples sont présentés afin de démontrer la validité et les capacités de la méthode.
ACKNOWLEDGEMENTS

The author wishes to express his sincere appreciation to Professor B.R. Baliga for his encouragement, support and advice throughout the course of this work.

The author would also like to extend many thanks to Ms. Assunta Cerrone for typing this manuscript.

This research project was performed under auspices of the Department of Mechanical Engineering of McGill University, whose support is much appreciated.
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<td>A</td>
<td>Surface area of container; coefficient in interpolation functions, Eqns. (3-8) and (3-9).</td>
</tr>
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<td>ADDT&lt;sub&gt;j&lt;/sub&gt;</td>
<td>Area of control volume, associated with node j, divided by the time step ( \Delta t ).</td>
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<tr>
<td>B</td>
<td>Coefficient in interpolation function, Eqns. (3-8) and (3-9).</td>
</tr>
<tr>
<td>Bi</td>
<td>Biot number, ( hL/k ).</td>
</tr>
<tr>
<td>C</td>
<td>Coefficient in interpolation function, Eqns. (3-8) and (3-9).</td>
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<tr>
<td>C</td>
<td>Specific heat.</td>
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<td>D</td>
<td>Coefficient in interpolation function, Eqn. (3-9).</td>
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<td>E&lt;sub&gt;i&lt;/sub&gt;</td>
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<td>h</td>
<td>Convective heat transfer coefficient.</td>
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<td>i</td>
<td>Specific enthalpy</td>
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<tr>
<td>k</td>
<td>Thermal conductivity.</td>
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<tr>
<td>L</td>
<td>Half width of square container.</td>
</tr>
<tr>
<td>n</td>
<td>Unit normal to control surface.</td>
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<tr>
<td>P</td>
<td>Pressure</td>
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<tr>
<td>Q</td>
<td>Surface integrated heat transfer rate.</td>
</tr>
<tr>
<td>q</td>
<td>Local heat flux.</td>
</tr>
<tr>
<td>R</td>
<td>Radius of conduits.</td>
</tr>
<tr>
<td>S</td>
<td>Center-to-center distance between conduits.</td>
</tr>
<tr>
<td>SYMBOL</td>
<td>DESCRIPTION</td>
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<td>-----------------------------------------------------------------------------</td>
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<tr>
<td>( \text{Ste} )</td>
<td>Stefan number for liquid, ( c \frac{(T_o - T_{\text{sat}})}{\lambda} ).</td>
</tr>
<tr>
<td>( \text{Ste}_s )</td>
<td>Stefan number for solid, ( c_s \frac{(T_{\text{sat}} - T)}{\lambda} ).</td>
</tr>
<tr>
<td>( s )</td>
<td>Arc length along control surface.</td>
</tr>
<tr>
<td>( T )</td>
<td>Temperature.</td>
</tr>
<tr>
<td>( T_o )</td>
<td>Initial temperature.</td>
</tr>
<tr>
<td>( T_{\text{sat}} )</td>
<td>Saturation temperature.</td>
</tr>
<tr>
<td>( T )</td>
<td>Cooling fluid temperature.</td>
</tr>
<tr>
<td>( t )</td>
<td>Time.</td>
</tr>
<tr>
<td>( u )</td>
<td>Specific internal energy.</td>
</tr>
<tr>
<td>( V )</td>
<td>Volume of the control volume.</td>
</tr>
<tr>
<td>( S_V )</td>
<td>Surface area (or perimeter) of the control volume.</td>
</tr>
<tr>
<td>( v_n^* )</td>
<td>Local velocity of interface in the direction of ( n^* ).</td>
</tr>
<tr>
<td>( x, y )</td>
<td>Spatial coordinates.</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>Thermal diffusivity, ( (k/\rho c) ).</td>
</tr>
<tr>
<td>( \xi, \eta )</td>
<td>Dimensionless spatial coordinates, ( x/L ) and ( y/L ) or ( x/R ) and ( y/R ).</td>
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<td>( \theta )</td>
<td>Dimensionless enthalpy, Eqn. (3-3).</td>
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<td>( \lambda )</td>
<td>Latent heat of fusion.</td>
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<td>( \psi )</td>
<td>Angular position along conduit surface.</td>
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<tr>
<td>( \rho )</td>
<td>Density.</td>
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<tr>
<td>( \gamma )</td>
<td>Ratio of specific heats, ( c_s/c ).</td>
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<td>( \Gamma )</td>
<td>Ratio of thermal diffusivities, ( \alpha/\alpha_s ).</td>
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<td>( \phi, \phi' )</td>
<td>Dimensionless temperatures, Eqns. (3-3) and (4-8).</td>
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<tr>
<td>( \tau )</td>
<td>Dimensionless time, ( (\tau \alpha/L^2) ).</td>
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<td>SUBSCRIPTS</td>
<td>DESCRIPTION</td>
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<tr>
<td>------------</td>
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</tr>
<tr>
<td>l</td>
<td>Liquid phase.</td>
</tr>
<tr>
<td>s</td>
<td>Solid phase.</td>
</tr>
<tr>
<td>w</td>
<td>Wall of container or conduit.</td>
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<tr>
<td>m</td>
<td>Time level.</td>
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<tr>
<td>*</td>
<td>Saturated state.</td>
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1-1 AIMS OF THE THESIS AND MOTIVATION

Numerous technologically important problems involve unsteady heat conduction in materials with or without phase change. Examples of such problems can be found in such diverse areas as the freezing and thawing of foodstuffs and soils, the solidification of castings, the heating and melting of the anode in high intensity electric arcs, the storage of thermal energy in phase change materials (PCM's), and the production of silicon crystals for the electronics industry (1-4). A majority of such problems are multidimensional, and they involve irregular domain shapes. Further, all problems involving phase change are characterized by one or more interfaces, or phase boundaries, whose positions and shapes vary with time; mathematically, therefore, these problems are nonlinear. The main aim of this thesis is the formulation and application of a general numerical method for the solution of such problems.

To date, several analytical, semianalytical, and numerical methods for unsteady heat conduction in materials with or without phase change have been proposed in the
published literature (1-13). In general, analytical and semianalytical methods have a limited range of applicability. Numerical methods, on the other hand, enjoy a great deal of versatility, and they are better suited for the solution of the practical problems mentioned above (1,10). Most of the available numerical methods, however, suffer from severe complications, or fail completely, when they are applied to problems which involve irregular-shaped and multiply-connected domains. The method proposed in this thesis is free from these difficulties.

The above-mentioned unsteady phase-change problems are often three-dimensional; an adequate description of such problems requires at least three space coordinates. In this thesis, however, because of the limitations imposed by the available resources of computer time and storage, attention will be focused on the formulation of a numerical method for unsteady plane two-dimensional problems. The aim, nevertheless, is to propose a method whose key ideas can be easily extended to unsteady three-dimensional problems. It is to be noted in this connection that two-dimensional formulations can adequately model many practical problems (4). Further, three-dimensional effects can often be accounted for by performing fairly simple calculations with the results of a two-dimensional model (14).
The method proposed in this thesis is formulated to handle liquid-solid (freezing) and solid-liquid (melting) phase-change problems; it can handle problems that involve both subcooled solid regions and superheated liquid regions. Problems involving evaporation or boiling (liquid-gas phase change) are not within the scope of this thesis. Further, the proposed method is strictly applicable only to problems which allow the following assumptions: (a) equilibrium solidification with a smooth interface; (b) constant density in each phase; (c) negligible influence of density difference between solid and liquid phases; (d) uniform thermal conductivity and specific heat in each phase. A brief examination of the validity of these assumptions is presented in the next paragraph.

Supercooling, or metastable states, may be encountered in some phase-change materials (PCM's), but there are numerous PCM's, especially high temperature PCM's, which suffer very little or no supercooling. Further, most of the important PCM's used in thermal energy storage units conform to assumption (a) very well (20). The main influence of assumption (b) is the exclusion of natural convection effects in the liquid phase. In many problems, during both melting and freezing, however, it is quite likely that heat will be transported by natural convection in the liquid phase (15).
The study of this complicated problem is not within the scope of this thesis. Thus in problems which involve significant natural convection effects, the results of the proposed method can be used only as conservative predictions of the actual phenomena (20). Often, in phase change problems, the density difference between solid and liquid phases could lead to shrinkage cavities. Such shrinkage cavities, however, usually occur in the interior of the PCM, and not near the heat transfer surfaces (20). As a consequence, they exert very little influence on the bulk of the heat transfer process (20), and assumption (c) is quite valid. If the range of operating temperatures is narrow, a condition met in numerous practical phase change problems, assumption (d) is justifiable. Further, this assumption is involved in the proposed method mainly for convenience in its formulation, and, as will be evident in subsequent chapters, it is not too difficult to do away with this assumption.

The building and testing of a general computer program incorporating the proposed method formed an important part of the work reported in this thesis. It was done mainly to enable the application of the proposed method to a wide variety of one- and two-dimensional test problems. The results of four such problems, selected to illustrate the different capabilities of the proposed method, are reported.
in this thesis.

1-2 SYNOPIS OF AVAILABLE METHODS

As was mentioned in the previous section, several analytical, semianalytical, and numerical methods for unsteady heat conduction in materials with or without phase change are currently available in the published literature. A review of most of these methods can be found in Refs. (1,2,10,11), so it will not be repeated here. Only a few numerical methods that are relevant to the work reported in this thesis will be briefly discussed in this section. It is usual to group the numerical methods for phase-change problems into two categories: temperature models and enthalpy models (10). This categorization is adopted in the following discussion.

In numerical methods based on the temperature model, as the name implies, the temperature of the PCM is the sole dependent variable, and energy conservation equations are written separately for the solid and liquid phases; the requirements of continuity of temperature and energy conservation are used to match the solutions at the interfaces, or phase boundaries. In all such methods, one of the main difficulties is the handling of the time varying phase boundary, and a number of different techniques have been devised to solve it. One approach is based on the so-called
quasi-steady assumption: over a small time interval, the phase boundary, which is at the saturation temperature, is assumed to be fixed in space, and the temperature distributions in the liquid and solid phases are solved: then the phase boundary is relaxed, or adjusted, to a new position using an energy balance condition, and the procedure is repeated (5). Another approach is to model the latent heat effect as a large thermal capacity over a small temperature range, which includes the saturation temperature, and smooth out the values of thermal conductivity and specific heat (6-8). Often, a coordinate transformation is used to fix the phase boundary and map the domain onto a regular-shaped region, if required (9). Methods based on these techniques suffer from some shortcomings. The quasi-steady approach is a tedious method, especially in multidimensional problems; it usually requires adjustments of the grid at each time step, and this, in turn, necessitates the interpolation of the dependent variables (5). Some of these methods cannot handle problems that involve a discrete phase-change, or saturation, temperature (8). Methods that rely on transformations to fix the phase boundary become very complicated, or fail completely, when multiply-connected domains are encountered. Kushner (11) has proposed a "synthesized-phase boundary method" which appears to be free from the aforementioned difficulties; a finite element method based on the Galerkin formulation is
used in this method. Bonnerot and Jamet (12) have also proposed a finite element method for phase change problems; in their method, at each time step, the position of the nodes is allowed to change so as to approximate the phase boundary by a piecewise-linear curve.

In the enthalpy models, the specific enthalpy is used as a dependent variable along with the temperature. The phase boundary position and shape are not explicitly determined, and the problem is made equivalent to one of nonlinear heat conduction without phase change. Although the phase boundary is not tracked explicitly, its position can be determined approximately by an examination of the enthalpy distribution. Of the available enthalpy models (10, 13), the one proposed by Shamsundar and Sparrow (10) appears to be the most versatile. It is based on a finite difference formulation, however, so it is not well suited for the solution of problems with irregular domain shapes. Further, it is limited to freezing problems in which the entire liquid phase is initially in a saturated state. In a subsequent paper, Shamsundar and Srinivansan (4) have extended this method to account for superheat effects: using a suitable method, the single phase conduction, or convection, problem is solved and the time required for the initiation of solidification is determined: at this stage, all residual superheat effects
are ignored, the entire liquid phase is assumed to be at the saturation temperature, and the phase change problem is solved using the method described in Ref. (10). This method could get quite inaccurate if significant superheat or high cooling rates are involved, and it is fairly tedious to start with. An integrated method that can deal with superheated liquid phase and subcooled solid phase, simultaneously, is desirable.

1-3 AN OVERVIEW OF THE PROPOSED METHOD

In the proposed method, a fully-implicit finite element method is used in conjunction with an enthalpy model. Its formulation was done in three stages: first, a simplified version of the control-volume based finite element method developed by Baliga and Patankar (16) was constructed and modified for the solution of unsteady heat conduction problems; then the enthalpy model of Shamsundar and Sparrow (10) was extended to enable the handling of problems involving superheated liquid phase; finally, the aforementioned finite element method and enthalpy model were amalgamated. This strategy allowed the realization of the aims stated in Section 1-1. Further, as will be evident in subsequent chapters, this approach allows an easy interpretation of the formulation in terms of physically meaningful quantities such
as fluxes, sources, temperature, and enthalpy. The key ideas of the formulation are summarized below.

First, the domain is discretized into a finite number of elements: two types of elements are considered in this thesis, three-node triangular elements and four-node rectangular elements. Following this, each node is associated with a polygonal-shaped control volume. These control volumes are obtained by joining the centroids of the elements to the midpoints of the corresponding sides. Suitable interpolation functions are then selected for the dependent variables: in triangular elements, the temperature is interpolated linearly, and in rectangular elements, it is interpolated bilinearly; the nodal values of the enthalpy are assumed to prevail over their associated control volumes; the properties of the PCM are stored at the centroids of the elements, and their values are assumed to prevail over the elements. Next, the first law of thermodynamics, in the form of an integral enthalpy equation (10), is imposed on each of the control volumes in the domain. The interpolation functions described above are then used to obtain a set of algebraic discretization equations that approximate the integral enthalpy equations. Another set of algebraic equations is provided by the known enthalpy versus temperature relationship for the PCM under consideration. These two
coupled sets of algebraic equations are solved by a modified version of the Gauss-Seidel iterative method. Following this, auxiliary computations are done to obtain spatially local and total heat fluxes at the domain boundaries, solidification fraction, and interface positions, all as functions of time. The formulation of the proposed method is geared to handle three different types of boundary conditions: specified temperature boundaries, specified heat flux boundaries, and convectively cooled or heated boundaries. Radiation boundary conditions, if encountered, can be linearized and handled iteratively as convection boundary conditions.

1-4 SURVEY OF THE THESIS

The aims of this thesis and the motivation behind it were discussed in Section 1-1. A synopsis of currently available methods and an overview of the proposed method were also presented in preceding sections of this chapter. A brief survey of the rest of this thesis is presented in this section.

Chapter II is devoted mainly to the presentation and discussion of the enthalpy model used in the construction of the proposed method. First, the governing equations of the enthalpy model and the temperature model are presented. Following this, the equivalence of the proposed enthalpy
model and the more familiar temperature model is demonstrated.

The formulation of a general control-volume based finite element method, incorporating the above mentioned enthalpy model, is presented in Chapter III. The discussion is keyed to five basic building blocks which are used to construct the proposed method. First, the domain discretization procedure is described. Then, a specialization of the enthalpy model to enable its amalgamation with the control-volume based finite element method is presented. A discussion of suitable interpolation functions for the dependent variables and the PCM properties follows. Next, attention is focused on the derivation of the discretization equations. Finally, the procedure used to solve the discretization equations is described.

The proposed method has been incorporated in a couple of general computer programs, and it has been successfully applied to a wide variety of one- and two-dimensional test problems. The results of four illustrative examples of such problems are presented in Chapter IV. In Chapter V, the last chapter of this thesis, the key ideas and results of this thesis are summarized and commented upon, and some ideas for the improvement and extension of the proposed method are presented.
CHAPTER II

PROBLEM FORMULATION

The mathematical formulation of the two-dimensional phase-change problem depicted schematically in Fig. 1a is the subject of this chapter. The calculation domain is irregular in shape and multiply-connected. It is assumed that the densities of the solid and liquid phase are identical and uniform; natural convection effects are ignored, and it is assumed that the energy transfer inside the calculation domain is by conduction only. Other thermophysical properties of the solid and liquid phases may not be the same, and they may vary with temperature.

As discussed in Chapter I, the currently available solution methods for this problem can be grouped into two categories. All methods based on the enthalpy model are grouped in one category, and those based on the temperature model are assigned to the other. In this chapter, both the enthalpy model and the temperature model are presented. It is also shown that the mathematical formulation of the enthalpy model is equivalent to the set of equations used in the temperature model; namely, the partial differential equations that describe energy conservation in the solid and liquid regions, and at the solid-liquid interface.
2-1 GOVERNING EQUATIONS

2-1-1 Enthalpy Model

Consider an irregular-shaped control volume, V, which is fixed in space; such a control volume is shown in Fig. 1b. If there are no sources of energy inside V, and no external work is performed on it, the first law of thermodynamics gives:

\[
\frac{d}{dt} \int_V \rho u \, dV = \int_{\partial V} K \nabla T \cdot \hat{n} \, ds
\]

(2-1)

where \( \rho \) is the density, \( u \) is the specific internal energy, and \( K \) is the thermal conductivity. This equation is applicable to control volumes in single phase regions and also to control volumes through which the solid-liquid interface passes, see Fig. 1c. For the problem under consideration, the pressure \( p \), is independent of time. Therefore:

\[
\frac{d}{dt} \int_V p \, dV = 0
\]

(2-2)

The specific enthalpy, \( i \), is defined by

\[
i = u + p/\rho
\]

(2-3)
In Eqn. (2-1), if ρu is replaced by (ρi-p), then the following form of energy conservation equation is obtained:

$$\frac{d}{dt} \int_{V} \rho_i \, dV = \int_{\partial V} K \, \text{grad} \, T \cdot \mathbf{n} \, ds$$

(2-4)

This is the so-called enthalpy equation (7).

2-1-2 Temperature Model

In this model, the conventional forms of energy conservation equations are used. Thus, in the solid:

$$\rho C_p \frac{\partial T}{\partial t} = \text{div}(K_s \, \text{grad} \, T)$$

(2-5)

and in the liquid:

$$\rho C_p \frac{\partial T}{\partial t} = \text{div}(K_l \, \text{grad} \, T)$$

(2-6)

At the solid-liquid interface(s), \( T = T_{sat} \), and an energy balance condition applies:

$$(K_s T/\partial n^*)_s - (K_l T/\partial n^*)_l - \rho \lambda V^* = 0$$

(2-7)

In Eqn. (2-7), \( \lambda \) is the enthalpy of fusion, and \( V^* \) is the local
velocity of the interface(s) normal to itself.

2-2 EQUIVALENCE OF THE ENTHALPY MODEL AND THE TEMPERATURE MODEL

Shamsundar and Sparrow (7) have proved the equivalence of the enthalpy model and the temperature model. A similar proof is presented below.

In order to show the equivalence of Eqn. (2-4) to the equations of the temperature model, it will first be applied to a control volume without an interface, and then to a control volume which contains the interface.

For the case where the control volume does not contain the interface, both \((\rho i)\) and \((K \text{ grad } T)\) are continuous throughout \(V\) and \(\partial V\), so the divergence theorem can be applied to the right-hand side of Eqn. (2-4). Thus,

\[
\int_V \frac{\partial}{\partial t} (\rho i) \, dV = \int_V \text{div}(K \text{ grad } T) \, dV \quad (2-8)
\]

Eqn. (2-8) may be rewritten as:

\[
\int_V \left[ \frac{\partial}{\partial t} (\rho i) - \text{div}(K \text{ grad } T) \right] \, dV = 0 \quad (2-9)
\]
Eqn. (2-9) applies to any control volume, \( V \), within a single phase region. Therefore,

\[
\frac{\partial}{\partial t} (\rho i) - \text{div}(K \text{ grad } T) = 0 \quad (2-10)
\]

The specific enthalpy is related to temperature by the equation \( \Delta i = c_d T \). Thus equation (2-10) may be rewritten as:

\[
\rho c \frac{\partial T}{\partial t} = \text{div}(K \text{ grad } T) \quad (2-11)
\]

This is the conventional form of the heat conduction equation for a single phase region.

Eqn. (2-4) will now be applied to a control volume, containing the interface. At time \( t \), the interfacial surface \( \Sigma \) divides the control volume into two regions; solid and liquid. It also divides the surface area of \( V \), into two portions, \( \partial V_s \) and \( \partial V_L \). In this case, \( (K \text{ grad } T) \) and \( i \) change discontinuously across the moving surface \( \Sigma \).

For convenience in the following discussion, the problem of freezing is considered. After a small increment in time, \( \delta t \), the volume of solid increases, while the volume of liquid decreases. Consequently, the interface moves through a volume \( \delta V \) to a new position \( \Sigma' \). A derivation of the energy conservation condition at the interface is presented below.
At time $t$, 

$$\int_V \rho_i \, dV = \int_{V_s} (\rho_i)_s \, dV + \int_{V_L} (\rho_i)_L \, dV =$$

$$\int_{V_s} (\rho_i)_s \, dV + \int_{V_s + \delta V} (\rho_i)_s \, dV + \int_{V_L - \delta V} (\rho_i)_L \, dV$$

(2-12)

And at time $t + \delta t$, 

$$\int_V \rho_i \, dV = \int_{V_s + \delta V} (\rho_i)_s \, dV + \int_{V_L - \delta V} (\rho_i)_L \, dV =$$

$$\int_{V_s} (\rho_i)_s \, dV + \int_{V_s} (\rho_i)_s \, dV + \int_{V_L - \delta V} (\rho_i)_L \, dV$$

(2-13)

The following operations are now performed: subtract Eqn. (2-12) from Eqn. (2-13), and divide by $\delta t$; then take the limit as $\delta t$ approaches zero, and note that as $\delta t \to 0$, $(V_L - \delta V) + V_L$. The resulting equation is:
\[
\frac{d}{dt} \int_V \rho_i \, dV = \frac{d}{dt} \int_{V_S} (\rho_i)_s \, dV + \frac{d}{dt} \int_{V_L} (\rho_i)_L \, dV + \lim_{\delta t \to 0} \int_{\delta V} \frac{(\rho_i)_{s,t+\delta t} - (\rho_i)_L,t}{\delta t} \, dV
\]

(2-14)

It is to be noted that as \( \delta t \to 0 \), the ratio \( dV/\delta t \) approaches \( V_i^* d\Sigma \), where \( V_i^* \) is the local velocity of the interface towards the liquid region; \( i_s \) and \( i_L \) approach their saturation values \( i_s^* \) and \( i_L^* \); \( \delta V \) shrinks to the surface \( \Sigma \), and the interface region becomes \( \Sigma \). Thus Eqn. (2-14) reduces to

\[
\frac{d}{dt} \int_V \rho_i \, dV = \frac{d}{dt} \int_{V_S} (\rho_i)_s \, dV + \frac{d}{dt} \int_{V_L} (\rho_i)_L \, dV + \int_{\Sigma} \rho (i_s^* - i_L^*) \, V_i^* d\Sigma
\]

(2-15)

By applying the enthalpy equation to the single phase regions in Eqn. (2-15), and introducing the enthalpy of fusion,

\( \lambda = (i_L^* - i_s^*) \), Eqn. (2-15) may be rewritten as:
\[
\frac{d}{dt} \int_V \rho i \, dV = \int_{\partial V} K \, \text{grad} \, T \cdot \hat{n} \, ds + 
\]

\[
\int_{\partial V}^\Sigma K \, \text{grad} \, T \cdot \hat{n} \, ds - \int_{\Sigma} \rho \lambda v^* \, d\Sigma 
\]

(2-16)

In the first term on the right-hand side of Eqn. (2-16), \( \hat{n} \) represents the outward normal to the solid region, whereas in the second term, it represents the outward normal to the liquid region. So if the local normal to \( \Sigma \) towards the liquid region is denoted by \( \hat{n}^* \), then in the second term, \( \hat{n} = -\hat{n}^* \). By splitting up the integrals in Eqn. (2-16), and combining the terms involving the control volume surface into one term, and those portions involving the interface into another, the following equation is obtained:

\[
\frac{d}{dt} \int_V \rho i \, dV = \int_{\partial V} K \, \text{grad} \, T \cdot \hat{n} \, ds + 
\]

\[
\int_{\Sigma} \left[ \left( K \frac{\partial T}{\partial n^*} \right)_s - \left( K \frac{\partial T}{\partial n^*} \right)_L - \rho \lambda v^* \right] \, d\Sigma 
\]

(2-17)

By subtracting the enthalpy equation from Eqn. (2-17), it is
established that the integral over $\Sigma$ is equal to zero. Since this applies to any position of the interface, $\Sigma$,

$$\left(K \frac{\partial T}{\partial n^\star} \right)_s - \left(K \frac{\partial T}{\partial n^\star} \right)_l - \rho \lambda v^\star \frac{n}{n} = 0$$

This is the conventional energy conservation condition of the interface.
CHAPTER III

FINITE ELEMENT FORMULATION OF THE ENTHALPY MODEL

In the finite element formulation, attention is focused on the values of the dependent variables at a finite number of points (nodes) inside the domain of interest. In this thesis, the control-volume approach proposed by Baliga and Patankar (16) is adopted: first, the domain is divided into finite elements, and then each node in the domain is associated with a polygonal control volume. The entire formulation is composed of five basic building blocks: a domain discretization scheme; a specialization of the enthalpy model to enable its amalgamation with the finite element method; selection of suitable interpolation functions; derivation of the discretization equations; and the solution of the discretization equations. Brief descriptions of each of these building blocks are presented in this chapter.

3-1 DOMAIN DISCRETIZATION

The domain of interest is first divided into three-node triangular elements or four-node quadrilateral elements. Following this, the centroids of the elements are joined to the midpoints of the corresponding sides to obtain polygonal control volumes surrounding each node in the calculation domain.
Sample domain discretizations are shown in Figs. 2 and 3.

The selection of a suitable element, triangular or quadrilateral, depends on the problem being solved. The following observations have been made in this regard (16):

1. highly irregular-shaped domains can be more easily divided into triangles than into quadrilaterals;
2. curved boundaries can be better approximated by triangular elements than by quadrilateral ones;
3. for the same number of nodes, triangular elements provide greater flexibility than quadrilateral elements in the distribution of the nodes inside the calculation domain; and
4. in certain problems, those possessing some natural symmetry surfaces, for instance, schemes using triangular discretization are more prone to grid generated asymmetries than those using quadrilateral discretization.

3-2 SPECIALIZATION OF THE ENTHALPY MODEL

Consider the polygonal control volume, V, associated with a node j, as shown in Figs. 2b and 3b. The total enthalpy, $I$, contained in V is given by

$$ I = \int_{V} \rho_{i} \, dV \quad (3-1) $$

Let $i_{s}^{*}$ and $i_{l}^{*}$ denote the saturated state enthalpies of the
solid and liquid phases, respectively. Then if

$$\int_V \rho_i \, dV < 1 < \int_V \rho_l \, dV$$

it may be concluded that the solid-liquid interface passes through the control volume V. In this case, it is assumed that the temperature at the node j is $T_{\text{sat}}$. An error is introduced by this assumption, but it decreases as the size of V is reduced; it may be regarded as a discretization error. When

$$\int_V \rho_i \, dV < 1 \quad \text{or} \quad 1 > \int_V \rho_l \, dV$$

the entire control volume V lies in a single phase region, and the specific enthalpy at node j is obtained from the equation

$$i = I/\rho V$$

(3-2)

The known $i$ versus $T$ relationship for the phase change material can then be used to determine the temperature at node j.

At this stage, the nondimensionalization suggested by Shamsundar and Sparrow (10) is adopted:
\[ \theta = \frac{1}{\rho V} \int_V \frac{\rho (i-i*)}{\lambda} dV; \quad \phi = \frac{c(T-T_{sat})}{\lambda} \] (3-3)

Here, \( \theta \) is a nondimensional enthalpy and \( \phi \) is a nondimensional temperature. It is now assumed, mainly for convenience, that aside from the enthalpy, the properties of the phase change material are independent of temperature. Then in terms of \( \theta \) and \( \phi \), the enthalpy equation can be written as

\[ (V/L^2) \frac{\partial \theta}{\partial \tau} = \int_{\partial V} \Gamma \text{grad} \phi \cdot \hat{n} ds \] (3-4)

In Eqn. (3-4), \( \tau = \frac{t \alpha_s}{L^2} \), where \( L \) is a characteristic length, and \( \Gamma = \frac{\alpha}{\alpha_s} \). Therefore, in the solid phase \( \Gamma = 1 \) and in the liquid phase \( \Gamma = \frac{\alpha_L}{\alpha_s} \). The two-dimensional regions depicted in Figs. 2 and 3 are assumed to have unit depth, therefore \( (V/L^2) \) is equal to the nondimensional area of the control volume surrounding node \( j \).

The \( \theta \) variable is negative within the solid region and greater than unity in the liquid. For a control volume through which the interface passes, \( 0 \leq \theta \leq 1 \), and the value of \( \theta \) is equal to the fraction of the control volume which is in liquid state. Further, from the assumptions and definitions stated above, the following relationship between \( \theta \) and \( \phi \) can be deduced:
\[ \phi = 0 \text{ for } \theta < 0; \quad \phi = 0 \text{ for } 0 \leq \theta \leq l; \]

and

\[ \phi = \theta - l \text{ for } \theta > l \quad (3-5) \]

For concreteness in the specification of the initial and the boundary conditions, the following problem is assumed; the phase change material is initially in a superheated liquid state at temperature \( T_0 \), and convective cooling is imposed on the domain boundaries. Then, at \( \tau = 0 \),

\[ \phi = \text{Ste}_s \Delta c \frac{(T_0 - T_{sat})}{\lambda} \quad (3-6) \]

If a control volume has a portion of its surface lying on the boundary, Eqn. (3-4) takes the form

\[ (V/L^2) \frac{\partial \theta}{\partial \tau} = \int_{\partial V_i} \text{grad} \phi \cdot \mathbf{n} ds - \int_{\partial V_o} \text{Bi} (\gamma \phi + \text{Ste}_s) ds \quad (3-7) \]

Where \( \text{Bi} \) is the Biot number \((hL/K_s)\), \( \text{Ste}_s \) is a Stefan number for the solid \((c_s(T_{sat} - T_w)/\lambda)\), \( \gamma \) is the ratio \((c_s/c)\), \( \partial V_i \) is the portion of \( \partial V \) lying inside the domain, and \( \partial V_o \) is the portion corresponding to the domain boundary.
INTERPOLATION FUNCTIONS

The derivation of algebraic approximations to Eqns. (3-4) and (3-7) requires the specification of interpolation functions for the dependent variables $\theta$ and $\phi$, and the ratios $\Gamma = \alpha/\alpha_s$ and $\gamma = c_s/c$.

If triangular elements are used, the dependent variable $\phi$ is interpolated linearly in each element. For example, in the typical element depicted in Fig. 2c, $\phi$ is given by

$$\phi = Ax + By + C$$

(3-8)

The constants $A$, $B$, and $C$, can be easily determined in terms of $\phi_1$, $\phi_2$, and $\phi_3$, and the nodal coordinates (APPENDIX II).

The nondimensional enthalpy, on the otherhand, is interpolated via the so-called staircase functions in each control volume; the nodal values of $\theta$ are assumed to prevail over the associated polygonal control volumes. In this regard, it is to be noted that linear interpolation for $\theta$ was also experimented with, but the results generated by such schemes were, in many instances, prone to spurious, grid-dependent, variations.

In problems where rectangular elements are used, $\phi$ is interpolated by the bilinear function in each element. Thus, in the typical element depicted in Fig. 3c,
\[ \phi = Ax + By + Cxy + D \quad (3-9) \]

Again, the constants \( A, B, C, \) and \( D \) can be determined in terms of \( \phi_1, \phi_2, \phi_3, \) and \( \phi_4, \) and the nodal coordinates (APPENDIX III). The nodal values of \( \theta \) are again assumed to prevail over the associated polygonal control volumes.

It is important to note that for arbitrary quadrilaterals, the bilinear interpolation function given in Eqn. (3-9) would not be continuous from one element to an adjacent element. Therefore, bilinear interpolation may be used only on rectangular elements. For a more general quadrilateral, however, it is still possible to change coordinates in such a way that it becomes a rectangle, and then bilinear functions in the new coordinates are admissible. Such a coordinate transformation can itself be described by a bilinear function. Thus the same polynomials are used for the transformation of coordinates as for the interpolation function within each element; such a procedure is labelled as an isoparametric technique (17, 18).

Isoparametric transformations allow the use of general quadrilateral elements, but they complicate the derivation of the discretization equations (18). For this reason, only rectangular elements are used in this thesis.

The centroidal values of \( \Gamma \) and \( \gamma, \) in the case of both triangular and rectangular elements, were stored, and they were assumed to prevail over the corresponding elements.
each time step, these centroidal values were obtained by taking the arithmetic mean of the corresponding nodal values. In the case of nodes at which $0 < \theta < 1$, the weighted averages of the liquid phase and solid phase values of $\Gamma$ were assigned. This smoothing out procedure is akin to the practices adopted in other investigations (8).

3-4 DISCRETIZATION EQUATIONS

These are algebraic approximations to Eqns. (3-4) and (3-7), applied to each control volume in the calculation domain. Only a brief description of the derivation of these equations for triangular elements is presented in this section. This description is broken into two parts: the first part deals with internal nodes, and the other with boundary nodes. A similar procedure is used to obtain the discretization equations for rectangular elements (APPENDIX V).

3-4-1 Internal Nodes

These are nodes in the interior of the calculation domain. When applied to the polygonal control volume associated with a typical node $l$, see Fig. 2b, the enthalpy equation for internal nodes may be written as:
Using the linear interpolation function introduced in Eqn. (3-8)

\[ \vec{\nabla} \phi = A \vec{i} + B \vec{j} \]  

and

\[
\int_a^c \vec{\nabla} \phi \cdot \hat{n} ds + \int_o^c \vec{\nabla} \phi \cdot \hat{n} ds = A(y_c - y_a) - B(x_c - x_a) \]  

Eqn. (3-12) is valid only if the node numbering is done in the counter-clockwise fashion illustrated in Fig. 2c. The constants A and B are linear functions of \( \phi_1 \), \( \phi_2 \), and \( \phi_3 \); therefore, the right-hand side of Eqn. (3-12) can be expressed as a linear function of the nodal values of \( \phi \).

The unsteady term, involving \( \theta \), is approximated by a simple one-step finite difference scheme:

\[ \frac{d\theta}{d\tau} = \frac{(\theta^m_{l} - \theta^{m-1}_{l})}{\Delta\tau} \]  

(3-13)
In this equation, $\theta^m_1$ and $\theta^{m-1}_1$ are the values of $\theta_1$ at time levels $m$ and $m-1$, respectively, and $\Delta \tau$ is the nondimensional time step, $(\tau^m_1 - \tau^{m-1}_1)$.

Expressions similar to Eqns. (3-12) and (3-13) can be derived for the contributions of all other elements associated with node 1. Such expressions, when substituted into Eqn. (3-10) yield the complete discretization equation for node 1.

The complete discretization equation for a typical internal node $i$, for both triangular and quadrilateral elements, can be cast in the following general form:

$$\text{ADDT}_i \theta^m_i + a_i \phi^m_i = \text{ADDT}_i \theta^{m-1}_i + \sum_{\text{neighbors of node } i} a_n \phi^m_n + b_i$$

(3-14)

The term AD$I_i$ in Eqn. (3-14) denotes the control volume area divided by the time step $\Delta \tau$. It is to be noted that a fully implicit scheme is used to obtain Eqn. (3-14). Further, it can be proved that the coefficient $a_i$ is positive definite, for both triangular and rectangular elements (APPENDIX VI).

3-4-2 Boundary Nodes

Nodes which lie on the boundary of the domain are termed boundary nodes. Similarly, element sides which lie along the domain boundary are called boundary sides. Further,
elements which have at least one boundary side are labelled as boundary elements. Two typical boundary nodes, along with their associated elements and control volumes, are depicted in Fig. 4: (a) A boundary node with two associated boundary elements and two (or more) associated internal elements; (b) A boundary node with only one associated boundary element.

The discussion presented below will be keyed to the boundary node shown in Fig. 4a; this is a more general situation than the one depicted in Fig. 4b.

The nondimensional form of the enthalpy equation, Eqn. (3-4), when applied to the control volume associated with node 1 in Fig. 4a, takes on the following form:

\[
\left[ \text{Area}_{1aoc} \frac{\partial \theta}{\partial t} - \left[ R_0 \left( \int_0^C \hat{v}_\phi \cdot \hat{n} \, ds + \int_0^C \hat{v}_\phi \cdot \hat{n} \, ds \right) \right] \right] + \\
\left[ \text{similar contributions from internal elements} \right] + \\
\left[ \text{associated with the boundary node } 1 \right] = \\
\left[ \text{Area}_{1ghi} \frac{\partial \theta}{\partial t} - \left[ R_h \left( \int_g^h \hat{v}_\phi \cdot \hat{n} \, ds + \int_h^i \hat{v}_\phi \cdot \hat{n} \, ds \right) \right] \right] + \\
\int_1^a q^* \, ds + \int_1^a q^* \, ds
\]

(3-15)
the term q* in this equation represents a nondimensionalized heat flux; it is normal to the boundary and enters into the domain.

The unsteady terms in Eqn. (3-15) are approximated by a one-step finite difference scheme, akin to the one presented in Eqn. (3-13). The terms related to heat conduction across the surface of the control volume lying inside the calculation domain are approximated by algebraic expressions similar to those given in Eqns. (3-11) and (3-12). In the integrals related to heat transfer across the boundary sides associated with node 1, it is assumed that an average value of the heat flux q* prevails over the portion of the control volume surface that lies on the domain boundary. The aforementioned approximations can be substituted into Eqn. (3-15), and a fully-implicit formulation can be used to obtain the following discretization equation:

$$\text{ADDT}_1 \theta_1^m + a_1 \phi_1^m = \text{ADDT}_1 \theta_1^{m-1} + \sum_{\text{neighbors of node 1}} a_n \phi_n^m + b_1 + (\ell_1 + \ell_2)q^*$$

(3-16)

So far in this discussion on the discretization equations for boundary nodes, nothing explicit has been said about the actual boundary condition at node 1; all that has been said is that q* is the average heat flux that prevails at node 1.
This was mainly to keep the derivation of Eqn. (3-16) as general as possible. At this stage, however, an explicit discussion of boundary conditions is in order. Three commonly encountered boundary conditions, namely, specified temperature, specified heat flux, and specified convective cooling, are discussed below under separate subheadings.

**Specified Temperature:** If a temperature is specified at node 1, the corresponding nondimensional temperature is given by

\[
\phi_1 = \frac{c(T_{\text{given}} - T_{\text{sat}})}{\lambda}
\]  

(3-17)

The value of the nondimensional enthalpy at node 1, \( \theta_1 \), depends on the value of \( \phi_1 \), and Eqn. (3-5) can be used to obtain it. Thus, if the material at node 1 is subcooled solid, \( \phi_1 < 0 \) and \( \theta_1 = \phi_1 \). If \( \phi_1 > 0 \), the material at node 1 is in a superheated liquid state, and \( \theta_1 = \phi_1 + 1 \). If \( \phi_1 = 0 \), the material in the control volume associated with node 1 is in a saturated state, and all that can be said about \( \theta_1 \) is that \( 0 \leq \theta_1 \leq 1 \): additional information about the material in (C.V.)_1 is needed before a specific value can be assigned to \( \theta_1 \). For a specified temperature boundary condition, therefore, the discretization equation (3-16) is replaced by the following set of equations.
The discretization equation (3-16) can be used to obtain the average nondimensional heat flux at node 1 after the entire $\phi$ and $\theta$ fields have been calculated: thus,

$$q_1^* = \left[ \text{ADDC}_1(\theta_1^m - \theta_1^{m-1}) + a_1\phi_1^m - \sum_{\text{neighbors of node } 1} a_n\phi_n^m - b_1 \right] / (\lambda_1 + \lambda_2) $$ (3-19)

**Specified Heat Flux:** If a heat flux is specified at node 1, the corresponding nondimensional heat flux is calculated as follows:

$$q_1^* = \left( q_{\text{given}}Lc_s \right) / (\lambda x_s) $$ (3-20)
This value of $q_1^*$ is substituted into Eqn. (3-16) to obtain the complete discretization equation for node 1.

**Specified Convective Cooling:** In this case the surrounding cooling fluid temperature, $T_\infty$, and a heat transfer coefficient, $h_1$, are specified. Thus the heat flux at node 1 is given by

$$q_1 = h_1 [T_\infty - T_1]$$

or

$$q_1 = h_1 [T_\infty - \frac{\lambda}{c} \phi_1 - T_{\text{sat}}] \quad (3-21)$$

The nondimensional heat flux at node 1 is given by:

$$q_1^* = \frac{(q_1 L c_s)}{(\lambda K_s)}$$

$$= \frac{h_1 L}{K_s} \left[ \frac{c_s (T_\infty - T_{\text{sat}})}{\lambda} - \left( \frac{c_s}{c} \right) \phi_1 \right]$$

or

$$q_1^* = -B_i (S_{\text{e}} + \gamma \phi_1) \quad (3-22)$$

Eqn. (3-22), when substituted into Eqn. (3-16), yields the following discretization equation for node 1:
ADDT_1 \theta_1^m + [a_1 + (l_1 + \varepsilon_2) Bi_1 \gamma] \phi_1^m = ADDT_1 \theta_1^{m-1} + \sum_{\text{neighbors of node 1}} a_n \phi_1^m + [b_1 - (l_1 + \varepsilon_2) Bi_1 \text{Ste}_s] \tag{3-23}

Comments: Often, the conditions on the surface of (C.V.)_1 that lies on the boundary of the domain are a combination of the three conditions discussed above. In such cases, an appropriate combination of the aforementioned procedures is used to obtain the corresponding discretization equation for node 1.

Solution of the Discretization Equations

At each time step, a modified Gauss-Seidel iterative procedure, similar to that proposed by Shamsundar and Sparrow (10), is used to solve the discretization equations. This is a so-called point-by-point scheme. Its application to the discretization equations associated with a typical node i is described below; the equations associated with all other nodes are handled in an analogous manner. Let

\[ E_i = ADDT_1 \theta_i^{m-1} + \sum_{\text{neighbors of node } i} a_n \phi_n^m + b_i \tag{3-24} \]
Then Eqn. (3-14) can be written as:

$$\text{ADDT}_i \theta_i^m + a_i \phi_i^m = E_i$$  \hspace{1cm} (3-25)

Another equation relating $\theta_i^m$ to $\phi_i^m$ is given by Eqn. (3-5).

Thus,

$$\phi_i^m = \theta_i^m \text{ for } \theta_i^m < 0,$$

$$\phi_i^m = 0 \text{ for } 0 \leq \theta_i^m \leq 1,$$  \hspace{1cm} (3-26)

and

$$\phi_i^m = \theta_i^m - 1 \text{ for } \theta_i^m > 1$$

The procedure to extend the solution from time level $(m-1)$ to time level $m$ will now be described. To start the calculation, all $\phi^m$ values are assigned the corresponding $\phi^{m-1}$ values, and the value of $E_i$ is computed. Following this, the calculation proceeds along one of the following three streams, based on the value of $E_i$.

(i) $E_i < 0$

Noting that $\text{ADDT}_i$ and $a_i$ are both positive definite, $\theta_i^m$ (or $\phi_i^m$) has to be negative in this case. Thus,
\[ \phi_i^m = \theta_i^m = E_i / (ADDT_i + a_i) \quad (3-27) \]

(ii) \( 0 \leq (E_i / ADDT_i) \leq 1 \)

In this case,

\[ \theta_i^m = E_i / ADDT_i \quad (3-28) \]

and

\[ \phi_i^m = 0 \]

(iii) \( (E_i / ADDT_i) > 1 \)

This implies a superheated liquid state at node \( i \). Thus,

\[ \theta_i^m' = (E_i + a_i) / (ADDT_i + a_i) \quad (3-29) \]

and

\[ \phi_i^m = \theta_i^m - 1 \]

Using this procedure, the old, or guessed, values of \( \theta_i^m \) and \( \phi_i^m \) are replaced by their newly calculated values. Then the values of \( \theta^m \) and \( \phi^m \) at all other nodes in the calculation domain are updated in a similar manner; the sequence in which these nodal values are updated is chosen so as to 'sweep' the domain in an alternating manner. This entire procedure is repeated until some convergence criteria are satisfied. Once this is achieved, the solution at time level \( m \) is assumed to
be known, and the solution proceeds to time level $(m + 1)$.

On the basis of numerous numerical experiments, it has been established that this iterative solution procedure is stable even with coarse spatial discretization and large time steps. As pointed out by Shamsundar and Sparrow (10), a straightforward analytical examination of the stability of this scheme is not possible because of the nonlinearity of the discretization equations.
CHAPTER IV

APPLICATION OF THE METHOD TO SAMPLE PROBLEMS

As mentioned in the introduction, the method described in this work has been successfully applied to a wide variety of one- and two-dimensional problems. The results of four illustrative problems are presented in this chapter. The first two problems involve heat conduction in regular- and irregular-shaped domains, without phase change: the first deals with unsteady heat conduction in a square domain; and steady heat conduction in a concrete slab is studied in the second problem. The last two problems involve heat conduction in a square domain with change of phase: first, the freezing of a liquid which is initially in a saturated state is studied; then the freezing of an initially superheated liquid phase is investigated.

In all these problems, the thermal resistance of the container walls is assumed to be negligible. Further, in problems involving the freezing of a phase change material (PCM), the properties of the PCM are assumed to be constant.

4-1 UNSTEADY HEAT CONDUCTION IN A SQUARE DOMAIN

Problem Statement

This problem involves the investigation of unsteady
heat conduction, without phase change, in a long solid cylinder with a square cross section. A cross-sectional view of the cylinder is depicted in Fig. 5a.

As is evident from Fig. 5a, this problem has a number of symmetry surfaces, so only one-eighth of the container need be analyzed. In this analysis, however, one-fourth of the container, shown shaded in Fig. 5a, is considered. This is because the computer program used to solve this problem is geared to handle rectangular domains, and the square domain is treated as a particular case.

In this example, the domain is initially heated to a uniform temperature, $T_i$. Then, during $t \geq 0$, the boundaries of the cylinder are maintained at a uniform temperature $T_w$. Heat conduction in the axial direction is ignored and the problem is considered as two-dimensional. Further, it is assumed that the solid cylinder possesses constant material properties.

As is well known (19), this problem has an analytical solution in the form of Fourier series. The solution generated by the numerical method can therefore be checked by comparing it with the analytical solution.

**Governing Equation**

The following nondimensionalization is adopted in this
problem.

\[ \xi = \frac{X}{L}, \quad \eta = \frac{Y}{L}, \quad t = \frac{t\alpha}{L^2} \]

\[ \phi' = \frac{T - T_w}{T_i - T_w} \quad (4-1) \]

In terms of these nondimensional quantities, the integral energy conservation equation takes on the following form:

\[ \left(\frac{V}{L^2}\right) \frac{\partial \phi'}{\partial t} = \int_{\partial V} \text{grad } \phi' \cdot \text{d}\mathbf{s} \quad (4-2) \]

Eqn. (4-2) can be obtained from Eqn. (3-4) by setting \( \phi = \phi' \), and \( \Gamma = 1 \). The initial condition is:

at \( t = 0 \), \( \phi' = 1 \) \quad (4-3)

On the boundaries of the square cylinder, \( \phi' = 0 \). On the symmetry surfaces, however, \( \partial \phi'/\partial n = 0 \); this is because there is no heat transfer in a direction normal to a symmetry surface. A differential formulation of this problem could also be adopted. Then the nondimensionalized governing equation reduces to,
This equation, subject to the aforementioned initial and boundary conditions, can be solved by the method of separation of variables. The analytical solution is a double Fourier series (19).

\[ \phi' = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{16}{mn \pi^2} \cdot \sin(n\pi \xi) \cdot \sin(m\pi \eta) \cdot \exp[-\pi^2 \cdot \tau (m^2+n^2)] \quad (4-5) \]

The non-dimensional surface integrated heat flux is given by:

\[ \frac{Q}{K(T_i - T_w)} = \int_0^{0.5} \left( \frac{\partial \phi'}{\partial \xi} \right)_{\xi=0} \, d\eta \quad (4-6) \]

The analytical solution, Eqn. (4-5), can be used in this equation to obtain

\[ \frac{Q}{K(T_i - T_w)} = \sum_{n=1}^{\infty} \sum_{m=1}^{\infty} \frac{16}{m^2 \pi^2} \cdot \exp[-\pi^2 \tau (m^2+n^2)] \quad (4-7) \]
Numerical Details

Three-node triangular elements were used to discretize the calculation domain, and the line-by-line method was used to solve the discretization equations.

All computations were done with a nonuniform grid; a higher concentration of grid lines was used in the vicinity of the specified-temperature boundaries than in the region adjacent to the symmetry boundaries. The actual distribution of the grid lines was done according to the following equations:

\[ \xi_i = 0.5 \left( \frac{i-1}{20} \right)^{1.5} \quad i = 1, 2, \ldots, 20, 21 \]

and

\[ \eta_j = 0.5 \left( \frac{j-1}{20} \right)^{1.5} \quad j = 1, 2, \ldots, 20, 21 \]

The temperature profile undergoes rapid changes, thus it has steep gradients, early in the cooling process, especially in the vicinity of the specified temperature boundaries. The nonuniform grid described above enables an accurate treatment of such changes; this conclusion is based on the results that are discussed in the following section.

Results

Plots of the nondimensional temperature along the
boundary are presented in Fig. 6. The variation of
t nondimensional surface integrated heat flux with time is
depicted in Fig. 7. The continuous lines represent the
analytical solution, and the finite element solution is
presented in the form of black dots (●).

As is evident from these figures, the numerical solution
matches the analytical solution very well.

4-2 HEAT CONDUCTION IN A CONCRETE SLAB CONTAINING AN ARRAY
OF CONDUITS FOR ELECTRIC POWER CABLES AND COOLING WATER

Problem Statement: This problem involves the calculation
of heat conduction, without phase change, in a very long
slab of concrete containing an array of conduits for electric
power cables and cooling water: it is relevant to utility
companies that employ underground electric power transmission
cables. A cross-section of the concrete slab is shown in Fig.
8a. It is assumed that the array is large enough to be
considered as an infinite one. The cable conduits and the
cooling water conduits are arranged in an alternating pattern
and their centers form regular squares. The radius of the
conduits is denoted by R and the distance between their centers
by S.

The conduit arrangement depicted in Fig. 8a results in
numerous symmetry surfaces. Thus the analysis can be limited
to only a small portion of the concrete slab. This is depicted in Fig. 8b. Initially, the entire concrete slab is assumed to be at the cooling water temperatures, \( T = T_0 \).

At \( t = 0 \), the power cables are energized. It is assumed that the ohmic heating of the cables imposes a constant (and uniform) heat flux, \( q \), at the cable conduit surface. The surface temperature of the cooling water conduit is assumed to remain constant at \( T_0 \).

Results were obtained for \( S/R \) ratios of 2.5, 3.0, and 4.0.

**Governing Equations**: The following nondimensionalization is adopted in this problem:

\[
\xi = \frac{X}{R}, \quad \eta = \frac{Y}{R}, \quad \tau = \frac{t \alpha}{R^2}
\]

and

\[
\phi' = \frac{(T-T_0)}{(qR/k)}
\]  \( (4-8) \)

In terms of these nondimensional quantities, the integral energy conservation equation in the concrete takes on the following form:

\[
(V/R^2) \frac{\partial \phi'}{\partial t} = \int_{\partial V} \text{grad} \ \phi' \cdot \mathbf{n} d\mathbf{s}
\]  \( (4-9) \)

The initial condition is:
For a node on the cable conduit surface:

\[
(V/R^2) \frac{\partial \phi'}{\partial t} = \int_{\partial V_i} \text{grad} \phi' \cdot \hat{n} ds + \sum \phi_i
\]  

(4-11)

and for a node on the cooling water conduit:

\[
\phi' = 0
\]

(4-12)

By setting \( \theta = \phi = \phi' \), \( \Gamma = 1 \), and other minor modifications, Eqns. (3-4) to (3-7) can be specialized to Eqns. (4-9) to (4-12).

Numerical Details: Triangular elements were used to discretize the calculation domain. The circular conduit surfaces were approximated by piece-wise linear curves. A typical discretization, for \( S/R = 4 \), is shown in Fig. 9.

Results: Plots of the steady-state nondimensional temperature of the cable conduit surface, for three different values of the ratio \( S/R \), are presented in Fig. 10. These results were considered the most important from an applications point of view.

The lowest value of \( (T-T_o)/(qR/k) \) is obtained with \( S/R = 2.5 \). This is because the cooling water conduit is
closest to the cable conduit for this case. It is also seen that the surface temperature of the cable conduit is highest at $\psi = 45^\circ$ and lowest at $\psi = 0^\circ$. The difference between these values decreases as the S/R value increases, the temperature distribution becoming almost uniform for S/R = 4. Again, this is an expected result.

4-3 FREEZING IN A SQUARE DOMAIN SUBJECTED TO CONVECTIVE COOLING

Problem Statement: In this problem, the freezing of a phase change material in a long container of square cross section is investigated. A cross-sectional view of the container is depicted in Fig. 5a. The walls of the container are subjected to convective cooling during the period $t > 0$. The heat transfer coefficient, $h$, and the cooling fluid temperature, $T_\infty$, are assumed to be spatially uniform and constant with time.

The calculation domain in this problem has a number of symmetry surfaces. Thus only one-eighth of the total domain need be analyzed. One-fourth of the domain is considered in this analysis, however, for the same reasons as those stated in section 4-1.

Two different classes of illustrative examples are considered within the context of this problem. In one, the
PCM is initially in a saturated liquid state, \( T_0 = T_{\text{sat}} > T_\infty \); a superheated liquid phase, \( T_0 > T_{\text{sat}} > T_\infty \), is the initial condition in the other. This classification is adopted in the following discussion.

4-3-1 Saturated Liquid Phase

**Governing Equations:** Eqns. (3-4) to (3-7) describe this problem completely. As the problem involves constant properties, \( \Gamma = 1 \) throughout the container. Further, the PCM is initially in a saturated liquid state, so \( \text{Ste}_s = 0 \). In addition, it is to be noted that though Eqn. (3-7) models convectively cooled boundaries, it can be applied to symmetry boundaries by setting \( \text{Bi} = 0 \).

Two combinations of \( \text{Bi} \) and \( \text{Ste}_s \) were investigated; \( \text{Bi} = 1.0, \text{Ste}_s = 0.05 \), and \( \text{Bi} = 10.0, \text{Ste}_s = 0.1 \). These cases are of intermediate and high difficulty with respect to the numerical solution procedure (10). They are also likely to be encountered in the design of solar energy storage devices (10). This problem has been solved by Shamsundar and Sparrow (10); their results were used to check the accuracy of the results produced by this analysis.

**Numerical Details:** The calculation domain and its discretization are shown in Fig. 5b; \( \xi = X/L \) and \( \eta = Y/L \). All computations were done with \( \Delta \xi = \Delta \eta = 0.05 \). For the case
of \( Bi = 1.0, \) \( Ste_s = 0.05, \) \( \Delta \tau = 0.1 \) was used for all computations; \( \Delta \tau = 0.02 \) was used for the case of \( Bi = 10.0, \) \( Ste_s = 0.1. \)

At each time step, the iterative solution procedure described in chapter II was stopped when all \( \theta \) and \( \phi \) values had converged to at least four significant figures.

**Results:** Spatially local and total heat transfer results and the solidification fraction were obtained as functions of time.

The distribution of the nondimensional wall heat flux, \( q_w/h[T_{sat} - T_{\infty}] \), for the case of \( Bi = 1.0, Ste_s = 0.05, \) is displayed in Fig. 11. Noting that \( q_w = h[T_w - T_{\infty}] \), it is easy to see that the curves also represent the nondimensional surface temperature, \( (T_w - T_{\infty})/(T_{sat} - T_{\infty}) \). The curves are parameterized by values of the product \( Ste_s \tau \). The product \( Ste_s \tau \), rather than \( \tau \), is used because it correlates, approximately, the results for different values of \( Ste_s \); thus, the results in Fig. 11 apply strictly to \( Ste_s = 0.05 \) only, but they are roughly representative of problems with \( 0.01 \leq Ste_s \leq 0.1 \).

The results presented in Fig. 11 indicate that as the freezing progresses, the wall heat flux decreases faster at the corner of the container than in the vicinity of the symmetry boundaries. This is a consequence of the higher thermal resistance of the thicker solid layer at the corner.
which, because of heat loss from the two adjacent faces, freezes faster. During the initial phase of the solidification, this effect is evident only in the immediate vicinity of the corner, and the heat flux is uniform away from this region. As the solidification continues, the flat portions of the heat flux curves diminish in width and finally disappear, indicating fully two-dimensional heat transfer.

Shamsundar and Sparrow (10) have presented results similar to those in Fig. 11. Their results match those of this analysis so closely that it was impossible to separate the two in Fig. 11.

The variations of the nondimensional surface-integrated heat flux, $Q/hA(T_{\text{sat}} - T_\infty)$, and the solidification fraction with $St_T$ are shown in Fig. 12. For the case of $\Bi = 1$, it is seen that the surface-integrated heat flux decreases almost linearly with time to a value of about 0.3 at the end of solidification. Thereafter, there is no latent heat available, and $Q$ drops off very rapidly; the heat flux is entirely fed by changes in sensible heat content. In the $\Bi = 10$ case, $Q$ drops to a small value in a brief period at the start of the solidification and decreases relatively slowly thereafter: this indicates that the high initial values of $Q$ cannot be sustained, even with the aid of the latent heat liberated by the solidification process: smaller
values of $Q, Q/hA[T_{\text{sat}} - T_{\infty}] < 0.2$, are fairly well sustained by the liberation of latent heat. Again, these results coincide exactly, within plotting accuracy, with the corresponding results reported in Ref. (10).

4-3-2 Superheated Liquid Phase

**Governing Equation:** This problem is completely described by Eqns. (3-4) to (3-7). Constant properties are involved, therefore $\Gamma = 1$ throughout the container. Further, the PCM is initially in a superheated liquid state, so $T_o > T_{\text{sat}}$, and $\text{Ste}_L > 0$.

**Numerical Details:** Two combinations of $\text{Bi}, \text{Ste}_S$, and $\text{Ste}_L$ were investigated; $\text{Bi} = 1.0$, $\text{Ste}_S = 0.05$, $\text{Ste}_L = 0.2$, and $\text{Bi} = 10.0$, $\text{Ste}_S = 0.1$, $\text{Ste}_L = 0.2$. For the first case, $\Delta \tau = 0.1$ was used for all computations; $\Delta \tau = 0.02$ was used for the second case. In both cases, $\Delta \xi = \Delta \eta = 0.05$.

The iterative solution procedure described in Chapter II was employed to solve this problem too. As was done in the previous problem, at each time step, the iteration procedure was terminated when all $\theta$ and $\phi$ values had converged to at least four significant figures.

**Results:** Again, spatially local and total heat transfer results and the solidification fraction were obtained as functions of time.
Plots of nondimensional wall heat flux, for the case of $Bi = 1.0$, $Ste_s = 0.05$, $Ste_L = 0.2$ are presented in Fig. 13. The curves are parameterized by values of the product $Ste_s \cdot \tau$. The variations of the nondimensional surface integrated heat flux and the solidification fraction with $Ste_s \cdot \tau$ are shown in Fig. 14.

The curves presented in Fig. 13 indicate that for $Ste_s \cdot \tau < 0.05$, the nondimensional wall heat flux, $q_w/h(T_{sat}-T_\infty)$, is greater than one, and relatively uniform, away from the corners; in the vicinity of the corners it dips below one. This is because the liquid phase is initially in a superheated state ($Ste_L = 0.2$), and for $Ste_s \cdot \tau < 0.05$, freezing does not commence, as is evident from Fig. 14, so $T_w > T_{sat}$. Further, as was stated in the discussion of the problem involving saturated liquid phase ($Ste_L = 0$), the PCM in the vicinity of the corner cools faster than that away from it, because of heat loss from the two adjacent faces.

For the case of $Bi = 1.0$, the nondimensional surface integrated heat flux, $Q/hA(T_{sat}-T_\infty)$, decreases rapidly during the initial transient: solidification does not commence until $Ste_s \cdot \tau = 0.05$, thus latent heat is not available. Beyond $Ste_s \cdot \tau = 0.05$, it decreases relatively gradually, and almost linearly, to a value of about 0.3 at the end of solidification. Thereafter, the latent heat is again unavailable, and $Q$ drops off rapidly. For the case of $Bi = 10$, solidification starts
almost immediately after the start of the cooling process. The high initial values of Q, however, cannot be sustained. During the period $0 < \text{Ste}_s < 0.1$, $Q/hA(T_{\text{sat}} - T_\infty)$ drops rapidly. Beyond this period, it decreases gradually until the solidification process is complete, and then it again drops off steeply.

To the best knowledge of the author, this superheated liquid problem has not been dealt with in the published literature. Therefore, the aforementioned results could be considered as an augmentation of the currently available data on heat transfer phenomena.
CHAPTER V

CONCLUSION

This chapter is divided into two main sections. First, the work presented in the earlier chapters is briefly reviewed and commented upon. Following this, some ideas for extending this work are presented.

5-1 REVIEW OF THE THESIS

In this thesis, an extended version of the enthalpy model of Shamsundar and Sparrow (10) has been merged with a fully implicit control-volume based finite element method, akin to that proposed by Baliga and Patankar (16). This has resulted in a method that has the capability of solving unsteady heat conduction problems which involve solid-liquid phase change and irregular multiply-connected domains. To the best knowledge of the author, this is the first time that the enthalpy model has been incorporated in a general numerical method with the aforementioned capabilities.

The proposed method can handle unsteady, and steady, heat conduction in a variety of problems, with or without solid-liquid phase change; four illustrative examples have been presented in Chapter IV. In problems involving phase
change, the method is capable of dealing simultaneously with superheated liquid and subcooled solid regions. This represents an extension of the capabilities of the enthalpy model proposed by Shamsundar and Sparrow (10).

An analytical investigation of the order of accuracy (21) of the proposed method is extremely difficult, if not impossible, to carry out. This is mainly because the problems of interest are unsteady, multidimensional and non-linear. For steady-state problems of this nature, an empirical investigation of the order of accuracy is possible using a modified version of the Richardson extrapolation technique (16, 21). This technique could, in principle, be applied to unsteady problems too, but it would involve significantly greater costs. The difficulty is that a spatial discretization (ΔX, ΔY) and a time discretization (Δt) are involved, and a considerable computational effort is required to isolate their individual influences on the order of accuracy of the proposed method. For this reason, such an investigation was not undertaken in this thesis. Instead, the proposed method was applied to numerous test problems. The results of four such problems were discussed in Chapter IV, and their validity was established by comparing them with corresponding solutions available in the published literature.

As was stated earlier in this discussion, the main advantage of the proposed method over a corresponding finite
difference formulation is its ability to handle irregular multiply-connected domains. It is to be noted that this advantage is obtained at the expense of greater complexity in the computer code and, consequently, larger computer times for the same number of nodes and time steps. The increase in computer times, however, is not drastic. For example, in the problem involving freezing of a superheated liquid P.C.M. in a convectively cooled container of square cross section, discussed in Chapter IV, the proposed method required about 1.4 times the computer time needed by a corresponding finite difference scheme (22); the number of nodes, time steps, and iterations were kept the same, and both methods were run on the AMDHAL V7 computer using a FORTRAN H compiler.

5-2 SOME IDEAS FOR THE EXTENSION AND IMPROVEMENT OF THE WORK PRESENTED IN THIS THESIS

The formulation of the proposed method is geared to the use of either triangular or rectangular elements. As was stated in earlier chapters, there are advantages and disadvantages associated with each of these elements, and the selection of one or the other is mainly dictated by the nature of the problem of interest. Indeed, a combination of triangular and rectangular elements may be desirable in some problems. Thus a method that could simultaneously employ
triangular and rectangular elements would be more versatile than the formulation presented in this thesis. Such a method may be constructed using the following guidelines: divide the given domain into a suitable number of rectangular and triangular subdomains; discretize each subdomain into similar shaped elements; derive discretization equations for the nodes inside each subdomain, using the formulation presented in this thesis. Nodes lying on the interfaces between subdomains could be associated with both triangular and rectangular elements, and a special procedure would have to be devised to assemble the corresponding discretization equations.

In its present form, the proposed method is capable of solving only plane two-dimensional problems. However, it could be relatively easily modified to enable the solution of two-dimensional axisymmetric problems. Such an extension would use elements generated by revolving triangular, or rectangular, elements through 360 degrees about the axis of symmetry.

The proposed method can solve unsteady heat conduction in problems involving solid-liquid phase change; it cannot handle natural convection in such problems. However, in phase change problems that involve a superheated liquid phase, natural convection effects are often very significant (5,11,15). Thus the proposed method is not strictly applicable to such problems. The formulation of a method that can efficiently
handle such complex natural convection phenomena would represent a significant contribution to the currently available repertoire of numerical methods.

Numerous test problems have been successfully solved using the proposed method; four such problems have been discussed in Chapter IV. The results seem encouraging enough to warrant the application of this method to more challenging and practical problems.
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APPENDIX I

GENERAL FORM OF THE GOVERNING EQUATIONS

The general form of the governing equation for a steady state heat conduction problem can be written as follows:

\[ \nabla \cdot (\Gamma \nabla \phi) + S_\phi = 0 \]  (A1-1)

where \( \phi \) is a general dependent variable, \( \Gamma \) is the thermal conductivity, and \( S_\phi \) is the 'source term'.

When applied to two dimensional problems in Cartesian coordinates, and \( \Gamma = 1 \), Eqn. (A1-1) reduces to:

\[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + S_\phi = 0 \]  (A1-2)

For unsteady state problems, the general form of the governing equation can be written as follows:

\[ \nabla \cdot (\Gamma \nabla \phi) + \frac{\partial (\beta \phi)}{\partial t} + S_\phi = 0 \]  (A1-3)

In this equation, \( \beta = \rho c \).
For two dimensional problems in Cartesian coordinates, and \( r = 1 \), Eqn. (A1-3) reduces to:

\[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \Phi_\phi = \frac{3(\partial \phi)}{\partial \tau}. \]  

(A1-4)
APPENDIX II

COEFFICIENTS IN THE LINEAR INTERPOLATION FUNCTION

For triangular elements, the dependent variable $\phi$ is interpolated linearly in each element as follows:

$$\phi = Ax + By + C \quad (A2-1)$$

The constants $A$, $B$, and $C$, are determined in terms of $\phi_1$, $\phi_2$, and $\phi_3$, and the nodal coordinates. Applied to the nodes $(1,2,3)$ of a typical triangular element, Eqn. (A2-1) can be written in a matrix form as:

$$
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\phi_3
\end{bmatrix} =
\begin{bmatrix}
x_1 & y_1 & 1 \\
x_2 & y_2 & 1 \\
x_3 & y_3 & 1
\end{bmatrix}
\begin{bmatrix}
A \\
B \\
C
\end{bmatrix} \quad (A2-2)
$$

Eqn. (A2-2) can be solved to obtain $A$, $B$, and $C$:

$$A = \frac{1}{\text{DET}} \left[ (y_2 - y_3)\phi_1 + (y_3 - y_1)\phi_2 + (y_1 - y_2)\phi_3 \right] \quad (A2-3)$$

$$B = \frac{1}{\text{DET}} \left[ (x_3 - x_2)\phi_1 + (x_1 - x_3)\phi_2 + (x_2 - x_1)\phi_3 \right] \quad (A2-4)$$
\[ C = \frac{1}{\text{DET}} \left[ (x_2y_3 - y_2x_3) \Phi_1 + (x_3y_1 - x_1y_3) \Phi_2 + (x_1y_2 - x_2y_1) \Phi_3 \right] \quad (A2-5) \]

where

\[ \text{DET} = (x_1y_2 - y_1x_2) + (y_1x_3 - x_1y_3) + (x_2y_3 - x_3y_2) \quad (A2-6) \]
APPENDIX III

COEFFICIENTS IN THE BILINEAR INTERPOLATION FUNCTION

In problems where quadrilateral elements are used, the dependent variable \( \phi \) is interpolated by the bilinear function in each element as follows:

\[
\phi = Ax + By + Cxy + D \tag{A3-1}
\]

where \( A, B, \) and \( C \) are determined in terms of \( \phi_1, \phi_2, \phi_3 \) and \( \phi_4 \) and the nodal coordinates. Equations (A3-1) can be applied to the nodes 1, 2, 3 and 4 of a typical element to obtain the following matrix equation:

\[
\begin{bmatrix}
\phi_1 \\
\phi_2 \\
\phi_3 \\
\phi_4
\end{bmatrix} =
\begin{bmatrix}
x_1 Y_1 & x_1Y_1 & 1 \\
x_2 Y_2 & x_2 Y_2 & 1 \\
x_3 Y_3 & x_3 Y_3 & 1 \\
x_4 Y_4 & x_4 Y_4 & 1
\end{bmatrix}
\begin{bmatrix}
A \\
B \\
C \\
D
\end{bmatrix} \tag{A3-2}
\]

Let

\[
\text{DET} = \begin{vmatrix}
(x_1-x_2) & (y_1-y_2) & (x_1y_1-x_2y_2) \\
(x_2-x_3) & (y_2-y_3) & (x_2y_2-x_3y_3) \\
(x_3-x_4) & (y_3-y_4) & (x_3y_3-x_4y_4)
\end{vmatrix} \tag{A3-3}
\]
or in a compact form,

\[
\begin{vmatrix}
  a_1 & b_1 & c_1 \\
  a_2 & b_2 & c_2 \\
  a_3 & b_3 & c_3
\end{vmatrix} = \text{DET} \tag{A3-4}
\]

The expressions for \(a_1, a_2, \ldots, c_2, c_3\) may be deduced by comparing Eqns. (A3-3) and (A3-4) with one another. Eqn. (A3-2) can be solved to obtain \(A, B,\) and \(C\):

\[
A = \frac{1}{\text{DET}} \left[ [b_2 c_3 - c_2 b_3] \phi_1 + [b_3 (c_1 + c_2) - c_3 (b_1 + b_2)] \phi_2 + [b_1 (c_2 + c_3) - c_1 (b_2 + b_3)] \phi_3 + [b_2 c_1 - c_2 b_1] \phi_4 \right] \tag{A3-5}
\]

\[
B = \frac{1}{\text{DET}} \left[ [c_2 a_3 - a_2 c_3] \phi_1 + [c_3 (a_1 + a_2) - a_3 (c_1 + c_2)] \phi_2 + [a_1 (a_2 + a_3) - a_1 (c_2 + c_3)] \phi_3 + [c_2 a_1 - a_2 c_1] \phi_4 \right] \tag{A3-6}
\]

\[
C = \frac{1}{\text{DET}} \left[ [a_2 b_3 - b_2 a_3] \phi_1 + [a_3 (b_1 + b_2) - b_3 (a_1 + a_2)] \phi_2 + [a_1 (b_2 + b_3) - b_1 (a_2 + a_3)] \phi_3 + [a_2 b_1 - b_2 a_1] \phi_4 \right] \tag{A3-7}
\]
The expressions for $A$, $B$, and $C$ can be cast in the following compact form:

\[
A = A_1^1 \phi_1 + A_2^2 \phi_2 + A_3^3 \phi_3 + A_4^4 \phi_4 \quad (A3-8)
\]

\[
B = B_1^1 \phi_1 + B_2^2 \phi_2 + B_3^3 \phi_3 + B_4^4 \phi_4 \quad (A3-9)
\]

\[
C = C_1^1 \phi_1 + C_2^2 \phi_2 + C_3^3 \phi_3 + C_4^4 \phi_4 \quad (A3-10)
\]

Again, by matching the set of equations (A3-5) to (A3-7) with the corresponding set of equations (A3-8) to (A3-10), the expressions for $A_1$, $A_2$, ..., $C_3$, $C_4$ can be deduced.
APPENDIX IV

ELEMENT CONTRIBUTIONS TO THE INTEGRAL CONSERVATION EQUATION FOR $\phi$: TRIANGULAR ELEMENTS

In this work, the control-volume based finite element method (16) is applied. The domain of interest is divided into three-node triangular elements. Each node in the domain is surrounded by a control volume, as shown in Fig. 2.

The 'enthalpy equation', when applied to C.V. 1, see Fig. 2b, associated with node 1, may be written as follows:

$$\frac{3}{3} \int (\beta \theta) dV - \left( \int_0^\theta \dot{\Phi} \cdot n ds + \int_0^\theta \dot{\Phi} \cdot n ds \right) -$$

$$\int_{laoc} S_\phi dV + \text{[similar contributions from other elements associated with node 1]} = 0$$

(A4-1)

The first term on the left-hand side of Eqn. (A4-1) can be approximated by:

$$\int_{laoc} \frac{\beta (\theta m - \theta m - 1)}{\Delta \tau} dV = \frac{\beta}{\Delta \tau} \frac{A \epsilon}{3} \left( \theta m - \theta m - 1 \right)$$

(A4-2)
where $A_e$ is the area 123 and is given by:

$$
A_e = \text{ABS} \left( \begin{vmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \end{vmatrix} \right) / 2 \quad (A4-3)
$$

In Eqn. (A4-2), $\theta_1^m$ and $\theta_1^{m-1}$ are the values of $\theta_1$ at time levels $m$ and $(m-1)$, respectively, and $\Delta \tau$ is the nondimensional time step, $(\tau_m - \tau_{m-1})$.

Using the linear interpolation function introduced in Eqn. (A2-1),

$$
\ddot{\psi}_\phi = A^i + B^j \quad (A4-4)
$$

Let

$$
\hat{n}_{oa} = \frac{(y_a - y_0)\hat{i} - (x_a - x_0)\hat{j}}{|\hat{o}a|} \quad (A4-5)
$$

and

$$
\hat{n}_{oc} = \frac{(y_c - y_0)\hat{i} - (x_c - x_0)\hat{j}}{|\hat{o}c|} \quad (A4-6)
$$
Then
\[ \Gamma \int_a^b \nabla \cdot \mathbf{r}_{oa} \, ds = \frac{\Gamma}{|oa|} \int_a^b \left[ (y_a - y_o)A - (x_a - x_o)B \right] ds \quad (A4-7) \]

Noting that the integrand on the right-hand side of Eqn. (A4-7) is a constant, the equation may be reduced to
\[ \Gamma \int_a^b \nabla \cdot \mathbf{r}_{oa} \, ds = \Gamma \left[ A(y_a - y_o) - B(x_a - x_o) \right] \quad (A4-8) \]

The expressions for A and B, Eqns. (A2-3) and (A2-4), may be introduced into Eqn. (A4-8) to give
\[ \Gamma \int_a^b \nabla \cdot \mathbf{r}_{oa} \, ds = \frac{\Gamma}{\text{DET}} \left[ (y_a - y_o)(y_2 - y_3) + (x_a - x_o)(x_2 - x_3) \right] \phi_1 + \]
\[ + \frac{\Gamma}{\text{DET}} \left[ (y_a - y_o)(y_3 - y_1) + (x_a - x_o)(x_3 - x_1) \right] \phi_2 + \]
\[ + \frac{\Gamma}{\text{DET}} \left[ (y_a - y_o)(y_1 - y_2) + (x_a - x_o)(x_1 - x_2) \right] \phi_3 \quad (A4-9) \]
Similarly,

\[
\Gamma \int_0^C \nabla \phi \cdot \mathbf{n_{oc}} \, ds = \frac{\Gamma}{\text{DET}} \left[ (y_c-y_o)(y_2-y_3) + (x_c-x_o)(x_2-x_3) \right] \phi_1 + \\
\frac{\Gamma}{\text{DET}} \left[ (y_c-y_o)(y_3-y_1) + (x_c-x_o)(x_3-x_1) \right] \phi_2 + \\
\frac{\Gamma}{\text{DET}} \left[ (y_c-y_o)(y_1-y_2) + (x_c-x_o)(x_1-x_2) \right] \phi_3
\]  

(A4-10)

The integral involving the source term is approximated by the following algebraic expression,

\[
\int_{\text{laoc}} S_\phi \, dV = \int_{\text{laoc}} (S_c + S_p \phi_1) \, dV 
\]  

(A4-11)

where \( S_c \) and \( S_p \) are stored at the centroid, \( o \), and they are assumed to be constant over the element. Let \( \phi_1 \) prevail over the area \( \text{laoc} \) and consider unit thickness. Then Eqn. (A4-11) may be written as:

\[
\int_{\text{laoc}} (S_c + S_p \phi_1) \, dV = \frac{A_e}{3} S_c + \frac{A_e}{3} S_p \phi_1 
\]  

(A4-12)
With respect to C.V. 1, \( \mathbf{n}_{oa} \) is directed inwards and \( \mathbf{n}_{oc} \) is directed outwards. It is to be noted that to ensure the validity of the last statement, it is mandatory to number the element nodes in a counter-clockwise manner as shown in Fig. 2. Therefore, the following terms can be rearranged and cast as follows:

\[
-\Gamma \int_a^b \nabla \phi \cdot \mathbf{n} ds + \int_0^c \nabla \phi \cdot \mathbf{n} ds - \int_{loac} S_\phi dV =
\]

\[
\frac{\Gamma}{\text{DET}} \left[ (Y_2 - Y_3)(y_a - y_c) + (x_2 - x_3)(x_a - x_c) \right] - \frac{Ae}{3} S_p \phi_1 +
\]

\[
\frac{\Gamma}{\text{DET}} \left[ (Y_3 - Y_1)(y_a - y_c) + (x_3 - x_1)(x_a - x_c) \right] \phi_2 +
\]

\[
\frac{\Gamma}{\text{DET}} \left[ (Y_1 - Y_2)(y_a - y_c) + (x_1 - x_2)(x_a - x_c) \right] \phi_3 - \frac{Ae}{3S_c} (A4-13)
\]

This equation can be written in the following compact form:

\[
-\Gamma \int_a^b \nabla \phi \cdot \mathbf{n} ds + \int_0^c \nabla \phi \cdot \mathbf{n} ds - \int_{loac} S_\phi dV =
\]

\[
C1(1) \phi_1 + C1(2) \phi_2 + C1(3) \phi_3 + \text{CONT} \]  
(A4-14)
Using Eqns. (A4-2) and (A4-14), the element contribution to the enthalpy equation (A4-1) can be written as:

\[
\frac{\partial}{\partial t} \int_{\Omega} (\beta \phi) \, dV - \int_{\Omega} \left( \int_0^t \mathbf{v} \cdot \mathbf{n} \, ds + \int_0^t \mathbf{v} \cdot \mathbf{n} \, ds \right) - \int_{\Omega} S \, dV = \\
C_I(1) \phi_{1m} + C_I(2) \phi_{2m} + C_I(3) \phi_{3m} + \text{CONT} l + \frac{Ae \beta}{3 \Delta t} \theta_{1m} - \frac{Ae \beta}{3 \Delta t} \theta_{1m-1}
\]

(A4-15)

In Eqn. (A4-15), all spatial terms, that is all terms not involving the time derivative, are approximated at time level \( m \). In other words, a fully-implicit scheme is employed to obtain the discretization equations.
APPENDIX V

ELEMENTS CONTRIBUTIONS TO THE INTEGRAL CONSERVATION
EQUATION FOR φ: QUADRILATERAL ELEMENTS

As was mentioned before, the selection of a suitable element, triangular or quadrilateral, depends on the problem being solved. In this appendix, the contribution of a quadrilateral element to the control volume associated with node 1, see Fig. 3c, is presented. The enthalpy equation may be written as follows:

\[
\frac{2}{\phi} \int_{\text{load}} (\beta \theta) dV - \Gamma \left[ \int_a \nabla \phi \cdot n ds + \int_0^d \nabla \phi \cdot n ds \right] = 0
\]

\[
\int_{\text{load}} \Phi ds + \text{[similar contributions from other elements associated with node 1]} = 0 \quad (A5-1)
\]

The first term on the left-hand side of Eqn. (A5-1) can be approximated by a simple one step finite difference scheme:

\[
\int_{\text{load}} \frac{\beta(\theta_1^{m-1} - \theta_1^{m-1})}{\Delta \tau} dV = \frac{\beta}{\Delta \tau} \cdot \text{Area}_{\text{load}}[\theta_1^{m-1} - \theta_1^{m-1}] \quad (A5-2)
\]
Using the bilinear interpolation function given in Eqn. (A3-1),

\[ \hat{\mathbf{v}} = (A + Cy) \hat{i} + (B + Cx) \hat{j} \]  

(A5-3)

Let

\[ \hat{n}_{oa} = (y_a \hat{i} - x_a \hat{j})/|oa| \]  

(A5-4)

and

\[ \hat{n}_{od} = (y_d \hat{i} - x_d \hat{j})/|od| \]  

(A5-5)

It is to be noted here that local, or element, coordinates are being used in this derivation; thus the coordinates of the centroid, \( o \), are \( (x_o = 0, y_o = 0) \). Further, \( \hat{n}_{oa} \) and \( \hat{n}_{od} \) point inwards and outwards, respectively, with respect to C.V. 1; the counter-clockwise node numbering shown in Fig. 3 is mandatory. Then,

\[ \Gamma \int_a^b \hat{\mathbf{v}} \cdot \hat{n}_{oa} \, ds = \frac{\Gamma}{|oa|} \int_0^a [(A + Cy) y_a - (B + Cx) x_a] \, ds \]  

(A5-6)

The integrand on the right-hand side of Eqn. (A5-6) is a
linear function in $x$ and $y$. Thus,

$$\Gamma \int_{a}^{b} \tilde{\nabla} \phi \cdot \hat{n}_{ao} \, ds = \Gamma \left[ A + \frac{Cy}{2} \right] y_a - \Gamma \left[ B + \frac{Ck}{2} \right] x_a \quad (A5-7)$$

The expressions for $A$, $B$, and $C$, given by Eqns. (A3-8) to (A3-10), may be introduced into Eqn. (A5-7) to obtain

$$-\Gamma \int_{a}^{b} \tilde{\nabla} \phi \cdot \hat{n}_{ao} \, ds = \Gamma \left[ B^1 x_a + C^1 \left( \frac{x_a^2 - y_a^2}{2} \right) - A^1 y_a \right] \phi_1 +$$

$$\Gamma \left[ B^2 x_a + C^2 \left( \frac{x_a^2 - y_a^2}{2} \right) - A^2 y_a \right] \phi_2 +$$

$$\Gamma \left[ B^3 x_a + C^3 \left( \frac{x_a^2 - y_a^2}{2} \right) - A^3 y_a \right] \phi_3 +$$

$$\Gamma \left[ B^4 x_a + C^4 \left( \frac{x_a^2 - y_a^2}{2} \right) - A^4 y_a \right] \phi_4 \quad (A5-8)$$

Similarly,
\[-r \int_0^d \nabla \phi \cdot \vec{r}_o \, ds = r \left[ B^1 x_d + c^1 \left( \frac{x_d^2 - y_d^2}{2} \right) - A^1 y_d \right] \phi_1 +
\r \left[ B^2 x_d + c^2 \left( \frac{x_d^2 - y_d^2}{2} \right) - A^2 y_d \right] \phi_2 +
\r \left[ B^3 x_d + c^3 \left( \frac{x_d^2 - y_d^2}{2} \right) - A^3 y_d \right] \phi_3 +
\r \left[ B^4 x_d + c^4 \left( \frac{x_d^2 - y_d^2}{2} \right) - A^4 y_d \right] \phi_4 \quad (A5-9)\]

The integral involving the source term is approximated by the following algebraic expression:

\[
\int_{\text{laod}} S_\phi \, dV = \int_{\text{laod}} (S_c + S_p \phi) \, dV \quad (A5-10)
\]

In quadrilateral elements, just as in triangular ones, \( S_c \) and \( S_p \) are stored at the centroid, \( o \), and they are assumed to be constant over the element. Further, in Eqn. (A5-10) \( \phi_1 \) is assumed to prevail over the area \( \text{laod} \). Thus,

\[
\int_{\text{load}} S_\phi \, dV = S_c \, \text{Area}_{\text{laod}} + S_p \phi_1 \cdot \text{Area}_{\text{laod}} \quad (A5-11)
\]
The area of the quadrilateral lao is defined by adding the areas of the triangles lao, and ldo in the following way:

\[ \text{Area}_{lao} = \frac{\text{ABS(DET1)}}{2} \quad (A5-12) \]

Where

\[ \text{DET1} = \begin{vmatrix} x_1 & y_1 & 1 \\ x_a & y_a & 1 \\ x_o & y_o & 1 \end{vmatrix} \quad (A5-13) \]

By taking the origin at point o, the centroid of the quadrilateral, Eqn. (A5-13) reduces to:

\[ \text{DET2} = x_1 y_a - y_1 x_a \quad (A5-14) \]

Similarly,

\[ \text{Area}_{ldo} = \frac{\text{ABS(DET2)}}{2} \quad (A5-15) \]

Where

\[ \text{DET2} = x_1 y_d - y_1 x_d \quad (A5-16) \]
The area load is therefore given by

\[ \text{Area}_{\text{load}} = \text{Area}_{\text{load}} + \text{Area}_{\text{load}} \]  \hspace{1cm} (A5-17)

Thus,

\[ \left[ \int_{a}^{d} \hat{v}_{\phi} \cdot \hat{n} \, ds \right] - \int_{\text{load}} S_{\phi} \, dv = \]

\[ \text{Cl}(1)\phi_{1} + \text{Cl}(2)\phi_{2} + \text{Cl}(3)\phi_{3} + \text{Cl}(4)\phi_{4} + \text{CONT} \]  \hspace{1cm} (A5-18)

The coefficients of \( \phi_{1}, \phi_{2}, \phi_{3} \) and \( \phi_{4} \) in Eqn. (A5-18) can be deduced by using Eqns. (A5-8), (A5-9) and (A5-11).

Finally, using Eqns. (A5-2) and (A5-18), the element contribution to the enthalpy equation (A5-1) can be written as:

\[ \frac{\partial}{\partial t} \int_{\text{load}} (\beta \theta) \, dv - \left[ \int_{a}^{d} \hat{v}_{\phi} \cdot \hat{n} \, ds + \int_{b}^{c} \hat{v}_{\phi} \cdot \hat{n} \, ds \right] - \int_{\text{load}} S_{\phi} \, dv = \]

\[ \text{Cl}(1)\phi_{1}^{m} + \text{Cl}(2)\phi_{2}^{m} + \text{Cl}(3)\phi_{3}^{m} + \text{Cl}(4)\phi_{4}^{m} + \text{CONT} + \frac{\beta}{\Delta t} \cdot \text{Area}_{\text{load}} \theta_{1}^{m} - \]

\[ \frac{\beta}{\Delta t} \cdot \text{Area}_{\text{load}} \theta_{1}^{m-1} \]  \hspace{1cm} (A5-19)
It is to be noted that a fully-implicit scheme is used to obtain the discretization equations.
APPENDIX VI

ON THE POSITIVE DEFINITENESS OF THE COEFFICIENT $a_i$ IN THE DISCRETIZATION EQUATION

The complete discretization equation for a typical node $i$, for both triangular and rectangular elements, can be cast in the following general form (Eqn. 3-14):

$$ADDT_i \theta_i^m + a_i \phi_i^m = ADDT_i \theta_i^{m-1}$$

$$+ \sum_{\text{neighbors of node } i} a_n \phi_n^m + b_i \quad (A6-1).$$

This discretization equation is assembled by adding the appropriate contributions of all elements associated with node $i$.

For triangular elements, see Fig. 2, using the derivations in Appendix IV, the coefficient $a_i$ in Eqn. (A6-1) may be expressed as

$$a_i = \sum_{\text{elements associated with node } i} \left[ \frac{1}{\text{DET}} (y_2-y_3)(y_a-y_c) + (x_2-x_3)(x_a-x_c) \right] \frac{AE}{3} S_p \quad (A6-2).$$
The source term $S_p$ is either zero or negative ($<0$). The coordinates of the element mid-side points can be expressed in terms of the coordinates of the nodal points. Thus Eqn. (A6-2) may be rewritten as follows:

$$a_i = \sum_{\text{elements associated with node } i} \left[ \frac{\Gamma}{\text{DET}} \left( \frac{(y_2-y_3)^2}{2} + \frac{(x_2-x_3)^2}{2} \right) + (AS)^2 \right]_{n,i}$$  \hspace{1cm} (A6-3)

It is to be noted that

$$(AS)^2 = -\frac{A_e}{3} s_p; \quad \frac{(x_2-x_3)}{2} = (x_a-x_c); \quad \frac{(y_2-y_3)}{2} = (y_a-y_c)$$

Let

$$c_{n,i} = \frac{\Gamma}{\text{DET}} \left[ \frac{(y_2-y_3)^2}{2} + \frac{(x_2-x_3)^2}{2} \right] + (AS)^2$$  \hspace{1cm} (A6-4)

Then

$$a_i = \sum_{\text{elements associated with node } i} c_{n,i}$$  \hspace{1cm} (A6-5)
It is clear from Eqn. (A6-4) that the $C_{n,i}$ are positive definite. Therefore $a_i$ is also positive definite.

The proof for rectangular elements is similar to the one given above for triangular elements. The algebra is considerably more complicated, however, so it is not presented in this thesis.
APPENDIX VII

LISTING OF COMPUTER PROGRAM AND SAMPLE EXECUTION

In this appendix, a computer program for the prediction of unsteady heat conduction in materials with or without solid-liquid phase change is listed along with a sample run. The program is written in the FORTRAN language, and it incorporates the four-node rectangular finite element formulation presented in the main body of this thesis. The sample run was executed using the FORTRAN-H compiler on the AMDHAL V7 computer; it corresponds to the superheated liquid phase problem discussed in Chapter IV, section 4-3-2.

An overall flow diagram of the computer program is presented on the following page. Then, the listing and sample run are presented. Brief descriptions of the tasks performed by the various subroutines and algorithms that make up the program are provided by the comment cards in the program itself.
MASTER PROGRAM: SET OF CALLING AND CONTROL STATEMENTS GEARED TO PROBLEM OF INTEREST

CALL DATAI
CALL GRID
CALL START
CALL COEFF
CALL PRINT

SUPPRESS PRINTING OF COEFFICIENTS AND NODAL COORDINATES IF DESIRED

ISTEP = ISTEP + 1
TIME = TIME + DT

DETAILED OUTPUT DESIRED?

YES

ITERATION MONITOR ON
CALL SOLVE
ITERATION MONITOR OFF
CALL PRINT

GENERAL SUBROUTINES
COEFF
SOLVE
PRINT

NO

ADJUST NUMBER OF ITERATIONS IN SOLVE IF NEEDED

MORE TIME STEPS DESIRED?

YES

STOP

OVERALL FLOW DIAGRAM OF THE COMPUTER PROGRAM
LEVEL 2.1.0 (JUNE 78) 05/360 FORTRAN II EXTENDED DATE 80.109/22.56.43 PAGE 1

REQUESTED OPTIONS:
OPTIONS IN EFFECT: NAME(MAIN) OPTIMIZE(2) LINECOUNT(60) SIZE(MAX) AUTODRL(NONE)
SOURCE ECN2IC NOLIST NODERECK OBJECT NOMAP NOFORMAT GOSTMT NOXREF NOANSF NOTERM IBM FLAG(1)

******************************************************************************
** Finite Element Program for the Prediction of Unsteady Heat Conduction in Materials With or Without Phase Change.**
******************************************************************************

C

C IMPLICIT REAL*(A-H,O-Z)
C LOGICAL LSOLVE,LPINT,LMONIT
C COMMON/CNTL/, LSOLVE(2), LPINT(2), LMONIT, IPRINT, ISTEP
C COMMON F(23,23), G(22,22), BCTA(22,22), SC(22,22), SP(22,22)
C COMMON AC(23,23), AN(23,23), AS(23,23), ASW(23,23), COM(23,23)
C COMMON X(23,23), Y(23,23), ARC(23), AR(23), CV(23,23), DT,TIME,
C IATOT
C COMMON LI, L2, M2, NF, NTER

C CALL DATAI
C CALL GRID
C CALL START
C 30 FORMAT(1H1,2X,'ISTEP=',5X, 'TIME=',6.D10, 4)
C CALL COPER
C CALL PRINT
C IPRINT=1
C 10 ISTEP=ISTEP+1
C TIME=TIME+DT
C ISTEP.EQ.30 OR ISTEP.EQ.50 OR ISTEP.EQ.100 OR ISTEP.EQ.175 OR
C ISTEP.EQ.200 GO TO 100
C CALL SOLVE
C GO TO 110
C 100 ISTEP=ISTEP
C 110 WRITE(6,30) ISTEP, TIME
C CALL PRINT
C CONTINUE
C IF(ISTEP.GT.10) NITER=50
C IF(ISTEP.GT.30) NITER=30
C IF(ISTEP.GT.200) GO TO 20
C 20 CONTINUE
C STOP
C END

*OPTIONS IN EFFECT* NAME(MAIN) OPTIMIZE(2) LINECOUNT(60) SIZE(MAX) AUTODRL(NONE)

*OPTIONS IN EFFECT* SOURCE ECN2IC NOLIST NODERECK OBJECT NOMAP NOFORMAT GOSTMT NOXREF NOANSF NOTERM IBM FLAG(1)
LEVEL 2.3.0 (JUNE 78)  05/360 FORTRAN H EXTENDED
REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) OPTIMIZE(2) LINECOUNT(60) SIZE(MAX) AUTODUBL(NONE)
SOURCE ESCDOC NOLIST OBJECT OPTION NOFORMAT GOSTMT N0XREF NOALC N0ANSF N0TERM IBM FLAG(I)

C                 ****************************************
C     SUBROUTINE USER
C                 ****************************************
ISN 0002
C
C
ISN 0003  IMPLICIT REAL*(A-H,O-Z)
ISN 0004  LOGICAL LSOLVE,LPRT,LMONIT
ISN 0005  COMMON/DERV/STE,SL,FLUX,B
ISN 0006  COMMON/CNTL/LSOLVE(2),LPRT,LMONIT,IPRT,ISTEP
ISN 0007  COMMON F(23,23),GAM(22,22),BETA(22,22),SI(22,22),SP(22,22)
ISN 0008  COMMON AC(23,23),AN(23,23),AS(23,23),AE(23,23),AM(23,23)
           IAVE(23,23),ANW(23,23),ASW(23,23),AVE(23,23),AMW(23,23)
ISN 0009  COMMON X(23,23),Y(23,23),ARC(23),A(23),R(23),C(23),V(23,23),OT,TIME,
           LAT
ISN 0010  COMMON LI,M1,L2,MP,NF,NITER
           ************************************************
ISN 0011  ENTRY DATA!
           ********
           DEFAULT VALUES
ISN 0012  LSOLVE(1)=.FALSE.
ISN 0013  LSOLVE(2)=.FALSE.
ISN 0014  LPRT(1)=.FALSE.
ISN 0015  LPRT(2)=.FALSE.
ISN 0016  LMONIT=.FALSE.
ISN 0017  NITER=5
ISN 0018  IPRT=5
ISN 0019  DT=1.00
ISN 0020  TIME=0.00
ISN 0021  DT=1.00
ISN 0022  ISTEP=0
ISN 0023  STEL=0.00
ISN 0024  FLUX=0.00
ISN 0025  BI=0.00
ISN 0026  ATOTS=0.00
ISN 0027  RETURN
ISN 0028  ENTRY GRID
           *****************
           GENERATION OF X AND Y VALUES OF ALL THE NODES
           ***********************************************
ISN 0029  LI=21
ISN 0030  M1=21
ISN 0031  L2=LI-1
ISN 0032  M2=M1-1
ISN 0033  XL=1.00
ISN 0034  YL=1.00
ISN 0035  PW=1.0
```
LEVEL 2.3.0 (JUNF 78) USR 05/36 G FORTRAN H EXTENDED

| SN 0036 | PWY=1.0 |
| SN 0037 | DO 10 J=1, L1 |
| SN 0038 | XCOOT=(DFLOAT(-1)/DFLOAT(L2))**PWY*XL |
| SN 0039 | DO 10 J=1, L1 |
| SN 0040 | XCOOT |
| SN 0041 | 10 CONTINUE |
| SN 0042 | DO 11 J=1, M1 |
| SN 0043 | YCOOR=(DFLOAT(J-1)/DFLOAT(M2))**PWY*YL |
| SN 0044 | DO 11 J=1, L1 |
| SN 0045 | Y(J)=YCOOR |
| SN 0046 | 11 CONTINUE |
| SN 0047 | DO 100 J=1, M2 |
| SN 0048 | 100 ARC(J)=SQRT((X(1,J+1)-X(1,J))*+*(Y(1,J+1)-Y(1,J))*+2.00 |
| SN 0049 | DO 100 J=1, L2 |
| SN 0050 | 110 ARC(X)=SQRT((X(I+1,1)-X(I,1))*+2*(Y(I+1,1)-Y(I,1))*+2)/2.00 |
| SN 0051 | RETURN |
| SN 0052 | C ENTRY START |
| SN 0053 | C PROBLEM INITIAL VALUES, AND DATA |
| SN 0054 | LPRINT(1)=.TRUE. |
| SN 0055 | LPRINT(2)=.TRUE. |
| SN 0056 | STE=0.000 |
| SN 0057 | STEL=0.200 |
| SN 0058 | DT=0.100 |
| SN 0059 | RI=1.00 |
| SN 0060 | NI=75 |
| SN 0061 | IPRINT=2 |
| SN 0062 | C STARTING GUESS VALUES FOR ALL NONDIMENSIONAL |
| SN 0063 | C TEMPERATURES AND ENTHALPY VALUES IN THE DOMAIN |
| SN 0064 | DO 20 I=1, L1 |
| SN 0065 | DO 20 J=1, M1 |
| SN 0066 | FI(I,J)=STE |
| SN 0067 | DFI(I,J)=STE |
| SN 0068 | CONTINUE |
| SN 0069 | 20 RETURN |
| SN 0070 | C ENTRY DENSE |
| SN 0071 | C ********** |
| SN 0072 | DD 330 10=1,L2 |
| SN 0073 | DD 300 J0=1,M2 |
| SN 0074 | CONTINUE |
| SN 0075 | RETURN |
| SN 0076 | C ENTRY GMSOR |
| SN 0077 | C ********** |
| SN 0078 | DD 400 J0=1,M2 |
| SN 0079 | DD 400 10=1,L2 |
```
ENTRY BOUND
*******
INCLUSION OF BOUNDARY CONTRIBUTIONS

CON(1:1)=CON(1:1)-ARC(1)*BI*STE-ARCX(1)*BI*STE
DO 520 J=2,M2
520 CON(1,J)=CON(1,J)-(ARC(J-1)+ARC(J))*BI*STE,
CON(2,J)=CON(2,J)-ARCX(J-1)+ARCX(J)*BI*STE
DO 530 I=2,L2
530 CONTINUE
CON(L1,1)=CON(L1,1)-ARCX(L2)*BI*STE
RETURN
END
LEVEL 2, 3.0 (JUN 78)

REQUESTED OPTIONS:

OPTIONS IN EFFECT:

NAME(MAIN) OPTIMIZE(2) LINECOUNT(60) SIZE(MAX) AUTOLOG(NONE)
SOURCE FORMAT NOLIST NONFICK OBJCFT NOMAP NOFORMAT GOSTMT NOXREF NOALC NOANSF NOTERM IBM FLAG(I)

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SUBROUTINE SOLVE

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! implicit real(a-h,o-z) !

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LEVEL 2.1.0 (JUNE 78)  SOLVE  05/360 FORTRAN IV EXTENDED  DATE 80.109/22.56.47  PAGE 2

ISN 0049  50 IF(I1.NE.1) GO TO 52
ISN 0051  52 F(I1,2)=(CEN+AC(I1,1))*ARC(I1)*BI
ISN 0052  GO TO 51
ISN 0053  52 F(I1,2)=(CEN+AC(I1,1))*ARC(I2)*BI
ISN 0055  53 F(I1,2)=B/(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0056  GO TO 53
ISN 0057  53 F(I1,2)=B/(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0058  53 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0059  53 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0060  54 GO 50 J=2-M0
ISN 0061  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0062  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0063  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0064  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0065  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0066  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0067  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0068  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0069  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0070  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0071  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0072  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0073  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0074  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0075  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0076  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0077  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0078  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0079  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0080  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0081  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0082  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0083  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0084  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0085  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0086  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0087  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0088  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0089  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0090  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0091  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0092  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0093  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0094  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0095  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0096  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0097  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0098  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0099  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0100  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0101  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0102  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0103  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0104  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0105  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0106  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0107  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0108  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0109  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0110  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0111  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0112  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0113  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0114  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0115  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0116  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0117  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0118  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
ISN 0119  54 F(I1,1)=(CEN+AC(I1,1)+ARC(I2)*BI)
LEV1L 2.3.0 (JUNE 78) SOLVE 05/360 FORTRAN I EXTENDED DATE 80.102/12.56.47 PAGE 4

LEVEL 2.3.0 (JUNE 78) SOLVE 05/360 FORTRAN I EXTENDED

SN 0106
GO TO 170

SN 0107
200 IF(J .GE. 1) GO TO 201

SN 0108
F(I,J-I,2)=S/(CEN+AC(I,J,1)+ACX(I,1)+ARCX(I,1)+BI)

SN 0109
F(I,J-I,J)=F(I,J-2)

SN 0110
GO TO 170

SN 0111
201 F(I,J,J-2)=S/(CEN+AC(I,J,1))

SN 0112
F(I,J,J-1)=F(I,J-2)

SN 0113
170 CONTINUE

SN 0114
CEN=CEN+V(L,J)/GT

SN 0115
B=CONT(L,J)*CEN+F(L,J,1)+AUX(L,J)+F(L,J,1)

SN 0116
1 F(J ,GE. 1) GO TO 210

SN 0117
G=SL+AS(L,J)*((L,J,1)+AS(L,J)*F(L,J-1,1))

SN 0118
IF(J.GE.41) GO TO 220

SN 0119
210 B=AN(L,J)*F(I,J,J-1)+AUX(L,J)*F(I,J,J-1)

SN 0120
220 IF(B.LT.0.00) GO TO 230

SN 0121
FTEM=V/CEN

SN 0122
F(I,J,J-1) = FTEM

SN 0123
GO TO 170

SN 0124
IF TEMP.LE.1.00) GO TO 360

SN 0125
GO TO 750

SN 0126
750 F(I,J,J-2)=(B+AC(L,J,1)+ARCX(L,2)+BI)/(CEN+AC(L,J,1)+ARCX(L,2)+BI)

SN 0127
F(I,J,J) = F(I,J,J-2)

SN 0128
CONTINUE

SN 0129
GO TO 170

SN 0130
230 IF(J .GE. 1) GO TO 231

SN 0131
F(I,J-1,2)=S/(CEN+AC(L,J,1)+ARCX(L,2)+BI)

SN 0132
F(I,J-1,J)=F(I,J,2)

SN 0133
GO TO 170

SN 0134
231 F(I,J-1,J)=F(I,J,2)

SN 0135
130 CONTINUE

SN 0136
IF(J .NOT.LOWNJ) GO TO 10

SN 0137
10 CONTINUE

CC LOAD NEW F(I,J,2) INTO F2OLD I.E. F(I,J,3)

SN 0138
DD 300 IN=1,L1

SN 0139
DD 300 J=1,M1

SN 0140
F(I,J,3)=F(I,J,2)

SN 0141
CONTINUE

SN 0142
RETURN

SN 0143
END

*OPTIONS IN EFFECT NAME=MAIN OPTIMIZE=2 LINECOUNT=60 SIZE=MAX AUTOOBJ=NONE

*OPTIONS IN EFFECT SOURCE EBCDIC NOLIST NODECK OBJECT NOMAP NODUMP GOSTMT NODUMP NOMEAS NOSDS NETERM IBM FLAG

*STATISTICS SOURCE STATEMENTS = 230, PROGRAM SIZE = 4798, SUBPROGRAM NAME = SOLVE

*STATISTICS NO DIAGNOSTICS GENERATED

******* END OF COMPILATION ******

64K BYTES OF CORE NOT USED
SUBROUTINE COEFF
***
C
C IMPLICIT REAL*8(A-H,O-Z)
C
C COMMON/LSOLVE,PRINT,LMONIT
C COMMON/PRINT,LSOLVE,PRINT,LMONIT,IPRINT,ISTEP
C COMMON(F(2,22,22),GAM(22,22),BETA(22,22),SC(22,22),SP(22,22)
C COMMON(AC[23,23],AN[23,23],AS[23,23],AE[23,23],AM[23,23]
C COMMON(X[23,23],Y[23,23],ARC[23],CV[23,23],DT,TIME)
C
C COMMON L1,M1,L2,M2,NF,NITER
C
C DIMENSION XE(4),YE(4),XM(4),YM(4),A(4),B(4),C(4),D(4),CA(4),CB(4),
C COMMON X(4),Y(4),XM(4),YM(4),A(4),B(4),C(4),D(4),CA(4),CB(4)
C
C DO 1 NF=1,2
C IF(3LSOLVE(NP)) GO TO 2
C GO TO 1
C CALL DENSE
C CALL GANSOR
C DO 5 J=1,41 A(J,J)=0.1
C DO 6 J=1,41 A(J,J)=0.1
C DO 7 J=1,41 A(J,J)=0.1
C DO 8 J=1,41 A(J,J)=0.1
C DO 9 J=1,41 A(J,J)=0.1
C DO 10 J=1,41 A(J,J)=0.1
C Continue DO 10 J=1,41 A(J,J)=0.1
C DO 10 J=1,41 A(J,J)=0.1
C DO 10 J=1,41 A(J,J)=0.1
C DO 10 J=1,41 A(J,J)=0.1
C DO 10 J=1,41 A(J,J)=0.1
C EACH ELEMENT COORDINATES
C
C X0=(X[I,J]+X[I,J+1]+X[I+1,J]+X[I+1,J+1])/4.0
C Y0=(Y[I,J]+Y[I,J+1]+Y[I+1,J]+Y[I+1,J+1])/4.0
C XE(I,J)=X0
C YE(I,J)=Y0
C XE(2)=X0
C YE(2)=Y0
C XE(3)=X0
LEVEL 2.3.0 (JUNE 78)  COEFF  05/360 FORTRAN-H EXTENDED  DATE 80.109/22.56.51  PAGE 2

ISN 0043  YE(3)=Y(I)*X(J+1)+Y(I+1)-YO
ISN 0045  XF(J)=X(I)+J+1-X0
ISN 0046  XM(1)=(XE(I)+XE(I+1))/2-DO
ISN 0047  YM(1)=(YE(I)+YE(I+1))/2-DO
ISN 0048  XM(2)=X(I)+X(I+1)-X0
ISN 0049  YM(2)=(YE(I)+YE(I+1))/2-DO
ISN 0050  XM(3)=(XE(I)+XE(I+1))/2-DO
ISN 0051  YM(3)=(YE(I)+YE(I+1))/2-DO
ISN 0052  XM(4)=(XE(I)+XE(I+1))/2-DO
ISN 0053  YM(4)=(YE(I)+YE(I+1))/2-DO

C C COEFFICIENTS IN THE EXPRESSIONS FOR
C C TRANSPORT ACROSS C.V. FACES

ISN 0054  GAMMD=GA(M+J)/DET
ISN 0055  SPE=SP(I,J)
ISN 0056  SCE=SC(J,I)
ISN 0057  BETA=RETA(I,J)
ISN 0058  DO 30 L=1,4
ISN 0059  DO 30 K=1,4
ISN 0060  COEFF(CD(K)*XM(L)+CC(K)*(XM(L)+2)*YM(L)+Z2-YM(L)*2)/2.00-C(A(K)+YM(L))
ISN 0061  IGAMMD
ISN 0062  IF(L.EQ.1) A(K)=-COEFF
ISN 0063  IF(L.EQ.2) B(K)=-COEFF
ISN 0064  IF(L.EQ.3) C(K)=-COEFF
ISN 0065  IF(L.EQ.4) D(K)=-COEFF
ISN 0066  30 CONTINUE
C C COMPUTATION OF ELEM-AREAS

ISN 0067  AREA(I)=(DABS(XE(I)+YM(I)+YM(I+1)+DABS(XE(I)+YM(I+1))
LEVEL 2.3.0 (JUNE 78) COEFFICIENTS FORTRAN H EXTENDED

Date 00-109/22-56-51 Page 3

ISN 00001
1-VE(1)*XN(1)/2.00

ISN 00002
AF(1)*DABS(X(1)-.Y(1))*DABS(VE(1)-X(1))

ISN 00003
1-VE(1)*XN(1)/2.00

ISN 00004
AF(1)*DABS(X(1)-.Y(1))*DABS(VE(1)-X(1))

LOADING OF ELEMENT CONTRIBUTIONS TO C.V. 1

ISN 00005
AC(I,J)=AC(I,J)+D(I)-A(1)*R(I,J)

ISN 00006
ASEC(I,J)=ASEC(I,J)+Z(R(I,J))

LOADING OF ELEMENT CONTRIBUTIONS TO C.V. 2

ISN 00007
AM(I,J)+AM(I,J)+D(I)-A(1)*R(I,J)

ISN 00008
AN(I,J)=AN(I,J)+D(I)-A(1)*R(I,J)

LOADING OF ELEMENT CONTRIBUTIONS TO C.V. 3

ISN 00009
CON(I,J)+CON(I,J)+R(I,J)+R(I,J)

ISN 00010
CV(I,J)=CV(I,J)+R(I,J).

LOADING OF ELEMENT CONTRIBUTIONS TO C.V. 4

ISN 00011
AC(I,J)+AC(I,J)+D(I)-A(1)*R(I,J)

ISN 00012
ASEC(I,J)=ASEC(I,J)+Z(R(I,J))

CONTINUING

ISN 00013
DIM I,J

ISN 00014
END

OPTIONS IN EFFECT: NAMF(MAIN) OPTIMIZE(2) LIMECOUNT(60) SIZE(MAX) AUTODOU(NONE)

OPTIONS IN EFFECT: NOEQU NOSTD NODSAL OBJECT NODAUTO NOSDF NDTERM IAN FLAG(1)
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LEVEL 7-1.0 (JULY 70)

DS/360 FORTRAN H EXTENDED

DATE 09-109/22.56.03

PAGE 1

REQUESTED OPTIONS:

OPTIONS IN EFFECT: NAME(MAIN) OPTIMIZE(2) LIMINOUT(20) SIZE(MAX) AUTOORL(NONE)

SOURCE RECORD NO LIST NODECK OBJECT NOSAV NOFORMAT GOSTMT NODRVR NOALC NOANSF NOTERM IRM FLAG(I)

| ISN 0002 | C | SUBROUTINE PRINT
| ISN 0003 | C | IPLICIT REAL*8(A-H,O-Z)
| ISN 0004 | C | LOGICAL LSOLVE,LPRINT,LMONIT
| ISN 0005 | C | COMMON/PARAM/ STE, STEL, FLUX, BI
| ISN 0006 | C | COMMON/CONT/ LSOLVE(2), LPRINT(2), LMONIT, LPRINT, ISTEP
| ISN 0007 | C | COMMON C=(23,23), GAM(22,22), RPTA(22,22), SC(22,22), SP(22,22)
| ISN 0008 | C | COMMON AC(23,23), AN(23,23), AS(23,23), AE(23,23), AW(23,23)
| ISN 0009 | C | COMMON X(23,23), Y(23,23), ARC(23), ARCL(23), CV(23,23), DTIME, IATOT
| ISN 0010 | C | COMMON L1, M1, LZ, M2, NF, NITER

| ISN 0011 | C | IF(PRINT,L1,GO TO 98)

| ISN 0013 | C | WRITE(6,1009)
| ISN 0014 | C | 1009 FORMAT(/'T12,'(I,J)',5X,'AC',7X,'AN',7X,'AS',7X,'AE',7X,'AW',
| ISN 0015 | C | 17X,'ANE',6X,'ANW',6X,'ASM',6X,'AON',6X,'CV',6X,'AREAS',/) |
| ISN 0016 | C | DO 101 I=1,L1 |
| ISN 0017 | C | DO 101 J=1,L1 |
| ISN 0018 | C | WRITE(6,1010) I,J,AC(I,J),AN(I,J),AS(I,J),AE(I,J),AW(I,J),ANE(I,J),ANW(I,J),ASM(I,J),AON(I,J),CV(I,J)
| ISN 0019 | C | 1010 FORMAT(T12,12,1,12X,2F7.2,2X,F7.2,2X,F7.2,2X,F7.2,2X,F7.2,2X,F7.2,2X,F7.2,2X)
| ISN 0020 | C | CONTINUE |
| ISN 0021 | C | IF(PRINT,L2,GO TO 98)

| ISN 0023 | C | WRITE(6,200)
| ISN 0024 | C | 200 FORMAT(IH)
| ISN 0025 | C | K=0
| ISN 0026 | C | DT(210 J=1,W1)
| ISN 0027 | C | K=W1
| ISN 0028 | C | IF(K.LE.5) GO TO 200
| ISN 0029 | C | K=1
| ISN 0030 | C | WRITE(6,200)
| ISN 0031 | C | 200 WRITE(6,200) J
| ISN 0032 | C | IEND=0
| ISN 0033 | C | 230 IF(IEND.EQ.L1) GO TO 210
| ISN 0034 | C | IEND=IEND+1
| ISN 0035 | C | IF(IEND.LT.L1) IFEND=L1
| ISN 0036 | C | WRITE(6,290)
| ISN 0037 | C | WRITE(6,250) (I,I=16,IFNG,IFNO)
| ISN 0038 | C | WRITE(6,260) (K(I,J),I=16,END,END) |
LEVEL 2.3.0 (JUNE 78)

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DATE 06.103/22.56.93

PAGE 2

ISN 0043
WRITE(6,279) Y(I1,J1),I1=IPG,1END
ISN 0044
GO TO 210
ISN 0045
210 CONTINUE
ISN 0046
220 FORMAT(J= 1,5X,J= '+13')
ISN 0047
240 FORMAT(1H1)
ISN 0048
250 FORMAT(1X,' ',1X=12(14.5X))
ISN 0049
260 FORMAT(1X,Y=' ',IP12D9.2)
ISN 0050
270 FORMAT(1X,Y=' ',IP12D9.2)
ISN 0051
97 CONTINUE
ISN 0052
IP(ISTEP,NE,0) GO TO 3000

C COMPUTATION AND OUTPUT SEQUENCE FOR SURFACE INTEGRATED

C HEAT FLUX AND SOLIDIFICATION FRACTION

C

ISN 0054
WRITE(6,30) ISTEP,TIME
ISN 0055
30 FORMAT(1H1,2X,'ISTEP=',15.5X,'TIME=',D10.4)
ISN 0056
070=1.00
ISN 0057
SFRAO=O.00
ISN 0058
GO TO 3010
ISN 0059
3000 KIN=0.00
ISN 0060
210 DO 3020 =I,LI
ISN 0061
211 DO 3020 J=1,4
ISN 0062
ADD=K(J,J,2)
ISN 0063
IF(ADE+LT.0.00) ADD=0.00
ISN 0064
212 IF(ADE+GT.1.00) ADD=1.00
ISN 0065
DI=SUM+CV(I,J)+ADD
ISN 0066
213 SUM=SUM+CV(I,J)+ADD
ISN 0067
3020 CONTINUE
ISN 0068
SFRAO=(ATOT-SUM)/ATOT
ISN 0069
070=ARC(I)/(1.00+FT(I,1,1)/STE)
ISN 0070
220 DO 3030 J=2,ME
ISN 0071
221 IF(LPQINTINF) GO TO 2200
ISN 0072
3030 CONTINUE
ISN 0073
070=ARC(I)/(1.00+FT(I,1,1)/STE)
ISN 0074
230 WRITE(6,3030) SFRAO,OTOT
ISN 0075
3030 FORMAT(1H1,2X,'SFRAC,OTOT
ISN 0076
3030 FORMAT(/',2X,'THE SOLIDIFICATION FRACTION=',IP014.7,5X

C SURFACE INTEGRATED HEAT TRANSFER

C

ISN 0077
240 DO 3040 NF=1,2
ISN 0078
241 DO TO (195,205,2)
ISN 0079
242 WRITE(6,900)
ISN 0080
900 FORMAT('THE TEMPERATURE FIELD')
ISN 0081
GO TO 25
ISN 0082
905 WRITE(6,910)
ISN 0083
910 FORMAT(1H1,'THE ENTHALPY FIELDC')
ISN 0084
GO TO 25
ISN 0085
25 CONTINUE
ISN 0086
IP(LPRINT(NF)) GO TO 3010

C OUTPUT SEQUENCE FOR DEPENDENT VARIABLES

C

ISN 0087
GO TO 2090
ISN 0088
2010 WRITE(6,2090)
ISN 0089
2020 WRITE(6,2090) NF
ISN 0090
IPEG=1
ISN 0091
2040 CONTINUE
ISN 0092
1PEG=1PEG+12
ISN 0093
1END=1PEG+11
ISN 0094
1F(1END-GT,L1) TEND=L1
ISN 0095
WRITE(6,2020)
ISN 0096
WRITE(6,2050) (I1=1PEG,1END)
ISN 0078 WRITE(6,2060)
ISN 0079 JPL=NN[N+1]
ISN 0100 DO 2070 J=1,N+1
ISN 0101 JF=J..J
ISN 0102 WRITE(6,2080) J,(F(I,J,NF),I=IBEG,IEG)
ISN 0103 2070 CONTINUE
ISN 0104 IF(ENF.LT.LT.LI) GO TO 2040
ISN 0105 2080 CONTINUE
ISN 0106 2040 FORMAT(HO)
ISN 0107 2030 FORMAT(I0X,'NF=',I2)
ISN 0108 2050 FORMAT(I0X,'=I16.11110)
ISN 0110 2050 FORMAT(I0X,1HJ)
ISN 0111 2000 FORMAT(I0X,12.3X,IP12010.3)
ISN 0112 RETURN
C
******************************************************************************
ISN 0113 FND

*OPTIONS IN EFFECT*NAME(MAIN) OPTIMIZE(2) LINECOUNT(60) SIZE(MAX) AUTODIM(NONE)
*OPTIONS IN EFFECT*SOURCE EBCDIC NOLIST NODECK OBJECT NOUNAP NOFORMAT GOSTMT NOXREF NOALC NOANSF NOTERM IBM FLAG(I)
*STATISTICS* SOURCE STATEMENTS = 112, PROGRAM SIZE = 2612, SUBPROGRAM NAME = PRINT
*STATISTICS* NO DIAGNOSTICS GENERATED
***** END OF COMPI LATION *****
*STATISTICS* NO DIAGNOSTICS THIS STEP

LEVEL 2.3.0 (JUNE 78) PRINT OS/360 FORTRAN H EXTENDED DATE 00.109/22.56.53 PAGE 3
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Figure 1. Typical multiply-connected irregular-shaped domain; (a) solid-liquid interfaces; (b) control volume in single-phase region; (c) control volume containing a portion of an interface.
Figure 2. Discretization using three-node triangular elements: (a) calculation domain; (b) elements and control volume associated with a node $j$; (c) typical element.
Figure 3. Discretization using four-node rectangular elements: (a) calculation domain; (b) elements and control volume associated with node j; (c) typical element.
Figure 4. Typical boundary nodes: (a) boundary node 1 with two associated boundary elements and two associated internal elements; (b) boundary node 1 with one associated boundary element.
Figure 5. Unsteady heat conduction, with or without phase change, in a long cylinder of square cross-section: (a) cross-sectional view; (b) calculation domain and its discretization.
Figure 6. Unsteady heat conduction without phase change in a long cylinder of square cross-section: temperature variation along the boundary.
Figure 7. Unsteady heat conduction without phase change in a long cylinder of square cross-section: variation of surface integrated heat flux with time.
Figure 8. Heat conduction in a concrete slab containing an array of power cable conduits and cooling water conduits: (a) cross-sectional view, \( @ \) implies cable conduit, \( 0 \) implies cooling water conduit; (b) typical calculation domain.
Figure 9. Domain discretization used in the concrete slab problem.
Figure 10. Concrete slab problem: cable conduit wall temperature distribution.
Figure 11. Freezing in a square domain: heat flux distribution on the boundary, $Ste_L = 0.0$, $Ste_s = 0.05$, $Bi = 1.0$. 
Figure 12. Freezing in a square domain: variation of surface-integrated heat transfer rate and frozen fraction with $\text{Ste}_s \tau$. $\text{Ste}_s = 0.05$.
Figure 13. Freezing in a square domain: heat flux distribution on the boundary, $St_e = 0.2$, $St_s = 0.05$, $Bi = 1.0$
Figure 14. Freezing in a square domain: variation of surface integrated heat transfer rate and frozen fraction with $\text{St}e_{S}; \text{St}e_{J} = 0.2$