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Jay I. Frankel

Jay I. Frankel, Major Professor

We have read this thesis
and recommend its acceptance:

Majed Kyzhani

Roger V. Asimelli

Accepted for the Council:

Lew Minkel

Associate Vice Chancellor and
Dean of The Graduate School

A Weighted Residual Approach for Solving a
One-Dimensional Inverse Solidification Design
Problem Involving a Pure Melt

A Thesis
Presented for the
Master of Science
Degree
The University of Tennessee, Knoxville

Ryan Christopher McMahon

August 1996

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DEDICATION

This thesis is dedicated to my family, whose support has been invaluable to me.

ACKNOWLEDGMENTS

I would like to thank many people at the University of Tennessee for making my time here both rewarding and enjoyable. I would like to thank my advisor, Dr. Jay Frankel, for his guidance and especially his patience in helping me complete this thesis. Our countless conversations about this project as well as other subjects has been an enjoyable experience for me. I would also like to thank the members of my Thesis Committee, Dr. Rao Arimilli and Dr. Majid Keyhani, for serving on my committee as well as instructing me in many of my classes while here at Tennessee. Their instruction has given me a new understanding and appreciation of heat transfer. I also have to thank my fellow graduate students who, together, helped break the monotony of schoolwork and research.

This work was funded, in part, by the National Science Foundation(CTS-9510441). I also wish to thank the Department of Mechanical Engineering for providing me with partial funding. Completing this work would have been difficult without it.

ABSTRACT

Inverse solidification design studies are critical for assuring a desired solid-liquid interfacial motion that promotes certain morphological characteristics during a particular solidification process. Knowledge of this motion is important since it is well known that the interfacial motion is directly related to the quality of the casting. This problem involves the determination of an unknown time-dependent boundary condition that produces a prescribed solid-liquid interfacial motion in a pure material. Though clearly conceived, this problem is considered mildly ill-posed since it has been shown that small changes in the input data can have a profound effect on its solution. Additionally, previous investigations have typically produced unstable numerical results that require some sort of stabilizing scheme in order to arrive at reliable numerical results. The solution method offered in the present work uses a novel collocation method where the unknown temperatures are expanded in terms of global basis functions. All known auxiliary conditions are incorporated into the expansions forming a set of trial functions for each region. The method of weighted residuals, particularly orthogonal collocation, is used to resolve the expansion coefficients using a single matrix inversion. This is shown possible if the time variable is treated in an elliptic fashion. This novel adaption stabilizes the numerical solution in a natural manner since all future information is incorporated into the numerical scheme. This method has the potential to produce benchmark results. Numerical accuracy of the proposed method is demonstrated by comparison to an exact solution for a one-phase test case where the solid-liquid interface moves with a constant velocity. A two-phase investigation reveals that the time collocation method produces accurate numerical results to both direct and inverse problems.

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List of Symbols

Roman

$a_j(\bar{\Delta})$	Time dependent expansion coefficients, Eq.(3.3.1)
$a_j^{N+1}(\bar{\Delta})$	Approximate time dependent expansion coefficients in the solid region, Eq.(3.3.27)
A	Cross-sectional area (m^2), Eq.(2.1.8)
b_{nm}	Defined in Eq.(4.1.15)
c_m^k	Expansion coefficients for the solid region, Eq.(3.3.41)
C_p	Specific heat ($J/kg \cdot K$), Eq.(2.1.1)
$d_i(\bar{\Delta})$	Time-dependent expansion coefficients for the liquid region, Eq.(3.3.3)
$d_i^{N+1}(\bar{\Delta})$	Approximate time-dependent expansion coefficients for the liquid region, Eq.(3.3.4)
$\hat{f}(x_\ell)$	Initial temperature profile in the liquid region, Eq.(2.1.19)
$\bar{f}(\eta_\ell)$	Dimensionless temperature profile in the liquid region, Eq.(2.2.9)
$f(\tau_\ell)$	Mapped initial temperature profile in the liquid, Eq.(3.2.33)
g	Ratio of reference temperatures($T_{ref,\ell}/T_{ref,s}$)
g_j^k	Expansion coefficients in liquid region, Eq.(3.3.19)
h	Specific enthalpy (J/kg), Eq.(2.1.10)
$h(\bar{\Delta})$	Mapped position of the solid-liquid interface, Eq.(3.2.18)
$\dot{h}(\bar{\Delta})$	Mapped velocity of the solid-liquid interface, Eq.(3.3.34)

k	Thermal conductivity ($W/m \cdot K$), Eq.(2.1.1)
L	Length (m), Eq.(2.1.1)
L_ℓ	Differential operator for the liquid region, Eq.(4.1.1)
L_s	Differential operator for the solid region, Eq.(4.2.1)
N	Number of terms used in the spatial series representations, Eq.(3.3.2)
q''	Heat flux (W/m^2), Eq.(2.1.5)
$\dot{Q}$	Rate of energy transfer due to moving interface, (W), Eq.(2.1.7)
Q	Dimensionless heat flux, Eq.(2.2.4)
P	Ratio of the thermal diffusivities, Eq.(3.2.29)
P_k	Number of temporal terms for the liquid region, Eq.(3.3.19)
r	Ratio of thermal conductivities(k_ℓ/k_s)
R_k	Number of temporal terms for the solid region, Eq.(3.3.41)
R_ℓ^N	Residual function for the liquid region, Eq.(4.1.4)
R_s^N	Residual function for the solid region, Eq.(4.2.4)
$s(t)$	Position of solid-liquid interface (m), Eq.(2.1.2)
Ste	Stefan number, Eq.(2.2.6)
t	Dimensional time (s), Eq.(2.1.1)
t_{max}	Maximum time of solidification, (s), Eq.(2.1.1)
T	Dimensional temperature ($^{\circ}C$), Eq.(2.1.1)
T_i	Initial temperature of the liquid region ($^{\circ}C$, Eq.(5.3.1)

T_{melt}	Melting temperature ($^{\circ}C$), Eq.(2.1.6)
T_{ref}	Reference temperature (K), defined in text on page 13
U	Velocity of the solid-liquid interface (m/s), Eq.(2.1.10)
x	Dimensional space (m), Eq.(2.1.1)
<i>Greek</i>	
α	Thermal diffusivity (m^2/s), Eq.(2.1.2)
$\beta_k^N(\tau_s)$	Spatial trial functions for the solid region, Eq.(3.3.39)
δ	Dirac delta function, Eq.(4.1.5)
$\gamma_{\hat{n}\hat{m}}$	Defined in Eq.(4.2.15)
Δ	Dimensionless time, Eq.(2.2.1)
Δ_{max}	Maximum dimensionless time, Eq.(2.2.5)
$\bar{\Delta}$	Mapped Dimensionless time, Eq.(3.1.11)
ζ_j	Expansion coefficients for the least square curve fit used on the experimental data [25], Eq.(5.2.1)
η	Dimensionless space, Eq.(2.2.1)
θ	Dimensionless temperature, Eq.(2.2.1)
θ_i	Dimensionless temperature based on the initial hot temperature of the liquid when superheat is present, Eq.(5.3.1)
$\tilde{\theta}^{N+1}$	Approximation for temperature, Eq.(3.3.2)
$\mu(\Delta)$	Dimensionless position of solid-liquid interface, Eq.(2.2.1)

ρ	Density (kg/m^3), Eq.(2.1.1)
$\rho_k^N(\tau_\ell)$	Spatial trial functions for the liquid region, Eq.(3.3.16)
τ	Mapped dimensionless space, Eq.(3.2.1)
$\Phi_{mk}^{\hat{n}\hat{m}}$	Defined in Eq.(4.2.14)
Ω_{jk}^{nm}	Defined in Eq.(4.1.14)

Subscript

s	Associated with the solid region.
ℓ	Associated with the liquid region.

Abbreviations

IHCP	Inverse Heat Conduction Problem
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Chapter 1

Introduction

In this chapter, the significance of the Inverse Solidification Design Problem is discussed. A background and literature review discusses the beginnings of the problem and the current techniques that are used in its solution. This chapter concludes with a brief discussion on the scope of research to be presented in this work.

1.1 The Inverse Solidification Design Problem

In today's society, there is a constant need for engineered materials to keep up with the demands of advancing technologies. For example, today's technologies require metals to have high strength at high temperatures and plastics to have high strength while being inexpensive. There is a constant search for processes that produce materials with these desirable properties. Certain steps in the manufacturing

process, such as heat treatment and shaping techniques, often yield these desirable properties in materials. The key here is that there may be one or many steps involved in obtaining the final desired properties. As the number of steps increase, the final manufacturing cost tends to become expensive. It would thus be beneficial to have materials with the desirable properties before it undergoes any sort of machining or finishing process. By instilling these properties in the material when it is cast, the need for extra manufacturing steps can be eliminated while obtaining the desired material properties.

If it is known that a certain solid-liquid interfacial profile produces a desirable morphology in a material, the question arises on how to remove heat at the cooling face in order to sustain this prescribed motion. This is the foundation of the Inverse Solidification Design Problem, i.e., to design a transient boundary condition that yields a prescribed interfacial profile which in turn promotes the desired material properties.

1.2 Background and Literature Review

The Inverse Solidification Design Problem is also referred to as the inverse Stefan problem. The Stefan problem is defined as a heat transfer problem with a change of phase taking place at a single temperature for a pure melt [1]. This problem is also characterized by a distinct interface that moves [1] either into the liquid region for a

solidification process or into the solid region for a melting process. The solution to the direct Stefan problem involves solving a non-linear, coupled system of equations for the solid-liquid interfacial motion given prescribed boundary and initial conditions. The inverse Stefan problem differs in that the motion of the solid-liquid interface is given and one must determine the unknown boundary condition or boundary conditions that assure this motion. This specification of the interfacial motion causes the inverse problem to become an uncoupled linear problem, when constant material properties are assumed, instead of the coupled non-linear direct problem. The inverse problem is also mildly ill-posed, meaning that small changes in the input can cause dramatic changes in the output. The focus of the current research is to illustrate that a weighted method can solve the inverse problem in an accurate and stable manner.

The history of the direct or classic Stefan problem is one which spans more than a century. Early analytical work was conducted as early as 1831 [2] while the turn of the century saw such people as Stefan and Neumann publish their work on the subject [2]. The work by Crank [3] is recommended to the interested reader and a more detailed literature review on the direct problem can be found in the work by Özişik [2], and Yao and Prusa [4].

Interest in the inverse Stefan problem stems from another type of inverse problem: that is, the inverse heat conduction problem or IHCP. This problem is based on determining some surface phenomenon, such as temperature or fluxes, using internal

discrete temperature measurements such as those obtained from a thermocouple. Early work on this problem was done by Stolz [5] involving numerical solutions for simple shapes. This work [5] includes several examples for solving IHCP's some of which include trial and error, simplification of the problem to a direct one, numerical inversion of a suitable direct problem, and a graphical method. The procedure used by Stolz determined an important characteristic of the inverse problem, namely that small time steps produce oscillations in the solution. This differs from the direct problem where smaller time steps generally produce accurate results.

Another author who has done extensive work on the IHCP is Beck [6]. Beck developed a time-marching scheme that uses regularization and sensitivity analysis. This technique is generally used in practice today. Other works by Beck [7, 8], using his time marching method, show how incorporating more future data helps to stabilize a numerical solution. Beck also demonstrates the so-called "time-step paradox" discovered by Stolz [5]. Beck has also published a paper on the criteria for comparison of the methods used in solution of the IHCP [9]. This work also presents illustrative examples on the time-step problem as well as the effects of using the future data in developing the solution. Other examples for solving the IHCP include: the finite difference method [10], eigenvalue reduction [11], the Laplace transform method [12], an integral method [13], and exact solutions [14].

The inverse Stefan or solidification problem is similar to the IHCP with the ex-

ception that the inverse Stefan problem has a moving boundary that must be dealt with. In the IHCP, the measured data at some internal location is usually temperature while with the inverse Stefan design problem, the measured data is the location of the solid-liquid interface which is used to determine the temperature history of the cooling surface. This problem has drawn considerable attention due to its potential impact on the materials industry as well as other areas where phase-change problems are important.

There has been considerable research into the solution of this problem and many methods have been proposed and used, with various degrees of success. Beck's future-time method [6] with regularization and sensitivity analysis has also been used in resolving inverse Stefan problems. Some other examples of solution techniques for the inverse solidification problem include integral formulations [1, 15–19] and finite difference techniques [20]. The use of finite elements and deforming finite elements has been used extensively by Zabaras [18, 21, 22] and his co-workers on the inverse solidification problem. Exact solutions for this type of problem are not as numerous as numerical solutions. Carslaw and Jaeger [23] relate an exact solution for the temperature at the cooling face for a single-phase constant velocity case.

Recently, Frankel and Keyhani [24] proposed a new approach for solving the inverse Stefan design problem. This approach involves a Weighted-Residual method applied to a one-phase pure material where time is treated in an elliptic fashion. This

method produces accurate numerical results and the authors clearly illustrate the ill-posed nature of the problem.

1.3 Scope of Research

In this study, a mathematical model is formulated and a stable and accurate numerical method is proposed for a two-phase Inverse Solidification Design Problem having constant properties. A fixed-domain approach is proposed and applied to the two-phase problem. The specified interfacial boundary condition, the remaining auxiliary conditions, and the heat equation for each region are then mapped onto a computational domain that supports Chebyshev polynomials as the basis functions. The solution for the temperature distribution in each region is then expressed in terms of series expansions where all known auxiliary conditions are exactly satisfied since they are incorporated into the trial functions. Orthogonal collocation and matrix inversion are then used to solve for the expansion coefficients using the symbolic software *Mathematica*TM, v.2.2. This approach accounts for all time and space, and requires only a single matrix inversion for determining the expansion coefficients. This approach is in stark contrast to traditional time-marching methods. The solutions are then compared to existing analytical solutions where available, and also to some recent experimental results obtained by Wesley [25].

Chapter 2

Mathematical Formulation

In this chapter, the mathematical formulation of the governing equations and their associated auxiliary conditions is presented. This chapter also addresses key assumptions that have been imposed on the mathematical model as well as presenting the dimensionless forms of the governing equations.

2.1 Dimensional Equations

A brief discussion on the governing mathematical description of the two-phase Inverse Stefan Design Problem is now presented. Figure 2.1.1 displays the physical geometry of the problem to be considered. This figure depicts a one-dimensional system involving only the x -direction. In order to proceed with the mathematical description of this system, several key assumptions must be discussed. It has

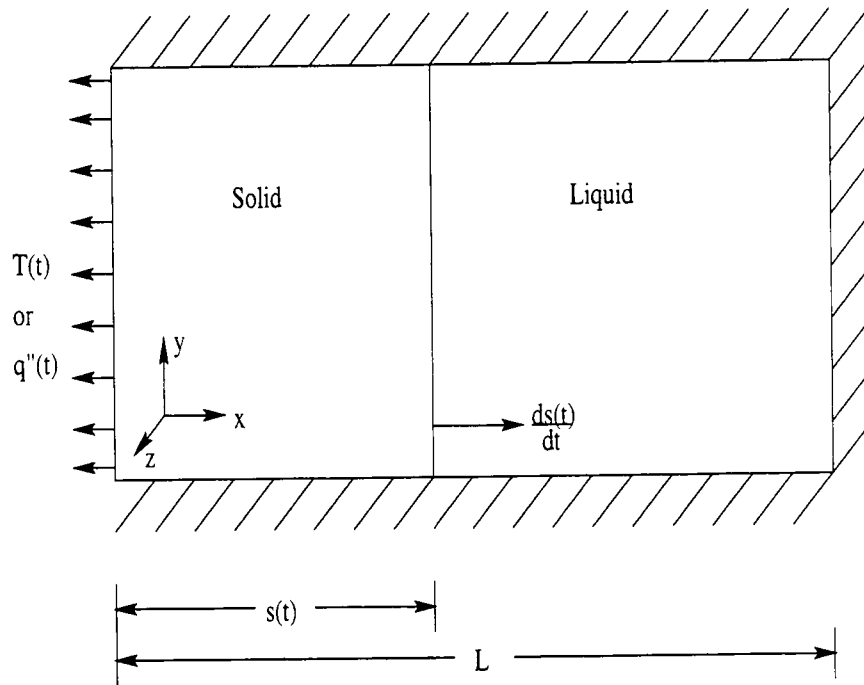


Figure 2.1.1: Schematic of the solidification process.

already been mentioned that the system is one-dimensional in the x -direction. Another key assumption to be made for this problem is that the thermal properties are constant though possibly distinct in each region with the exception of the density. If the densities were dissimilar in each region, a convective term would appear in the governing field description for the liquid region [23]. It is also assumed that perfect thermal contact exists at both the interface ($x = s(t)$) and at the cooling face ($x = 0$). It can also be assumed that there is no internal heat generation during the solidification process in either region. With these assumptions, the one-dimensional, constant property, sourceless form of the energy equation reduces to [2, 23]

$$k \frac{\partial^2 T}{\partial x^2} = \rho C_p \frac{\partial T}{\partial t}, \quad x \in (0, L), \quad t \in (0, t_{max}). \quad (2.1.1)$$

Let the thermal diffusivity be defined as $\alpha = k/\rho C_p$ and the dimensional form of the heat equation for the solid region becomes

$$\frac{1}{\alpha_s} \frac{\partial T_s}{\partial t}(x_s, t) = \frac{\partial^2 T_s}{\partial x_s^2}(x_s, t), \quad x_s \in (0, s(t)), \quad t \in (0, t_{max}), \quad (2.1.2)$$

while the heat equation for the liquid region becomes

$$\frac{1}{\alpha_\ell} \frac{\partial T_\ell}{\partial t}(x_\ell, t) = \frac{\partial^2 T_\ell}{\partial x_\ell^2}(x_\ell, t), \quad x_\ell \in (s(t), L), \quad t \in (0, t_{max}). \quad (2.1.3)$$

Here the subscripts s and ℓ denote the solid and liquid regions, respectively.

The two field equations described in Eqs. (2.1.2) and (2.1.3) are subject to a set of auxiliary conditions. These auxiliary conditions are a combination of boundary and

initial conditions. Recall from Chapter 1 that the objective of this inverse analysis involves determining an unknown surface condition at $x = 0$; that is, either

$$T_s(0, t) = ? \quad t \in [0, t_{max}], \quad (2.1.4)$$

or

$$q_s''(0, t) = ? \quad t \in [0, t_{max}], \quad (2.1.5)$$

that produces the desired interfacial motion, $s(t)$.

The interfacial and end boundary conditions are expressible in terms of conventional forms [26]. The interfacial condition at $x = s(t)$ requires two mathematical relations. The first is obtained by using the assumption that perfect thermal contact is present at the solid-liquid interface. This allows for temperature continuity at the interface and can be written mathematically as

$$T_s(s(t), t) = T_\ell(s(t), t) = T_{melt}. \quad (2.1.6)$$

The second interfacial condition is derived through an energy balance [26]. This energy balance is written as

$$\dot{Q}_{in_{Cond}} + \dot{Q}_{in_{Conv}} - \dot{Q}_{out_{Cond}} - \dot{Q}_{out_{Conv}} = 0, \quad (2.1.7)$$

where

$$\dot{Q}_{in_{Cond}} = A_\ell k_\ell \left(\frac{\partial T_\ell}{\partial x_\ell}(s(t), t) \right), \quad (2.1.8)$$

$$\dot{Q}_{out_{Cond}} = A_s k_s \left(\frac{\partial T_s}{\partial x_s}(s(t), t) \right), \quad (2.1.9)$$

and the “apparent” convective terms are given as

$$\dot{Q}_{in_{Conv}} = \rho U_\ell A_\ell h_\ell, \quad (2.1.10)$$

$$\dot{Q}_{in_{Conv}} = \rho U_s A_s h_s, \quad (2.1.11)$$

where $U_i (i = s, \ell)$ represents the velocities in each region, $h_i (i = s, \ell)$ denotes the specific enthalpies of each region, and $A_i (i = s, \ell)$ are the cross-sectional areas of the individual regions. Substituting Eqs.(2.1.8-2.1.11) into Eq.(2.1.7), the boundary condition becomes

$$A_\ell k_\ell \left(\frac{\partial T_\ell}{\partial x_\ell}(s(t), t) \right) - A_s k_s \left(\frac{\partial T_s}{\partial x_s}(s(t), t) \right) + \rho U_\ell A_\ell h_\ell - \rho U_s A_s h_s = 0. \quad (2.1.12)$$

Conservation of mass at the interface can be written as [26]

$$\rho U_\ell A_\ell = \rho U_s A_s, \quad (2.1.13)$$

which, when incorporated into Eq.(2.1.12), leads to

$$k_\ell \left(\frac{\partial T_\ell}{\partial x_\ell}(s(t), t) \right) - k_s \left(\frac{\partial T_s}{\partial x_s}(s(t), t) \right) + \rho U_s h_\ell - \rho U_s h_s = 0, \quad (2.1.14)$$

or

$$k_\ell \left(\frac{\partial T_\ell}{\partial x_\ell}(s(t), t) \right) - k_s \left(\frac{\partial T_s}{\partial x_s}(s(t), t) \right) + \rho U_s h_{s\ell} = 0, \quad (2.1.15)$$

where $h_{s\ell}$ is the latent heat of fusion, and is defined as $h_{s\ell} = h_\ell - h_s$. The velocities that appear in Eq.(2.1.14) and Eq.(2.1.15) are known to be equivalent and can be written as

$$U_s = U_\ell = \frac{ds(t)}{dt}. \quad (2.1.16)$$

Upon substituting Eq.(2.1.16) into Eq.(2.1.15), the boundary condition at the solid-liquid interface can be written as

$$k_\ell \left(\frac{\partial T_\ell}{\partial x_\ell} \right)_{x_\ell=s(t)} - k_s \left(\frac{\partial T_s}{\partial x_s} \right)_{x_s=s(t)} + \rho h_{sf} \left(\frac{ds(t)}{dt} \right) = 0. \quad (2.1.17)$$

This is the conventional interfacial conservation of energy statement when $\rho_\ell = \rho_s = \rho$.

The insulated boundary condition at $x = L$ is given by

$$\left(\frac{\partial T_\ell}{\partial x_\ell} (L, t) \right) = 0. \quad (2.1.18)$$

The initial condition for this problem involves the premelt temperature in the liquid, i.e.,

$$T_\ell(x_\ell, 0) = \hat{f}(x_\ell), \quad x_\ell \in [0, L], \quad (2.1.19)$$

where $\hat{f}(x_\ell)$ is determined from the pure conduction solution (in the absence of convection) of the liquid when the temperature of the cooling face is lowered to the melt temperature in some manner. By requiring continuity of temperature for all $t > 0$ in the solid, the solid initial condition is taken as

$$T_s(x_s, 0) = T_{melt}, \quad x_s \in [0, s(t)]. \quad (2.1.20)$$

2.2 Dimensionless Equations

The governing heat equations defined by Eqs.(2.1.2) and (2.1.3) and their auxiliary conditions, Eqs.(2.1.6,2.1.17-2.1.20), are now cast in dimensionless form using the fol-

lowing dimensionless variables: $\eta_s = x_s/L$, $\eta_\ell = x_\ell/L$, $\Delta = \alpha_s t/L^2$, $\mu(\Delta) = \bar{s}(\Delta)/L$. $\theta_s(\eta_s, \Delta) = (\bar{T}_s(\eta_s, \Delta) - T_{melt})/T_{ref,s}$, and $\theta_\ell(\eta_\ell, \Delta) = (\bar{T}_\ell(\eta_\ell, \Delta) - T_{melt})/T_{ref,\ell}$. Here, $\bar{T}_s(\eta_s, \Delta) = T_s(\eta_s L, \Delta L^2/\alpha_s)$ and $\bar{T}_\ell(\eta_\ell, \Delta) = T_\ell(\eta_\ell L, \Delta L^2/\alpha_\ell)$. The reference temperatures in θ_s and θ_ℓ are $T_{ref,s} = h_{sl}/C_{ps}$ and $T_{ref,\ell} = h_{sl}/C_{p\ell}$. The dimensionless heat flux $Q(\eta, \Delta)$ is $q''LC_p/(kh_{sl})$. These dimensionless variables are now used to rewrite the governing equations in an equivalent dimensionless form. Substituting the proper variables into the governing equation for the solid region shown in Eq.(2.1.2), the dimensionless heat equation becomes

$$\frac{\partial \theta_s}{\partial \Delta} = \frac{\partial^2 \theta_s}{\partial \eta_s^2}, \quad \eta_s \in (0, \mu(\Delta)), \quad \Delta > 0. \quad (2.2.1)$$

Following a similar procedure, the dimensionless heat equation in the liquid region. described in Eq.(2.1.3), becomes

$$\left(\frac{\alpha_s}{\alpha_\ell}\right) \left(\frac{\partial \theta_\ell}{\partial \Delta}\right) = \frac{\partial^2 \theta_\ell}{\partial \eta_\ell^2}, \quad \eta_\ell \in (\mu(\Delta), 1), \quad \Delta > 0. \quad (2.2.2)$$

Using the previously defined dimensionless quantities, and following the order from Section 2.1 for the auxiliary conditions, the corresponding dimensionless form of the auxiliary conditions can now be developed. The desired function of interest in the inverse problem either involves the dimensionless surface temperature at $\eta_s = 0$.

$$\theta_s(0, \Delta) = ? \quad (2.2.3)$$

or the dimensionless surface heat flux

$$Q(0, \Delta) = -\frac{\partial \theta_s}{\partial \eta_s}(0, \Delta) = ?, \quad (2.2.4)$$

for the cooling surface. The continuity condition for temperature at the interface, described in Eq.(2.1.6), becomes

$$\theta_s(\mu(\Delta), \Delta) = \theta_\ell(\mu(\Delta), \Delta) = 0, \quad \Delta \in [0, \Delta_{max}]. \quad (2.2.5)$$

The interface boundary condition displayed in Eq.(2.1.17) becomes

$$\left(\frac{k_\ell}{k_s}\right) \left(\frac{T_{ref,\ell}}{T_{ref,s}}\right) \frac{\partial \theta_\ell}{\partial \eta_\ell}(\eta_\ell, \Delta) - \frac{\partial \theta_s}{\partial \eta_s}(\eta_s, \Delta) + \frac{1}{Ste_s} \frac{\partial \mu(\Delta)}{\partial \Delta} = 0, \\ \eta_s \in [0, \mu(\Delta)], \quad \eta_\ell \in [\mu(\Delta), 1], \quad \Delta \in [0, \Delta_{max}]. \quad (2.2.6)$$

This equation has a new non-dimensional variable called the Stefan number [26] which is defined as

$$Ste_s = \frac{C_{ps} T_{ref,s}}{h_{s\ell}}. \quad (2.2.7)$$

Notice that the Stefan number becomes unity based on the definition of $T_{ref,s} = h_{s\ell}/C_{ps}$. The insulated boundary condition shown in Eq.(2.1.18) can be written in the dimensionless form

$$\frac{\partial \theta_\ell}{\partial \eta_\ell}(1, \Delta) = 0, \quad \Delta \in [0, \Delta_{max}]. \quad (2.2.8)$$

Finally, the initial conditions shown in Eqs.(2.1.19) and (2.1.20) can be established as

$$\theta_\ell(\eta_\ell, 0) = \bar{f}(\eta_\ell), \quad \eta_\ell \in [\mu(\Delta), 1]. \quad (2.2.9)$$

and

$$\theta_s(\eta_s, 0) = 0, \quad \eta_s \in [0, \mu(\Delta)], \quad (2.2.10)$$

respectively.

Now that the governing equations and necessary auxiliary conditions have been expressed in dimensionless form, it is time to recast these equations in a form conducive to the chosen solution method. The proposed method makes use of the Chebyshev polynomials [27] which are a family of orthogonal polynomials defined on the interval -1 to 1 . Since these functions exist on this $[-1, 1]$ region, it is necessary to map the governing equations and auxiliary conditions to this domain. This is the topic of the next chapter

Chapter 3

Series Solution using Chebyshev Polynomials

In this chapter, a brief description is given on the mathematical characteristics of Chebyshev polynomials. The governing mathematical formulations developed in Chapter 2 are then mapped into a computational region convenient for implementation of expansions based on Chebyshev polynomials. Once this is completed, the series solutions are derived for both the liquid and solid regions.

3.1 Chebyshev Polynomials

Chebyshev polynomials are a family of orthogonal polynomials [27, 28] defined on a region of $[-1, 1]$. There are two principal kinds of Chebyshev polynomials.

Chebyshev polynomials of the first kind and Chebyshev polynomials of the second kind. Chebyshev polynomials of the first kind are emphasized in the present work. The first four polynomials are

$$T_0(x) = 1,$$

$$T_1(x) = x,$$

$$T_2(x) = 2x^2 - 1,$$

$$T_3(x) = 4x^3 - 3x.$$

A plot showing the first four Chebyshev polynomials is displayed in Figure 3.1.1. As indicated in this figure, the polynomials are bounded by ± 1 in the region involving $x \in [-1, 1]$. In general, the n^{th} order Chebyshev polynomial can be expressed in terms of trigonometric functions as [28]

$$T_n(x) = \cos(n \cos^{-1} x), \quad (3.1.1)$$

or in terms of the two-term recursive formula [28, 29] as

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x), \quad n \geq 1. \quad (3.1.2)$$

These polynomials are known to possess similar convergence properties as the Fourier series but with a faster rate of convergence [28].

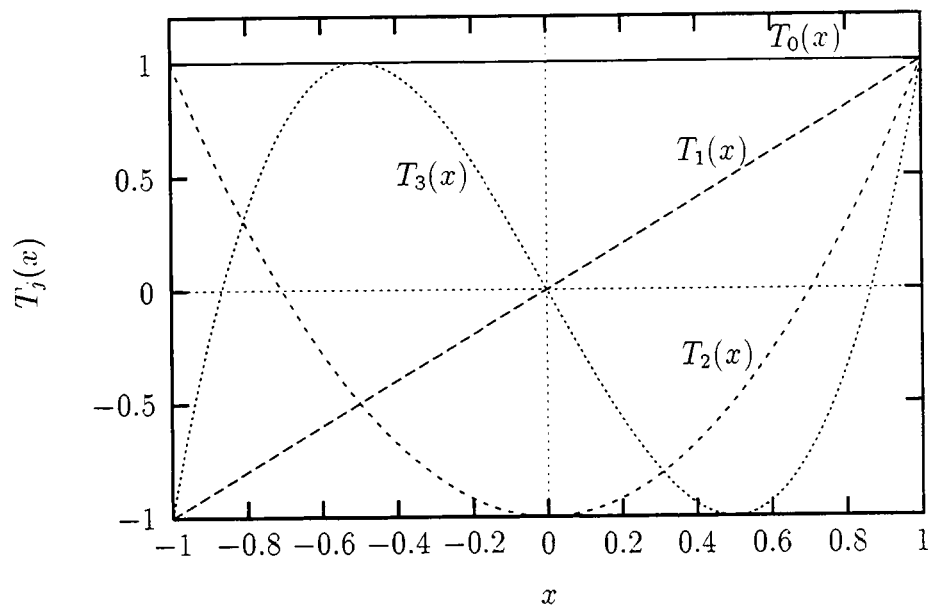


Figure 3.1.1: Chebyshev polynomials of the first kind.

3.2 Mapping of Equations

The governing heat equations must be transformed into a region where the Chebyshev polynomials can be used as the basis functions for the expansions. This is accomplished by using a linear transformation on the spatial and temporal variables, η_s , η_ℓ , and Δ , respectively. It is noted that both the solid and liquid regions are to be mapped to spatial regions confined within $[-1,1]$. For the solid region, the linear transformation for the spatial variables η_s is given by

$$\tau_s = A\eta_s + B, \quad \tau_s \in [-1, 1], \quad \eta_s \in [0, \mu(\Delta)], \quad (3.2.1)$$

where τ_s is the mapped spatial variable and A and B are presently unknown and are not necessarily constants. By requiring that the spatial domain of τ_s to be confined within ± 1 , the appropriate sides of the η_s domain are mapped to the τ_s domain in accordance to

$$-1 = A(0) + B, \quad (3.2.2)$$

$$1 = A(\mu(\Delta)) + B. \quad (3.2.3)$$

Solving for A and B yields $B = -1$ and $A = 2/\mu(\Delta)$. This allows the transformation shown in Eq.(3.2.1) to be written as

$$\tau_s = \frac{2}{\mu(\Delta)}\eta_s - 1, \quad \tau_s \in [-1, 1], \quad (3.2.4)$$

or inversely as

$$\eta_s = \frac{(\tau_s + 1)\mu(\Delta)}{2}, \quad \eta_s \in [0, \mu(\Delta)]. \quad (3.2.5)$$

The transformation for the liquid region is done in a similar manner. Applying the proper mappings to the linear transformation

$$\tau_\ell = C\eta_\ell + D, \quad \tau_\ell \in [-1, 1], \quad \eta_\ell \in [\mu(\Delta), 1], \quad (3.2.6)$$

yields

$$-1 = C\mu(\Delta) + D, \quad (3.2.7)$$

$$1 = C(1) + D, \quad (3.2.8)$$

and solving for the unknowns functions produces $C = -2/(\mu(\Delta) - 1)$ and $D = 1 + 2/(\mu(\Delta) - 1)$. Thus, the transformation for the liquid region becomes

$$\tau_\ell = \frac{-2\eta_\ell}{\mu(\Delta) - 1} + 1 + \frac{2}{\mu(\Delta) - 1}, \quad \tau_\ell \in [-1, 1], \quad (3.2.9)$$

or inversely

$$\eta_\ell = 1 + \frac{\mu(\Delta) - 1}{2}(1 - \tau_\ell), \quad \eta_\ell \in [\mu(\Delta), 1]. \quad (3.2.10)$$

The transformation for the temporal variable is also done following a similar logic.

Defining

$$\bar{\Delta} = E\Delta + F, \quad \bar{\Delta} \in [-1, 1], \quad \Delta \in [0, \Delta_{max}], \quad (3.2.11)$$

where both E and F are unknown and making the required mappings yields

$$-1 = E(0) + F, \quad (3.2.12)$$

$$1 = E(\Delta_{max}) + F. \quad (3.2.13)$$

Solving these equations for the two unknowns renders $F = -1$ and $E = 2/\Delta_{max}$.

This leads to the transformation for the temporal variable defined as

$$\bar{\Delta} = \frac{2}{\Delta_{max}}\Delta - 1, \quad \bar{\Delta} \in [-1, 1], \quad (3.2.14)$$

or inversely

$$\Delta = \frac{(\bar{\Delta} + 1)\Delta_{max}}{2}, \quad \Delta \in [0, \Delta_{max}]. \quad (3.2.15)$$

All of the independent variables have now been mapped to regions involving $[-1, 1]$. It is now necessary to transform the governing heat equations and auxiliary conditions. This is done by taking the necessary derivatives and substituting them into the governing field descriptions. Recalling Eq.(2.2.1) and Eq.(2.2.2), it is evident that a first derivative in time and a second derivative in space are needed that introduce the new computational domain. This is accomplished with the aid of the chain rule for differential calculus [30] and the previously defined transformations.

Starting with the solid region, the time derivative becomes

$$\frac{\partial}{\partial \Delta} = \frac{\partial}{\partial \bar{\Delta}} \frac{\partial \bar{\Delta}}{\partial \Delta} + \frac{\partial}{\partial \tau_s} \frac{\partial \tau_s}{\partial \Delta}. \quad (3.2.16)$$

Taking the proper derivatives of the variables given in Eqs.(3.2.4) and (3.2.14) and substituting them into Eq.(3.2.16) produces

$$\frac{\partial}{\partial \Delta} = \frac{2}{\Delta_{max}} \frac{\partial}{\partial \bar{\Delta}} - \frac{2}{\Delta_{max}} \frac{dh(\bar{\Delta})}{d\bar{\Delta}} \frac{(1 + \tau_s)}{h(\bar{\Delta})} \frac{\partial}{\partial \tau_s}, \quad (3.2.17)$$

and introducing

$$h(\bar{\Delta}) = \mu((\bar{\Delta} + 1) \frac{\Delta_{max}}{2}), \quad (3.2.18)$$

which represents a newly defined function describing the interfacial motion. The first derivative of the spatial variable can be written as

$$\frac{\partial}{\partial \eta_s} = \frac{\partial}{\partial \tau_s} \frac{\partial \tau_s}{\partial \eta_s} + \frac{\partial}{\partial \bar{\Delta}} \frac{\partial \bar{\Delta}}{\partial \eta_s}, \quad (3.2.19)$$

which reduces to

$$\frac{\partial}{\partial \eta_s} = \frac{\partial}{\partial \tau_s} \frac{2}{h(\bar{\Delta})}, \quad (3.2.20)$$

since

$$\frac{\partial \bar{\Delta}}{\partial \eta_s} = 0, \quad (3.2.21)$$

as indicated by Eq.(3.2.14). The second derivative in space can be written as

$$\frac{\partial^2}{\partial \eta_s^2} = \frac{\partial}{\partial \tau_s} \frac{\partial}{\partial \eta_s}, \quad (3.2.22)$$

which clearly produces

$$\frac{\partial^2}{\partial \eta_s^2} = \frac{4}{h^2(\bar{\Delta})} \frac{\partial^2}{\partial \tau_s^2}. \quad (3.2.23)$$

The necessary substitutions can now be made into Eq.(2.2.1) in order to obtain the correct form for the transformed coordinates in the solid region. Substituting Eqs.(3.2.17) and (3.2.23) into Eq.(2.2.1) produces

$$\begin{aligned} \frac{\partial^2 \theta_s}{\partial \tau_s^2}(\tau_s, \bar{\Delta}) &= \frac{h(\bar{\Delta})}{2\Delta_{max}} \left(h(\bar{\Delta}) \frac{\partial \theta_s}{\partial \bar{\Delta}}(\tau_s, \bar{\Delta}) - (\tau_s + 1) \frac{dh(\bar{\Delta})}{d\bar{\Delta}} \frac{\partial \theta_s}{\partial \tau_s}(\tau_s, \bar{\Delta}) \right). \\ &\tau_s \in [-1, 1] \quad \bar{\Delta} \in [-1, 1]. \end{aligned} \quad (3.2.24)$$

where $\theta_s(\tau_s, \bar{\Delta}) = \theta_s(\frac{2}{\mu(\bar{\Delta})}\eta_s - 1, \frac{2}{\Delta_{max}}\bar{\Delta} - 1)$.

Next, the process is repeated for the liquid region; that is, the proper derivatives from the coordinate transformations defined in Eqs.(3.2.9) and (3.2.10) must be obtained. The time derivative needed in this case is given as

$$\frac{\partial}{\partial \Delta} = \frac{\partial}{\partial \bar{\Delta}} \frac{\partial \bar{\Delta}}{\partial \Delta} + \frac{\partial}{\partial \tau_\ell} \frac{\partial \tau_\ell}{\partial \Delta}. \quad (3.2.25)$$

Using Eqs.(3.2.9) and (3.2.14) and transforming the independent variables into the new domain produces

$$\frac{\partial}{\partial \Delta} = \frac{2}{\Delta_{max}} \left(\frac{\partial}{\partial \bar{\Delta}} + \frac{(1 - \tau_\ell)}{(h(\bar{\Delta}) - 1)} \frac{dh(\bar{\Delta})}{d\bar{\Delta}} \frac{\partial}{\partial \tau_\ell} \right). \quad (3.2.26)$$

Following a similar procedure as previously outlined in arriving at $\partial/\partial \eta_s$, the spatial derivative in the liquid domain can be written as

$$\frac{\partial}{\partial \eta_\ell} = \frac{-2}{(h(\bar{\Delta}) - 1)} \frac{\partial}{\partial \tau_\ell}, \quad (3.2.27)$$

and the necessary second derivative becomes

$$\frac{\partial^2}{\partial \eta_\ell^2} = \frac{\partial}{\partial \eta_\ell} \frac{\partial}{\partial \eta_\ell} = \frac{4}{(h(\bar{\Delta}) - 1)^2} \frac{\partial^2}{\partial \tau_\ell^2}. \quad (3.2.28)$$

The governing equation for the liquid region is now ready to be expressed in terms of the transformed coordinates. Substituting Eq.(3.2.26) and Eq.(3.2.28) into Eq.(2.2.2), the governing heat equation for the liquid region becomes

$$\begin{aligned} \frac{\partial^2 \theta_\ell}{\partial \tau_\ell^2}(\tau_\ell, \bar{\Delta}) &= P \frac{(h(\bar{\Delta}) - 1)}{2\Delta_{max}} \left((h(\bar{\Delta}) - 1) \frac{\partial \theta_\ell}{\partial \bar{\Delta}}(\tau_\ell, \bar{\Delta}) + \frac{dh(\bar{\Delta})}{d\bar{\Delta}} (1 - \tau_\ell) \frac{\partial \theta_\ell}{\partial \tau_\ell}(\tau_\ell, \bar{\Delta}) \right) \\ &\quad \tau_\ell \in [-1, 1], \quad \bar{\Delta} \in [-1, 1], \quad (3.2.29) \end{aligned}$$

where $\theta_\ell(\tau_\ell, \bar{\Delta}) = \theta_\ell(\frac{-2\eta_\ell}{\mu(\bar{\Delta})-1} + 1 + \frac{2}{\mu(\bar{\Delta})-1}, \frac{2}{\Delta_{max}}\bar{\Delta} - 1)$ and $P = \alpha_s/\alpha_\ell$.

The boundary condition that describes temperature continuity at the interface shown in Eq.(2.2.5) becomes

$$\theta_s(1, \bar{\Delta}) = \theta_\ell(-1, \bar{\Delta}) = 0 \quad (3.2.30)$$

The transformed interface boundary condition described in Eq.(2.2.6) becomes

$$-\frac{k_\ell T_{ref,\ell}}{k_s T_{ref,s}} \frac{1}{(h(\bar{\Delta}) - 1)} \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) - \frac{1}{h(\bar{\Delta})} \frac{\partial \theta_s}{\partial \tau_s}(1, \bar{\Delta}) + \frac{1}{Ste_s} \frac{1}{\Delta_{max}} \frac{dh(\bar{\Delta})}{d\bar{\Delta}} = 0, \quad (3.2.31)$$

while the insulated end condition shown in Eq.(2.2.8) is now expressable as

$$\frac{\partial \theta_\ell}{\partial \tau_\ell}(1, \bar{\Delta}) = 0. \quad (3.2.32)$$

Finally, the initial conditions in Eqs. (2.2.9) and (2.2.10) for the solid and liquid regions map to

$$\theta_\ell(\tau_\ell, 0) = f(\tau_\ell) \quad (3.2.33)$$

and

$$\theta_s(\tau_s, 0) = 0 \quad (3.2.34)$$

The governing heat equations and auxiliary conditions have now been mapped to the new computational domain $[-1, 1]$. Next, the expansion solutions for each region will be formulated using the previously described Chebyshev polynomials, beginning with the liquid region.

3.3 Series Expansions

The solution to Eq.(3.2.24) and Eq.(3.2.29) can, in general, be written in the expansion form as

$$\theta(\tau, \bar{\Delta}) = \sum_{j=0}^{\infty} a_j(\bar{\Delta}) T_j(\tau), \quad (3.3.1)$$

where $T_j(\tau)$ is the j^{th} order Chebyshev polynomial of the first kind and $a_j(\bar{\Delta})$ are the unknown time-varying expansion coefficients. Since the summation in Eq.(3.3.1) cannot be computationally evaluated to an infinite number of terms, a truncated form must be used to approximate $\theta(\tau, \bar{\Delta})$. This approximation takes the form of

$$\theta(\tau, \bar{\Delta}) \approx \tilde{\theta}^{N+1}(\tau, \bar{\Delta}) = \sum_{j=0}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j(\tau), \quad (3.3.2)$$

where $a_j^{N+1}(\bar{\Delta}) \approx a_j(\bar{\Delta})$ for sufficiently large N . This concept is used for both the solid and liquid regions.

In the next section, uniform representations based on series expansions are developed for the temperature distributions in both the liquid and solid regions. Before developing these expansions, it is observed that uncoupling of the solutions between the solid and liquid regions exists. That is, it is possible to set up a two-point boundary value problem in the liquid region using Eq.(3.2.29) as the differential equation and Eq.(3.2.30) and Eq.(3.2.32) as the boundary conditions. Once the temperature distribution in the liquid region is known, the temperature distribution in the solid region can be resolved. This is in contrast to the direct Stefan problem that requires

the simultaneous solution of both regions. Owing to this uncoupling, the solution to the liquid region is developed first.

3.3.1 Expansion Solution for the Liquid Region

The basic expansion shown in Eq.(3.3.1) is rewritten for the liquid region as

$$\theta_\ell(\tau_\ell, \bar{\Delta}) = \sum_{i=0}^{\infty} d_i(\bar{\Delta}) T_i(\tau_\ell), \quad (3.3.3)$$

where the basis set $\{T_j(\tau_\ell)\}_{j=0}^{\infty}$ are represented in terms of Chebyshev polynomials of the first kind. In practice, the infinite series representation shown in Eq.(3.3.3) must be truncated after a finite number of terms, say $N + 2$. Thus the approximation to $\theta_\ell(\tau_\ell, \bar{\Delta})$ is denoted as $\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta})$ and given by

$$\theta_\ell(\tau_\ell, \bar{\Delta}) \approx \tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = \sum_{i=0}^{N+1} d_i^{N+1}(\bar{\Delta}) T_i(\tau_\ell), \quad (3.3.4)$$

where $d_i^{N+1}(\bar{\Delta})$ are the unknown time-varying expansion coefficients. It is hoped that as N increases to a sufficiently large value, $d_i^{N+1}(\bar{\Delta}) \approx d_i(\bar{\Delta})$. With this basis set, effective trial functions can be developed by incorporating all known auxiliary conditions. In order to arrive at a desirable set of trial functions, it is possible to incorporate all known auxiliary conditions directly into the assumed expansion. By doing so, all auxiliary conditions are exactly satisfied, thereby reducing introduced errors. This direct inclusion of the auxiliary conditions also tends to accelerate the convergence rate of the series representation for the solution.

Applying the known boundary condition at the interface ($\tau_\ell = -1$) displayed in Eq.(3.2.30) to Eq.(3.3.4) yields the following,

$$\theta_\ell(-1, \bar{\Delta}) = \tilde{\theta}_\ell^{N+1}(-1, \bar{\Delta}) = 0 = \sum_{i=0}^{N+1} d_i^{N+1}(\bar{\Delta}) T_i(-1). \quad (3.3.5)$$

Recognizing that $T_i(-1) = (-1)^i$ for $i = 0, 1, 2, \dots, N+1$, [28] and solving for d_0^{N+1} produces

$$d_0^{N+1}(\bar{\Delta}) = - \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) (-1)^i. \quad (3.3.6)$$

This knowledge can be directly incorporated into Eq.(3.3.4) by isolating the leading term $i = 0$, i.e.,

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = d_0^{N+1}(\bar{\Delta}) T_0(\tau_\ell) + \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) T_i(\tau_\ell). \quad (3.3.7)$$

Knowing $T_0(\tau_\ell) = 1$, $\tau_\ell \in [-1, 1]$ and upon substituting Eq.(3.3.6) into Eq.(3.3.7), the following is obtained,

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = - \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) (-1)^i + \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) T_i(\tau_\ell), \quad (3.3.8)$$

or

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) \left(T_i(\tau_\ell) - (-1)^i \right). \quad (3.3.9)$$

Next, the insulated boundary condition displayed in Eq. (3.2.32) is applied to Eq.(3.3.9). Doing so yields

$$\frac{\partial \theta_\ell}{\partial \tau_\ell}(1, \bar{\Delta}) = \frac{\partial \tilde{\theta}_\ell^{N+1}}{\partial \tau_\ell}(1, \bar{\Delta}) = 0 = \sum_{i=1}^{N+1} d_i^{N+1}(\bar{\Delta}) T'_i(1). \quad (3.3.10)$$

Releasing the $i = 1$ term shown in Eq.(3.3.10) and knowing $T_1'(1) = 1$, $d_1^{N+1}(\bar{\Delta})$ can be expressed as

$$d_1^{N+1}(\bar{\Delta}) = - \sum_{i=2}^{N+1} d_i^{N+1}(\bar{\Delta}) T_i'(1). \quad (3.3.11)$$

Again, this finding can be directly imported into the expansion represented by Eq.(3.3.9). To incorporate this knowledge, the $i = 1$ term is released in Eq.(3.3.9) to get

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = d_1^{N+1}(\bar{\Delta}) (\tau_\ell + 1) + \sum_{i=2}^{N+1} d_i^{N+1}(\bar{\Delta}) (T_i(\tau_\ell) - (-1)^i). \quad (3.3.12)$$

Substituting Eq.(3.3.11) for $d_1^{N+1}(\bar{\Delta})$ into Eq.(3.3.12) produces

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = \sum_{i=2}^{N+1} d_i^{N+1}(\bar{\Delta}) (T_i(\tau_\ell) - (-1)^i - (\tau_\ell + 1) T_i'(1)). \quad (3.3.13)$$

For notational convenience, let $k = i - 1$, then Eq.(3.3.13) becomes

$$\tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = \sum_{k=1}^N d_{k+1}^{N+1}(\bar{\Delta}) (T_{k+1}(\tau_\ell) - (-1)^{k+1} - (\tau_\ell + 1) T_{k+1}'(1)). \quad (3.3.14)$$

It is now time to account for the known initial condition. Before proceeding further, the notation is simplified by letting

$$\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta}) = \tilde{\theta}_\ell^{N+1}(\tau_\ell, \bar{\Delta}) = \sum_{k=1}^N b_k^N(\bar{\Delta}) \rho_k^N(\tau_\ell), \quad (3.3.15)$$

where

$$\rho_k^N(\tau_\ell) = T_{k+1}(\tau_\ell) - (-1)^{k+1} - (\tau_\ell + 1) T_{k+1}'(1), \quad (3.3.16)$$

and

$$b_k^N(\bar{\Delta}) = d_{k+1}^{N+1}(\bar{\Delta}), \quad k = 1, 2, \dots, N. \quad (3.3.17)$$

The initial condition for the liquid region is the temperature profile of the liquid at the moment solidification begins at the cooling face. This initial condition is established in Eq.(3.2.33) as

$$\theta_\ell(\tau_\ell, -1) = \tilde{\Theta}_\ell^N(\tau_\ell, -1) = f(\tau_\ell), \quad \tau_\ell \in [-1, 1], \quad (3.3.18)$$

where $f(\tau_\ell)$ is the temperature profile of the liquid. Before applying the initial condition to Eq.(3.3.15), the functional form of the time-varying expansion coefficients must be assumed. This can be done by expressing the time-varying expansion coefficients in Eq.(3.3.17) as

$$b_k^N(\bar{\Delta}) = \sum_{j=0}^{P_k} g_j^k T_j(\bar{\Delta}), \quad k = 1, 2, \dots, N, \quad \bar{\Delta} \in [-1, 1], \quad (3.3.19)$$

which allows Eq.(3.3.15) to be written as

$$\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta}) = \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=0}^{P_k} g_j^k T_j(\bar{\Delta}). \quad (3.3.20)$$

For the sake of generality, define the upper limit in the summation as P_k , $k = 1, 2, \dots, N$. The initial condition shown in Eq.(3.3.18) is now applied to Eq.(3.3.20).

Doing so produces

$$\theta_\ell(\tau_\ell, -1) = \tilde{\Theta}_\ell^N(\tau_\ell, -1) = f(\tau_\ell) = \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=0}^{P_k} g_j^k T_j(-1). \quad (3.3.21)$$

Releasing the $j = 0$ term in the time-series expansion produces

$$f(\tau_\ell) = \sum_{k=1}^N \rho_k^N(\tau_\ell) \left(g_0^k + \sum_{j=1}^{P_k} g_j^k (-1)^j \right), \quad (3.3.22)$$

where $T_j(-1) = (-1)^j$, $j = 0, 1, 2, \dots, P_k$. Upon distributing, it is determined that

$$f(\tau_\ell) = \sum_{k=1}^N \rho_k^N(\tau_\ell) g_0^k + \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=1}^{P_k} g_j^k (-1)^j, \quad (3.3.23)$$

or

$$\sum_{k=1}^N \rho_k^N(\tau_\ell) g_0^k = f(\tau_\ell) - \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=1}^{P_k} g_j^k (-1)^j. \quad (3.3.24)$$

This result is now incorporated into Eq.(3.3.20) by first releasing the $j = 0$ term,

namely

$$\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta}) = \sum_{k=1}^N g_0^k \rho_k^N(\tau_\ell) + \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=1}^{P_k} g_j^k T_j(\bar{\Delta}), \quad (3.3.25)$$

since $T_0(\bar{\Delta}) = 1$ and observing the common occurrence of terms in Eqs.(3.3.24) and (3.3.25), the expansion becomes

$$\theta_\ell(\tau_\ell, \bar{\Delta}) \approx \tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta}) = f(\tau_\ell) + \sum_{k=1}^N \rho_k^N(\tau_\ell) \sum_{j=1}^{P_k} g_j^k (T_j(\bar{\Delta}) - (-1)^j), \quad \tau_s \in [-1, 1], \bar{\Delta} \in [-1, 1]. \quad (3.3.26)$$

Equation (3.3.26) represents the expansion form of the solution for the liquid region and contains the yet to be determined constants $\{g_j^k\}$, $j = 1, 2, \dots, P_k$, $k = 1, 2, \dots, N$. These constants will be determined using a Weighted Residual method which is the topic of Chapter 4.

3.3.2 Expansion Solution for Solid Region

Next, the expansion solution for the solid region is developed in the same manner as the liquid solution. The approximate solution for the solid region is assumed to be

of the form

$$\theta_s(\tau_s, \bar{\Delta}) \approx \tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta}) = \sum_{j=0}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j(\tau_s), \quad (3.3.27)$$

subject to the boundary conditions displayed in Eq.(3.2.30) and Eq.(3.2.31), namely

$$\theta_s(1, \bar{\Delta}) = \tilde{\theta}_s^{N+1}(1, \bar{\Delta}) = 0, \quad (3.3.28)$$

and

$$-\frac{k_\ell T_{ref,\ell}}{k_s T_{ref,s}} \left(\frac{1}{h(\bar{\Delta}) - 1} \right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) - \frac{1}{h(\bar{\Delta})} \frac{\partial \tilde{\theta}_s^{N+1}}{\partial \tau_s}(1, \bar{\Delta}) + \frac{1}{Ste_s} \frac{1}{\Delta_{max}} \frac{dh(\bar{\Delta})}{d\bar{\Delta}} = 0$$

$$\bar{\Delta} \in [-1, 1], \quad (3.3.29)$$

respectively. Subjecting Eq.(3.3.27) to the boundary condition shown in Eq.(3.3.28)

produces

$$\theta_s(1, \bar{\Delta}) = \tilde{\theta}_s^{N+1}(1, \bar{\Delta}) = 0 = \sum_{j=0}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j(1), \quad \bar{\Delta} \in [-1, 1]. \quad (3.3.30)$$

Releasing the $j = 0$ term in the summation and recognizing that $T_j(1) = 1$ for $j = 0, 1, 2, \dots, N+1$, the leading term of the expansion can be expressed in terms of the others as

$$a_0^{N+1}(\bar{\Delta}) = - \sum_{j=1}^{N+1} a_j^{N+1}(\bar{\Delta}). \quad (3.3.31)$$

Substitute Eq.(3.3.31) into Eq.(3.3.27) obtains

$$\tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta}) = \sum_{j=1}^{N+1} a_j^{N+1}(\bar{\Delta}) (T_j(\tau_s) - 1). \quad (3.3.32)$$

Next, the boundary condition shown in Eq.(3.3.29) is used by taking the first derivative of $\tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta})$ with respect to τ_s and evaluating at $\tau_s = 1$ to produce

$$\frac{\partial \tilde{\theta}_s^{N+1}}{\partial \tau_s}(1, \bar{\Delta}) = \sum_{j=1}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j'(1), \quad (3.3.33)$$

where $T_j'(\tau_s) = dT_j/d\tau_s$. Substituting Eq.(3.3.33) into Eq.(3.3.29), and letting $r = k_\ell/k_s$, $g = T_{ref,\ell}/T_{ref,s}$, $\dot{h}(\bar{\Delta}) = dh/d\bar{\Delta}$, the following is obtained

$$-\left(\frac{r g}{h(\bar{\Delta}) - 1}\right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) - \frac{1}{h(\bar{\Delta})} \sum_{j=1}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j'(1) + \frac{\dot{h}(\bar{\Delta})}{Ste_s} \frac{1}{\Delta_{max}} = 0, \quad \bar{\Delta} \in [-1, 1]. \quad (3.3.34)$$

Releasing the $j = 1$ term in Eq.(3.3.34) and noting that $T_1'(\tau_s) = 1$ for $\tau_s \in [-1, 1]$, $a_1^{N+1}(\bar{\Delta})$ can be expressed as

$$\begin{aligned} a_1^{N+1}(\bar{\Delta}) &= -\left(\frac{h(\bar{\Delta}) r g}{h(\bar{\Delta}) - 1}\right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) \\ &\quad - \sum_{j=2}^{N+1} a_j^{N+1}(\bar{\Delta}) T_j'(1) + \frac{\dot{h}(\bar{\Delta}) h(\bar{\Delta})}{2 Ste_s} \frac{2}{\Delta_{max}}. \end{aligned} \quad (3.3.35)$$

Releasing the $j = 1$ term in Eq.(3.3.32) for the expansion of $\tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta})$ and acknowledging that $T_1(\tau_s) = \tau_s$, it is seen that

$$\tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta}) = a_1^{N+1}(\bar{\Delta})(\tau_s - 1) + \sum_{j=2}^{N+1} a_j^{N+1}(\bar{\Delta})(T_j'(\tau_s) - 1). \quad (3.3.36)$$

Substituting Eq.(3.3.35) into Eq.(3.3.36) for $a_1^{N+1}(\bar{\Delta})$ and collecting terms produces

$$\tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta}) = \frac{\dot{h}(\bar{\Delta}) h(\bar{\Delta})}{Ste_s} \frac{(\tau_s - 1)}{\Delta_{max}} - h(\bar{\Delta}) \left(\frac{r g (\tau_s - 1)}{h(\bar{\Delta}) - 1}\right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta})$$

$$+ \sum_{j=2}^{N+1} a_j^{N+1}(\bar{\Delta})(T_j(\tau_s) - 1 - (\tau_s - 1)T'_j(1)). \quad (3.3.37)$$

Next, for notational convention, define $k = j - 1$ and rewrite Eq.(3.3.37) as

$$\begin{aligned} \tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) &= \tilde{\theta}_s^{N+1}(\tau_s, \bar{\Delta}) = \frac{\dot{h}(\bar{\Delta})h(\bar{\Delta})}{Ste_s} \frac{(\tau_s - 1)}{\Delta_{max}} \\ &- h(\bar{\Delta}) \left(\frac{r g(\tau_s - 1)}{h(\bar{\Delta}) - 1} \right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) + \sum_{k=1}^N z_k^N(\bar{\Delta}) \beta_k^N(\tau_s), \\ &\tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1], \end{aligned} \quad (3.3.38)$$

where

$$\beta_k^N(\tau_s) = T_{k+1}(\tau_s) - 1 - (\tau_s - 1)T'_{k+1}(1), \quad \tau_s \in [-1, 1], \quad k = 1, 2, \dots, N, \quad (3.3.39)$$

and

$$z_k^N(\bar{\Delta}) = a_{k+1}^N(\bar{\Delta}). \quad (3.3.40)$$

Observe that at this time, the temperature gradient $\partial \theta_\ell / \partial \tau_\ell$ is unresolved and can be expressed by the previously derived approximation, i.e., $\partial \tilde{\Theta}_\ell^N / \partial \tau_\ell(-1, \bar{\Delta})$.

At this point, the time dependency of the problem can now be addressed. Up to this point, the time dependency has been embodied through the expansion coefficients $z_k^N(\bar{\Delta})$. Assume that $z_k^N(\bar{\Delta})$ can be expanded as

$$z_k^N(\bar{\Delta}) = \sum_{m=0}^{R_k} c_m^k T_m(\bar{\Delta}), \quad k = 1, 2, \dots, N, \quad (3.3.41)$$

where $T_m(\bar{\Delta})$ is the m^{th} Chebyshev polynomial of the first kind in the time variable and $c_m^k, m = 0, 1, \dots, R_k, k = 1, 2, \dots, N$ are unknown constants. Substituting Eq.(3.3.41) into Eq.(3.3.38) produces

$$\begin{aligned} \tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) &= \frac{\dot{h}(\bar{\Delta})h(\bar{\Delta})}{Ste_s} \frac{(\tau_s - 1)}{\Delta_{max}} - h(\bar{\Delta}) \left(\frac{r g(\tau_s - 1)}{h(\bar{\Delta}) - 1} \right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}) \\ &+ \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=0}^{R_k} c_m^k T_m(\bar{\Delta}), \quad \tau_s \in [-1, 1], \bar{\Delta} \in [-1, 1]. \end{aligned} \quad (3.3.42)$$

The initial condition given in Eq.(3.2.34) becomes

$$\theta_s(\tau_s, -1) = \tilde{\Theta}_s^N(\tau_s, -1) = 0, \quad (3.3.43)$$

and is applied to Eq.(3.3.42) to obtain

$$\begin{aligned} 0 &= -h(-1) \left(\frac{r g(\tau_s - 1)}{h(-1) - 1} \right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, -1) \\ &+ \frac{\dot{h}(-1)h(-1)}{Ste_s} \frac{(\tau_s - 1)}{\Delta_{max}} + \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=0}^{R_k} c_m^k (-1)^m. \end{aligned} \quad (3.3.44)$$

For the physical situation involving continuity in temperature along the boundary at $\eta_s = -1$, one assumes $h(-1) = 0$ and $\dot{h}(-1) < \infty$, thereby reducing Eq.(3.3.44) to

$$0 = \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=0}^{R_k} c_m^k (-1)^m. \quad (3.3.45)$$

or upon releasing the $m = 0$ term

$$0 = \sum_{k=1}^N c_0^k \beta_k^N(\tau_s) + \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=1}^{R_k} c_m^k (-1)^m \quad (3.3.46)$$

The expansion shown in Eq.(3.3.42) is now manipulated in order to release terms that can be either dropped or re-substituted in some other form. First, rewrite Eq.(3.3.42) in compact form as

$$\tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) = f_s(\tau_s, \bar{\Delta}) + \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=0}^{R_k} c_m^k T_m(\bar{\Delta}), \quad \tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1], \quad (3.3.47)$$

where

$$f_s(\tau_s, \bar{\Delta}) = \frac{\dot{h}(\bar{\Delta})h(\bar{\Delta})}{Ste_s} \frac{(\tau_s - 1)}{\Delta_{max}} - h(\bar{\Delta}) \left(\frac{rg(\tau_s - 1)}{h(\bar{\Delta}) - 1} \right) \frac{\partial \theta_\ell}{\partial \tau_\ell}(-1, \bar{\Delta}). \quad (3.3.48)$$

and then release the $m = 0$ term to get

$$\tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) = f_s(\tau_s, \bar{\Delta}) + \sum_{k=1}^N \beta_k^N(\tau_s) \left(c_0^k + \sum_{m=1}^{R_k} c_m^k (-1)^m \right), \quad (3.3.49)$$

since $T_0(\tau_s) = 1$, $\tau_s \in [-1, 1]$ and $T_m(-1) = (-1)^m$, $m = 1, 2, \dots, R_k$. Therefore,

Eq.(3.3.49) can be written as

$$\begin{aligned} \tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) = f_s(\tau_s, \bar{\Delta}) + \sum_{k=1}^N c_0^k \beta_k^N(\tau_s) + \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=1}^{R_k} c_m^k (-1)^m, \\ \tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1]. \end{aligned} \quad (3.3.50)$$

The findings from the initial condition shown in Eq.(3.3.46) are now substituted into

Eq.(3.3.50) to get

$$\theta_s(\tau_s, \bar{\Delta}) \approx \tilde{\Theta}_s^N(\tau_s, \bar{\Delta}) = f_s(\tau_s, \bar{\Delta}) + \sum_{k=1}^N \beta_k^N(\tau_s) \sum_{m=1}^{R_k} c_m^k (T_m(\bar{\Delta}) - (-1)^m),$$

$$\tau_s \in [-1, 1], \bar{\Delta} \in [-1, 1]. \quad (3.3.51)$$

At this point, the approximation for $\theta_\ell(\tau_\ell, \bar{\Delta})$, i.e., $\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})$ is substituted into the right hand side of Eq.(3.3.51). Since the liquid region solution is uncoupled, it is clear that this function,

$$\frac{\partial \theta_\ell}{\partial \tau_\ell} \approx \frac{\partial \tilde{\Theta}_\ell^N}{\partial \tau_\ell}, \quad (3.3.52)$$

is known and can be expressed in terms of the series displayed in Eq.(3.3.26).

The solutions for both regions are now expressed in the form of expansions. The solution for the solid region contains the derivative of the liquid solution, therefore it is necessary to first solve for the temperature distribution in the liquid region and then solve for temperature distribution in the solid region. This can be done since the solution for the liquid phase is uncoupled from the solid region. This solution is differentiated and evaluated at the interface and then used in arriving at the temperature distribution in the solid region. It is clear that the only remaining obstacle in arriving at a numerical solution for the temperature distribution in both regions lies in obtaining the expansion coefficients $\{g_j^k\}, j = 1, 2, \dots, P_k, k = 1, 2, \dots, N$ for the liquid region and $\{c_m^k\}, m = 1, 2, \dots, R_k, k = 1, 2, \dots, N$ for the solid region. This is the focus of the next chapter, which details the implementation of the Weighted

Residual method for determining the expansion coefficients.

Chapter 4

Numerical Implementation

In this chapter, numerical values for the expansion coefficients indicated in Eqs.(3.3.26) and (3.3.51) are obtained. The solution for the liquid region is presented first, since it has been shown that the solutions uncouple and that the liquid region can be solved as a two-point boundary value problem. The solid solution, which requires the solution for the liquid region, is then be presented.

4.1 Liquid Solution

The mapped mathematical description for the liquid region was derived in Section 3.2 and is shown in Eq.(3.2.29). Let the differential operator for the transformed heat

equation in the liquid region be defined as L_ℓ and given by

$$L_\ell = \frac{\partial^2}{\partial \tau_\ell^2} - P \frac{(h(\bar{\Delta}) - 1)}{2\Delta_{max}} \left((h(\bar{\Delta}) - 1) \frac{\partial}{\partial \bar{\Delta}} + (1 - \tau_\ell) \frac{dh(\bar{\Delta})}{d\bar{\Delta}} \frac{\partial}{\partial \tau_\ell} \right),$$

$$\tau_\ell \in [-1, 1], \quad \bar{\Delta} \in [-1, 1]. \quad (4.1.1)$$

Thus, rewriting Eq.(3.2.29) with the definition shown in Eq.(4.1.1) produces

$$L_\ell[\theta_\ell(\tau_\ell, \bar{\Delta})] = 0, \quad \tau_\ell \in [-1, 1], \quad \bar{\Delta} \in [-1, 1]. \quad (4.1.2)$$

Since the present analysis develops an approximate solution to $\theta_\ell(\tau_\ell, \bar{\Delta})$, namely

$\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})$, Eq.(4.1.2) must now be written as

$$L_\ell[\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})] \approx 0. \quad (4.1.3)$$

In order for Eq.(4.1.3) to maintain the equality sign shown in Eq.(4.1.2), a residual function must be introduced to Eq.(4.1.3). This allows for the re-introduction of the equality, namely

$$R_\ell^N(\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})) = -L_\ell[\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})], \quad \tau_\ell \in [-1, 1], \quad \bar{\Delta} \in [-1, 1], \quad (4.1.4)$$

where $R_\ell^N(\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta}))$ is the local residual function. A zero residual for the entire computational domain indicates that the approximation has indeed recreated the exact solution. The Weighted Residual approach is based on minimizing the residual in some sense [31]. An excellent exposition on the Weighted Residual method is offered by Finlayson [31]. For computational simplicity, the approach taken here

involves the use of orthogonal collocation, which requires the residual to be evaluated only at the collocation points [31]. Galerkin or least squares methods could also be used, however the computational cost in terms of CPU time will increase.

The weighted residual statement for the collocation method is [31]

$$\left\langle R_\ell^N(\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})), \delta(\tau_\ell - \tau_{\ell,m})\delta(\bar{\Delta} - \bar{\Delta}_n) \right\rangle_1 = 0, \quad n = 1, 2, \dots, P_m; \quad m = 1, 2, \dots, N, \quad (4.1.5)$$

where the weight function is unity, δ is the Dirac delta function [31], $\tau_{\ell,m}$ is the m^{th} spatial collocation point in the liquid region, and $\bar{\Delta}_n$ is the n^{th} collocation point in the temporal domain. Equation (4.1.5) can clearly be reduced to a compact statement [31] based on the mathematical properties of the Dirac delta function. This compact form is

$$R_\ell^N(\tilde{\Theta}_\ell^N(\tau_{\ell,m}, \bar{\Delta}_n)) = 0, \quad n = 1, 2, \dots, P_m; \quad m = 1, 2, \dots, N. \quad (4.1.6)$$

For this study, the collocation points $\bar{\Delta}_n$ and $\tau_{\ell,m}$ are defined by the open rules [32] as

$$\bar{\Delta}_n = \cos\left(\frac{(2n-1)\pi}{2P_m}\right), \quad n = 1, 2, \dots, P_m, \quad (4.1.7)$$

and

$$\tau_{\ell,m} = \cos\left(\frac{(2m-1)\pi}{2N}\right), \quad m = 1, 2, \dots, N. \quad (4.1.8)$$

Substituting Eq.(3.3.26) into Eq.(4.1.4) produces

$$R_\ell^N(\tilde{\Theta}_\ell^N(\tau_\ell, \bar{\Delta})) = -L_\ell[f(\tau_\ell)] - \sum_{k=1}^N \sum_{j=1}^{P_k} g_j^k L_\ell [\rho_k(\tau_\ell)(T_j(\bar{\Delta}) - (-1)^j)],$$

$$\tau_\ell \in [-1, 1], \bar{\Delta} \in [-1, 1]. \quad (4.1.9)$$

It is known from Eq.(4.1.6) that the residual function is zero at the collocation points given by $\tau_{\ell,m}$ and $\bar{\Delta}_n$ for $m = 1, 2, \dots, N$ and $n = 1, 2, \dots, P_m$. Thus Eq.(4.1.9) reduces to

$$L_\ell[f(\tau_{\ell,m})] + \sum_{k=1}^N \sum_{j=1}^{P_k} g_j^k L_\ell [\rho_k(\tau_{\ell,m})(T_j(\bar{\Delta}_n) - (-1)^j)] = 0,$$

$$n = 1, 2, \dots, P_m; \quad m = 1, 2, \dots, N. \quad (4.1.10)$$

Rearranging Eq.(4.1.10) gives

$$-L_\ell[f(\tau_{\ell,m})] = \sum_{k=1}^N \sum_{j=1}^{P_k} g_j^k L_\ell [\rho_k(\tau_{\ell,m})(T_j(\bar{\Delta}_n) - (-1)^j)],$$

$$n = 1, 2, \dots, P_m; \quad m = 1, 2, \dots, N, \quad (4.1.11)$$

which can be written in matrix form as

$$A\bar{x} = \bar{b}. \quad (4.1.12)$$

Here A is the coefficient matrix, $\bar{b}$ is a column vector, and $\bar{x}$ is a column vector containing the unknown expansion coefficients. Matrix inversion can now be used for determining the unknown expansion coefficients $\{g_j^k\}$, $j = 1, 2, \dots, P_k$, $k = 1, 2, \dots, N$, for the liquid region. The matrix form of Eq.(4.1.11) allows for all space and time

to be accounted for at once. Accounting for all of space and time at once is a novel concept as applied to solving parabolic differential equations. Traditional doctrine involves time-marching methods while here time is treated in an elliptic fashion which takes into account all future information [6].

In order to begin setting up the necessary matrices, a decision must be made on how Eq.(4.1.11) is to be evaluated. One method is to fix space and move in time or to fix time and move in space. Either is acceptable and for this study, space is held fixed while moving in time. Using shorthand notation, Eq.(4.1.11) is written as

$$\sum_{k=1}^N \sum_{j=1}^{P_k} g_j^k \Omega_{jk}^{nm} = -b_{nm}, \quad n = 1, 2, \dots, P_m; \quad m = 1, 2, \dots, N, \quad (4.1.13)$$

where g_j^k are the unknown expansion coefficients and Ω_{jk}^{nm} is given by

$$\Omega_{jk}^{nm} = L_\ell \left[\rho_k(\tau_{\ell,m})(T_j(\bar{\Delta}_n) - (-1)^j) \right], \quad (4.1.14)$$

while b_{nm} is

$$b_{nm} = L_\ell[f(\tau_{\ell,m})], \quad m = 1, 2, \dots, P_m; \quad n = 1, 2, \dots, N. \quad (4.1.15)$$

Observe that $-b_{nm}$ is actually independent of n which comes from the initial condition in the liquid being a function of space only. This allows us to write $-b_{nm} = -\hat{b}_m$. The indices n and m represent the n^{th} and m^{th} collocation points while j is the index from the inner summation in Eq.(4.1.11) and k is the index from the outer summation in Eq.(4.1.11).

We can now set up the coefficient matrix A . It is noted that for a given row in the coefficient matrix, the same collocation points are used in evaluating Eq.(4.1.14). As one moves down a given row, the jk indices remain the same for each column. An example of a general coefficient matrix is

$$A = \begin{pmatrix} \begin{pmatrix} \Omega_{11}^{11} & \cdots & \Omega_{P_1 1}^{11} \\ \vdots & \ddots & \vdots \\ \Omega_{11}^{P_1 1} & \cdots & \Omega_{P_1 1}^{P_1 1} \end{pmatrix} & \cdots & \begin{pmatrix} \Omega_{1N}^{11} & \cdots & \Omega_{P_N N}^{11} \\ \vdots & \ddots & \vdots \\ \Omega_{1N}^{P_1 1} & \cdots & \Omega_{P_N N}^{P_1 1} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ \begin{pmatrix} \Omega_{11}^{1N} & \cdots & \Omega_{P_1 1}^{1N} \\ \vdots & \ddots & \vdots \\ \Omega_{11}^{P_N N} & \cdots & \Omega_{P_1 1}^{P_N N} \end{pmatrix} & \cdots & \begin{pmatrix} \Omega_{1N}^{1N} & \cdots & \Omega_{P_N N}^{1N} \\ \vdots & \ddots & \vdots \\ \Omega_{1N}^{P_N N} & \cdots & \Omega_{P_N N}^{P_N N} \end{pmatrix} \end{pmatrix}. \quad (4.1.16)$$

Notice that within each subgroup, the value for k remains the same, while the index j moves through its entire range, $j = 1, 2, \dots, P_{m=N}$. Also notice that for each row, the collocation points m and n do not change. The associated matrix representing

the expansion coefficients, $\bar{x}$, is

$$\bar{x} = \begin{pmatrix} \begin{pmatrix} g_1^1 \\ \vdots \\ g_{P_1}^1 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} g_1^N \\ \vdots \\ g_{P_{m=N}}^N \end{pmatrix} \end{pmatrix}, \quad (4.1.17)$$

while the $\bar{b}$ vector takes the form

$$\bar{b} = \begin{pmatrix} \begin{pmatrix} -\hat{b}_1 \\ \vdots \\ -\hat{b}_1 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} -\hat{b}_N \\ \vdots \\ -\hat{b}_N \end{pmatrix} \end{pmatrix}. \quad (4.1.18)$$

Now that the coefficient matrix and associated vectors are set up, matrix inversion is used to determine $\bar{x}$ using

$$\bar{x} = [A]^{-1}\bar{b}. \quad (4.1.19)$$

With the expansion coefficients known for the liquid region, Eq.(3.3.26) can be ex-

panded to determine the temperature profile in the liquid region. Since the temperature profile in the liquid region is necessary for the solution to the solid region and it is now known, the solution for the solid region may now be examined.

4.2 Solid Solution

The steps involved in determining the expansion coefficients for the solid region are similar to the ones used in arriving at the expansion coefficients for the liquid region. Let the differential operator for the solid region be defined as

$$L_s = \frac{\partial^2}{\partial \tau_s^2} - \frac{h(\bar{\Delta})}{2\Delta_{max}} \left(h(\bar{\Delta}) \frac{\partial}{\partial \bar{\Delta}} - (\tau_s + 1) \dot{h}(\bar{\Delta}) \frac{\partial}{\partial \tau_s} \right),$$

$$\tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1], \quad (4.2.1)$$

thus Eq.(3.2.24) can be expressed as

$$L_s[\theta_s(\tau_s, \bar{\Delta})] = 0, \quad \tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1]. \quad (4.2.2)$$

Since the solution being developed is an approximation, $\tilde{\Theta}_s^N(\tau_s, \bar{\Delta})$, Eq.(4.2.2) becomes

$$L_s[\tilde{\Theta}_s^N(\tau_s, \bar{\Delta})] \approx 0. \quad (4.2.3)$$

Introducing the residual function to Eq.(4.2.3) permits the re-introduction of the equal sign, namely

$$R_s^N(\tilde{\Theta}_s^N(\tau_s, \bar{\Delta})) = -L_s[\tilde{\Theta}_s^N(\tau_s, \bar{\Delta})], \quad \tau_s \in [-1, 1], \quad \bar{\Delta} \in [-1, 1]. \quad (4.2.4)$$

The Weighted Residual statement for the solid region can be written as [31]

$$\left\langle R_s^N(\tilde{\Theta}_s^N(\tau_s, \bar{\Delta})), \delta(\tau_s - \tau_{s,\hat{m}}) \delta(\bar{\Delta} - \bar{\Delta}_{\hat{n}}) \right\rangle_1 = 0, \quad \hat{n} = 1, 2, \dots, R_{\hat{m}}; \quad \hat{m} = 1, 2, \dots, N, \quad (4.2.5)$$

which reduces to

$$R_s^N(\tilde{\Theta}_s^N(\tau_{s,\hat{m}}, \bar{\Delta}_{\hat{n}})) = 0, \quad \hat{n} = 1, 2, \dots, R_{\hat{m}}; \quad \hat{m} = 1, 2, \dots, N, \quad (4.2.6)$$

due to the mathematical properties of the Dirac delta function [31]. The collocation points for the solid region are also given by the open rule [32] as

$$\bar{\Delta}_{\hat{n}} = \cos\left(\frac{(2\hat{n} - 1)\pi}{2R_{\hat{m}}}\right), \quad \hat{n} = 1, 2, \dots, R_{\hat{m}}, \quad (4.2.7)$$

$$\tau_{s,\hat{m}} = \cos\left(\frac{(2\hat{m} - 1)\pi}{2N}\right), \quad \hat{m} = 1, 2, \dots, N. \quad (4.2.8)$$

Substituting Eq.(4.2.4) into Eq.(4.2.5) allows us to write

$$L_s[\tilde{\Theta}_s^N(\tau_{s,\hat{m}}, \bar{\Delta}_{\hat{n}})] = 0, \quad \hat{n} = 1, 2, \dots, R_{\hat{m}}; \quad \hat{m} = 1, 2, \dots, N. \quad (4.2.9)$$

Substituting Eq.(3.3.51) into Eq.(4.2.9) and rearranging produces

$$L_s[f(\tau_{s,\hat{m}}, \bar{\Delta}_{\hat{n}})] + \sum_{k=1}^N \sum_{m=1}^{R_k} c_m^k L_s[\beta_k^N(\tau_{s,\hat{m}})(T_m(\bar{\Delta}_{\hat{n}}) - (-1)^m)] = 0, \quad \hat{n} = 1, 2, \dots, R_{\hat{m}}; \quad \hat{m} = 1, 2, \dots, N. \quad (4.2.10)$$

or

$$\sum_{k=1}^N \sum_{m=1}^{R_k} c_m^k L_s[\beta_k^N(\tau_{s,\hat{m}})(T_m(\bar{\Delta}_{\hat{n}}) - (-1)^m)] = -L_s[f(\tau_{s,\hat{m}}, \bar{\Delta}_{\hat{n}})], \quad (4.2.11)$$

which is in the form of

$$C\bar{w} = \bar{v}, \quad (4.2.12)$$

where C is the coefficient matrix, $\bar{w}$ is the vector containing the unknown expansion coefficients, and $\bar{v}$ is a known column vector.

Equation (4.2.11) is now cast into shorthand form in order to set up the necessary matrices. This shorthand form is

$$\sum_{k=1}^N \sum_{m=1}^{R_k} c_m^k \Phi_{mk}^{\hat{n}\hat{m}} = -\gamma_{\hat{n}\hat{m}}, \quad \hat{n} = 1, 2, \dots, R_{\hat{m}} \quad \hat{m} = 1, 2, \dots, N, \quad (4.2.13)$$

where

$$\Phi_{mk}^{\hat{n}\hat{m}} = L_s[\beta_k^N(\tau_{s,\hat{m}})(T_m(\bar{\Delta}_{\hat{n}}) - (-1)^m)], \quad (4.2.14)$$

and

$$-\gamma_{\hat{n}\hat{m}} = -L_s[f(\tau_{s,\hat{m}}, \bar{\Delta}_{\hat{n}})]. \quad (4.2.15)$$

The subscripts $\hat{m}$ and $\hat{n}$ represent the $\hat{m}^{th}$ and $\hat{n}^{th}$ collocation points, respectively. The subscript m is the index on the inner summation and k is the index on the outer summation.

A single matrix inversion is used for determining all of the unknown expansion coefficients. Setting up the matrices proceeds exactly as it did for the liquid region.

The general form of the coefficient matrix for the solid region is

$$C = \begin{pmatrix} \begin{pmatrix} \Phi_{11}^{11} & \cdots & \Phi_{R_1 1}^{11} \\ \vdots & \ddots & \vdots \\ \Phi_{11}^{R_1 1} & \cdots & \Phi_{R_1 1}^{R_1 1} \end{pmatrix} & \cdots & \begin{pmatrix} \Phi_{1N}^{11} & \cdots & \Phi_{R_N N}^{11} \\ \vdots & \ddots & \vdots \\ \Phi_{1N}^{R_1 1} & \cdots & \Phi_{R_N N}^{R_1 1} \end{pmatrix} \\ \vdots & \ddots & \vdots \\ \begin{pmatrix} \Phi_{11}^{1N} & \cdots & \Phi_{R_1 1}^{1N} \\ \vdots & \ddots & \vdots \\ \Phi_{11}^{R_N N} & \cdots & \Phi_{R_1 1}^{R_N N} \end{pmatrix} & \cdots & \begin{pmatrix} \Phi_{1N}^{1N} & \cdots & \Phi_{R_N N}^{1N} \\ \vdots & \ddots & \vdots \\ \Phi_{1N}^{R_N N} & \cdots & \Phi_{R_N N}^{R_N N} \end{pmatrix} \end{pmatrix}, \quad (4.2.16)$$

The associated vector, $\bar{w}$, becomes

$$\bar{w} = \begin{pmatrix} \begin{pmatrix} c_1^1 \\ \vdots \\ c_{R_1}^1 \end{pmatrix} \\ \vdots \\ \begin{pmatrix} c_1^N \\ \vdots \\ c_{R_m}^N \end{pmatrix} \end{pmatrix}, \quad (4.2.17)$$

and $\bar{v}$ is

$$\bar{v} = \begin{pmatrix} \begin{pmatrix} -\gamma_{11} \\ \vdots \\ -\gamma_{R_1 1} \end{pmatrix} \\ \vdots \\ \begin{pmatrix} -\gamma_{1N} \\ \vdots \\ -\gamma_{R_m N} \end{pmatrix} \end{pmatrix}. \quad (4.2.18)$$

The expansion coefficients are now determined from matrix inversion

$$\bar{w} = [C]^{-1} \bar{v}. \quad (4.2.19)$$

The expansion coefficients for both the solid and liquid regions are now known, and thus the temperature distribution for both regions, are available. With these temperature distributions known, the analytical and numerical models are ready to be verified by comparing the results generated from Eq.(3.3.26) and Eq.(3.3.51) to known exact solutions and to experimental results [25].

Chapter 5

Results

In this chapter, several test cases are considered to numerically verify the model described in Chapter 4. The first case to be considered involves a one-phase, half-space problem where the solid-liquid interface moves with a constant velocity. The exact solution for this case is presented in Carslaw and Jaeger [23] and is used to determine the accuracy of the numerical model for two different pure materials. The second test case involves another one-phase problem where the interfacial motion is described, in an approximate manner, from experimental data [25]. The last case to be examined involves a two-phase, constant velocity situation where the time collocaton method is used to solve the direct problem in the liquid region before solving for the inverse problem in the solid region.

5.1 One-Phase, Constant-Velocity Motion

Some solidification processes require rapid solidification in order to prevent unwanted nucleation and to insure that the desired properties are present in the cast material [33]. A solid-liquid interface that moves with a constant-velocity is one possible way to obtain a rapid solidification time. It is also an ideal test case since an exact analytic solution for a one-phase problem is available and presented in Carslaw and Jaeger [23]. The availability of an exact solution allows for a descriptive error analysis to be performed. Frankel and Keyhani [24] demonstrated that convergence takes place at an exponential rate for this case and that the maximum error takes place at t_{max} as a result of the open rule being used for determining the collocation points. The exact solution in dimensional form [23] is given by

$$T(x, t) = T_{melt} + \frac{h_{s\ell}}{C_{ps}} \left[1 - e^{\frac{V^2}{\alpha}t - \frac{V}{\alpha}x} \right], \quad x \leq Vt, \quad (5.1.1)$$

and

$$T(x, t) = T_{melt}, \quad x \geq Vt, \quad (5.1.2)$$

where C_{ps} is the specific heat for the solid region, $h_{s\ell}$ is the latent heat of fusion, T_{melt} is the melt temperature, α is the thermal diffusivity, and V is the interfacial velocity. Since the temperature of interest is at $x = 0$, Eq.(5.1.1) reduces to

$$T_c(t) = T(0, t) = T_{melt} + \frac{h_{s\ell}}{C_{ps}} \left[1 - e^{\frac{V^2}{\alpha}t} \right], \quad t > 0. \quad (5.1.3)$$

Non-dimensionalization and mapping of Eq.(5.1.3) yields

$$\theta_s(-1, \bar{\Delta}) = 1 - \exp \left[V^2 \left(\frac{L}{\alpha_s} \right)^2 \frac{\Delta_{max}}{2} (\bar{\Delta} + 1) \right], \quad \bar{\Delta} \in [-1, 1]. \quad (5.1.4)$$

Two materials, n-octadecane and aluminum, are used to compare the numerical model with Eq.(5.1.4) for a solidification time t_{max} , of 3000 seconds for n-octadecane and 20 seconds for aluminum. The numerical model reduces to a one-phase problem by setting the initial condition in the liquid region to zero ($f(\tau_\ell) = 0$). This eliminates the liquid region from the model and it is only necessary to solve for expansion coefficients in the solid region. To make the problem a half-space problem, the length L is chosen to be large enough such that it is considerably larger than the maximum amount of material that will form during the solidification time span.

5.1.1 N-Octadecane

The first material to be considered is n-octadecane which is a 99% pure wax. The thermal and physical properties [34,35] of this material that are used in the numerical and exact solutions are: $T_{melt} = 28.15^\circ C$, $h_{s\ell} = 241,730 J/kg$, $\rho_\ell = 774 kg/m^3$, $\rho_s = 814 kg/m^3$, $k_\ell = 0.15 W/(m \cdot K)$, $k_s = 0.43 W/(m \cdot K)$, $\bar{C}_{p\ell} = 2,233 J/(kg \cdot ^\circ C)$, and $\bar{C}_{ps} = 1,823 J/(kg \cdot ^\circ C)$. These two values for the specific heats are taken as averaged values for this test case.

Two different velocities are examined to determine how the boundary condition behaves when the velocity is increased. One expects that as the velocity increases,

a larger temperature drop over the same amount of time results. The first test case uses an interfacial velocity of 0.002 mm/s which grows 6 mm of solid material in 3000 seconds. Figure 5.1.1 is a plot of the dimensionless surface temperature history for the solid showing graphical convergence of the numerical solution for $N=R=8$. Figure 5.1.2 is a plot of this converged solution compared with the exact solution, Eq.(5.1.4). This plot shows that the converged numerical solution for the surface temperature appears almost linear and is graphically identical to the exact the exact solution for this velocity. This surface temperature history corresponds to a dimensional temperature drop from $T_{melt} = 28.15^{\circ}\text{C}$ to approximately 22.5°C . This represents a realistic temperature drop over the 3000 seconds of solidification time.

The second velocity to be considered using n-octadecane is 0.004 mm/s which results in 12 mm of solid material after 3000 seconds of solidification time. Figure 5.1.3 is a plot showing that the numerical solution for the surface temperature has again converged using $N=R=8$. A comparison of the converged numerical solution and the exact solution is shown in Figure 5.1.4. This plot shows that the numerical solution has again graphically matched the exact solution and that the temperature drop required during the indicated solidification time has increased by a factor of four when the velocity is doubled. The dimensional temperature drop resulting from this velocity is from 28.15°C to approximately 4°C . This is a realistic temperature drop and a relatively linear surface temperature history is obtained.

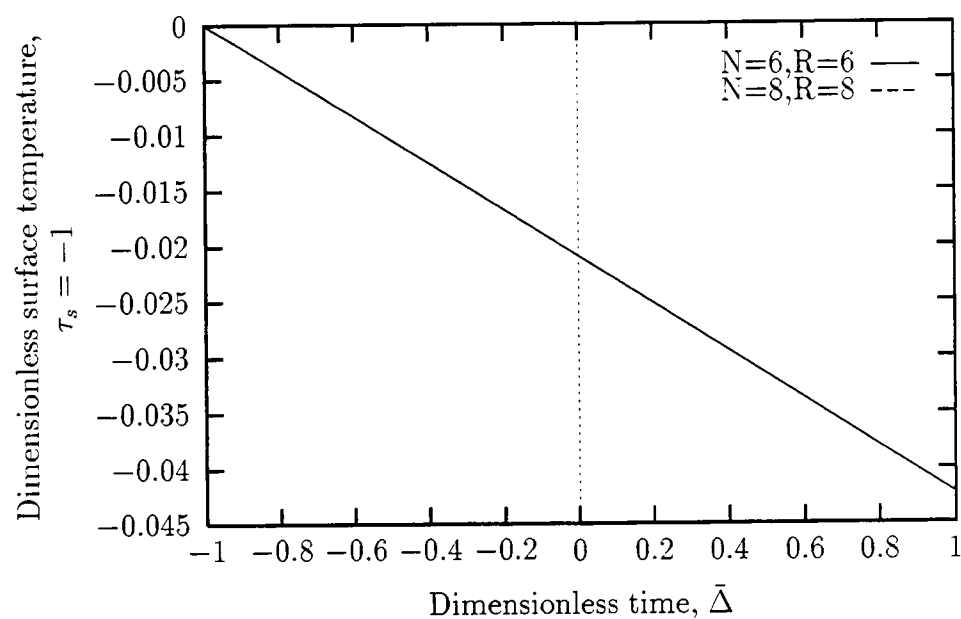


Figure 5.1.1: Dimensionless surface temperature history for n-octadecane showing convergence of the numerical solution for $N=R=8$ using a constant velocity of 0.002 mm/s .

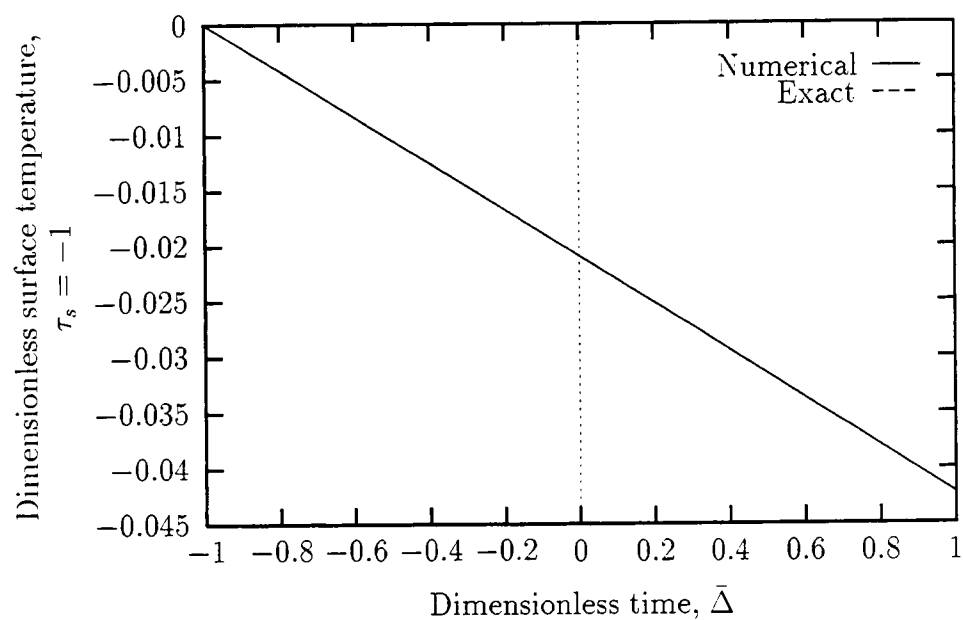


Figure 5.1.2: Comparison of the exact solution, Eq.(5.1.4), and the numerical solution for n-octadecane with a constant velocity of 0.002 mm/s .

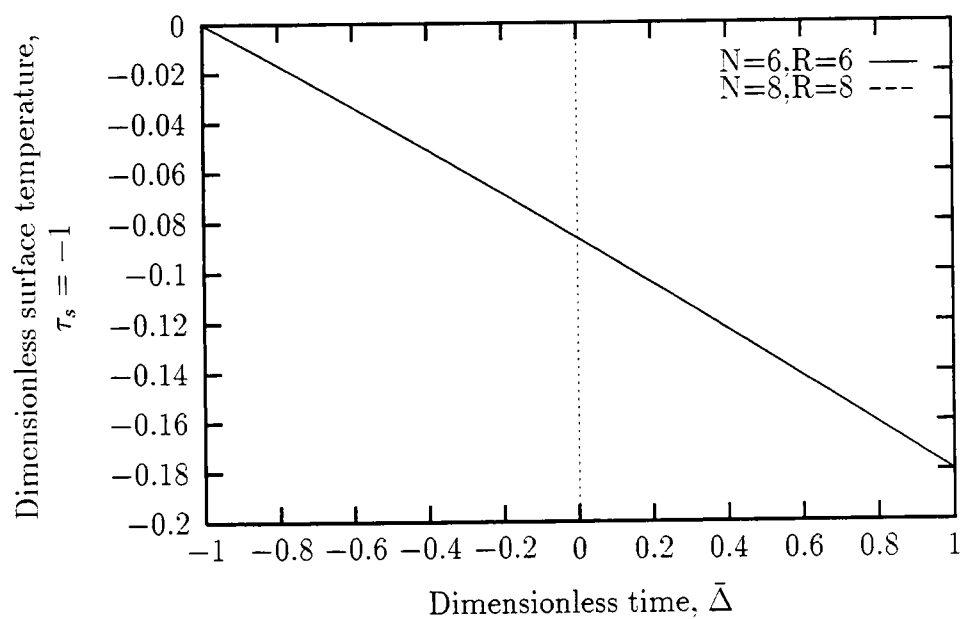


Figure 5.1.3: Dimensionless surface temperature history for n-octadecane showing convergence of the numerical solution for $N=R=8$ using a constant velocity of 0.004 mm/s .

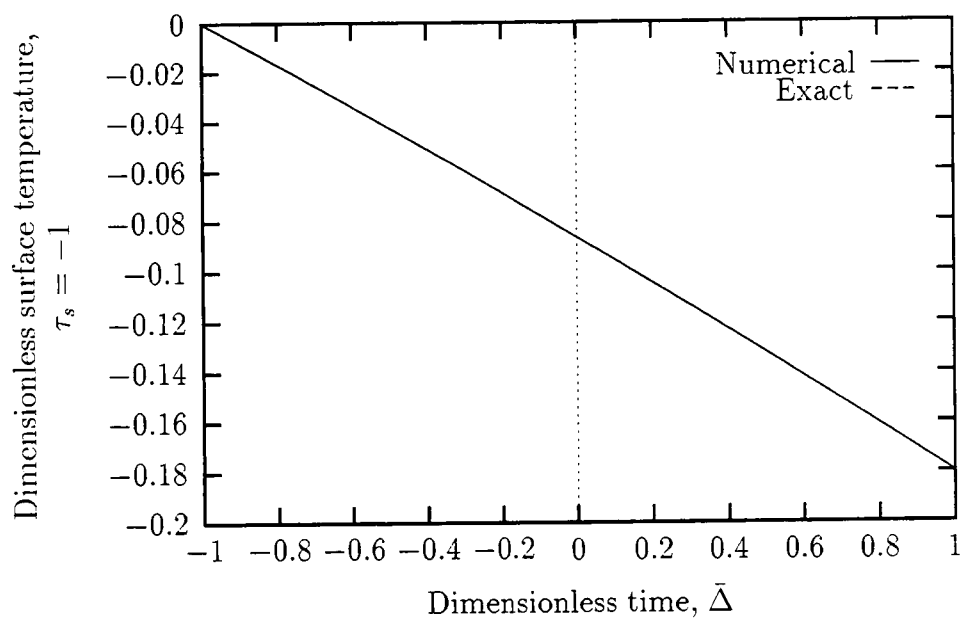


Figure 5.1.4: Comparison of the exact solution, Eq.(5.1.4), and the numerical solution for n-octadecane with a constant velocity of 0.004 mm/s .

These two cases show that further increases in the velocity can quickly yield a required temperature drop which is physically unrealistic for a solidification time of 3000 seconds. In order to obtain faster velocities for this material, the solidification time will have to be decreased.

5.1.2 Aluminum

The properties of pure aluminum [36] used in this analysis are: $\rho = 2702 \text{ kg/m}^3$, $C_{ps} = 903 \text{ J/kg} \cdot \text{K}$, $k_s = 237 \text{ W/m} \cdot \text{K}$, $k_\ell = 237 \text{ W/m} \cdot \text{K}$, $h_{sl} = 395,000 \text{ J/kg}$, $T_{melt} = 660^\circ\text{C}$, and $C_{p\ell} = 903 \text{ J/kg} \cdot \text{K}$. The velocity to be considered for the aluminum is 1 mm/s which yields 20 mm of solid material after 20 seconds of solidification time. Figure 5.1.5 is a plot showing the convergence of the numerical solution for the surface temperature when $N=R=10$. Figure 5.1.6 is a comparison of the numerical solution to the exact solution given by Eq.(5.1.4). This plot shows that the two are graphically identical and again the surface temperature history appears linear. A dimensional surface temperature drop from 660°C to 561°C is required to sustain the constant velocity of 1 mm/s over the 20 seconds of solidification time. This situation portrays a realistic interfacial velocity and an attainable temperature drop at the cooling face for the 20 second solidification time.

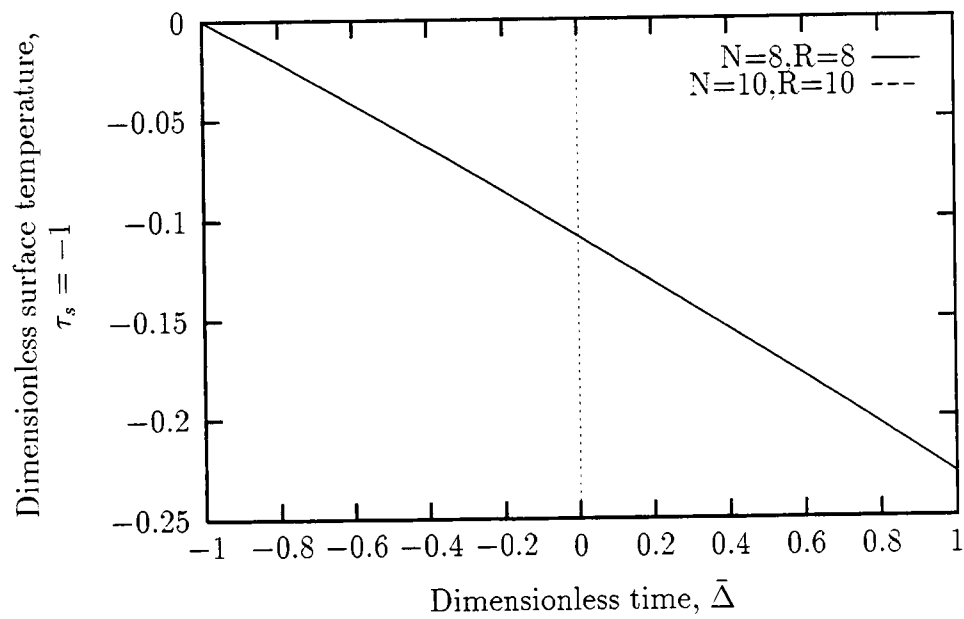


Figure 5.1.5: Dimensionless surface temperature history for aluminum showing convergence of the numerical solution for $N=R=10$ using a constant velocity of 1 mm/s .

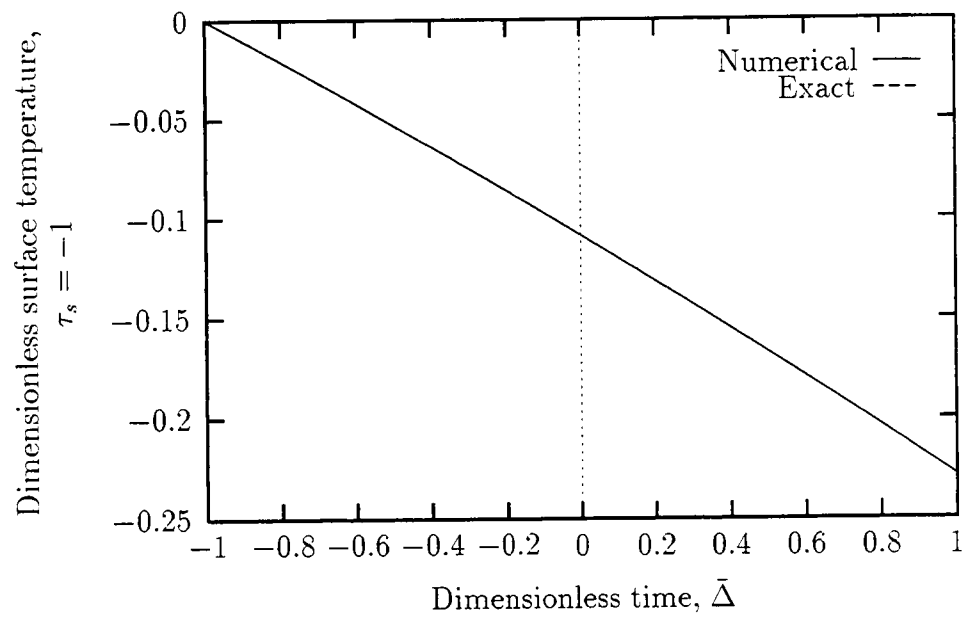


Figure 5.1.6: Comparison of the exact solution, Eq.(5.1.4), and the numerical solution for aluminum with a constant velocity of 1 mm/s .

5.2 Experimental Data

The next case to be considered uses experimental data from a nearly one-phase experiment [25] using n-octadecane as the solidifying material. Details describing the experimental set-up and data acquisition procedures can be found in Wesley [25]. The purpose of this comparison is to clearly indicate that these problems are ill-posed in that a small perturbation in the input data can have profound effects in the numerical solution. Frankel and Keyhani [24] present a clear example indicating this feature of inverse solidification design studies. In general, this type of analysis makes use of a given analytic function for the interfacial velocity and there is no need to curve fit data.

The discussed data comes from an experiment that involves dropping the temperature at the cooling face from the initial temperature of $\approx 28.20^\circ\text{C}$ to a value of 3°C in a rapid, i.e., direct manner in order to approximate a step-change. The experimentally obtained position for the solid-liquid interface is shown in Figure 5.2.1 for a time duration of 1250 seconds. This plot shows that the interfacial position profile exhibits an approximate $\sqrt{t}$ behavior that is predicted by the exact solution [2.26] for a step change in the boundary temperature. In order to incorporate this information into the present model, the data must be curve-fitted. A smooth function and not discrete data is the necessary form of the input for the proposed method. Since the profile exhibits an apparent $\sqrt{t}$ behavior, the function that the data is to be fitted to

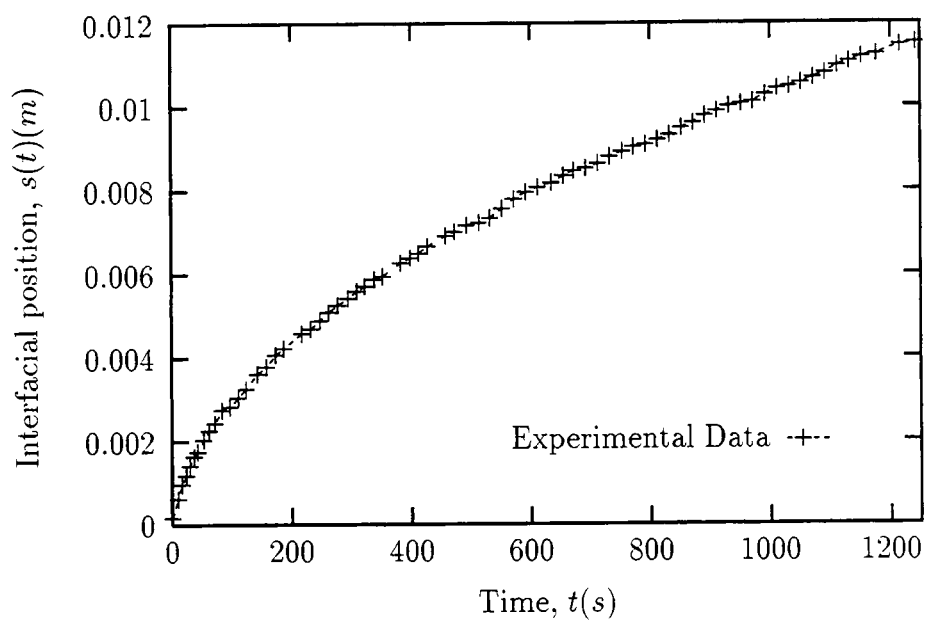


Figure 5.2.1: Position data taken from Wesley [25] for the solid-liquid interface for a one-phase experiment using n-octadecane.

should contain such a term. This choice reduces oscillations in the curve-fit when compared to a purely polynomial representation for $s(t)$. The dimensional form chosen is

$$s(t) = A(\sqrt{t + \epsilon} - \sqrt{\epsilon}) + \sum_{j=1}^{\sigma} \zeta_j t^j, \quad (5.2.1)$$

where the coefficients A and ζ_j are determined from a least-squares, curve-fit algorithm. This perturbed form containing ϵ is used since a true $\sqrt{t}$ profile has an infinite velocity at $t = 0$. Recall from Chapter 4 that the differential operator for the solid region shown in Eq.(4.2.1) contains the product of the velocity and the position evaluated at $\bar{\Delta} = -1$. This corresponds to the position and velocity of the front at time $t = 0$. If a true square root function were used, then this product would be indeterminate at $\bar{\Delta} = -1(t=0)$ due to $h(-1)$ being zero and $\dot{h}(-1)$ being infinite. This dilemma can be mathematically resolved with the aid of L'Hopital's rule. However, since the true physical problem does not have a true jump condition, this approximation appears justifiable. Including this constant ϵ allows the $\sqrt{t}$ form to be used, but the velocity is no longer infinite at $t = 0$. This also serves to simplify the problem while retaining it for illustrative purposes.

Figure 5.2.2 is a plot of the curve-fit along with the experimental data using a value of $\epsilon = 2$. This value is chosen since it yields the minimum value in the variance. This plot shows that for $\sigma = 3$, the curve-fit appears to be representative of the experimental data. Figure 5.2.3 shows the velocity of the interface using the curve

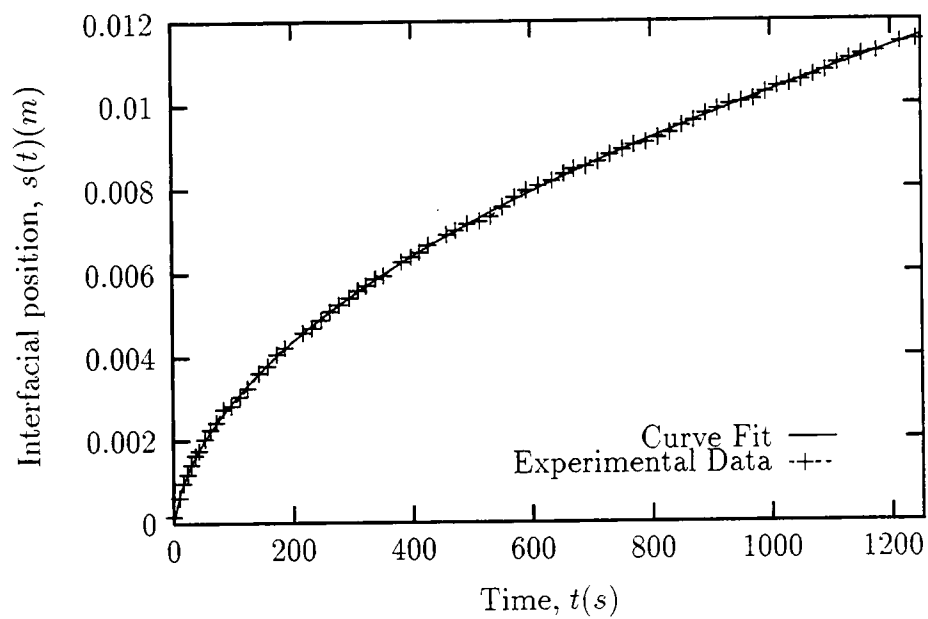


Figure 5.2.2: Experimental data with the curve fit given by Eq.(5.2.1).

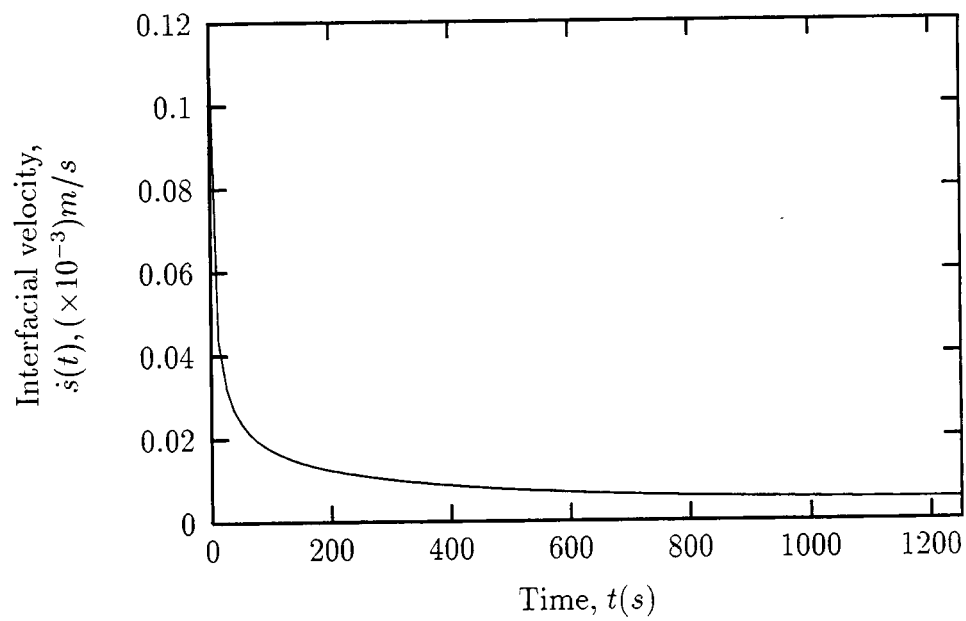


Figure 5.2.3: Velocity profile for the curve-fit given by Eq.(5.2.1).

fit. This form of the curve-fitting function eliminates the infinite velocity at $t = 0$. Using the interfacial profile shown in Figure 5.2.2 and a solidification time of 900 seconds, the numerical prediction for the surface temperature history is shown in Figure 5.2.4. An average value for C_{ps} ; namely $C_{ps} = 1805 \text{ J/kg} \cdot \text{K}$ is used when considering the temperature range to be confined between 3°C and 28.15°C . This plot shows that the numerical solution achieves graphical convergence for $N=R=18$. This plot also indicates that there are some small fluctuations present in the converged numerical solution. This is due to using polynomials to approximate a solution which undergoes such a sharp change in shape and due to the ill-posed nature of the problem.

A plot of the converged numerical solution and the experimentally measured surface temperature is shown in Figure 5.2.5. Again, details for how this data is acquired can be found in Wesley [25]. This plot indicates that the measured surface temperature levels off at a value of 3°C while the numerical solution predicts a value of approximately 2°C . This plot reveals that the numerical solution predicts a step-like change although the cold plate temperature is predicted to be 1°C lower than the measured value. Recall that the numerical results are based on a constant property model. This may be the source of the discrepancy between the numerical results and the thermocouple data. Taking into account the variable properties of n-octadecane leads to a more accurate numerical prediction [37] when compared to the experimental results for this test case. Another source of potential discrepancy arises in the

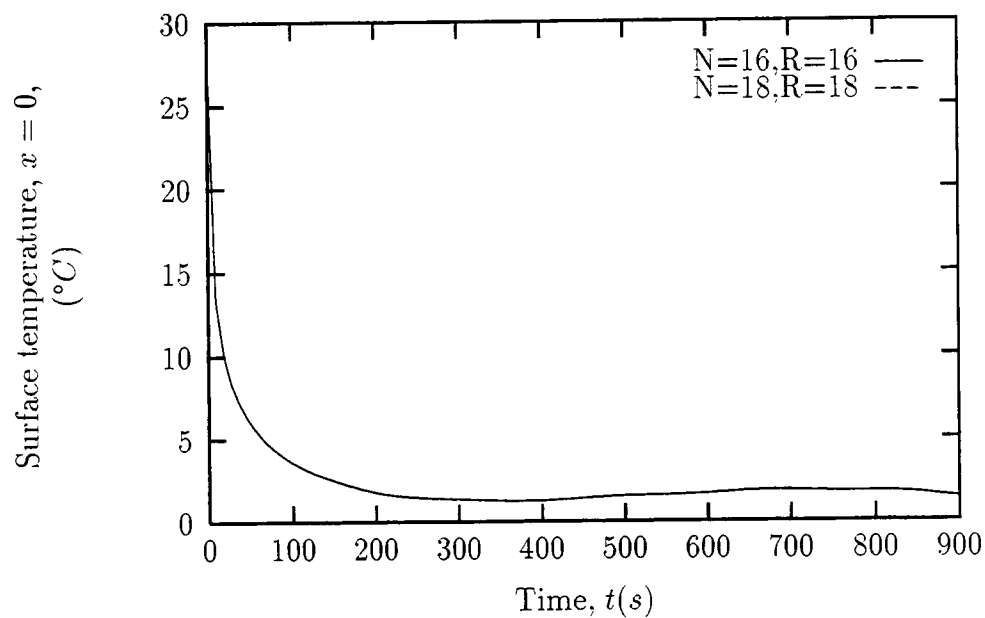


Figure 5.2.4: Converged numerical results for the surface temperature history using the curve-fit given by Eq.(5.2.1) when $C_{ps} = 1805 \text{ J/kg} \cdot \text{K}$, $\rho_s = 814 \text{ kg/m}^3$, $h_{sl} = 241,730 \text{ J/kg}$, and $k_s = 0.43 \text{ W/(m} \cdot \text{K)}$ [34,35].

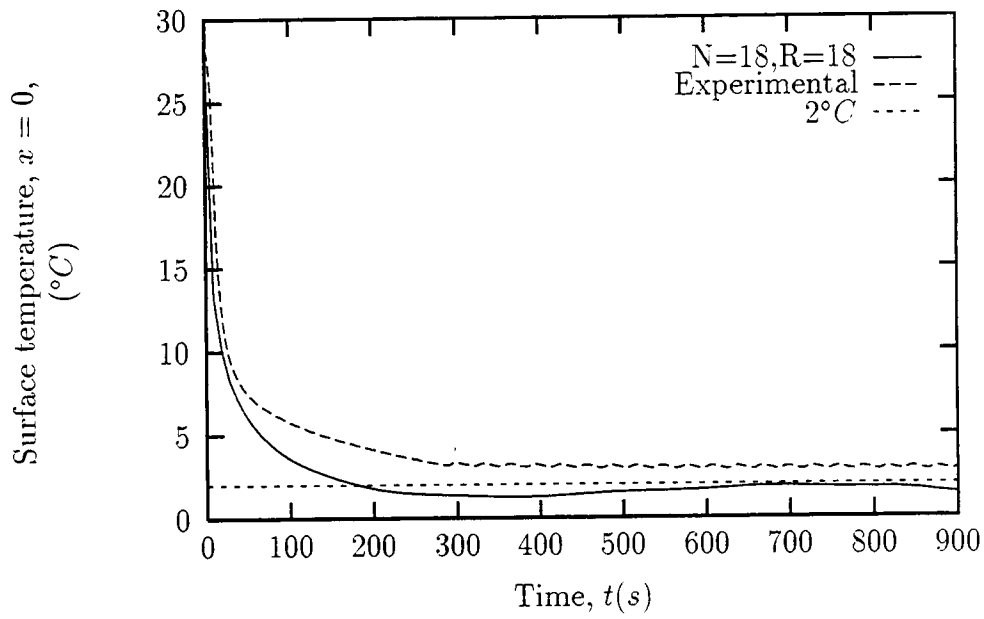


Figure 5.2.5: Comparison of the experimental temperature history and the numerical solution when $C_{ps} = 1805 \text{ J/kg} \cdot \text{K}$, $\rho_s = 814 \text{ kg/m}^3$, $h_{se} = 241,730 \text{ J/kg}$, and $k_s = 0.43 \text{ W/(m} \cdot \text{K)}$ [34,35].

curve fitted interfacial data. The uncertainty in the measurement of $s(t)$ is large at the beginning of the experiment, which will affect the solution through the curve fit. The “tailing down” effect observed in the approximate solution for $t > 800s$ may be attributed to the least-squares curve fit of the data. The key point about the presented results using experimental data is that numerical convergence is obtained, no time-step instabilities are present, and of course, validation of the theory.

5.3 Two-Phase, Constant-Velocity Motion

The final case to be considered involves the constant property two-phase problem that has a solid-liquid interface moving at a constant velocity. This case shows that treating time in an elliptic fashion is successful when applied to a direct problem as well as an inverse problem. Recall that the solution for the temperature in the solid region shown in Eq.(3.3.51) includes a derivative of the temperature in the liquid region evaluated at the interface($\tau_\ell = -1$). Also recall that the liquid region is a direct two-point boundary value problem that can be solved for using many conventional methods. This test case will solve for the liquid solution using the same time collocation method that is used for the inverse solution in the solid region. In order to determine if solving the direct problem with this method is successful, n-octadecane will be used with one level of superheat. The velocities and solidification times will be the same as those used in the one-phase test cases.

Before continuing with the results for the two-phase problem, the initial condition used for these results must be addressed. In the previous two cases, the initial condition for the liquid regions was zero since the liquid region was initially at the melt temperature. In the present case, there is some degree of superheat present and therefore a temperature gradient exists in the liquid region. The profile used for each test case is given by

$$f(\tau_\ell) = \theta_\ell(\tau_\ell) = -\frac{\theta_i}{e^{\nu L} - 1 - \nu L e^{\nu L}} - \frac{\theta_i \nu L e^{\nu L} \tau_\ell}{e^{\nu L} - 1 - \nu L e^{\nu L}} + \frac{\theta_i e^{\nu L} \tau_\ell}{e^{\nu L} - 1 - \nu L e^{\nu L}} \quad \tau_\ell \in [-1, 1], (5.3.1)$$

where $\theta_i = (T_i - T_{melt})/T_{ref,\ell}$, T_i is the initial temperature of the liquid, and ν is a constant. This profile is shown in Figures 5.3.1 for n-octadecane, using various values of ν when given a fixed length L as dictated by the provided geometry. This profile serves to preserve the physics of the premelt period without undue complication, i.e., removes the need to use slowly converging infinite series [2]. This profile is one that could exist if the cooling face was dropped from the initial temperature T_i to the melt temperature T_{melt} which is a realistic profile to have in the liquid region. The constant ν that appears in Eq.(5.3.1) governs how far into the liquid the changes in the boundary temperature are felt. This constant depends on the properties of the material and how the boundary temperature is dropped from the initial temperature T_i to the melt temperature T_{melt} . A large negative value for this constant causes the profile to approach that of a jump boundary condition while a small negative value

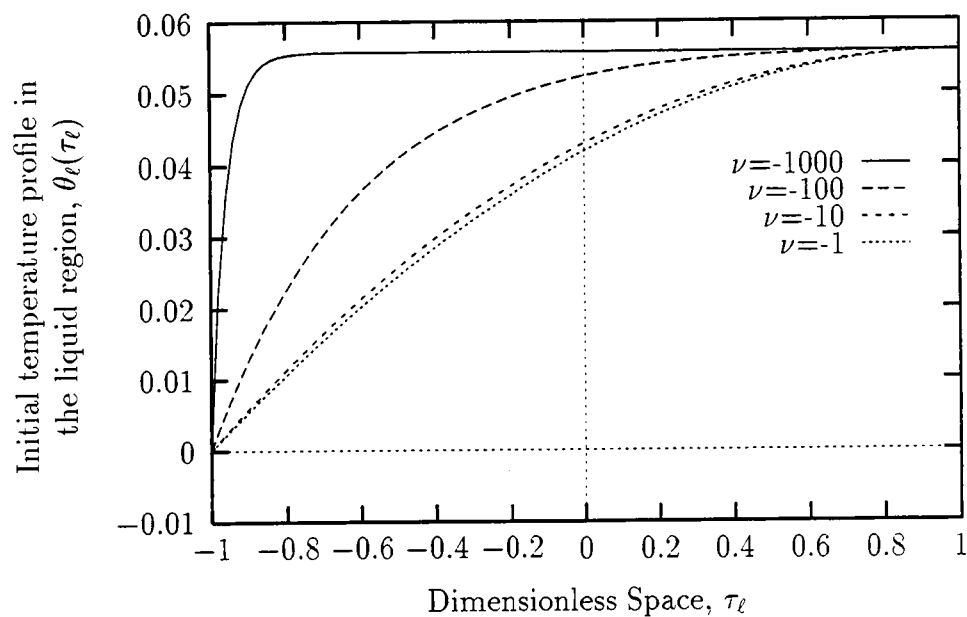


Figure 5.3.1: Initial temperature profile, Eq.(5.3.1), in liquid n-octadecane with 6°C of superheat for various values of ν .

results in a near linear profile as shown in Figure 5.3.1.

5.3.1 N-Octadecane

This material is considered in the presence of superheat in order to determine the effect on the temperature history at the cooling face and to demonstrate the use of the numerical scheme of Chapter 4 as applied to a direct problem, which is the liquid region. The level of superheat to be used is 6°C . This represents a superheat level that is 21% of the melt temperature, T_{melt} . The length L , used for these results is chosen to be sufficiently larger than the amount of material that will solidify. The initial condition is given by Eq.(5.3.1) where $\nu = -100$.

Figure 5.3.2 shows the converged results for the surface temperature history of the solid using 6°C of superheat and a velocity of 0.002 mm/s and $t_{max}=3000\text{ s}$. These results are generated using $N=R=12$ in the solid region. The solution appears linear during the solidification time and corresponds to a temperature drop from 28.15°C to 22.3°C . The temperature gradients in the liquid that are used to produce the temperature histories in Figure 5.3.2 are shown in Figure 5.3.3. It is seen that the results for the temperature gradient have not yet fully converged owing to the visibly small oscillations, but it is still possible to obtain graphically converged results in the desired surface temperature history for the solid. The results for the surface temperature history in the solid and the liquid temperature gradient for a velocity of

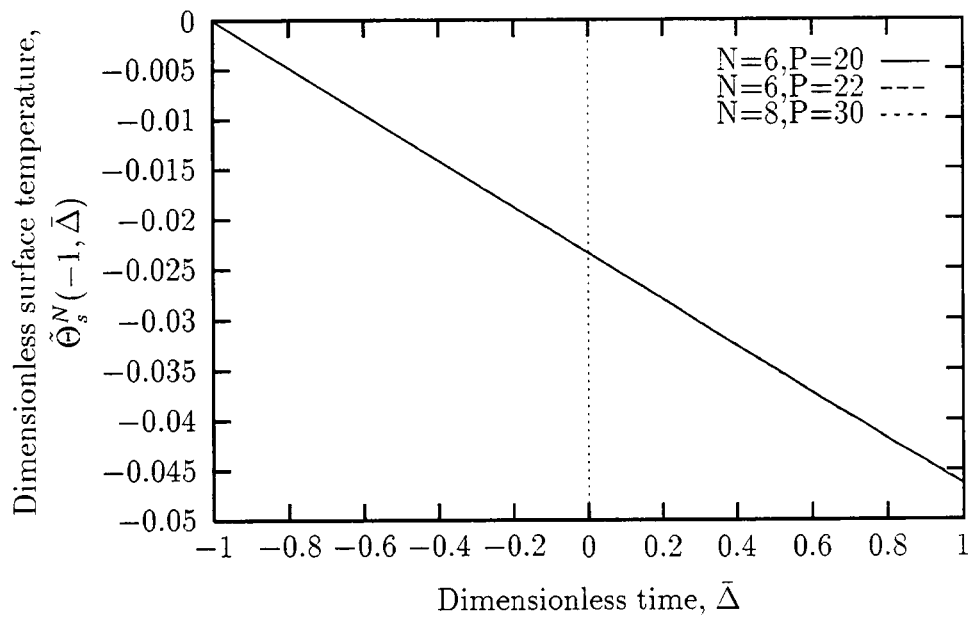


Figure 5.3.2: Dimensionless surface temperature history for n-octadecane with 6°C superheat showing convergence for $N=R=12$ in the solid region and using a constant velocity of 0.002 mm/s and $t_{max} = 3000\text{ s}$.

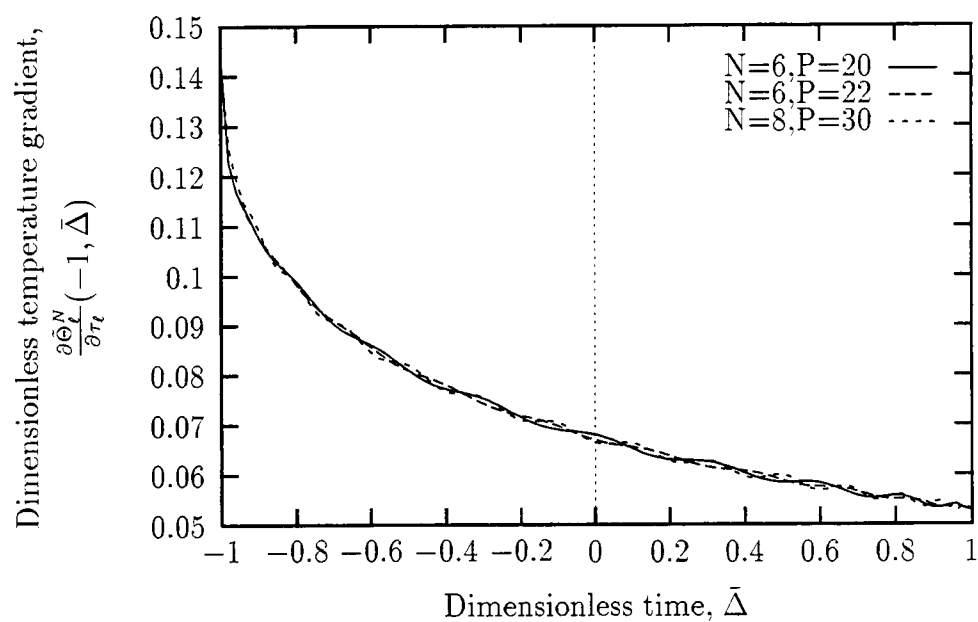


Figure 5.3.3: Temperature gradients at the liquid side of the interface for varying values of N and P in the liquid region and using a constant velocity of 0.002 mm/s with 6°C superheat and $t_{max} = 3000\text{s}$.

0.004 mm/s and 6°C of superheat are shown in Figures 5.3.4 and 5.3.5, respectively. These results exhibit similar trends as those for the previously discussed case. Figure 5.3.4 indicates, in dimensional values, a temperature drop from 28.15°C to approximately 3°C . Again the temperature gradient in the liquid region shows some oscillations for different values of N and P yet the solid solution has graphically converged. This is explained by examining the interfacial boundary condition given by Eq.(2.1.17). This boundary condition can be rewritten to relate the heat flux in the solid region evaluated at the interface to the heat flux at the interface for the liquid region plus a constant multiplied by the velocity of the front. In relative terms, the magnitude of the flux in the liquid will be much smaller than the term containing the velocity. This dominance of the term containing the velocity allows for the presence of the small oscillations shown in Figures 5.3.3 and 5.3.5 and still obtaining converged results in the solid region. However, this may not always be the case. There may arise certain cases where the magnitude of the flux in the liquid may be of equal magnitude as the term containing the velocity. In this case, converged results for the temperature gradient in the liquid may be necessary for converged results in the solid region.

The results presented in this chapter provide some interesting information about the convergence and stability qualities of the proposed numerical method as well as the accuracy of the Weighted Residual approach. Additionally, some insight into the

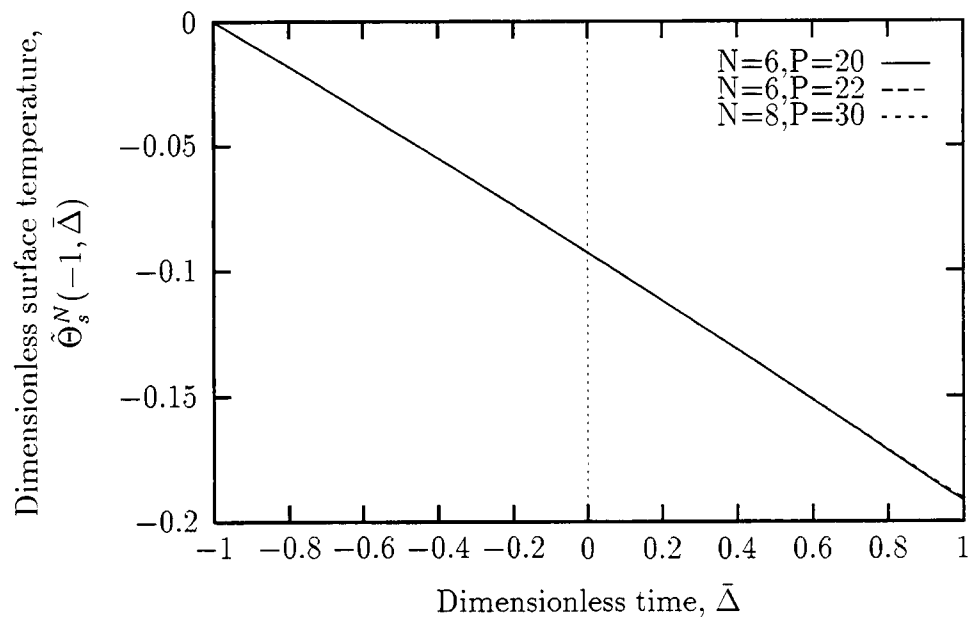


Figure 5.3.4: Dimensionless surface temperature history for n-octadecane with 6°C superheat showing convergence for $N=R=12$ in the solid region and using a constant velocity of 0.004 mm/s and $t_{max} = 3000\text{ s}$.

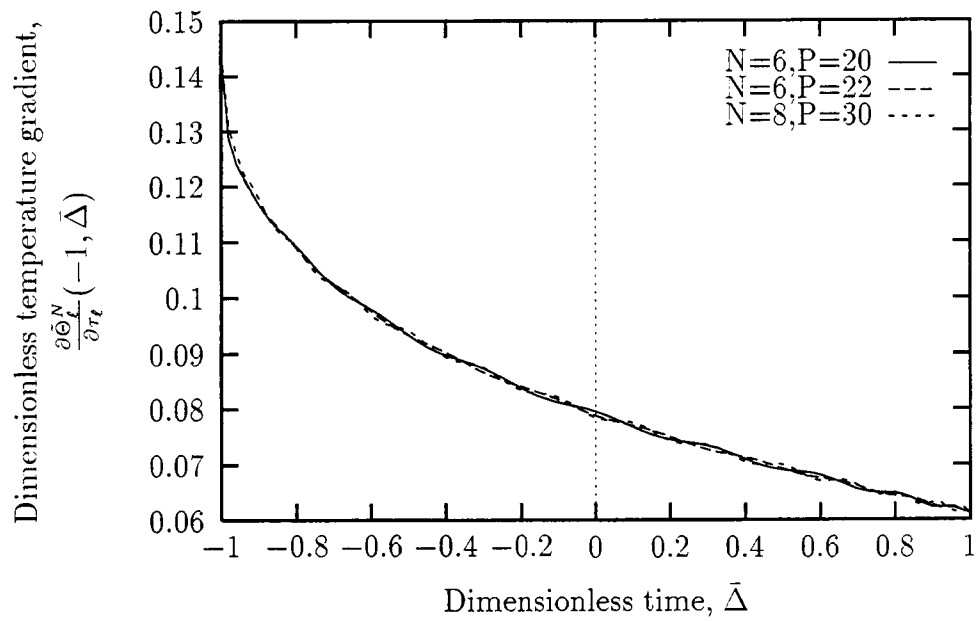


Figure 5.3.5: Temperature gradients at the liquid side of the interface for varying values of N and P in the liquid region and using a constant velocity of 0.004 mm/s with 6°C superheat and $t_{max} = 3000\text{s}$.

effects of varying the degree of superheat and velocity of the interface are related at a physical level.

Chapter 6

Conclusions

In this chapter, some concluding remarks integrating the results of the previous chapters are related.

6.1 Concluding Remarks

The successful implementation of a novel Weighted Residual method for resolving one-dimensional, pure melt inverse solidification design problems demonstrates that an accurate and stable solution methodology is available for such mildly ill-posed inverse problems. Highly favorable numerical results are yielded when compared to an existing exact solution involving a one-phase, half-space problem with a prescribed constant interfacial velocity [23]. Two pure materials, n-octadecane and aluminum, are numerically investigated to indicate the effect of the interfacial velocity on the

required surface temperature history at the cooling face in order to provide such a motion. Convergence in the numerical solutions for the surface temperature is obtained for both materials in which vastly different thermal properties exist.

Using experimental data for the interfacial motion required a least-square procedure to be developed in order to manipulate the discrete data into a usable analytic form as required for the present approach. The predicted surface temperature is similar to the measured surface temperature. The numerical solution predicts a cold temperature that is approximately 1°C lower than the experimental data. This discrepancy between the two results can most likely be attributed to the assumption of constant properties and the curve fit used to describe the interfacial motion. It is well known [24] that the solutions of ill-posed problems are sensitive to the input set. Thus, the implemented curve fit can potentially have a profound effect on the outcome. It should be noted that for the indicated curve fit, numerically converged results are obtained. In other words, the numerical solution for the surface temperature history using a curve fitted interfacial position function generated from experimental data converged using $N=R=18$ terms in the solid region and shows no signs of numerical instability.

The two-phase results revealed some physical information about the nature of the solution when superheat is present in the liquid. The most significant aspect is that the time collocation method worked for the direct problem allowing for all time and

space to be accounted for in one matrix inversion, thus eliminating conventional time-step methods. Another important finding is that the presence of small oscillations in the liquid region produces graphically converged results in the solid region. This type of behavior is not typically expected since the problem is mildly ill-posed. Also, the initial condition in the liquid region has the potential to effect the convergence of the solution in the solid region. In the presence of a steep temperature gradient in the liquid region near the interface, large oscillations in the solution for the temperature gradient at the solid-liquid interface can result if the approximation is terminated too early. Thus, when such situations occur, additional terms in the series expansion for the liquid region are required in order to resolve the solution for the liquid temperature gradient at the interface.

Overall, the proposed method of Weighted Residuals produces stable and accurate results for the chosen test cases. The method did not possess any inherent instabilities like those present in conventional methods [16].

Chapter 7

Recommendations and Future Research

In this chapter, recommendations for the proposed method are discussed as well as avenues of future research.

7.1 Recommendations

There are several recommendations that can be made concerning the current method for solving inverse solidification design problems. The first concerns the computer(platform) and software(language) that is used for the numerical calculations. The results presented in this work are generated using a Silicon Graphics workstation with 48MB of RAM and using the symbolic software language *Mathematica*TM.

Memory requirements, using *Mathematica*, grow as the order of the approximation is increased. At some point, this dilemma overtakes the available memory on the platform. This problem is removed if a high-level programming language is used. This software is relatively slow and cannot handle large arrays that may be required to handle solidification problems having high velocities, large degrees of superheat, and initial conditions that have steep temperature gradients. The majority of the CPU effort comes from the construction of the coefficient matrices shown in Eq.(4.1.16) and Eq.(4.2.16), where numerous symbolic manipulations are performed. The actual solution of the system of equations for the expansion coefficients is relatively fast compared to the “building” of the actual coefficient matrices. A higher level language, such as C or FORTRAN, is better suited for these types of calculations. Recent discussions with Osborne [38] reveal that it is possible to use 32 collocation points in time and space, and obtain the expansion coefficients in approximately 10 seconds using FORTRAN on a 120MHz Pentium PC with 40MB of RAM. This includes setting up a 1024 by 1024 coefficient array and inverting it to arrive at the expansion coefficients. Such a calculation is impossible using *Mathematica*TM, v2.2 on the present platform.

Another recommendation involves the choice of the basis functions. If some prior knowledge is known about the physics of the problem and its solution, then the basis functions may include this information in the form of special functions which have

similar characteristics. An example of this would be the addition of an exponential term in the expansion solution where the solution is expected to have rapid changes in shape as was shown in the case of the experimental data. This could accelerate the convergence rate of the solution. This is just an example and other forms could easily be incorporated into the expansion solution.

7.2 Future Research

Future work in the area of the Inverse Solidification Design Problem has many possible directions. The results presented here show that the method is successful in solving the one-dimensional, constant property case. The next step is to incorporate variable temperature-dependent properties into the one-dimensional model. Then, it is suggested to investigate two-dimensional cases with constant and variable properties. Other variations that can be incorporated into the mathematical model include a variable cross-sectional area as well as the inclusion of convective effects.

Once the method has been proven for multi-dimensional cases having variable properties, the next major step is to incorporate it into a solidification problem involving binary melts or alloys. This type of problem presents a new challenge since solidification now takes place over a range of temperatures, creating a "mushy" zone [39]. This problem is important since most high-strength, high-temperature applications use alloys. In the present problem, only the interfacial motion is prescribed

which is used to determine the unknown temperature history at the cooling face. In the binary melt problem, the motion is specified as well as the temperature gradient in the mush zone. Certain combinations of the temperature gradient G and velocity V are known to produce certain morphologies in binary materials [39]. These two variables are used in the determination of the unknown boundary conditions for the binary melt inverse problem.

These examples show that there are many different aspects of the Inverse Solidification Design Problem that can be investigated using the numerical method proposed here. The incorporation of this method, along with the recommendations mentioned earlier, represent the next challenge.

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VITA

Ryan Christopher McMahon was born in Columbia, South Carolina on July 27, 1971. He was raised in the small rural community of Leesville, SC and graduated from Batesburg-Leesville High school in May of 1989. While in high school he spent the summers driving tractors in the local peach fields. This experience and having to work 12 hour days in the hot sun quickly made him realize that continuing his education was a decision he could not go wrong with. He chose to enter Clemson University in the fall of 1989 to pursue a Bachelors degree in Mechanical Engineering. While attending Clemson, his summers were spent working at AlliedSignal in Columbia, SC. This experience was very valuable to him as he gained some insight into what a lot of engineers do in industry and it did not appeal to him. Upon graduation from Clemson in 1993, he had no desire to have a job which did not utilize his skills like the ones he saw while at AlliedSignal and he felt that he was no different from any of his fellow graduates. He made a decision to continue on to graduate school, but not without a well-deserved break. He spent the next seven months in Charleston, SC playing on the beaches and working as a bartender in order to save money for graduate school. Working the late hours of a bartender and always smelling of smoke **really** made him see the appeal of an advanced degree and he entered the Masters degree program at the University of Tennessee in August of 1994. While at the University of Tennessee, he chose to concentrate his studies in the Thermal Science area and after

two years, recieved his Master's degree in Mechanical Engineering in August of 1996. Upon receiving his Master's degree, he again headed to the beaches of Charleston for some much needed rest and relaxation. After several weeks in Charleston he moved to West Palm Beach, Florida to join the Externals group at Pratt & Whitney as an Associate Engineer.