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**LA THÈSE A ÉTÉ
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**A Finite Element Formulation for
Heat Transfer Incorporating
Latent Heat Effects**

by

Robert C. House
B. Eng. (Mechanical)

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 and Aeronautical Engineering
Carleton University
Ottawa, Ontario
Canada
December, 1986

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Incorporating Latent Heat Effects,*
submitted by
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Thesis Supervisor

Chairman

Department of Mechanical
and Aeronautical Engineering

Carleton University

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ABSTRACT

The effects of latent heat of fusion and heat of transformation are significant in many manufacturing processes. A formulation that can model discontinuous temperature gradients in the material is required to represent these effects accurately in a thermal analysis. A finite element formulation with this capability was obtained by converting the existing code in ASGARD (a finite element analysis program) to a specific energy formulation. A nonlinear incremental iterative solution technique was used to solve the heat equation after it had been integrated in time. The resulting code was successfully tested on a solidification problem. Future research will apply the code to practical problems.

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List of Symbols

- $B, B(T)$ - the total load vector
 C, C_{ij} - capacitive stiffness matrix
 c - volumetric specific heat capacity (J/m^3C)
 D - a conductivity matrix
 DT_i - the total change in temperature in an increment
 DU_i - the total change in freezing index in an increment
 $e(t)$ - the specific energy (J/m^3)
 e_0 - the initial specific energy (J/m^3)
 F_i - a load vector comprising part of B
 H - a convection contribution to the load vector
 H^*, H^*_{ij} - the combined convective radiative contribution to the effective stiffness matrix
 h - convection coefficient
 h^* - combined radiation and convection coefficient
 i, j - pointers for node numbers and equation numbers
 K, K_{ij} - conductive stiffness matrix
 K_{eff} - effective stiffness matrix
 k_n - thermal conductivity in the n direction (W/mC)
 l - latent heat of transformation (J/m^3)
 N_i - basis function for the i^{th} node
 N - basis function vector
 N^T - transpose of the basis function vector
 n - indicates a direction of the outward normal (unit vector)
 Q - q integrated in time (J)
 Q^s - q^s integrated in time (J)
 Q^b - q^b integrated in time (J)
 q - the heat flux (W/m^2)
 q^s - the heat flux through the surface (W/m^2)
 q^b - the heat generated in the body (W/m^3)

- q_i - point heat source at the i^{th} node (W)
- R, R_i - a load vector excluding point loads,
after Chapter 3 it is a time integrated load vector
- r - heat generated per unit volume (W/m^3)
- s - indicates a surface
- T - temperature in time and space (C)
- T_{∞} - ambient temperature for radiation and convection (C)
- T_{TR} - transition temperature (C)
- T_0 - initial temperature of the body (C)
- t - the time (s)
- u - freezing index (J/m)
- u_i - freezing index at the i^{th} node (J/m)
- U_1 - freezing index for fixed temperature boundary (J/m)
- U_{∞} - freezing index for ambient temperature (J/m)
- x, y, z - space coordinates (m)
- Γ_j - indicates j^{th} surface with an applied boundary condition
- ΔT_i - the most recently computed correction to T_i (C)
- Δt - time increment size (s)
- Δu_i - most recently computed correction to u_i (J/m)
- ϵ - emissivity
- η - a term to prevent division by zero in the homographic approximation
- θ - a weighting factor for time integration
- κ - 'convective' coefficient for radiation term
- Λ - a primitive of k with respect to T
- μ - fraction of the phase transformed
- σ - Stefan-Boltzmann's constant ($5.689 \times 10^{-8} W/m^2 K^4$)
- τ - parameter for time integration
- Ω - the domain or volume of the body being analysed

Chapter 1

Introduction

There are many applications in modern engineering which involve heat transfer and phase transformations. Freezing water is an example of a common engineering problem in which the latent heat of fusion is an important component. Welding is another example of melting, solidification and several solid state transformations [1]. Casting processes similarly involve melting and solidification. In these two common manufacturing processes, a significant error in the thermal analysis can occur unless the latent heats for phase changes are considered.

The mathematical problem of computing the temperature in a material that changes phase is referred to as a Stefan problem [2]. Stefan studied the one dimensional problem of a sheet of ice initially at 0 C. The temperature of one surface was raised to a fixed temperature. Stefan's problem was to compute the temperatures throughout the sheet of ice as it melted. In particular, the position of the internal boundary between the solid and liquid zones was to be computed as a function of time.

In materials that transform at a fixed temperature, there are three important conditions at this internal boundary: the temperature is the melting point; the temperature gradient across the boundary is discontinuous and the boundary moves with a velocity dependent on the latent heat and the flux extracted from the boundary. In alloys that transform over a temperature range, the boundary which divides the frozen and unfrozen zones is not sharp. This type of internal boundary has been described as a mushy zone [3], one which poses a particularly difficult problem. Solutions to the problem which do not properly account for latent heat of transformations and the temperature gradient discontinuity predict either incorrect heat fluxes, incorrect temperatures or both. Thus a correct solution for the Stefan problem is required in order to compute accurately the temperature and the heat flux in a realistic problem like welding.

This thesis is a part of a project to develop a state-of-the-art thermal stress analysis program called ASGARD at Carleton University. This nonlinear transient finite element

program can perform thermal analysis, linear elastic stress analysis, elasto-plastic stress analysis and thermo-elasto-plastic stress analysis. The capability to perform thermal analysis with latent heat and phase change effects included is needed to accurately predict the microstructure and associated properties that result from thermal processes such as welding, casting and heat treating. Thermal analysis is also needed to predict accurately the residual stresses in materials such as steel which undergo solid state transformations. The advantage of being part of such a project is that it enables one to do research on a complex formulation, such as the specific energy formulation, without the overhead of developing main utilities such as pre- and post-processors and solvers. It supports specialisation and depth of knowledge. The challenge of ASGARD is that one must interface with a large, complex and changing program.

The objective of this thesis is to develop a program for thermal analysis that includes phase change effects. The program builds upon existing ASGARD thermal analysis routines so that it can be easily coupled to other analyses which use the ASGARD program. The application of the program to industrial processes such as welding or casting is a future research objective.

This thesis developed a code in ASGARD based on the freezing index method approach originally outlined by Blanchard and Fremond [3]. The Stefan problem was solved correctly in tests performed to verify the code. However, these tests revealed that certain problems with convergence can arise if the approximation for the specific energy is not appropriate.

1.1 Previous Solutions

1.1.1 Previous Methods

An extensive literature exists on the Stefan problem [4, 5]. Much of the literature emphasizes analytical or classical solutions. Solutions of this type for simplistic problems are useful as rough estimates for real problems when a computer is not available. These classical solutions usually cannot be applied to real problems involving complex geometries, constitutive relations, initial conditions or boundary conditions because the equations become too complex.

The alternative to the classical solution is a numerical solution to the Stefan problem. There are several such methods available. The boundary integral equation method was

originally a classical solution technique. A numerical method based on this concept has been developed for the computer and is preferred by a few researchers. It can be used to solve transient field problems in areas such as stress analysis or heat transfer but its application to nonlinear problems has not been well developed. One of the oldest and most popular methods for thermal and fluid problems has been the finite difference method. It is limited, however, by the inability of a finite difference mesh to model geometric details with accuracy. Another approach initially developed for stress analysis and later expanded to other areas is the finite element method. It can be argued that the finite element method incorporates the capability of modeling complex geometry, nonlinear material properties and complex boundary and initial conditions more naturally than boundary integral and finite difference methods.

1.1.2 Selection of a Method

The process for selecting a numerical method was influenced by the requirement of interfacing with a thermo-elasto-plastic stress analysis program. The principal challenge posed by the boundary integral equation method and the finite difference method is that they are very rarely used for nonlinear stress analysis in industry. While both methods can be used in limited applications to perform stress analysis, the boundary integral method is most suited to linear problems and the finite difference method to simple geometries. Any kind of nonlinearity such as plasticity further complicates the already complicated mathematics and programming of the boundary integral equation method. Finite difference analysis of complex geometries often uses a special transformation to a rectangular mesh and new programming must be developed for each new geometry. Because of their limited industrial application and because they do not compute nonlinear stress problems effectively, these two methods would have posed a hindrance to the long-term goal of thermal analysis coupled to stress problems and thus they were not selected for this thesis. On the other hand, most commercial applications use the finite element method for solving problems involving stress analysis. Existing finite element stress analysis programs integrate naturally with a finite element solution to the Stefan problem. This transient finite element method has the capability of handling the nonlinearity and complex geometry involved in solving Stefan problems and was thus selected as the optimum method for this thesis.

1.1.3 Previous Techniques

The literature on the finite element method applied to the Stefan problem discusses several different fixed mesh techniques and moving mesh techniques. Each technique has its advantages and disadvantages which are discussed briefly here.

One common approach is to simulate the phase change effects by increasing the specific heat capacity in a temperature interval about the transformation temperature. This necessitates the use of very small time steps to capture the desired effect since large time increments can cause large temperature changes during the increment. If the time step is analyzed with the inflated specific heat, the temperature change due to latent heat will be underestimated; if the time step is analyzed with the normal specific heat, the latent heat effect may be missed entirely. These cases are the two extremities and a full spectrum of intermediate cases can occur.

Comini *et al.* [6] developed a method which averaged the modified specific heat in order to reduce the possibility of neglecting this modification during the time integration. However, this averaging technique can still neglect the change if the time step is too large [7].

Morgan *et al.* improved on Comini's work by including the latent heat effect in the enthalpy and using a backward difference scheme to calculate the specific heat [7]. If the time increment used in these calculations is too large, significant integration errors can still occur. As Keavey noted, this method fails entirely if the temperature is uniform or steady state [8].

Harder [9] solved the heat equation (presented in Chapter 2) with the time derivative of enthalpy instead of the time derivative of temperature. This is a more rigorous method, but it results in a new set of unknowns, the nodal enthalpies. Introducing new unknowns is a definite disadvantage.

Moving mesh methods have been developed for heat transfer with latent heats [10, 11, 12]. These methods move nodes to keep element boundaries at the boundary between phases. The discontinuity in the temperature gradient at the liquid-solid interface is accommodated by constraining it to the element boundaries. However, these methods fail

in mushy zones and zones which have no temperature gradient in the volume being transformed.

Rolph and Bathe associated a lumped mass with each node in a finite element mesh [13]. This method is similar to the actual physical process of freezing or melting, in that the temperature at each node is restrained to the transformation temperature until the heat of transformation has flowed into or out of the mass. Energy is conserved; however, the flux is incorrect because the temperature gradient is continuous in each element. In addition, the lumped mass formulation is suitable only for linear elements.

Another method applies the Kirchoff transformation to the heat equation. This method integrates the heat equation in time and thus converts the unknown variable, temperature, to a new unknown variable called the freezing index [14]. A variational inequality must be solved to determine the values of the freezing index [3]. Variational inequalities require special solution techniques which differ from the standard solution techniques of finite element analysis. Blanchard and Fremond [3] modified this technique, using the freezing index, but combining it with the homographic approximation to create a variational equality. This allows the freezing index to be determined by standard finite element techniques.

1.1.4 Selection of a Technique

Many factors come into a discussion concerning which solution technique is most suitable for solving Stefan problems while maintaining compatibility with conventional thermo-elasto-plastic stress analysis programs. Each of the aforementioned techniques has its own benefits and drawbacks. The easiest technique to program modifies the specific heat capacity [6, 7]. It is so easy to program that it has become the most popular method. The delta function shape of the modification, however, requires a fine mesh and small time increments. This leads to high computing costs if a high degree of accuracy is to be obtained. The improvements to this technique developed by Comini *et al* [6] and Morgan *et al* [7] do not totally alleviate this problem. They also require small time increments and a fine mesh to achieve accurate results. Attempts to analyse the heat equation after an enthalpy derivative is substituted for the temperature derivative in the time dependent term either generate a new set of unknowns [9] or else they degrade to a specific heat modification [8]. Neither of these options is appealing since the former compounds computational problems and the latter is subject to the constraints of small time increments and fine mesh. Moving

mesh methods have several disadvantages. The convective term in the governing equations leads to an asymmetric matrix which requires twice as much computer memory and four times as much computation as a symmetric solution. The method fails in zones which have no temperature gradient in the volume being transformed. The discontinuity in the temperature gradient must be confined to an element boundary and cannot exist within the interior of an element. For these reasons moving mesh methods were not pursued. However, the moving mesh concept is attractive for problems such as welding which involve moving heat sources. This technique should be considered for future development in conjunction with the specific energy method. Rolph and Bathe [13] require the addition of a heat flow vector to determine whether the material about a node is melting or solidifying. This technique does not calculate the heat flux correctly. It simply forces the temperature to remain at the transformation temperature until the latent heat is absorbed or released. Alternative procedures which transform the heat equation and use the freezing index instead of a temperature variable can compute temperature gradients and heat flux correctly. However, the direct application of the Kirchhoff transformation results in a variational inequality which is not compatible with standard finite element codes for stress analysis or heat transfer. Blanchard and Fremond [3] modified this technique to obtain a variational equality. The rigorous mathematical analysis of the relevant physics is expected to yield the most efficient and computationally accurate algorithm. Complexities in the mathematics and the programming, although difficult, are not insurmountable. This technique is compatible with ASGAR, and will mesh well with the overall goal of the project which is to develop a state-of-the-art program for weld analysis.

1.2 Implementation

In order to use the specific energy method of Blanchard and Fremond [3], the existing nonlinear heat transfer code in ASGAR had to be modified. ASGAR used a Picard iteration scheme for heat transfer analysis. The relevant equations used are described in Chapter 2. Blanchard and Fremond's technique requires a semi-direct method such as a modified Newton-Raphson iterative solver, similar to that developed by Bathe and Khoshgoftaar [14] or an iterative solver. The decision to use this solver was advantageous because the thermoplastic stress analysis segment of ASGAR already used a Newton method type of solver. The Newton method iterative solver is compatible with plans for

error analysis and residual calculations. Some Newton methods can reduce computing costs by avoiding factoring the global equation on each iteration. The equations for the Newton method of solution are described in Chapter 3.

Once the iterative solver was implemented, a specific energy method analogous to Blanchard and Fremond's freezing index was developed in Chapter 4. The equations developed in the previous chapters which had neglected the latent heat term were modified to include the latent heat of transformation. Blanchard and Fremond had assumed that the freezing (melting) point was zero degrees [3] in whatever system of units were used. This assumption was acceptable to them because they were dealing with freezing water in soils; whereas it is unacceptable for work with welding because the transition temperatures are usually not zero. The homographic approximation was thus generalized to apply for any transformation temperature. The equations for the specific energy method are developed in Chapter 4 and the implementation of these equations into ASGARD, is described in Chapter 5.

The resulting finite element formulation was tested with all of the test cases available. Results from these tests compared favourably to those results from the original form of the ASGARD thermal analysis program. Then the latent heat code was tested with a freezing water problem. The results agreed with the theoretical solution. All of these tests are described in Chapter 6. Conclusions based on the results in the previous chapters are presented in Chapter 7 and possibilities for future research to extend this work are discussed in Chapter 8.

Chapter 2

Nonlinear Transient Heat Transfer

2.1 Heat Equation

Heat flow in a conducting stationary material is described by the heat equation. The heat equation can be derived [15] by applying the law of conservation of energy to an elemental volume in which thermal conductivity and specific heat are defined. The resulting partial differential equation [15, 6, 17] for isotropic materials is:

$$\frac{\partial}{\partial x} \left(k_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left(k_y \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left(k_z \frac{\partial T}{\partial z} \right) + r = c \frac{\partial T}{\partial t} \quad (2.1)$$

where

k_n - thermal conductivity in the n direction (W/mC)

t - the time (s)

T - temperature in time and space (C)

r - heat generated per unit volume (W/m^3)

c - volumetric specific heat capacity (J/m^3C)

2.2 Boundary Conditions

The heat equation describes the temperature and heat flux within a body. On the boundary surrounding this domain, three types of boundary conditions may exist, the Dirichlet, the Neumann and the Fourier boundary conditions. The boundaries Γ_1 , Γ_2 and Γ_3 which have these boundary conditions applied to them are disjoint. The union of Γ_1 , Γ_2 and Γ_3 forms the complete boundary as illustrated in Figure 2-1.

The Dirichlet boundary condition requires that the value of the temperature be specified on the boundary.

$$T = T_1 \quad \text{on} \quad \Gamma_1 \quad (2.2)$$

Figure 2-1: Domain Ω , and Boundaries Γ_1 , Γ_2 and Γ_3 .

The Neumann boundary condition specifies the temperature gradient normal to the surface. This type of boundary condition can be further broken down into two cases.

Case a)

The insulated boundary condition is a surface on which the temperature gradient normal to the surface is zero. There is no heat flux across this boundary.

$$\frac{\partial T}{\partial n} = 0 \quad \text{on } \Gamma_1 \quad (2.3)$$

Case b)

The flux boundary condition exists when a known finite temperature gradient is prescribed over a surface indicating that q is the amount of heat per unit area per unit time that flows into the body.

$$-k \frac{\partial T}{\partial n} = q \quad \text{on } \Gamma_2 \quad (2.4)$$

The Fourier boundary condition defines a normal temperature gradient specified on a surface according to the convection or radiation boundary condition.

$$-k \frac{\partial T}{\partial n} = h(T - T_\infty) \quad \text{on } \Gamma_3 \quad (2.5)$$

For convection, h is simply the convective heat transfer coefficient, however, in the case of radiation, a 'convective' coefficient κ can be obtained from

$$\kappa = \epsilon \sigma (T^2 + T_{\infty}^2)(T + T_{\infty}) \quad (2.6)$$

This linearizes the radiation term. Substituting κ for h in Equation 2.5 gives the more familiar

$$-k \frac{\partial T}{\partial n} = \epsilon \sigma (T^4 - T_{\infty}^4) \quad (2.7)$$

describing the surface temperature gradient as a result of radiation.

The coefficients of the Fourier boundary condition from radiation and convection can be combined:

$$h^* = h + \kappa = h + \epsilon \sigma (T^2 + T_{\infty}^2)(T + T_{\infty}) \quad (2.8)$$

2.3 Finite Element Formulation

The Galerkin finite element method [8, 13] and Green's first identity [14, 16] can be applied to Equations 2.1 through 2.8 to obtain the equation for the i^{th} node:

$$\int_{\Omega} \left(\frac{\partial N_i}{\partial x} k_x \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} k_y \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} k_z \frac{\partial N_j}{\partial z} \right) d\Omega T_i + \int_{\Gamma} N_i (q + h^* (N_j T_j - T_{\infty})) d\Gamma + \int_{\Omega} N_i \left(Q - c N_j \frac{\partial T_j}{\partial t} \right) d\Omega = 0 \quad (2.9)$$

where

N_i - is the basis function associated with the i^{th} node

T_i - is the temperature at the i^{th} node

Simplifying and arranging this in matrix form gives:

$$C_{ij} T_{j,t} + (K_{ij} + H_{ij}^*) T_j + R_i = 0 \quad (2.10)$$

where

$$K_{ij} = \int_{\Omega} \left(\frac{\partial N_i}{\partial x} k_x \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} k_y \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} k_z \frac{\partial N_j}{\partial z} \right) d\Omega \quad (2.11)$$

$$H_{ij}^* = \int_{\Gamma} h^* N_i N_j d\Gamma \quad (2.12)$$

$$C_{ij} = \int_{\Omega} c N_i N_j d\Omega \quad (2.13)$$

$$R_i = \int_{\Gamma} (N_i q - N_i \alpha T_{\infty}) d\Gamma + \int_{\Omega} N_i Q d\Omega \quad (2.14)$$

Equation 2.10 must be integrated in time. This can be done with a semi-implicit time marching solution. The result of this method of time integration is the original formulation used by the nonlinear transient heat transfer analysis portion of ASGARD [18, 17]. The equation originally used by ASGARD was:

$$\left(\frac{C}{\Delta t} + (K + H^*)\theta \right) {}^{t+\Delta t}T_i + \left(\frac{-C}{\Delta t} + (K + H^*)(1 - \theta) \right) {}^tT_i + {}^{t+\Delta t}F_i\theta + {}^tF_i(1 - \theta) = 0 \quad (2.15)$$

where

- ${}^{t+\Delta t}T_i$ - temperature at the end of the time step at the i^{th} node
- tT_i - temperature at the beginning of the time step at the i^{th} node
- θ - weighting function for time integration: see Table 2.1

and

$$F_i = q_i + \int_{\Omega} q^b N_i^T d\Omega + \int_{\Gamma_2} q^s N_i^T d\Gamma + \int_{\Gamma_3} h^* T_{\infty} N_i^T d\Gamma \quad (2.16)$$

where

- q_i - a nodal point load (W)
- q^b - an internal heat generation rate (W/m³)
- q^s - applied surface heating flux (W/m²)

The solution can be an implicit, Galerkin, or Crank-Nicholson formulation depending on the value of θ as shown in Table 2.1. Hughes [19] points out the importance of evaluating the terms in the stiffness matrices (K and C), and the convection and radiation load vector at the intermediate temperature:

$${}^{t+\theta\Delta t}T_i = \theta {}^{t+\Delta t}T_i + (1 - \theta) {}^tT_i.$$

The contributions from point thermal loads, distributed surface flux loads and distributed volume sources are averaged between values at tT and at ${}^{t+\Delta t}T$ based on the value of θ [19].

TABLE 2.1 WEIGHTING FUNCTIONS

	0
Implicit	1
Galerkin	2/3
Crank-Nicholson	0.5

2.4 Nonlinear Analysis

If either K or C are functions of temperature, Equation 2.15 is nonlinear. It is also nonlinear if radiative boundary conditions are present. The Picard (direct) iteration in which C , K , and H^* are evaluated with the latest value of temperature is used to solve Equation 2.15. When the maximum temperature is less than an assigned tolerance, iteration is stopped. This is a crude measure of convergence.

Chapter 3

Incremental Iterative Solution

The iterative incremental method provides a structure for the use of modified Newton, Newton, and quasi-Newton semi-direct methods for solving nonlinear problems. In addition it is a step towards iterative methods such as the incomplete Cholesky conjugate gradient method which is showing promise for very large problems [20].

Although the formulation presented here will make it much easier to implement any of the above methods, only the Newton method is used in this thesis. The focus of this thesis is the element level operations needed for such solvers. Therefore the discussion of such solvers is minimal. No discussion of the advantages of these various solvers is presented since this would be beyond the scope of this thesis.

3.1 The Form of the Equations

An algorithm for an incremental iterative or semi-direct solver is described in Bathe and Khoshgoftaar's paper [14]. It contains a complete derivation of the finite element equations from the heat equation. This type of solver was required by a specific energy formulation of the type described by Blanchard and Fremond [3].

However, there is a simpler method of deriving these equations if a Picard iteration method already has been implemented. This is the form of the equations in Chapter 2.

Begin with Equation 2.15:

$$\left(\frac{C}{\Delta t} + (K + H^*)\theta \right)^{t+\Delta t} T_i + \left(\frac{-C}{\Delta t} + (K + H^*)(1 - \theta) \right)^t T_i + {}^{t+\Delta t} R_i \theta + {}^t R_i (1 - \theta) = 0 \quad (3.1)$$

The load term F_i of Equation 2.15 is changed to R_i to indicate that point loads are not included. The reasons for this change are discussed in Chapter 5.

$$R_i = \int_{\Omega} q^b N^T d\Omega + \int_{\Gamma_2} q^s N^T d\Gamma + \int_{\Gamma_3} h^* T_{\infty} N^T d\Gamma \quad (3.2)$$

Figure 3-1: Notation used for the Variables in a Time Increment

Then define

$$^{t+\Delta t}T_i = ^tT_i + \frac{DT_i + \Delta T_i}{\theta} \quad (3.3)$$

where

$$DT_i = \sum_{i=1}^n \Delta T_i = ^{t+\theta\Delta t}T_i^n - ^tT_i \quad (3.4)$$

and

$$\Delta T_i = ^{t+\theta\Delta t}T_i^{n+1} - ^{t+\theta\Delta t}T_i^n \quad (3.5)$$

provided that

$$^{t+\theta\Delta t}T_i^1 = ^tT_i \quad (3.6)$$

Figure 3.1 illustrates this notation in time-temperature space.

The form of the equations for the incremental iterative solution is obtained by substituting $T_i + \frac{DT_i + \Delta T}{\theta}$ for T_i and solving for ΔT_i . This gives :

$$\left(\frac{C}{\theta \Delta t} + K + H^* \right) \Delta T_i = \frac{-C}{\theta \Delta t} DT_i - K^{t+\theta \Delta t} T_i^n + R_{n+1} \theta + R_n (1 - \theta) + H \quad (3.7)$$

where

$$R = \int_{\Omega} q^t N^T d\Omega + \int_{\Gamma_2} q^s N^T d\Gamma \quad (3.8)$$

and

$$H = \int_{\Gamma_1} \left(h^* \left(N^{t+\theta \Delta t} T_i^n - T_{\infty} \right) \right) N^T d\Gamma \quad (3.9)$$

This is the final form of the equations for the method derived by Bathe and Khoshgoftar. The right hand side of Equation 3.7 is the residual or error in the energy. The change in temperature in an iteration ΔT_i , will reduce the residual in the energy to zero in a linear approximation. Since the error in Equation 3.7 is computed explicitly, this method is naturally compatible with more rigorous concepts of error and convergence. The equations for the Picard solver originally used in ASGARD were converted to this new form presented in Equations 3.7 through 3.9.

Chapter 4

Specific Energy Formulation

This chapter describes the development of the specific energy formulation originally presented by Blanchard and Fremond [3]. However, the derivation differs somewhat from theirs. In both cases the formulation is developed by integrating the heat equation in time. The concept of a freezing index is introduced. Then the finite element formulation is derived in the same manner as the finite element equations were derived for the heat equation in Chapter 3. The homographic approximation [3] relating the fraction of the phase transformed to the temperature is the key concept used to simplify the equations. Blanchard and Fremond's form is modified so that it applies at any transformation temperature and the equations are developed for the iterative incremental solver. This ends the derivation of the finite element formulation for the specific energy method.

4.1 Time Integrated Heat Equation

The specific energy is defined as:

$$e(T, \mu) = cT + l\mu \quad (4.1)$$

where

c - is the volumetric specific heat capacity (J/m^3C)

l - is the volumetric latent heat of transformation (J/m^3)

μ - is the fraction of the phase transformed

The thermal flux, q , is defined as:

$$q = -k(x, T) \text{grad } T \quad (4.2)$$

where

k - is the thermal conductivity (W/mC)

Equation 2.1 is integrated in time.

$$\frac{\partial}{\partial x} \int_0^t k_x \frac{\partial T}{\partial x} dr + \frac{\partial}{\partial y} \int_0^t k_y \frac{\partial T}{\partial y} dr + \frac{\partial}{\partial z} \int_0^t k_z \frac{\partial T}{\partial z} dr + \int_0^t r dr = \int_0^t \frac{\partial e}{\partial t} dr \quad (4.3)$$

Define a freezing index,

$$u(x, t) = \int_0^t \Lambda(x, T(x, r)) dr \quad (4.4)$$

where $\Lambda(x, y)$ is a primitive of $k(x, y)$ with respect to T . The mathematical concepts involved in this transformation are not elementary. A more complete discussion of the theory is given by Duvaut [21]. We have

$$Q = -\text{grad } u \quad (4.5)$$

$$T = (\Lambda)^{-1} \left(x, \frac{du}{dt} \right) \quad (4.6)$$

is the unique solution $\Lambda(x, T) = du/dt$. For example, if k is a constant:

$$u = k \int_0^t T dr \quad (4.7)$$

and

$$T = \frac{1}{k} \frac{du}{dt} \quad (4.8)$$

The conductivity k , however, does not need to have a constant value.

Equation 4.3 can be written as:

$$\frac{\partial}{\partial x} \left(\frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\partial u}{\partial y} \right) + \frac{\partial}{\partial z} \left(\frac{\partial u}{\partial z} \right) + R = e(t) - e(0) \quad (4.9)$$

or as:

$$e(t) + \text{div } Q = R + e(0) \quad (4.10)$$

where $Q = \int_0^t q dr$, $R = \int_0^t r dr$

4.2 Boundary Conditions

The essential or Dirichlet boundary conditions on Γ_1 (see Figure 2-1) are:

$$T = T_1 \quad \text{and} \quad u = U_1 = k \int_0^t T_1 dr \quad (4.11)$$

The natural or Neumann boundary conditions (prescribed flux) on Γ_2 and Γ_3 (see Figure 2-1) are:

$$-k \frac{\partial T}{\partial n} = q^* \quad \text{or} \quad \frac{\partial u}{\partial n} = Q^* = \int_0^t q^* d\tau \quad (4.12)$$

$$k \frac{\partial \theta}{\partial n} + h^*(T - T_\infty) = 0 \quad \text{or} \quad \frac{\partial u}{\partial n} + \frac{h^*}{k}(u - U_\infty) = 0 \quad (4.13)$$

where

$$U_\infty = k \int_0^t T_\infty d\tau \quad (4.14)$$

The initial condition is

$$e(T(x,0), \mu(x,0)) = e_0(x) \quad (4.15)$$

The unknowns are the freezing index, $u(x,t)$, and the fraction of the phase transformed, $\mu(x,t)$, at any point in the domain and at any time t .

4.3 Finite Element Formulation

The Galerkin finite element method and Green's identity [16] are applied to Equations 4.10 through 4.15 to obtain:

$$\begin{aligned} \int_{\Omega} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) d\Omega u_i + \\ \int_{\Gamma} N_i \left(Q^* + \frac{h^*}{k}(N, u, -U_\infty) \right) d\Gamma + \int_{\Omega} N_i \left(Q^* - e(t, \mu) + e(0) \right) d\Omega = 0 \end{aligned} \quad (4.16)$$

where

N_i - is the basis function associated with the i^{th} node

u_i - is the freezing index at the i^{th} node

Since specific energy can include latent heat effects, $e(t)$ may not be differentiable when the latent heat effects begin. To avoid this difficulty, the fraction of the phase transformed μ can be replaced with a continuous approximation; the homographic approximation defines the fraction of the phase transformed as:

$$\mu = \frac{1}{2} \left(\frac{T - T_{TR}}{\eta + |T - T_{TR}|} + 1 \right) \quad (4.17)$$

Figure 4-1: The Homographic Approximation: $T_{TR} = 0$

where T_{TR} is the transition temperature at which phase change occurs and η is a small parameter used to prevent division by zero. The homographic approximation makes the fraction transformed a function of temperature. The behaviour of this approximation for several values of η is shown in Figure 4-1. The smaller the value of η that is used, the steeper the slope of the approximation is at the transition temperature. This fact can cause convergence problems, if the value of η is too small.

When this approximation to the fraction of phase changed is substituted into Equation 4.1, the following expression for the specific energy is obtained:

$$e(T) = cT + \frac{l}{2} \left(\frac{T - T_{TR}}{\eta + |T - T_{TR}|} + 1 \right) \quad (4.18)$$

Now separate the T_{TR} terms from the T terms:

$$e(T) = cT + \frac{l}{2} \left(\frac{T}{\eta + |T - T_{TR}|} \right) + \frac{l}{2} \left(\frac{T_{TR}}{\eta + |T - T_{TR}|} \right) + \frac{l}{2} \quad (4.19)$$

and substitute into the last term of Equation 4.16:

$$\int_{\Omega} N_i \left(Q^b - \left(cT + \frac{l}{2} \left(\frac{T}{\eta + |T - T_{TR}|} \right) + \frac{l}{2} \left(\frac{T_{TR}}{\eta + |T - T_{TR}|} \right) + \frac{l}{2} \right) \right. \\ \left. + \left(cT_0 + \frac{l}{2} \left(\frac{T_0}{\eta + |T_0 - T_{TR}|} \right) + \frac{l}{2} \left(\frac{T_{TR}}{\eta + |T_0 - T_{TR}|} \right) + \frac{l}{2} \right) \right) d\Omega \quad (4.20)$$

Note that the $\frac{l}{2}$ terms cancel each other.

Then define the approximate temperature as:

$$T_i = \frac{1}{k} \frac{DU_i}{\theta \Delta t} \quad (4.21)$$

where

$$DU_i = \sum_{i=1}^{n+1} \Delta U_i = {}^{t+\theta \Delta t} u_i^{n+1} - {}^t u_i \quad (4.22)$$

and

$$\Delta U_i = {}^{t+\theta \Delta t} u_i^{n+1} - {}^{t+\theta \Delta t} u_i^n \quad (4.23)$$

provided that

$${}^{t+\theta \Delta t} u_i^1 = {}^t u_i \quad (4.24)$$

This notation is the same as that used for temperatures in Chapter 2 as shown in Figure 2-1. From this notation the Picard form of the equations, the equivalent of Equation 2.4, can be derived. Then the method used in Chapter 3 can be applied to obtain the final form of the Newton type iterative incremental method applied to Equation 4.10. It is presented here in its fully expanded form.

$$\int_{\Omega} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) d\Omega {}^{t+\theta \Delta t} u_i^n \\ + \int_{\Gamma} N_i \left(Q^s + \frac{h^*}{k} (N_j {}^{t+\theta \Delta t} u_j^n - U_{\infty}) \right) d\Gamma + \int_{\Omega} N_i \left(Q^b \right. \\ \left. - \left(c \frac{DU_i^n}{k \theta \Delta t} + \frac{l}{2} \left(\frac{\frac{DU_i^n}{k \theta \Delta t}}{\eta + \left| \frac{DU_i^n + \Delta U_i^{n+1}}{k \theta \Delta t} - T_{TR} \right|} \right) + \frac{l}{2} \left(\frac{T_{TR}}{\eta + \left| \frac{DU_i^n + \Delta U_i^{n+1}}{k \theta \Delta t} - T_{TR} \right|} \right) \right) \right. \\ \left. + \left(cT_0 + \frac{l}{2} \left(\frac{T_0}{\eta + |T_0 - T_{TR}|} \right) + \frac{l}{2} \left(\frac{T_{TR}}{\eta + |T_0 - T_{TR}|} \right) \right) \right) d\Omega \quad (4.25) \\ = \int_{\Omega} \left(c \frac{1}{k \theta \Delta t} + \frac{l}{2} \left(\frac{\frac{1}{k \theta \Delta t}}{\eta + \left| \frac{DU_i^n + \Delta U_i^{n+1}}{k \theta \Delta t} - T_{TR} \right|} \right) \right) d\Omega \Delta U_i^{n+1} \\ + \int_{\Omega} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) d\Omega \Delta U_i^{n+1} \\ + \int_{\Gamma} \frac{h^*}{k} N_i N_j d\Gamma \Delta U_i^{n+1}$$

The ΔU_i^{n+1} is unknown at the beginning of the $n+1$ iteration and therefore it was omitted from the denominator of the approximation when the code was written. It is suspected that neglecting this term can combine with the steep gradient at the transition temperature to cause poor convergence if η is not large enough.

Equation 4.25 is clearer and more compact when it is rearranged and presented in matrix form.

$$\left(\frac{C}{k\theta\Delta t} + K + H^* \right) \Delta U_i = \frac{-C}{\theta\Delta t} DU_i - K^{t+\theta\Delta t} u^n + R_{n+1}\theta + R_n(1-\theta) + H \quad (4.26)$$

where

$$C = \int_{\Omega} \frac{1}{k\theta\Delta t} \left(c + \frac{l}{2} \left(\frac{1}{\eta + \left| \frac{DU_i^*}{k\Delta t} - T_{TR} \right|} \right) \right) d\Omega \quad (4.27)$$

$$K = \int_{\Omega} \left(\frac{\partial N_i}{\partial x} \frac{\partial N_j}{\partial x} + \frac{\partial N_i}{\partial y} \frac{\partial N_j}{\partial y} + \frac{\partial N_i}{\partial z} \frac{\partial N_j}{\partial z} \right) d\Omega \quad (4.28)$$

$$H^* = \int_{\Gamma} \frac{h^*}{k} N_i N_j d\Gamma \quad (4.29)$$

$$R = \int_{\Gamma} N_i Q^a d\Gamma + \int_{\Omega} N_i Q^b d\Omega \quad (4.30)$$

$$H = \int_{\Gamma} \frac{h^*}{k} (N_j^{t+\theta\Delta t} u_j^n - U_{\infty}) d\Gamma \quad (4.31)$$

This new form of the specific energy equation is now available in ASGARD.

Chapter 5

Implementation

The implementation of the specific energy formulation proceeded in two stages. The first was to implement an iterative incremental solver for the equations described in Chapter 3. Temperature remained the independent variable and no latent heat effects were incorporated. This stage was accomplished by modifying the code for the iterative solver described in Chapter 2. The second stage was to modify the code for the equations given in Chapter 3 in order to implement the specific energy method described in Chapter 4. The independent variable became the freezing index, rather than the temperature. The temperature and the fraction of phase transformed were then computed from the freezing index.

5.1 Picard Solver

The thermal analysis code in ASGARD originally used a Picard solver. This type of solver computed the element stiffness matrix and load vector, assembled and solved the global set of equations and checked the maximum change in temperature at any node. If the temperature change exceeded the specified tolerance, this process was repeated. The equation solved was of the form:

$$K_{eff}(T)T = B(T) \quad (5.1)$$

where

$$K_{eff} = \left(\frac{C}{\Delta t} + (K + H^*)\theta \right) \quad (5.2)$$

is the effective stiffness matrix and

$$B(T) = \left(\frac{-C}{\Delta t} + (K + H^*)(1 - \theta) \right) T_i + {}^{t+\Delta t} F_i \theta + {}^t F_i (1 - \theta) \quad (5.3)$$

is the load vector. Both are defined by Equation 2.15 in Chapter 2. This solution algorithm had been used in ASGARD.

5.2 Iterative Incremental Solver

The iterative incremental method is a technique which calculates an increment (or a decrement) in temperature in each iteration. The iterative incremental solver computed the stiffness matrix and load vector, assembled and solved the global set of equations and computed a residual. The residual was sent back to the frontal solver to compute a correction to the temperature. The loop was repeated until the allowed number of iterations was exceeded. The algorithm can be represented by:

$$K_{eff}(T)\Delta T = (K_{eff}(T)T - B(T)) \quad (5.4)$$

where

$$K_{eff} = \left(\frac{C}{\theta \Delta t} + K + H^* \right) \quad (5.5)$$

is the effective stiffness matrix defined by Equation 3.7. This equation from Chapter 3 also defines the right hand side of Equation 5.4 as:

$$B(T) = \frac{-C}{\theta \Delta t} DT_i - K^{t+\theta \Delta t} T^n + R_{n+1}\theta + R_n(1 - \theta) + H \quad (5.6)$$

This form of iterative incremental solver is well suited to perform error calculations. The load vector, $B(T)$, is the difference between the external applied load and the internal heat flow resulting from the temperature distribution in the body. This imbalance is called the residual and it must be minimized. Any region of a finite element mesh where residuals were large would need to be refined. This has the potential for becoming a very efficient method of indicating areas of a mesh that need refinement.

There are certain difficulties, however, when point loads are included in the analysis. Point loads are not calculated for each element but are calculated for individual nodes which may belong to more than one element. At present, there is no rigorous mathematical method for dividing the point loads between elements. Another aspect of point loads is that they are a flux distribution that approximates a delta function. As such, the distribution of the energy in the point loads depends on the mesh. The delta function itself is a mathematical approximation used when the loading is very intense on an area that is less than the resolution of the mesh. It is preferable that the analyst specify the flux distribution so that the applied load is known more precisely. For these reasons point loads were excluded from the set of permissible load types.

The implementation of the iterative incremental solver required more changes than simply modifying the equations. First, nodes which were assigned temperatures were treated differently. This assigned temperature value could not change in time therefore the temperature change calculated at each of these fixed nodes was set at zero. Secondly, the assumption that the initial temperature at the beginning of a time increment was the same throughout the time increment meant that the capacitive contribution to the residual load was zero because the change in temperature before the program performed the first calculation for the change in temperature in an increment was also zero. Equations 3.4 and 3.6 can be manipulated to show this effect. Since there has been no temperature change in the time increment before the first iteration, the multiplication of the capacitance matrix can be avoided for the first iteration. Finally, the convection contribution to the load term had to be modified. It was corrected in every iteration since the most recent calculation of the temperature was used in the calculation of the energy residual. These changes as well as the changes necessary to convert Equation 2.15 to Equation 3.7 (see Chapter 3) were completed. The modified code was debugged by running the test problems described in Chapter 6. The new incremental iterative solver was then used as a basis for implementing the specific energy formulation.

5.3 Specific Energy Formulation

The implementation of the specific energy formulation was straightforward since the iterative incremental solver was already functioning. New variables were created in the property list to account for the latent heat and the phase change temperature. The code necessary to calculate the initial specific energy value was added to the program. The initial specific energy value was given by Equation 4.1 in Chapter 4. Then a simple trapezoidal time integration scheme based on the time increment size was employed (see Equation 4.14) to calculate the freezing index corresponding to the ambient temperatures. Finally, the new terms associated with the homographic approximation which are presented in Equation 4.26 (but not in Equation 3.7) were added to the code. The components of Equation 3.7 which were represented in Equation 4.26 were modified by dividing them by the thermal conductivity of the element. This completed the conversion of the temperature formulation to the specific energy formulation with a freezing index.

Chapter 6

Verification

A series of test cases designed to exercise all of the capabilities of the thermal analysis program were run in order to verify the accuracy of the iterative incremental solution and the specific energy formulation. Single element and multi-element tests were carried out. Static and transient problems were considered for the incremental solver but since the specific energy method cannot do static analysis because the time derivative of the freezing index is undefined, only transient problems were considered for the specific energy formulation. One new test case was designed to check the latent heat terms independently and the results of this test will be discussed in detail.

6.1 Single Element Static Tests

Test Case 1:

Temperature was prescribed on two opposite faces of a block. The other four faces were insulated.

Test Case 2:

A flux was prescribed on one face of a block. The temperature was fixed on the opposite face and all other faces were insulated.

Test Case 3:

Convection was applied to one face of a block. The opposite face was held at a fixed temperature and all of the other faces were insulated.

6.2 Transient Single Element Tests

Test Case 4:

Internal heat generation was applied to an element which was perfectly insulated on all surfaces.

Test Case 5:

A radiation test case was performed. This was a highly non-linear problem.

Radiation was applied to one surface of a single element block of initial temperature -173 C. All other surfaces were insulated. The temperature of the block was allowed to rise toward the ambient temperature of -73 C.

A theoretical solution was compared with both the old Picard iterative method and the new iterative incremental technique. Both the Picard method and the iterative incremental solution converged slowly. It had been expected that the new solver would converge more rapidly, but this was not the case - the old Picard method converged as well as the new algorithm. However, solvers with line search should converge more rapidly. Such solvers require minor code changes to the iterative incremental solver, but are not compatible with the Picard method.

6.3 Static Multi-element Tests

Test Case 6:

Four faces of a square block composed of three different element types were perfectly insulated. The three elements chosen were the four node and the eight node ~~perendipity~~ elements and a four to eight node grading element. The other two opposing faces were held at two different temperatures.

Test Case 7:

Three different element types (see Test Case 6) were used in the same block. Temperature was fixed on one side, a flux was applied on the opposite side and all other surfaces were insulated.

Test Case 8:

This case duplicated Test Case 7 but replaced the flux with a convective boundary condition.

6.4 Transient Multi-element Tests

Test Case 9:

Internal heat generation was applied to a block composed of three different element types (see Test Case 6). The block was insulated on all surfaces.

Test Case 10:

A five element bar with an initial temperature of zero had a convective load applied to its surfaces. The elements were all eight node serendipity elements.

Test Case 11:

Convection was applied to the tip of a bar (see Test Case 10) whose initial temperature was zero. All of the other surfaces were insulated.

Test Case 12:

The temperature at one end of a bar (see Test Case 10) was fixed at zero. The initial temperature in the bar was positive and non-zero. The temperature of the whole bar was then permitted to decay to zero.

All the above tests are standard ASGARD test cases, a description of which can be found in L. Beresford's thesis [17]. The new results obtained were compared with the results from the original ASGARD rununit which had used Picard iteration. The solutions compared exactly for all of the linear test cases and the solutions for the nonlinear radiation case were within the expected range.

6.5 Testing the Latent Heat Code

Test Case 13:

This test was specifically designed to assess the ability of the homographic approximation and the specific energy formulation to model a phase change. The problem was a one element test case in which the initial temperature was -100 C. All the faces of the element were insulated and it was heated by some means similar to microwave heating. The resulting thermal histories are shown in Figures 6-1 to 6-3. The latent heat was 80 J/m^3 and the specific heat was $1 \text{ J/m}^3\text{C}$.

Figure 6-1: Melting Solid - Effect of Time Increment: Δt

The results shown in Figure 6-1 indicate that the temperature rises to the transformation temperature and remains constant while the material transforms. This is in agreement with the theoretical results. The only difference is a slight rounding of the corners where the effects of the latent heat approximation begin and end. The rounded corners are related to the choice of η , where $\eta > 0$ is a small parameter used in the homographic approximation. This effect could be used to simulate alloy materials which change phase over a range of temperatures.

The time increment size has very little effect on the solution. The curves for $\Delta t = 1$ and $\Delta t = 2$ are almost superimposed on each other in Figure 6-1. The solution with a relatively large time increment of $\Delta t = 5$ which is illustrated in Figure 6-2 is accurate. The correct trend is predicted and the solution converges to the correct temperature after the latent heat energy has been absorbed. The choice of η , however, does affect the solution significantly. Not only does it affect

Figure 6-2: Melting Solid - Effect of Time Increment: $\Delta t = 5$

the amount of smoothing that occurs at the corners, but it also affects the rate of convergence. If the value of η chosen is too small, then the convergence will be very slow.

Figure 6-3 illustrates the effect of η in the homographic approximation. If η is too small, the slope of the approximation at the transition temperature is very large. This causes a numerical convergence problem. The program requires approximately twenty iterations to reach the correct solution. As long as η is reasonably large, in the order of 0.2, then convergence is relatively rapid and accurate. Even if the program does not converge to the correct temperature in the first time step after the latent heat effects end, it will reach the correct temperature value eventually. When η is small, a rapid temperature change occurs when the program corrects the solution. In Figure 6-3, when $\eta = 10^{-5}$ at 24 seconds, the temperature rises suddenly. This sudden change would be detrimental to the accuracy of the thermal

Figure 6-3: Melting Solid - Effect of η

solution in a large scale welding problem. The most effective choice of η for welding problems is not presently known. The underlying mathematics of the interaction between η and the solution deserves careful study in conjunction with computed results.

This test was also performed with the initial temperature at 100 C. Thereafter, heat was extracted. The results of this test were, as expected, the mirror image (about the 0 C line) of the results shown in Figure 6-1.

These results confirm that the code is stable and that it can model the latent heat effects with significant accuracy. The factor that requires attention is that a suitable value of η must be chosen to avoid difficulty with convergence. With this caveat, the method is a promising technique for modelling the effects of phase transformation.

Chapter 7

Conclusions

An effective numerical method for modelling phase change has been completed. This presents an opportunity for expanding the rigor of weld analysis to include latent heat effects more accurately and efficiently. This thesis not only achieved the original objective but it provided a path for future research.

The particular conclusions are:

1. ASGARD was converted from a Picard iterative solver to an iterative incremental solver.
2. The code for the iterative incremental solver was tested and proven to be fully functional.
3. The iterative incremental solver will facilitate coupling heat transfer analysis and thermo-elasto-plastic stress analysis because the numerical solution methods are now analogous.
4. A specific energy solution for the Stefan problem, similar to that used by Blanchard and Fremond, was selected for implementation. This method integrated the heat equation in time, transforming the unknown variable from the temperature to the freezing index.
5. The program ASGARD was used to facilitate implementation of the code for the specific energy solution of the Stefan problem.
6. The code for the specific energy formulation was tested for a full range of transient problems. The results were accurate and stable and concurred with theoretical solutions for the Stefan problem provided that a suitable value were assigned to η . Care must be taken that a reasonable value of η be chosen for the homographic approximation in order to assure rapid convergence.

Chapter 8

Future Research

Research is an attempt to understand the unknown. In striving to reach one objective, good research work will uncover many new and interesting leads and this is indeed the case with this thesis. These opportunities are briefly listed here:

1. Error analysis of the thermal results can now be performed more easily using residual calculations by the iterative incremental method. This method will allow further development in the fields of automatic mesh generation and adaptive finite element analysis.
2. Methods to assure rapid convergence to an accurate solution using the homographic approximation need to be developed. In particular, the optimal values of η and the time increment and mesh size should be studied in depth. Other variations of the iterative incremental solver such as the modified Newton-Raphson, the quasi-Newton or even the incomplete Cholesky gradient method should be tested.
3. The underlying mathematical assumptions of the specific energy formulation need to be investigated. This method may not treat the denominator of the homographic approximation in the best manner. Special flux-tracking algorithms, variable η values or limits on the value of the latent heat contribution to the capacitance matrix may be appropriate modifications to improve the solution.
4. The effect of latent heat on the thermal history of a weld should be investigated.
5. The ability of the specific energy method to predict the solidification zone from the freezing index needs to be researched. This could lead to improved prediction of weld pool shapes. If the specific energy method were coupled to a thermo-elasto-plastic stress analysis program, more accurate residual stress

calculations could be performed because the precise location of the weld pool would be known.

6. Improved thermal analysis will allow better microstructure predictions to be made. Coupling the thermal and microstructural analysis should be a goal of future research.
7. The specific energy formulation may facilitate the inclusion of plastic work (calculated by the stress analysis program) in the thermal analysis. If this were feasible, it would allow hot forging problems to be solved more accurately and easily.

Some of these items have already been partially researched and other research projects are just beginning. Other topics will have to wait until more resources are available before they can be given the attention that they deserve. As this research advances, the project to develop a state-of-the-art computer program approaches its goal. Looking back on the progress thus far reveals that some major obstacles have been overcome. This provides encouragement to continue searching for more rigorous, practical solutions to engineering analysis problems. The specific energy solution is one such answer for the Stefan problem.

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