A THEORETICAL ANALYSIS OF COMBINED MELTING AND VAPORIZATION USING THE BOUNDARY ELEMENT METHOD

by

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(ABSTRACT)

Melting and vaporization of solids occur very often in nature and in man-made processes. Many analytical and numerical solutions exist for solving the temperature field in the liquid and solid regions, but inaccuracies persist in tracking the phase change interfaces and the numerical solution of the temperature field is usually cumbersome. The Boundary Element Method is proposed as an accurate, efficient way to solve for the temperature field and the interface positions in a phase change problem involving combined melting and vaporization. When comparing to specific one-dimensional test cases, accurate results are obtained when using a sufficiently small time step. A comparison is made to existing data from a laser drilling experiment. The anticipated physical effects which occur on semi-infinite and finite domains are confirmed. Consequently, this method can be used to model natural and industrial phenomena involving phase change.
Acknowledgements

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NOMENCLATURE

PHYSICAL PARAMETERS

\( \alpha_s, \alpha_l \)  
Thermal diffusivity of solid, liquid

\( k_s, k_l \)  
Thermal conductivity of solid, liquid

\( \rho_s, \rho_l \)  
Density of solid, liquid

\( L_m, L_v \)  
Latent heat of melting, vaporization

\( T_{IN} \)  
Initial temperature

\( T_m, T_v \)  
Melt temperature, Vaporization temperature

\( x_o \)  
Origin of the total domain
\( x_L \) Location of the back wall

\( q_0(t) \) Applied heat flux at the origin

**DIMENSIONLESS PHYSICAL PARAMETERS**

\( A \) Thermal diffusivity

\( K \) Thermal conductivity

\( \beta_m, \beta_v \) Stefan \# of melting, vaporization

\( \theta_m \) Melt temperature

\( X_o \) Origin of the total domain

\( X_L \) Location of the back wall

\( Q_0(\tau) \) Applied heat flux at the origin
**PHYSICAL VARIABLES**

\[ x \quad \text{Position} \]

\[ t \quad \text{Time} \]

\[ T_s(x,t) \quad \text{Solid temperature at a given position and time} \]

\[ T_l(x,t) \quad \text{Liquid temperature at a given position and time} \]

\[ t_m \quad \text{Time at the onset of melting} \]

\[ t_v \quad \text{Time at the onset of vaporization} \]

\[ t_{melt} \quad \text{Time required to melt the entire domain} \]

\[ t_{abl} \quad \text{Time required to ablate the entire domain} \]

\[ s_m(t) \quad \text{Position of the melt front} \]

\[ s_v(t) \quad \text{Position of the vapor front} \]

\[ v_m(t), \quad \frac{ds_m}{dt} \quad \text{Velocity of the melt front} \]

\[ v_v(t), \quad \frac{ds_v}{dt} \quad \text{Velocity of the vapor front} \]
\( q_{im}(t) \) \hspace{1cm} \text{Heat flux entering the solid region at the melt front}

\( q_{in}(t) \) \hspace{1cm} \text{Heat flux leaving the liquid region at the melt front}

\( q_{lo}(t) \) \hspace{1cm} \text{Heat flux entering the liquid region at the vapor front}

\( x_0 \) \hspace{1cm} \text{Causal space variable}

\( t_0 \) \hspace{1cm} \text{Causal time variable}

\( G(x,t|x_0,t_0) \) \hspace{1cm} \text{Green's function}

\( \delta \) \hspace{1cm} \text{Dirac delta function}

\( \lambda \) \hspace{1cm} \text{Integration factor}

**DIMENSIONLESS PHYSICAL VARIABLES**

\( X \) \hspace{1cm} \text{Position}

\( \tau \) \hspace{1cm} \text{Time}

\( \theta_s(X, \tau) \) \hspace{1cm} \text{Solid temperature at a given position and time}

\( \theta_l(X, \tau) \) \hspace{1cm} \text{Liquid temperature at a given position and time}
\( \tau_m \)  
Time at the onset of melting

\( \tau_v \)  
Time at the onset of vaporization

\( \tau_{melt} \)  
Time required to melt the entire domain

\( \tau_{abl} \)  
Time required to ablate the entire domain

\( S_m(\tau) \)  
Position of the melt front

\( S_v(\tau) \)  
Position of the vapor front

\( V_m(\tau), \frac{dS_m}{d\tau} \)  
Velocity of the melt front

\( V_v(\tau), \frac{dS_v}{d\tau} \)  
Velocity of the vapor front

\( Q_{sm}(\tau) \)  
Heat flux entering the solid region at the melt front

\( Q_{lm}(\tau) \)  
Heat flux leaving the liquid region at the melt front

\( Q_{sl}(\tau) \)  
Heat flux entering the liquid region at the vapor front

\( X_0 \)  
Causal space variable

\( \tau_0 \)  
Causal time variable

\( G(X, \tau/X_0, \tau_0) \)  
Green’s function

NOMENCLATURE
**NUMERICAL INDICATORS**

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<td>General time step</td>
</tr>
<tr>
<td>( pp )</td>
<td>Current time step</td>
</tr>
<tr>
<td>( pp_m )</td>
<td>Time step at the onset of melting</td>
</tr>
<tr>
<td>( i )</td>
<td>Region indicator</td>
</tr>
<tr>
<td>( L^p )</td>
<td>Spatial integral of Green's function</td>
</tr>
<tr>
<td>( G^p )</td>
<td>Time integral of Green's function</td>
</tr>
<tr>
<td>( H^p )</td>
<td>Time integral of the gradient of the Green's function</td>
</tr>
<tr>
<td>([ A ]_i )</td>
<td>Coefficient matrix</td>
</tr>
<tr>
<td>([ X ]_i )</td>
<td>Matrix of unknown boundary values</td>
</tr>
<tr>
<td>([ B ]_i )</td>
<td>Matrix of known boundary values</td>
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1.0 INTRODUCTION

This chapter includes a description of the problem under investigation, the rationale for solving such a problem, the objectives of this thesis and a literature review.

1.1 PROBLEM DESCRIPTION

The type of problem under consideration is of a finite, one-dimensional medium, initially in the solid phase, exposed to a specified, time varying heat flux at one end and insulated at the other end (Fig. 1). As time passes, the end exposed to the heat flux experiences a temperature rise until its temperature meets the melt temperature, $T_m$, of the material, signaling the beginning of melting. The domain now includes liquid and solid regions, which are assumed to have constant, but not necessarily equal thermal and physical properties. While melting occurs, the
Figure 1. Phase change problem under consideration
end exposed to the heat flux continues to experience a temperature rise until its
temperature now meets the vaporization temperature, \( T_v \), of the material, signaling
the beginning of vaporization. The vapor is removed or ablated away. As
time passes, the problem may go through three distinct periods.

During Period 1 (Fig. 2), the temperature of the medium at the heated surface
gradually rises, from the initial body temperature \( T_b \), while still remaining less
than the melt temperature of the solid under consideration. Thus the entire me-
dium remains in the solid phase and pure conduction takes place. The unknowns
at the left and right boundaries are \( T_{sm} \) and \( T_{sr} \), respectively. Such a problem
may be classified as a Period 1 type problem until the onset of melting occurs
at the heated surface. At that time, \( t_m \), Period 2 begins.

During Period 2 (Fig. 2), two distinct regions now exist: 1) a solid region
bounded by the melt phase front, \( s_m \) and the insulated back wall, and 2) a liquid
region bounded by the heated surface and the melt phase front. The solid has
unknowns \( q_{sm} \) at its left boundary and \( T_{sl} \) at its right boundary. The liquid has
unknowns \( T_{lv} \) at its left boundary and \( q_{lm} \) at its right boundary. The temperature
of the evolving melt phase front is always the same as the melt temperature. The
melt front may possibly reach the back wall during Period 2, at a time defined
as \( t_{melt} \). At this time the solid region is melted away and only the liquid region
remains with unknowns \( T_{lv} \) at its left boundary and \( T_{ll} \) at its right boundary, the
insulated back wall. Such a problem may be classified as a Period 2 type problem.
Figure 2. The three distinct periods which the phase change problem undergoes.
until the onset of vaporization occurs at the heated surface. At that time, $t_v$, Period 3 begins.

During Period 3 (Fig. 2), two distinct regions now exist: 1) a solid region bounded by the melt phase front and the insulated back wall and 2) a liquid region bounded by the vapor phase front, $s_v$, and the melt phase front. The solid has unknowns $q_{lm}$ at its left boundary and $T_{dl}$ at its right boundary. The liquid has unknowns $q_{lv}$ at its left boundary and $q_{lm}$ at its right boundary. The temperature of the evolving vapor phase front remains constant at $T_v$. If total melting of the domain hasn’t already occurred in Period 2, it could occur some time during Period 3, leaving an all liquid domain. Under these conditions, at its left boundary, the liquid has $q_{lv}$ as the unknown, while $T_{dl}$ is the unknown on the right boundary. An interesting situation arises if $T_m = T_v$. If this condition is met, then vaporization occurs on an all solid domain with unknowns $q_{lv}$ at the left boundary and $T_{dl}$ at the right boundary. Regardless of any conditions, during Period 3 the vapor phase front continues to move to the right until it eventually reaches the insulated back wall. At this time, $t_{abl}$, the domain has been totally ablated away, and the problem under investigation has reached its conclusion. Periods 1, 2 and 3 are summarized in Fig. 2.
1.2 RATIONALE

Melting and vaporization of solids, especially metals, occur very often in both industrial processes and in nature. Undoubtedly the most common natural application involving phase change is the melting of ice. Specific industrial applications include laser cutting, laser drilling, laser welding, electroslag melting, scrap melting, zone melting, growth of pure crystals from melted materials, purification of metals, meltout in furnace valves, batch melting of glass, and thermal switching of glass. Many solution techniques, analytical and numerical, exist for solving such problems. Unfortunately, difficulties usually arise in predicting the movement of the melt and vapor phase fronts.

Of the existing numerical solutions, finite element and finite difference solutions accurately find the temperature distributions in two phase regions, with a moving boundary. However, these solutions are cumbersome because of the necessity to regenerate the domain’s mesh after each time step. Another drawback is the huge amount of computer memory needed to store the information for each mesh point. Using a numerical solution based on the Boundary Element Method (BEM) requires less memory because the mesh is only on the boundary of each region. For a one-dimensional material, the mesh becomes simply one element at each boundary.

Since the 1970’s, BEM has been used to numerically solve the temperature distribution for melting and solidification problems. Computer models based on
BEM are presently used to predict the behavior of prominent industrial processes listed above. However, these models either assume melting with immediate removal of the liquid material, melting without vaporization, or pure vaporization. Therefore a single phase region with one moving boundary is addressed. The BEM solution undertaken in this thesis finds the temperature distribution in a one-dimensional liquid-solid region with combined melting and vaporization.

1.3 THESIS OBJECTIVES

The lack of an existing BEM scheme which incorporates combined melting and vaporization, and the inefficient treatment of such a phase change problem by other numerical methods have been the primary motivations for undertaking this thesis. The main objectives of this thesis are: 1) to formulate an efficient numerical method (BEM) which can be implemented to solve one-dimensional heat transfer problems involving combined melting and vaporization, and 2) investigate the numerical and physical behavior of the combined melting and vaporization process.
1.4 LITERATURE REVIEW

This section consists of a review of literature pertaining to phase change problems. It includes a summary of existing analytical solutions, as well as numerical solutions using the finite difference, finite element and boundary element schemes.

1.4.1 Analytical solutions

A few exact analytical solutions exist for the melting of semi-infinite solids in one dimension under idealized conditions. Considering the case of melting with the immediate removal of the melt (ablation of the liquid), Landau [1] offered an analytical expression for the time required to initiate melting as well as steady state expressions for the temperature distribution and the melt front velocity. In the case of transient heat conduction involving two phases, others have assumed temperature distributions which satisfy the specified boundary and initial conditions, yielding solutions in the form of erf(x,t). Crank [2] considered a constant wall temperature boundary condition and provided the so called Neumann’s solution. Ozisik [3] assumed the solid remains at the initial temperature $T_{in} = T_{m}$. Carslaw and Jaeger [4] allowed for a constant or pulsed surface heat flux. Recently, Ku and Chan [5] used the Laplace transform method to arrive at expressions for the temperature distribution and liquid-solid interface position which agree exactly with those given in Ozisik [3] and Carslaw and Jaeger [4].

The embedding approach was used by Boley [10]. The liquid-solid domain is treated as a body of constant geometry, resulting in a coupled integro-differential problem in terms of the phase front location and an unknown fictitious heat flux.

1.4.2 Finite Difference

In the past, the most popular numerical method for solving phase change problems was undoubtedly the finite difference technique. A variety of approximation methods exist for modelling the interface motion, many of which are for multidimensional problems. The enthalpy method doesn't explicitly track the interface, which eliminates the need to solve two moving boundary problems for a melting
problem. The energy equation is discretized in terms of the two dependent variables, temperature $T$ and enthalpy $h$. This approach was used in implicit and explicit FD schemes by Crowley [11], and Furzeland [12] and implicitly by Longworth [13], Shamsundar and Sparrow [14] and Voller and Prakash [15]. Cao et al. [16] transformed the enthalpy method, making the enthalpy the only dependent variable. Unfortunately, FD schemes using the enthalpy model give oscillating values for temperatures near the phase front as well as for the phase front position. They also require much CPU time because of slow convergence and the use of fine spatial grids. Reductions in CPU time were made by Voller [17], whose rapid implicit FD scheme needed no under or over relaxation, by Raw and Schneider [18], who introduced a nonlinear iteration algorithm, and by Pham [19], who combined an implicit temperature method with the enthalpy method in a three-time-level FD scheme which did not require iterations. Other authors have made adjustments to the enthalpy method for more accurate tracking of the phase front position and less "waviness" in the temperature and heat flux histories. Consequently, accurate results are possible for spatial grids which are coarser than those used in the "weak" enthalpy formulations described above. The "strong" enthalpy formulation employed by Date [20], in particular, achieved these improvements by generalizing the relationship between enthalpy and temperature.

In another method used in FD schemes, several authors effectively immobilized the moving interface by a clever coordinate transformation. This method has been implemented by Hsu et al. [21] and Cohen [22], who applied it to time
varying applied heat fluxes for melting and vaporization problems. Kim and Kaviany [23] added an algorithm which removes the necessity to iterate.

The approximate analytical technique of embedding has been applied to FD schemes by Boley [24] for an ablation problem. Meyer [25] added the method of lines to the embedding method and was thus able to explicitly track the position of the melt front.

Other authors, such as Ehlrich [26] and Koh et al. [27], have used Taylor’s expansions in time and space near the moving interface. Mastanaiah [28] used a Taylor’s forward projection technique to account for nonlinearities. Gupta [29] incorporated a moving grid in his noniterative FD scheme.

The variable time step method chooses a time step such that the liquid-solid interface moves exactly one space mesh. Gupta and Kumar [30] and Douglas and Gallie [31] applied this method to FD schemes. Andrews and Attrey [32] used an iterative FD scheme to solve a phase change problem for a 1D semi-infinite domain exposed to a pulsed heat flux in which vaporization occurs without melting.

A variety of miscellaneous FD schemes also exist in the literature. An explicit temperature based method was used by Hsiao [33]. Bonacina et al. [34] approximated the latent heat effect by a large heat capacity over a small temperature range in their three time level implicit FD scheme. Goodrich [35] tracked the moving interface using a centered difference FD scheme using simple Gaussian
elimination at ordinary nodes. Finally, Griffith and Nassersharif [36] used the interface method to explicitly track the phase change boundary. Their method used a much coarser spatial mesh than that necessary for the enthalpy method to achieve the same accuracy.

1.4.3 Finite Element Method

The second major numerical method used for phase change problems is the Finite Element Method. A number of FEM schemes have been implemented using heat capacity methods, which account for latent heat effects by changing the heat capacity of the material during phase change. These schemes are easy to implement but are relatively inaccurate for fine grids and small time steps because the phase change interface is not tracked explicitly. Comini et al. [37] and Rolph and Bathe [38] both employed the effective capacity method in fixed grid FEM schemes. Pham [39] used a lumped capacitance approach, while Poirier and Salcudean [40] used an apparent heat capacity method. Runnels and Carey [41] recently made improvements to previous methods and introduced the “accelerated effective capacity” method and the “exact apparent capacity” method. Another recent method, the “exact specific heat” technique was developed by Bushko and Grosse [42] and removes the need to approximate the specific heat function. Hsiao and Chung [43] determined the specific heat for each phase in their modification of the equivalent heat capacity method and claimed accurate results for coarse grids and large time steps.
Another popular approximate method, which has been applied to FEM schemes as well as FD schemes (see above) is the enthalpy method. Ciavaldini [44] developed explicit and implicit FEM algorithms in his discretized “weak” enthalpy formulation. Ronel and Baliga [45] applied the enthalpy method to irregular shaped or multiply connected domains. Elliot and Ockendon [46] used a fixed grid scheme, but reported oscillations both in temperatures near the interface and in the interface position. Cames-Pintaux and Nguyen-Lamba [47] made improvements in the enthalpy method which reduce these oscillations. Comini et al. [48] used a three time level FEM scheme along with a corrector step which recovers the enthalpy balance from the problem formulation, thus minimizing the oscillations and reducing the necessary iterations for convergence. Zhong et al. [49] incorporated an eigenvalue method in their enthalpy method formulation and reported reasonably accurate results when using a coarse mesh and unconditional stability with respect to time step size. Crivelli and Idelsohn [50] integrated enthalpy on both sides of the phase change interface, causing temperature to be the only dependent variable. This is known as the temperature based enthalpy method.

Other miscellaneous techniques have been applied to FEM for phase change problems. The fixed grid embedding technique, using Green’s functions was employed by Patera [51], to more accurately track the liquid-solid interface. Bonnerot and Jamet [52,53] allowed the number of finite elements to remain constant but stretched each element at every time step once phase change enters the problem. They later applied the same method to allow the possibility of the
disappearance of a phase such as the completion of melting with or without vaporization of the liquid [54]. Jamet [55] first introduced finite element approximations which allow for choosing elements at each time step without using information from previous times. Finally, Lewis et al. [56] used an error estimation technique to adaptively reform the spatial mesh, where necessary, at each time step.

1.4.4 Boundary Element Method

The Boundary Element Method is an analytical/numerical technique which is gaining acceptance as a practical approach to solving phase change problems in heat transfer. This method consists of an exact problem formulation, the Boundary Integral Equation (BIE), which integrates the heat conduction equation over time and space, using the Green’s Function as a weight function. The Green’s Function (GF) incorporates the physics of the problem and reduces by one the dimensionality of the problem. The integral equations are discretized in time and in space over the domain boundaries in an implicit numerical scheme.

The first authors to apply a BIE formulation to melting/solidification problems were Chuang and Szekely [57], who used Gaussian quadrature to numerically integrate the integral equations. They considered a 1D slab immersed in its own melt and also considered the melting/solidification of cylinders [58]. Hassanein and Kucinski [59] used the Green’s Function method, which assumes a integral solution for the temperature distribution in terms of the GF, to solve 1D melting
and vaporization problems for a semi-infinite medium exposed to an intense applied heat flux. Ozisik [60] described how the Green’s Function method reformulates the general moving boundary problem into an equivalent heat conduction problem with a moving surface heat source.

Banerjee and Shaw [61] used the conventional BEM used in this paper to solve the melting of a 1D slab immersed in its own melt. Shaw [62] used the BEM to solve the ablation problem for a semi-infinite solid exposed to a time-varying applied heat flux. Brebbia et al. [63] thoroughly discussed the BIE formulation of Chuang and Szekely [57] and developed an iterative time stepping BEM scheme to solve a 1D melting problem. Heinlein et al. [64] used BEM for 1D solidification problems and claimed good agreement between their numerical results and experimental results.

Other authors have applied the BIE formulation to multidimensional phase change problems. O’Neill [65] first used a formulation based on a space-time GF, then based his second, more straightforward formulation, on the Laplace equation. His numerical scheme was non-iterative and yielded favorable results when compared to experiment. Sadegh et al. [66] made a quasi-steady approximation for the temperature distribution and used a spatially dependent GF. Their numerical solution is capable of using boundary elements which are either constant, linear, quadratic or higher-order. Coleman [67] implemented an iterative numerical scheme which evaluates all time integrals by the midpoint rule. Hong et al. [68] used an implicit BEM scheme to solve solidification problems
with complex geometries, but recommended small time steps to achieve accurate results. Zabaras and Mukherjee [69] developed a generalized implicit iterative BEM scheme which can be applied to a variety of phase change problems. It uses separate GF for the liquid and solid phases along with linear shape functions in space and time for the unknown temperatures and heat fluxes. Unfortunately they reported inaccurate results for the initial stages of the problem where a small level of solidification has taken place. Consequently, they used an equivalent heat capacity model for early times.
2.0 PHYSICAL MODEL

This chapter describes the physical model for a finite medium, initially in the solid phase, exposed to a surface heat flux accompanied by a change of phase. The governing equations and boundary conditions which apply to the problem during each period are given initially with real variables and then with dimensionless variables. Also included are any assumptions made during the analysis of the problem.

2.1 REAL VARIABLES

A variety of configurations could exist during the phase change problem under consideration, each with a different combination of boundary conditions. These possible configurations are described in the following sections.
2.1.1 Period 1: Pure conduction in the solid

Provided the initial body temperature is less than the melt temperature, the problem starts in Period 1 (see Fig. 2). The domain is all solid, one dimensional and the temperature distribution is time dependent. The temperature of the heated surface is less than the melt temperature, \( T_{im} < T_m \). Consequently, the governing equation during Period 1, in the solid, is the heat conduction equation.

\[
\frac{\partial^2 T_s}{\partial x^2} = \frac{1}{\alpha_s} \frac{\partial T_s}{\partial t}, \quad x_o \leq x \leq x_L. \quad [2.1]
\]

The left boundary of the solid is exposed to a time varying heat flux which may be either constant, pulsed (on and off) or any other specified variation. Therefore, the temperature gradient there is proportional to the applied heat flux.

\[-k_s \frac{\partial T_s}{\partial x} = q_o(t), \quad x = x_o \quad [2.2]\]

The right boundary of the solid is always insulated, thus

\[
\frac{\partial T_s}{\partial x} = 0, \quad x = x_L \quad [2.3]
\]

Initially the entire domain is isothermal, yielding

\[
T_s = T_{IN}, \quad t = 0 \quad [2.4]
\]
2.1.2 Period 2: Melting

Once the left boundary reaches the melt temperature, melting begins and a liquid region is introduced with its own governing equations and boundary conditions (see Fig. 2). The temperature at the left boundary of the liquid is greater than the melt temperature but less than the vaporization temperature, $T_m < T_v < T_i$. The time that melting begins is designated as $t_m$, while the time at which the melt front reaches the back wall is defined as $t_{mel}$. The liquid density $\rho_l$ is assumed to be equal to the solid density $\rho_s$, thus negating convection due to bulk motion of the liquid. There are also some changes in the boundary conditions of the solid region. The governing equation of the liquid region again is the heat conduction equation,

\[
\frac{\partial^2 T_l}{\partial x^2} = \frac{1}{\alpha_i} \frac{\partial T_l}{\partial t} , \quad x_o \leq x \leq s_m(t) \tag{2.5}
\]

The left boundary of the liquid is exposed to a uniform heat flux as the solid is in Period 1.

\[
-k_l \frac{\partial T_l}{\partial x} = q_o(t) , \quad x = x_o \tag{2.6}
\]

At the moving interface between the liquid and solid regions $s_m(t)$, the net sensible energy entering the phase front must equal the phase change energy. Also, the temperature at the melt front remains constant.
\[-k_f \frac{\partial T_l}{\partial x} + k_s \frac{\partial T_s}{\partial x} = \rho_s L_m \frac{ds_m}{dt}\]  \hspace{1cm} [2.7]

\[T_l = T_s = T_m, \quad x = s_m(t)\]  \hspace{1cm} [2.8]

The solid region is still governed by energy Eq. 2.1 and the boundary conditions given in Eqs. 2.3, 2.7 - 2.8 and the initial condition given in Eq. 2.4. However, the solid domain is now \(s_m(t) \leq x \leq x_L\).

**2.1.3 Period 2: Conduction in liquid after the completion of melting**

Melting of the entire domain is a possible occurrence in Period 2. If the melt front \(s_m(t)\) should reach the back wall of the total domain during Period 2, then only a liquid region remains. The liquid region is still governed by energy Eq. 2.5 over the interval \(x_o \leq x \leq x_L\) and has a boundary condition on its left side given by Eq. 2.6. However, the boundary condition on its right side changes to

\[\frac{\partial T_L}{\partial x} = 0, \quad x = x_L\]  \hspace{1cm} [2.9]

**2.1.4 Period 3: Combined melting and vaporization**

When the left boundary of the liquid reaches the vaporization temperature, \(T_v\), vaporization begins (see Fig. 2). If the melt front has not reached the back wall,
then both melting and vaporization occur together as \( t < t_{\text{melt}} \). The governing equation and boundary conditions of the solid region do not change when the problem goes from Period 2 to Period 3. The liquid domain does change to \( s_x(t) \leq x \leq s_m(t) \). The interface conditions at the melt front are still Eqs. 2.7 - 2.8. However, the conditions at the left boundary of the liquid, now identified as \( s_v(t) \), change due to the vaporization process. Again, a balance between sensible energy and phase change energy must be met while the front temperature remains constant.

\[
q_0(t) + k I \frac{\partial T_I}{\partial x} = \rho I L_v \frac{ds_v}{dt} \tag{2.10}
\]

\[
T_I = T_v, \quad x = s_v(t) \tag{2.11}
\]

**2.1.5 Period 3: Vaporization in liquid after the completion of melting**

If the melt front does not reach the back wall sometime during Period 2, then it could do so during Period 3, if enough heat is supplied. When this happens, at \( t = t_{\text{melt}} \), only the liquid region will remain and it will be governed by energy Eq. 2.5 over the interval \( s_x(t) \leq x \leq x_L \). The boundary conditions for the all liquid domain are given by Eqs. 2.9 - 2.11.
2.1.6 Period 3: Pure vaporization

If the special condition of $T_m = T_v$ is met, then pure vaporization occurs on an all solid domain, once the temperature of the solid at the heated surface, $T_{sm}$ reaches the vaporization temperature $T_v$. The solid region is governed by the energy Eq. 2.1 over the interval $s_m(t) \leq x \leq x_i$. The right boundary is subject to the condition given in Eq. 2.3. At the left boundary of the solid, there is a balance between the net sensible energy entering the phase front and the phase change energy. Also, the temperature at the phase front remains constant.

$$q_a(t) + k_s \frac{\partial T_s}{\partial x} = \rho_s L_v \frac{ds_m}{dt} \quad [2.12]$$

$$T_s = T_m = T_v, \quad x = s_m(t) \quad [2.13]$$

2.2 DIMENSIONLESS VARIABLES

The procedure for choosing a suitable group of dimensionless variables and parameters is given. An explanation of the physical meaning of each variable and parameter has been given in the nomenclature section.
2.2.1 Introduction

A set of reference quantities will now be chosen, which will then be used to construct dimensionless variables. The number of reference quantities must equal the number of independent dimensions the physical problem has. For the problem under investigation, there are four dimensions:

- length
- time
- temperature rise
- energy

A convenient set of reference quantities is:

- $k_s$
- $\alpha_s$
- $T_{IN} = \text{Temperature reference}$
- $\Delta T = T_r - T_{IN}$ \{ maximum temp. rise \}

$$v = \frac{q_s}{\rho_s[L_m + C_{ps}(T_m - T_{IN}) + L_v + C_{ps}(T_v - T_m)]}$$
where \( v \) is the quasi steady-state velocity of the melt and vapor fronts, for a semi-infinite medium when \( q_v(t) = q_o = \text{const.} \) (as derived in Appendix A). Using these reference quantities, the following dimensionless variables are now defined:

**Temperature variables** \((T_s - T_{IN} = \text{reference temperature rise})\)

- \( \theta_s = \frac{T_s - T_{IN}}{T_v - T_{IN}} \)
- \( \theta_l = \frac{T_l - T_{IN}}{T_v - T_{IN}} \)

**Time variables** \((\frac{P}{\alpha_s} = \text{reference time})\)

- \( \tau = \frac{t \alpha_s}{P} \)
- \( \tau_m = \frac{t_m \alpha_s}{P} \)
- \( \tau_v = \frac{t_v \alpha_s}{P} \)
- \( \tau_{\text{melt}} = \frac{t_{\text{melt}} \alpha_s}{P} \)
- \( \tau_{\text{abl}} = \frac{t_{\text{abl}} \alpha_s}{P} \)

**Distance variables** \((l = \frac{\alpha_s}{v} = \text{reference length})\)

- \( X = \frac{x}{l} \)
- \( S_m(\tau) = \frac{s_m(t)}{l} \)

2.0 PHYSICAL MODEL
- \( S_s(\tau) = \frac{s_s(t)}{l} \)

**Heat flux variables** \( \left( \frac{k_s(T_v - T_{IN})}{l} \right) = \text{reference heat flux} \)

- \( Q_s(\tau) = \frac{q_s l}{k_s(T_v - T_{IN})} \)

- \( Q(\tau) = \frac{q l}{k_s(T_v - T_{IN})} \)

With these dimensionless variables now defined, the following group of dimensionless parameters naturally arise:

**Thermal property parameters**

- \( K = \frac{k_l}{k_s} \)

- \( A = \frac{a_l}{a_s} \)

- \( \beta_m = \frac{C_p(T_v - T_{IN})}{L_m} \)

- \( \beta_v = \frac{C_p(T_v - T_{IN})}{L_v} \)

**Length parameters**

- \( X_o = \frac{x_o}{l} \)

- \( X_L = \frac{x_L}{l} \)
Temperature parameters

- $\theta_{IN} = \frac{T_{IN} - T_{IN}}{T_v - T_{IN}} = 0$

- $\theta_m = \frac{T_m - T_{IN}}{T_v - T_{IN}}$

- $\theta_v = \frac{T_v - T_{IN}}{T_v - T_{IN}} = 1$

2.2.2 Period 1: Pure conduction in the solid

The governing energy equation, boundary conditions and initial condition given by Eqs. 2.1 - 2.4 for a solid domain in Period 1 are converted to dimensionless form as:

\[
\frac{\partial^2 \theta_s}{\partial X^2} = \frac{\partial \theta_s}{\partial \tau}, \quad X_o \leq X \leq X_L \tag{2.14}
\]

\[- \frac{\partial \theta_s}{\partial X} = Q_o(\tau), \quad X = X_o \tag{2.15}\]

\[\frac{\partial \theta_s}{\partial X} = 0, \quad X = X_L \tag{2.16}\]

\[\theta_s = \theta_{IN} = 0, \quad \tau = 0 \tag{2.17}\]
2.2.3 Period 2: Melting

Once the left boundary reaches the melt temperature, at time \( \tau_m \), melting begins and a liquid region is introduced. Its governing energy equation and boundary conditions, given by Eqs. 2.5 - 2.8 are converted to dimensionless form as:

\[
\frac{\partial^2 \theta_l}{\partial X^2} = \frac{1}{A} \frac{\partial \theta_l}{\partial \tau} , \quad X_o \leq X \leq S_m(\tau) \tag{2.18}
\]

\[-K \frac{\partial \theta_l}{\partial X} = Q_o(\tau) , \quad X = X_o \tag{2.19}\]

\[-K \frac{\partial \theta_l}{\partial X} + \frac{\partial \theta_s}{\partial X} = \frac{1}{\beta_m} \frac{dS_m}{d\tau} , \quad X = S_m(\tau) \tag{2.20}\]

\[\theta_l = \theta_s = \theta_m \quad , \quad X = S_m(\tau) \tag{2.21}\]

The solid region is still governed by energy Eq. 2.14 but the domain is now \( S_m(\tau) \leq X \leq X_L \). Eq. 2.16 still serves as the boundary condition of the solid at its insulated surface.

2.2.4 Period 2: Conduction in liquid after the completion of melting

The governing energy equation for an all liquid domain in dimensionless form is given by Eq. 2.18 with the domain being \( X_o \leq X \leq X_L \). The left boundary is still
subject to the condition given by Eq. 2.19, while the right boundary now has the following condition:

\[
\frac{\partial \theta_l}{\partial X} = 0 , \quad X = X_L \tag{2.22}
\]

2.2.5 Period 3: Combined melting and vaporization

The solid region retains the same governing equation and boundary conditions in Period 3 as in Period 2. The liquid region's governing equation is also unchanged, however it is now on the interval \( S_c(\tau) \leq X \leq S_m(\tau) \). The interface conditions at the melt front are still Eqs. 2.20 - 2.21. However, the vaporization conditions at the left boundary, now \( S_c(\tau) \), become

\[
Q_o(\tau) + K \frac{\partial \theta_l}{\partial X} = \frac{1}{\beta_v} \frac{dS_v}{d\tau} \tag{2.23}
\]

\[
\theta_l = \theta_v = 1 \quad , \quad X = S_v(\tau) \tag{2.24}
\]

2.2.6 Period 3: Vaporization in liquid after the completion of melting

The problem reduces to vaporization of an all liquid domain. The liquid is governed by energy Eq. 2.18 on the interval \( S_c(\tau) \leq X \leq X_L \). The conditions on the left side of the domain are still given by Eqs. 2.23 - 2.24. The right side of the domain is subject to the condition given by Eq. 2.22.
2.2.7 Period 3: Pure vaporization

The governing energy equation for vaporization of an all solid domain in dimensionless form is the same as Eq. 2.14 but now applies to a domain of \( S_m(\tau) \leq X \leq X_L \). The initial condition remains Eq. 2.17 and the boundary condition on the right side is given by Eq. 2.16. However, the left side must obey the following conditions:

\[
Q_o(\tau) + \frac{\partial \theta_s}{\partial X} = \frac{1}{\beta_v} \frac{dS_m}{d\tau}
\]  \[2.25\]

\[
\theta_s = \theta_v = \theta_m = 1, \quad X = S_m(\tau)
\]  \[2.26\]

2.2.8 Equivalence of real and dimensionless values

With the governing equations, boundary conditions and initial condition now defined in terms of real variables (Eqs. 2.1 - 2.13) and dimensionless variables (Eqs. 2.14 - 2.26) the equivalence between real and dimensionless variables is summarized in Table 1. Also, the equivalence between real and dimensionless parameters is summarized in Table 2. When defining the thermal and physical properties of a given problem in terms of real variables, a total of eleven parameters must be defined. In dimensionless form, the same problem would be defined by seven distinct parameters.
Table 1. Equivalence of real and dimensionless variables

<table>
<thead>
<tr>
<th>Real Variables</th>
<th>Dimensionless Variables</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_s(x,t)$</td>
<td>$\theta_s(X, \tau)$</td>
</tr>
<tr>
<td>$T_r(x,t)$</td>
<td>$\theta_r(X, \tau)$</td>
</tr>
<tr>
<td>$s_m(t)$</td>
<td>$S_m(\tau)$</td>
</tr>
<tr>
<td>$s_v(t)$</td>
<td>$S_v(\tau)$</td>
</tr>
<tr>
<td>$x$</td>
<td>$X$</td>
</tr>
<tr>
<td>$t$</td>
<td>$\tau$</td>
</tr>
<tr>
<td>$l_m$</td>
<td>$\tau_m$</td>
</tr>
<tr>
<td>$l_v$</td>
<td>$\tau_v$</td>
</tr>
<tr>
<td>$l_{melt}$</td>
<td>$\tau_{melt}$</td>
</tr>
<tr>
<td>$l_{abl}$</td>
<td>$\tau_{abl}$</td>
</tr>
</tbody>
</table>
### Table 2. Equivalence of real and dimensionless parameters

<table>
<thead>
<tr>
<th>Real Parameters</th>
<th>Dimensionless Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{IN}$</td>
<td>0</td>
</tr>
<tr>
<td>$T_m$</td>
<td>$\theta_m = \frac{T_m - T_{IN}}{T_v - T_{IN}}$</td>
</tr>
<tr>
<td>$T_v$</td>
<td>1</td>
</tr>
<tr>
<td>$k_i$</td>
<td>$K$</td>
</tr>
<tr>
<td>$k_s$</td>
<td>1</td>
</tr>
<tr>
<td>$\alpha_i$</td>
<td>$A$</td>
</tr>
<tr>
<td>$\alpha_s$</td>
<td>1</td>
</tr>
<tr>
<td>$\rho L_m$</td>
<td>$\frac{1}{\beta_m} = \frac{L_m}{C_p(T_v - T_{IN})}$</td>
</tr>
<tr>
<td>$\rho L_v$</td>
<td>$\frac{1}{\beta_v} = \frac{L_v}{C_p(T_v - T_{IN})}$</td>
</tr>
<tr>
<td>$q_o(t)$</td>
<td>$Q_o(\tau)$</td>
</tr>
<tr>
<td>$X_L$</td>
<td>$X_L$</td>
</tr>
</tbody>
</table>

2.0 PHYSICAL MODEL
3.0 SOLUTION USING BEM

This chapter includes a derivation, in real variables, of the BEM integral equation for the boundary of a generalized region. This equation is then discretized for use in a numerical scheme. Given different boundary conditions, the integral equation is then rearranged so that the unknown boundary values (i.e., temperatures, heat fluxes, or phase boundaries) for a given region may be solved for. The chapter concludes with an explanation of the iteration scheme used to solve the discretized equations.

3.1 SELECTION OF THE GREEN'S FUNCTION

Consider a region, shown in Fig. 3, subject to the following heat conduction equation:
Figure 3. Generalized region with moving boundaries
\[
\frac{\partial^2 T}{\partial x^2} = \frac{1}{\alpha} \frac{\partial T}{\partial t} , \quad s_1(t) < x < s_2(t) , \quad t > 0
\] [3.1]

The Green’s function (GF), or fundamental solution is selected as energy Eq. 3.1 subjected to a pulsed, concentrated heat source,

\[
\frac{\partial^2 G}{\partial x^2} + \frac{1}{\alpha} \delta(x - x_0) \delta(t - t_0) = \frac{1}{\alpha} \frac{\partial G}{\partial t} , \quad t > t_0
\] [3.2]

\[
G(x,t/x_0,t_0) = 0 , \quad t < t_0
\] [3.3]

This auxiliary problem has a zero initial condition and has no constraining boundary conditions. The region is exposed to an impulsive point heat source \(q_0\), of strength unity, released instantaneously at time \(t_0\) and location \(x_0\). The Green’s function \(G(x,t/x_0,t_0)\), which satisfies the auxiliary problem yields the temperature distribution of the region in terms of the effect variables, \(x\) and \(t\).

Its notation has the following physical meaning:

\[
G(x,t/x_0,t_0) \equiv G(\text{effect/cause})
\] [3.4]

The GF also follows the reciprocity relation

\[
G(x,t/x_0,t_0) = G(x_0, - t_0/x, - t)
\] [3.5]

In view of this reciprocity condition, Eq. 3.2 can be written in terms of the causal variables, \(x_0\) and \(t_0\),

3.0 SOLUTION USING BEM
\[
\frac{\partial^2 G}{\partial x_0^2} + \frac{1}{\alpha} \delta(x - x_0)\delta(t - t_0) = -\frac{1}{\alpha} \frac{\partial G}{\partial t_0}, \quad t_0 > t
\]  

[3.6]

The Green's function which satisfies the auxiliary problem is [57]

\[
G(x, t|x_0, t_0) = \frac{1}{\sqrt{4\pi \alpha(t - t_0)}} \exp \left[ -\frac{(x - x_0)^2}{4\alpha(t - t_0)} \right]
\]  

[3.7]

### 3.2 DERIVATION OF THE BEM INTEGRAL

**EQUATION**

Express Eq. 3.1 in terms of the cause variables \(x_0, t_0\), then multiply by the Green's function and integrate over space and time to get,

\[
\int_0^{t^+} \int_{s_1(t_0)}^{s_2(t_0)} \left[ \frac{\partial^2 T}{\partial x_0^2} - \frac{1}{\alpha} \frac{\partial T}{\partial t_0} \right] G \, dx_0 \, dt_0 = 0,
\]  

[3.8]

where \(t^+ = t + \varepsilon\). The left side of Eq. 3.8 is split into two parts and each part is considered independently,

\[
I = \int_0^{t^+} \int_{s_1(t_0)}^{s_2(t_0)} \frac{\partial^2 T}{\partial x_0^2} G dx_0 dt_0
\]

### 3.0 SOLUTION USING BEM
\[
I = \int_0^t \left[ \left( \frac{\partial T}{\partial x_0} \right)_{x_0 = s_1(t_0)}^{s_2(t_0)} - \left( T \frac{\partial G}{\partial x_0} \right)_{x_0 = s_1(t_0)}^{s_2(t_0)} \right] dt_0 + \int_0^t \int_{s_1(t_0)}^{s_2(t_0)} T \frac{\partial^2 G}{\partial x_0^2} \, dx_0 \, dt_0
\]

(by Green's 2nd Theorem)

\[
I_1 = -\frac{1}{\alpha} \int_0^t \int_{s_1(t_0)}^{s_2(t_0)} \frac{\partial T}{\partial t_0} G \, dx_0 \, dt_0
\]

\[
= -\frac{1}{\alpha} \int_0^t \int_{s_1(t_0)}^{s_2(t_0)} \left[ \frac{\partial}{\partial t_0} (T G) - T \frac{\partial G}{\partial t_0} \right] \, dx_0 \, dt_0
\]

\[
= -\frac{1}{\alpha} \int_0^t \left[ \frac{d}{dt_0} \int_{s_1(t_0)}^{s_2(t_0)} T G \, dx_0 - (TG)_{x_0 = s_2(t_0)} \frac{ds_2}{dt_0} + (TG)_{x_0 = s_1(t_0)} \frac{ds_1}{dt_0} \right] \, dt_0
\]

\[
+ \frac{1}{\alpha} \int_0^t \int_{s_1(t_0)}^{s_2(t_0)} T \frac{\partial G}{\partial t_0} \, dx_0 \, dt_0
\]

(by the Leibnitz Rule)

Remembering that \( G = 0 \) for \( t_0 > t \), integral \( I_1 \) becomes

\[
I_1 = \frac{1}{\alpha} \int_{s_1(0)}^{s_2(0)} (TG)_{t_0 = 0} \, dx_0 + \frac{1}{\alpha} \int_0^t (TG)_{x_0 = s_2(t_0)} \frac{ds_2}{dt_0} \, dt_0
\]

3.0 SOLUTION USING BEM
\[- \frac{1}{\alpha} \int_{0}^{t} (TG)_{x_0 = s_{1(t_0)}} \frac{ds_1}{dt_0} dt_0 + \frac{1}{\alpha} \int_{0}^{t} \int_{s_{1(t_0)}}^{s_{2(t_0)}} T \frac{\partial G}{\partial t_0} dx_0 dt_0 \]

Combining integrals I and II yields

\[
\int_{0}^{t} \left[ \frac{\partial T}{\partial x_0} G - T \frac{\partial G}{\partial x_0} + \frac{1}{\alpha} T G \frac{ds_2}{dt_0} \right]_{x_0 = s_{2(t_0)}} dt_0
\]

\[
- \int_{0}^{t} \left[ \frac{\partial T}{\partial x_0} G - T \frac{\partial G}{\partial x_0} + \frac{1}{\alpha} T G \frac{ds_1}{dt_0} \right]_{x_0 = s_{1(t_0)}} dt_0
\]

\[+ \frac{1}{\alpha} \int_{s_{1(t_0)}}^{s_{2(0)}} (TG)_{t_0 = 0} dx_0\]

\[+ \int_{0}^{t} \int_{s_{1(t_0)}}^{s_{2(t_0)}} T(x_0, t_0) \left[ \frac{\partial^2 G}{\partial x_0^2} + \frac{1}{\alpha} \frac{\partial G}{\partial t_0} \right] dx_0 dt_0 = 0 \quad [3.9]\]

Inaccuracies would occur in the numerical scheme due to the terms containing the velocity \(\frac{ds}{dt_0}\), if the assumption of constant velocity over each discretized time interval is made. This was remedied by making the following transformation to the terms containing the phase front velocities:

3.0 SOLUTION USING BEM
\[
\int_0^{t^*} TG \frac{ds}{dt_0} dt_0 = \int_{s(0)}^{s(t^*)} TGds \tag{3.10}
\]

Substituting the Dirac delta function expression from Eq. 3.6 into the last term in Eq. 3.9 gives,

\[
\int_0^{t^*} \int_{s_1(t_0)}^{s_2(t_0)} T(x_0, t_0) \left[ \frac{\partial^2 G}{\partial x_0^2} + \frac{1}{\alpha} \frac{\partial G}{\partial t_0} \right] dx_0 dt_0
\]

\[
= -\frac{1}{\alpha} \int_0^{t^*} \int_{s_1(t_0)}^{s_2(t_0)} T(x_0, t_0) \delta(x - x_0) \delta(t - t_0) dx_0 dt_0 = -\frac{1}{\alpha} \lambda T(x, t)
\]

Notice that when the delta function is integrated over the time and spatial domains for which it is defined, the following property holds true:

\[
\int_0^{t^*} \int_{x_1}^{x_2} T(x_0, t_0) \delta(x - x_0) \delta(t - t_0) dx_0 dt_0 = \lambda T(x, t)
\]

where

\[
\lambda = \begin{cases} 
0, & x < x_1 \text{ or } x > x_2 \\
\frac{1}{2}, & x = x_1 \text{ or } x = x_2 \\
1, & x_1 < x < x_2
\end{cases}
\]
Substituting \( \frac{-q}{k} \) for \( \frac{\partial T}{\partial x_0} \), in Eq. 3.9, taking the limit as \( t^+ \to t \) and finally rearranging the integral equation in terms of the unknown temperature distribution yields the **BEM integral equation**:

\[
\lambda T(x,t) =
\]

\[
\frac{\alpha}{k} \int_0^t \left[ -qG - T_k \frac{\partial G}{\partial x_0} \right]_{s_0} = s_2(t_0) \, dt_0 - \frac{\alpha}{k} \int_0^t \left[ -qG - T_k \frac{\partial G}{\partial x_0} \right]_{s_0} = s_1(t_0) \, dt_0
\]

\[
+ \int_{s_2(0)}^{s_2(t)} (TG)_{s_0} = s_2(t_0) \, ds_2 - \int_{s_1(0)}^{s_1(t)} (TG)_{s_0} = s_1(t_0) \, ds_1 + \int_{s_1(0)}^{s_2(0)} (TG)_{t_0} = 0 \, dx_0
\]

\[3.11\]

The integration factor \( \lambda \) is defined as follows:

\[
\lambda = \begin{cases} 
\frac{1}{2} & \text{on region boundaries} \\
1 & \text{inside the region}
\end{cases}
\]

### 3.3 DISCRETIZATION OF THE BEM INTEGRAL EQUATION

For the implicit numerical scheme which will be used, the current time \( t \) will be defined as \( t^{np} \), where \( pp \) is the current time step. The temperatures, \( T \), and heat fluxes, \( q \) in Eq. 3.11 are assumed to be constant over the time interval...

---

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$t_p-1 < t_o \leq t_p$ and can be brought out in front of the integral. The discretization of all integrals now can take place, using a fully implicit scheme. The following types of integrals are required,

$$\int_0^t qG dt_0 =$$

$$\int_c^{t_p} qG dt_0 = \sum_{p=1}^{p_p} \left[ q^p \int_{t^p-1}^{t^p} G dt_0 \right] = \sum_{p=1}^{p_p} q^p G^p(x, t^p / x_0, t^p, t^p-1)$$

$$\int_0^t T \frac{\partial G}{\partial x_0} dt_0 =$$

$$\int_0^{t_p} T \frac{\partial G}{\partial x_0} dt_0 = \sum_{p=1}^{p_p} \left[ T^p \int_{t^p-1}^{t^p} \frac{\partial G}{\partial x_0} dt_0 \right] = \sum_{p=1}^{p_p} T^p H^p(x, t^p / x_0, t^p, t^p-1)$$

$$\int_{s(0)}^{s(t)} (TG)_{x_0 = s(t_0)} ds =$$

$$\int_{s(0)}^{s^{p_p}} (TG)_{x_0 = s(t_0)} ds = \sum_{p=1}^{p_p} \left[ T^p \int_{s^p-1}^{s^p} G ds \right] = \sum_{p=1}^{p_p} T^p L^p(x, t^p / s^{p-1}, s^p, t^p-1)$$

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The following definitions of the Green’s function integrals have been used for convenience; analytical expressions are given in Appendix B.

\[
G^p(x, t^{pp}/x_0, t^p, t^{p-1}) = \int_{t_0}^{t^p} G(x, t^{pp}/x_0, t_0) dt_0
\]

\[
H^p(x, t^{pp}/x_0, t^p, t^{p-1}) = \int_{t_0}^{t^p} \frac{\partial G}{\partial x_0} (x, t^{pp}/x_0, t_0) dt_0
\]

\[
L^p(x, t^{pp}/s^{p-1}, s^p, t^{p-1}) = \int_{s^{p-1}}^{s^p} G(x, t^{pp}/s, t^{p-1}) ds
\]

Note from Appendix B that when \( x = x_0 \), \( H^p(x_0, t^{pp}/x_0, t^p, t^{p-1}) = 0 \). The integral equation given in Eq. 3.11 can now be discretized with respect to time for any location \( x \)

\[
\lambda T^{pp}(x) = \frac{\alpha}{k} \sum_{p=1}^{pp} \left[ -q_2^p G^p(x, t^{pp}/s_2^p, t^p, t^{p-1}) - T_2^p k H^p(x, t^{pp}/s_2^p, t^p, t^{p-1}) \\
+ q_1^p G^p(x, t^{pp}/s_1^p, t^p, t^{p-1}) + T_1^p k H^p(x, t^{pp}/s_1^p, t^p, t^{p-1}) \\
+ \frac{k}{\alpha} T_2^p L^p(x, t^{pp}/s_2^{p-1}, s_2^p, t^{p-1}) - \frac{k}{\alpha} T_1^p L^p(x, t^{pp}/s_1^{p-1}, s_1^p, t^{p-1}) \right] \\
+ T_{IN} L^p(x, t^{pp}/s_1(0), s_2(0), 0) \tag{3.12}
\]
where $q_1$ and $T_1$ represent the heat flux and temperature, respectively at $x = s_1$. Similarly, $q_2$ and $T_2$ represent the heat flux and temperature at $x = s_2$. This discretized integral equation can be applied at $x = s_1$ to get

$$\frac{1}{2} T_1^{pp} =$$

$$\frac{\alpha}{k} \sum_{p=1}^{pp} \left[ - q_2^p G^p(s_1^{pp}, t^{pp} / s_2^p, t^p, t^{p-1}) - T_2^p k H^p(s_1^{pp}, t^{pp} / s_2^p, t^p, t^{p-1}) \right.$$

$$+ q_1^p G^p(s_1^{pp}, t^{pp} / s_1^p, t^p, t^{p-1}) + T_1^p k H^p(s_1^{pp}, t^{pp} / s_1^p, t^p, t^{p-1})$$

$$+ \frac{k}{\alpha} T_2^p L^p(s_1^{pp}, t^{pp} / s_2^p - 1, s_2^p, t^{p-1}) - \frac{k}{\alpha} T_1^p L^p(s_1^{pp}, t^{pp} / s_1^p - 1, s_1^p, t^{p-1}) \left. \right]$$

$$+ T_{IN} L^p(s_1^{pp}, t^{pp} / s_1(0), s_2(0), 0)$$

[3.13]

Similarly, the discretized integral equation at $x = s_2$ is

$$\frac{1}{2} T_2^{pp} =$$

$$\frac{\alpha}{k} \sum_{p=1}^{pp} \left[ - q_2^p G^p(s_2^{pp}, t^{pp} / s_2^p, t^p, t^{p-1}) - T_2^p k H^p(s_2^{pp}, t^{pp} / s_2^p, t^p, t^{p-1}) \right.$$

$$+ q_1^p G^p(s_2^{pp}, t^{pp} / s_1^p, t^p, t^{p-1}) + T_1^p k H^p(s_2^{pp}, t^{pp} / s_1^p, t^p, t^{p-1})$$

$$+ \frac{k}{\alpha} T_2^p L^p(s_2^{pp}, t^{pp} / s_2^p - 1, s_2^p, t^{p-1}) - \frac{k}{\alpha} T_1^p L^p(s_2^{pp}, t^{pp} / s_1^p - 1, s_1^p, t^{p-1}) \left. \right]$$

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\[ + T_{IN} L^p (s_2^{p}, t^{p}) / s_1(0), s_2(0), 0) \]  

[3.14]

### 3.4 DISCRETIZED BEM EQUATIONS FOR UNKNOWN BOUNDARY VALUES

Eqs. 3.13 and 3.14 can now be applied to either the solid or liquid and written in terms of unknown boundary values (i.e. temperatures or heat fluxes) for the numerous combinations of boundary conditions encountered in Periods 1, 2 and 3. This section contains a listing of the discretized BEM equations that are possible for each period. The evolution of unknown and known boundary temperatures and heat fluxes, as well as phase front positions and velocities during Periods 1 thru 3 are summarized in Table 3.

#### 3.4.1 Period 1: Pure conduction in the solid

Recalling the boundary conditions, and initial condition from Eqs. 2.2 - 2.4, the following parameters are known and unknown at \( t = t^p \), the current time step:

\[
\begin{align*}
    s_1 &= x_o \\
    q_1 &= q_o \quad \text{known} \\
    T_1 &= T_{sm} \quad \text{unknown} \\
    s_2 &= x_L \\
    q_2 &= 0 \quad \text{known} \\
    T_2 &= T_{st} \quad \text{unknown}
\end{align*}
\]
Table 3. Evolution of boundary values during Periods 1, 2 and 3

<table>
<thead>
<tr>
<th>Phase change fronts</th>
<th>Liquid</th>
<th>Solid</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$x = s_1$</td>
<td>$x = s_m$</td>
</tr>
<tr>
<td>$t$</td>
<td>$s_m$</td>
<td>$s_m$</td>
</tr>
<tr>
<td>$v_m$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$s_m$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_m$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q_m$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$T_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>$q_{m}$</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Period 1, conduction in solid:

Period 2, melting:

Period 2, conduction in liquid after melting:

Period 3, melting and vaporization:

Period 3, vaporization in liquid after melting:

Period 3, pure vaporization:

The discretized BEM equation at $x = s_1 = x_o$, given by Eq. 3.13, becomes:

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\[ \frac{1}{2} T_{sm}^{pp} = \]

\[ \frac{\alpha_s}{k_s} \sum_{p}^{pp} \left[ -T_{sl}^{p}k_s H_s^{p}(x_o, t^{pp}/x_L, t^p, t^{p-1}) + q_0^p G_s^{p}(x_o, t^{pp}/x_o, t^p, t^{p-1}) \right] \]

\[ + T_{IN} L_s^{p}(x_o, t^{pp}/x_o, x_L, 0) \]

where the discretized Green's Function integrals are expressed specifically for the solid phase by the subscript s. This equation is now rearranged with unknowns on the left and knowns on the right:

\[ \frac{1}{2} T_{sm}^{pp} + \alpha_s T_{sl}^{pp} H_s^{p}(x_o, t^{pp}/x_L, t^{pp}, t^{pp-1}) = \]

\[ \frac{\alpha_s}{k_s} \sum_{p}^{pp-1} \left[ q_0^p G_s^{p}(x_o, t^{pp}/x_o, t^p, t^{p-1}) - T_{sl}^{p}k_s H_s^{p}(x_o, t^{pp}/x_L, t^p, t^{p-1}) \right] \]

\[ + \frac{\alpha_s}{k_s} q_0^{pp} G_s^{p}(x_o, t^{pp}/x_o, t^{pp}, t^{pp-1}) + T_{IN} L_s^{p}(x_o, t^{pp}/x_o, x_L, 0) \]  \[ 3.15 \]

The second BEM equation given by Eq. 3.14 is at \( x = s_2 = x_L \):

\[ \frac{1}{2} T_{sl}^{pp} = \]
\[
\frac{\alpha_s}{k_s} \sum_{p=1}^{pp} \left[ q_p G_s(x_L, t^{pp} \mid x_o, t^p, t^{p-1}) + T_{sm}^p k_s H_s(x_L, t^{pp} \mid x_o, t^p, t^{p-1}) \right] \\
+ T_{IN} L_s^p(x_L, t^{pp} \mid x_o, x_L, 0) 
\]

As before, the equation is rearranged with unknowns on the left and knowns on the right.

\[- \alpha_s T_{sm}^p H_s(x_L, t^{pp} \mid x_o, t^{pp}, t^{pp-1}) + \frac{1}{2} T_{sl}^{pp} = \]

\[
\frac{\alpha_s}{k_s} \sum_{p=1}^{pp-1} \left[ q_p G_s(x_L, t^{pp} \mid x_o, t^p, t^{p-1}) + T_{sm}^p k_s H_s(x_L, t^{pp} \mid x_o, t^p, t^{p-1}) \right] \\
+ \frac{\alpha_s}{k_s} q_o^{pp} G_s(x_L, t^{pp} \mid x_o, t^{pp}, t^{pp-1}) + T_{IN} L_s^p(x_L, t^{pp} \mid x_o, x_L, 0) \quad [3.16] 
\]

### 3.4.2 Period 2: Melting

In this case, the domain consists of liquid and solid regions. Recalling the solid region boundary conditions from Eq. 2.3, and Eqs. 2.7 - 2.8, the following parameters are known and unknown for the solid region at \( t = t^{pp} \), the current time step:
\[ s_1 = s_m \left\{ \begin{array}{l}
T_1 = T_m \quad \text{known} \\
q_1 = q_{sm} \quad \text{unknown}
\end{array} \right. \]

\[ s_2 = x_L \left\{ \begin{array}{l}
q_2 = 0 \quad \text{known} \\
T_2 = T_{st} \quad \text{unknown}
\end{array} \right. \]

The discretized BEM equation at \( x = s_i = s_m \) becomes

\[
\frac{1}{2} T_m = \]

\[
\frac{\alpha_s}{k_s} \sum_{p=1}^{pp} \left( - T_{sL}^p k_s H_s^p (s_{m}^{pp}, t^{pp} | x, t^p, t^{p-1}) + q_{sm}^{pp} G_s^p (s_{m}^{pp}, t^{pp} | s_{m}, t^p, t^{p-1}) \right)
\]

\[
+ T_{sm}^p k_s H_s^p (s_{m}^{pp}, t^{pp} | s_{m}^{pp}, t^p, t^{p-1}) - \frac{k_s}{\alpha_s} T_m L_s^p (s_{m}^{pp}, t^{pp} | s_{m}^{pp}, t^p, t^{p-1}) \right]
\]

\[
+ T_{IN} L_s^p (s_{m}^{pp}, t^{pp} | x_0, x_L, 0)
\]

This equation is rearranged with unknowns on the left side and knowns on the right side:

\[
- \frac{\alpha_s}{k_s} q_{sm}^{pp} G_s^p (s_{m}^{pp}, t^{pp} | s_{m}^{pp}, t^{pp}, t^{pp-1}) + \alpha_s T_{sL}^{pp} H_s^p (s_{m}^{pp}, t^{pp} | x, t^p, t^{p-1}) =
\]

\[
\frac{\alpha_s}{k_s} \sum_{p=i}^{pp-1} \left( - T_{sL}^p k_s H_s^p (s_{m}^{pp}, t^{pp} | x, t^p, t^{p-1}) + q_{sm}^{pp} G_s^p (s_{m}^{pp}, t^{pp} | s_{m}, t^p, t^{p-1}) \right)
\]

\[
+ T_{sm}^p k_s H_s^p (s_{m}^{pp}, t^{pp} | s_{m}^{pp}, t^p, t^{p-1}) - \frac{k_s}{\alpha_s} T_m L_s^p (s_{m}^{pp}, t^{pp} | s_{m}^{pp}, t^p, t^{p-1}) \right]
\]

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\[- \frac{k_s}{\alpha_s} T_m L_s^p(s_m^{pp}, t^{pp} | s_m^{pp-1}, s_m^{pp}, t^{pp-1}) \]

\[+ T_{IN} L_s^p(s_m^{pp}, t^{pp} | x_o, x_i, 0) - \frac{1}{2} T_m \]

\[\text{[3.17]}\]

The BEM equation for the solid region at \( x = s_2 = x_L \) is

\[\frac{1}{2} T^{pp}_{sL} = \]

\[\frac{\alpha_s}{k_s} \sum_{p=1}^{pp} \left[ q_{sm}^p G_s^p(x_L, t^{pp} | s_m^{p}, t^p, t^{p-1}) + T_{sm}^p k_s H_s^p(x_L, t^{pp} | s_m^{p}, t^p, t^{p-1}) \right] \]

\[ - \frac{k_s}{\alpha_s} T_m L_s^p(x_L, t^{pp} | s_m^{p-1}, s_m^{p}, t^{p-1}) + T_{IN} L_s^p(x_L, t^{pp} | x_o, x_i, 0) \]

Now this equation is rearranged with unknowns on the left side:

\[- \frac{\alpha_s}{k_s} q_{sm}^{pp} G_s^p(x_L, t^{pp} | s_m^{pp}, t^{pp}, t^{pp-1}) + \frac{1}{2} T_{sL}^{pp} = \]

\[\frac{\alpha_s}{k_s} \sum_{p=1}^{pp} \left[ T_{sm}^p k_s H_s^p(x_L, t^{pp} | s_m^{p}, t^p, t^{p-1}) - \frac{k_s}{\alpha_s} T_m L_s^p(x_L, t^{pp} | s_m^{p-1}, s_m^{p}, t^{p-1}) \right] \]

\[+ \frac{\alpha_s}{k_s} \sum_{p=1}^{pp-1} [q_{sm}^p G_s^p(x_L, t^{pp} | s_m^{p}, t^p, t^{p-1})] + T_{IN} L_s^p(x_L, t^{pp} | x_o, x_i, 0) \]

\[\text{[3.18]}\]
Recalling the liquid region boundary conditions, Eqs 2.6 - 2.8, the following parameters are known and unknown for the current time step:

\[
\begin{align*}
    s_1 &= x_c & q_1 &= q_o & \text{known} \\
    T_1 &= T_{lv} & s_2 &= s_m & \text{unknown} \\
    \frac{T_2}{T_m} &= \text{known} \\
    q_2 &= q_{lm} & \text{unknown}
\end{align*}
\]

The discretized BEM equation at \( x = s_1 = x_c \) becomes

\[
\frac{1}{2} T_{lv}^{pp} =
\]

\[
\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ -q_l^{pp} G_l^p (x_o, t^{pp}|s_{m}^{p}, t^p, t^p - 1) - T_m k_l H_l^p (x_o, t^{pp}|s_{m}^{p}, t^p, t^p - 1) \right]
\]

\[
+ \frac{k_l}{\alpha_l} T_m L_l^p (x_o, t^{pp}|s_{m}^{p}, t^p, t^p - 1) + q_l^{pp} G_l^p (x_o, t^{pp}|x_o, t^p, t^p - 1)
\]

This equation is rearranged with unknowns on the left side and knowns on the right side:

\[
\frac{1}{2} T_{lv}^{pp} + \frac{\alpha_l}{k_l} q_l^{pp} G_l^p (x_o, t^{pp}|s_{m}^{p}, t^{pp}, t^{pp - 1}) =
\]

\[
\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ -T_m k_l H_l^p (x_o, t^{pp}|s_{m}^{p}, t^p, t^p - 1) + q_l^{pp} G_l^p (x_o, t^{pp}|x_o, t^p, t^p - 1) \right]
\]

\[
+ \frac{k_l}{\alpha_l} T_m L_l^p (x_o, t^{pp}|s_{m}^{p}, t^p, t^p - 1)
\]

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\[ + \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ - q_{lm}^p G_l^p (x_o, t^{pp} \mid s_m^p, t^p, t^{p-1}) \right] \] [3.19]

The BEM equation at for the liquid region at \( x = s_2 = s_m \) becomes

\[
\frac{1}{2} T_m = \]

\[
\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ - q_{lm}^p G_l^p (s_m^{pp}, t^{pp} \mid s_m^p, t^p, t^{p-1}) - T_m k_i H_i^p (s_m^{pp}, t^{pp} \mid s_m^p, t^p, t^{p-1}) \right] + k_i T_m L_i^p (s_m^{pp}, t^{pp} \mid s_m^{pp-1}, s_m^p, t^{p-1}) + q_o^p G_l^p (s_m^{pp}, t^{pp} \mid x_o, t^p, t^{p-1})
\]

\[+ T_i^p k_i H_i^p (s_m^{pp}, t^{pp} \mid x_o, t^p, t^{p-1})] \]

Again, rearranging the preceding equation with unknowns on the left side and knowns on the right side yields

\[- T_i^{pp} \alpha_l H_i^p (s_m^{pp}, t^{pp} \mid x_o, t^{pp}, t^{pp-1}) + \frac{\alpha_l}{k_l} q_{lm}^{pp} G_l^p (s_m^{pp}, t^{pp} \mid s_m^{pp}, t^{pp}, t^{pp-1}) = \]

\[
\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp-1} \left[ - q_{lm}^p G_l^p (s_m^{pp}, t^{pp} \mid s_m^p, t^p, t^{p-1}) + T_i^p k_i H_i^p (s_m^{pp}, t^{pp} \mid x_o, t^p, t^{p-1}) \right]
\]

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\[-T_m k_l H_1^p \left(s_{m}^{p}, t^{pp}/s_{m}^{p}, t^{p}, t^{p-1}\right) + \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[q_0^p G_1^p \left(s_{m}^{p}, t^{pp}/x_p, t^{p}, t^{p-1}\right)\right]

+ \frac{k_l}{\alpha_l} T_m L_1^p \left(s_{m}^{p}, t^{pp}/s_{m}^{p-1}, s_{m}^{p}, t^{p-1}\right) - \frac{1}{2} T_m \]  \hspace{1cm} [3.20]

Where \( p = pp_m \) denotes the time step in which melting first occurs. The liquid summations start at \( pp_m + 1 \) since the liquid did not exist before time step \( pp_m \).

The location of the melt front, \( s_m(t) \) is an additional unknown.

### 3.4.3 Period 2: Conduction in liquid after the completion of melting

In this case, the domain consists of only a liquid region. Recalling the liquid region boundary conditions from Eq. 2.6 and Eq. 2.9, the following parameters are known and unknown at \( t = tp \), the current time step:

\[
s_1 = x_o \begin{cases} 
q_1 = q_o \text{ known} \\
T_1 = T_{lv} \text{ unknown}
\end{cases}
\]

\[
s_2 = x_L \begin{cases} 
q_2 = 0 \text{ known} \\
T_2 = T_{ll} \text{ unknown}
\end{cases}
\]

The discretized BEM equation at \( x = s_1 = x_o \) becomes

\[
\frac{1}{2} T_{lv}^{pp} =
\]
\[
\frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp} \left[ -q_{lm}^p G_i^p (x_o, t^{pp} | s_m^p, t^p, t^{p-1}) - T_{IL}^p k_I H_i^p (x_o, t^{pp} | s_m^p, t^p, t^{p-1}) \right.
\]
\[+ \frac{k_l}{\alpha_l} T_{IL}^p L_i^p (x_o, t^{pp} | s_m^p, s_m^p, t^p, t^{p-1}) + q_o^p G_i^p (x_o, t^{pp} | x_o, t^p, t^{p-1}) \]

This equation is rearranged with unknowns on the left side and knowns on the right side:

\[
\frac{1}{2} T_{lv}^{pp} + \alpha_l T_{IL}^{pp} H_i^p (x_o, t^{pp} | x_l, t^{pp}, t^{pp-1}) = \frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp-1} \left[ - T_{IL}^p k_I H_i^p (x_o, t^{pp} | s_m^p, t^p, t^{p-1}) - q_{lm}^p G_i^p (x_o, t^{pp} | s_m^p, t^p, t^{p-1}) \right.
\]
\[+ \frac{k_l}{\alpha_l} T_{IL}^p L_i^p (x_o, t^{pp} | s_m^p, s_m^p, t^p, t^{p-1}) \]
\[+ \frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp} \left[ q_o^p G_i^p (x_o, t^{pp} | x_o, t^p, t^{p-1}) \right] \quad \text{(3.21)} \]

The BEM equation for an all liquid domain at \( x = s_2 = x_L \) is

\[
\frac{1}{2} T_{IL}^{pp} = \]
\[
\frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp} \left[ - q^p_{im} G^p_l (x_L, t^{pp}/s_m^p, t^p, t^{p-1}) - T^p_{il} \frac{k_l}{\alpha_l} H^p_l (x_L, t^{pp}/s_m^p, t^p, t^{p-1}) \right] \\
+ \frac{k_l}{\alpha_l} T^p_{il} L^p_l (x_L, t^{pp}/s_{m-1}^p, s_m^p, t^{p-1}) + q^p_o G^p_l (x_L, t^{pp}/x_o, t^p, t^{p-1}) \\
+ T^p_{io} k_l H^p_l (x_L, t^{pp}/x_o, t^p, t^{p-1}) \right] 
\]

Again, rearranging the preceding equation with unknowns on the left side and knowns on the right side yields

\[
- T^p_{iv} \alpha_l H^p_l (x_L, t^{pp}/x_o, t^{pp}, t^{pp-1}) + \frac{1}{2} T^p_{il} = 
\]

\[
\frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp-1} \left[ - q^p_{im} G^p_l (x_L, t^{pp}/s_m^p, t^p, t^{p-1}) + T^p_{ip} k_l H^p_l (x_L, t^{pp}/x_o, t^p, t^{p-1}) \right] \\
- T^p_{il} k_l H^p_l (x_L, t^{pp}/s_m^p, t^p, t^{p-1}) + \frac{k_l}{\alpha_l} T^p_{il} G^p_l (x_L, t^{pp}/s_{m-1}^p, s_m^p, t^{p-1}) \right] 
\]

\[
\frac{\alpha_l}{k_l} \sum_{p=pp_m+1}^{pp} \left[ q^p_o G^p_l (x_L, t^{pp}/x_o, t^p, t^{p-1}) \right] 
\]  

[3.22]
3.4.4 Period 3: Combined melting and vaporization

In this case, the domain consists of both a liquid and a solid region with moving vapor and melt phase fronts. Recalling the liquid region boundary conditions from Eqs. 2.7 - 2.8 and Eqs. 2.10 - 2.11, the following parameters are known and unknown at the current time step:

\[
\begin{align*}
    s_1 &= s_v \\
    q_1 &= q_{lv} \text{ unknown} \\
    T_1 &= T_v \text{ known} \\
    s_2 &= s_m \text{ unknown} \\
    T_2 &= T_m \text{ known} \\
    q_2 &= q_{lm} \text{ unknown}
\end{align*}
\]

The discretized BEM equation at \( x = s_1 = s_v \) becomes

\[
\frac{1}{2} T_v = \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ -q_{lm}^p G_l^p \left( s_v^{pp}, t^{pp}, s_m^p, t^p, t^{p-1} \right) - T_m k_l H_l^p \left( s_v^{pp}, t^{pp}, s_m^p, t^p, t^{p-1} \right) \right. \\
+ \frac{k_l}{\alpha_l} T_m L_l^p \left( s_v^{pp}, t^{pp}, s_m^{p-1}, s_m^p, t^p, t^{p-1} \right) + q_{lv}^p G_l^p \left( s_v^{pp}, t^{pp}, s_v^p, t^p, t^{p-1} \right) \\
+ T_{lv}^p k_l H_l^p \left( s_v^{pp}, t^{pp}, s_v^p, t^p, t^{p-1} \right) - \frac{k_l}{\alpha_l} T_v L_l^p \left( s_v^{pp}, t^{pp}, s_v^{p-1}, s_v^p, t^p, t^{p-1} \right) \left. \right]
\]

This equation is rearranged with unknowns on the left side and knowns on the right side:

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\[- \frac{\alpha_l}{k_l} q^{pp}_m G^p_l(s^{pp}_m, t^{pp} | s^{pp}_v, t^{pp}, t^{pp-1}) + \frac{\alpha_l}{k_l} q^{pp}_m G^p_l(s^{pp}_v, t^{pp} | s^{pp}_m, t^{pp}, t^{pp-1}) = \]

\[\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ - T_m k_l H^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) \right] + \frac{k_l}{\alpha_l} T_m L^p_l(s^{pp}_v, t^{pp} | s^{pp}_m, t^p, t^{p-1}) - \frac{k_l}{\alpha_l} T_m L^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) \]

\[+ \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp-1} \left[ - q^{pp}_m G^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) \right] + \frac{1}{2} T_m \quad [3.23] \]

The discretized BEM equation at \( x = s_2 = s_m \) becomes

\[\frac{1}{2} T_m = \]

\[\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ - q^{pp}_m G^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) - T_m k_l H^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) \right] \]

\[+ \frac{k_l}{\alpha_l} T_m L^p_l(s^{pp}_m, t^{pp} | s^{pp}_m, t^p, t^{p-1}) + q^{pp}_v G^p_l(s^{pp}_v, t^{pp} | s^{pp}_v, t^p, t^{p-1}) \]

\[+ T^p_v k_l H^p_l(s^{pp}_v, t^{pp} | s^{pp}_v, t^p, t^{p-1}) - \frac{k_l}{\alpha_l} T_v L^p_v(s^{pp}_v, t^{pp} | s^{pp}_v, t^p, t^{p-1}) \]
This equation is rearranged with unknowns on the left side and knowns on the right side:

\[-\frac{\alpha_l}{k_l} q_{lv}^{pp} G_l^p (s_m^{pp}, t^{pp}/s_v^{pp}, t^{pp}, t^{pp} - 1) + \frac{\alpha_l}{k_l} q_{lm}^{pp} G_l^p (s_m^{pp}, t^{pp}/s_m^{pp}, t^{pp}, t^{pp} - 1) =
\]

\[
\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ \frac{k_l}{\alpha_l} T_m L_l^p (s_m^{pp}, t^{pp}/s_m^{pp} - 1, s_m^{pp}, t^{p} - 1) \right]
\]

\[-\frac{k_l}{\alpha_l} T_v L_l^p (s_m^{pp}, t^{pp}/s_v^{pp} - 1, s_v^{pp}, t^{p} - 1) + T_v k_l H_l^p (s_m^{pp}, t^{pp}/s_v^{pp}, t^{p}, t^{p} - 1) \]

\[
+ \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp - 1} \left[ - q_{lm}^p G_l^p (s_m^{pp}, t^{pp}/s_m^{pp}, t^{p}, t^{p} - 1) \right]
\]

\[+ q_{lv}^p G_l^p (s_m^{pp}, t^{pp}/s_v^{pp}, t^{p}, t^{p} - 1) - T_m k_l H_l^p (s_m^{pp}, t^{pp}/s_m^{pp}, t^{p}, t^{p} - 1) \] - \frac{1}{2} T_m \quad [3.24]

During Period 3, the solid region has the same knowns and unknowns that it had during Period 2:

\[
s_1 = s_m \quad \left\{ \begin{array}{l}
T_1 = T_m \quad \text{known} \\
q_1 = q_{sm} \quad \text{unknown}
\end{array} \right.
\]

\[
s_2 = x_L \quad \left\{ \begin{array}{l}
q_2 = 0 \quad \text{known} \\
T_2 = T_{st} \quad \text{unknown}
\end{array} \right.
\]

Consequently, the discretized BEM equations at the boundaries of the solid region are given by Eqs. 3.17 and 3.18. Both the melt and vapor interfaces, \( s_m \) and \( s_v \), are unknown.

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3.4.5 Period 3: Vaporization in liquid after the completion of melting

In this case, because the melt front has reached the back wall, the entire domain is in the liquid phase. Recalling the liquid region boundary conditions from Eqs. 2.9 - 2.11, the following parameters are known and unknown at the current time step:

\[
 s_1 = s_v \begin{cases} 
 T_1 = T_v \text{ known} \\
 q_1 = q_{lv} \text{ unknown} 
\end{cases} \quad \{ 
 s_2 = x_L \begin{cases} 
 q_2 = 0 \text{ known} \\
 T_2 = T_{IL} \text{ unknown} 
\end{cases}
\]

The discretized BEM equation at \( x = s_1 = s_v \) becomes

\[
\frac{1}{2} T_v = \frac{\alpha_f}{k_f} \sum_{p = ppm+1}^{pp} \left[ - q_{lm}^p G_l^p \left( s_v^{pp}, t^{pp}/s_m^p, t^p, t^{p-1} \right) - T_{IL}^P k_f H_f^p \left( s_v^{pp}, t^{pp}/s_m^p, t^p, t^{p-1} \right) \right.
\]
\[
+ \frac{k_f}{\alpha_f} T_{IL}^P L_f^p \left( s_v^{pp}, t^{pp}/s_m^p, s_m^p, t^p, t^{p-1} \right) + q_{lv}^p G_l^p \left( s_v^{pp}, t^{pp}/s_v^p, t^p, t^{p-1} \right)
\]
\[
+ T_{lv}^P k_f H_f^p \left( s_v^{pp}, t^{pp}/s_v^p, t^p, t^{p-1} \right) - \frac{k_f}{\alpha_f} T_v L_f^p \left( s_v^{pp}, t^{pp}/s_v^p, s_v^p, t^p, t^{p-1} \right)
\]

This equation is rearranged with unknowns on the left side and knowns on the right side:

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\[- \frac{\alpha_l}{k_l} q_{i}^{pp} G_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{pp}, t^{pp} - 1) + \alpha_l T_{LL}^{pp} H_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{pp}, t^{pp} - 1) = \]

\[\frac{\alpha_l}{k_l} \sum_{p = pp_{m} + 1}^{pp - 1} \left[ - q_{i}^{p} G_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) + q_{i}^{p} G_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \right] \]

\[- T_{IL}^{p} k_{L} H_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) + \frac{k_{L}}{\alpha_l} T_{IL}^{p} L_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \]

\[+ T_{IL}^{p} k_{L} H_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \]

\[+ \frac{\alpha_l}{k_l} \sum_{p = pp_{m} + 1}^{pp} \left[ - \frac{k_{L}}{\alpha_l} T_{v} L_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \right] - \frac{1}{2} T_{v} \quad [3.25] \]

The discretized BEM equation at \( x = s_{2} = x_{l} \), becomes

\[\frac{1}{2} T_{IL}^{pp} = \]

\[\frac{\alpha_l}{k_l} \sum_{p = pp_{m} + 1}^{pp} \left[ - q_{i}^{p} G_{i}^{p} (s_{vp}^{pp}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) - T_{IL}^{pp} k_{L} H_{i}^{p} (x_{l}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \right] \]

\[+ \frac{k_{L}}{\alpha_l} T_{IL}^{p} L_{i}^{p} (x_{l}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) + q_{i}^{p} G_{i}^{p} (x_{l}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \]

\[+ T_{IL}^{p} k_{L} H_{i}^{p} (x_{l}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) - \frac{k_{L}}{\alpha_l} T_{v} L_{i}^{p} (x_{l}, t^{pp}, s_{vp}^{pp}, t^{p}, t^{p} - 1) \]

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This equation is rearranged with unknowns on the left side and knowns on the right side:

$$- \frac{\alpha_l}{k_l} q_{lv}^{pp} G_f^p (x_L, t^{pp} | s_v^{pp}, t^p, t^{pp} - 1) + \frac{1}{2} T_{IL}^{pp} =$$

$$\frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp - 1} \left[ - q_{lm}^p G_f^p (x_L, t^{pp} | s_m^p, t^p, t^{pp} - 1) + q_{lv}^p G_f^p (x_L, t^{pp} | s_v^p, t^p, t^{pp} - 1) \right]$$

$$- T_{IL}^p k_l H_f^p (x_L, t^{pp} | s_m^p, t^p, t^{pp} - 1) + \frac{k_l}{\alpha_l} T_{IL}^p L_f^p (x_L, t^{pp} | s_m^{p-1}, s_m^p, t^{pp} - 1) \right]$$

$$+ \frac{\alpha_l}{k_l} \sum_{p = pp_m + 1}^{pp} \left[ T_{lv}^p k_l H_f^p (x_L, t^{pp} | s_v^p, t^p, t^{pp} - 1) \right]$$

$$- \frac{k_l}{\alpha_l} T_v L_f^p (x_L, t^{pp} | s_v^{p-1}, s_v^p, t^{pp} - 1) \right]$$

[3.26]

The location of the vapor front, $s_v$, is an additional unknown.

### 3.4.6 Period 3: Pure vaporization

In this special case, where $T_m = T_v$, once $T_{sm}$ reaches the vapor temperature $T_v$, vaporization of the solid occurs without any melting. The domain consists of a solid region only. Recalling the solid region initial condition and boundary con-

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ditions from Eqs. 2.3 - 2.4 and Eqs. 2.12 - 2.13, the following parameters are known and unknown at the current time step:

\[
\begin{align*}
    s_1 &= s_m & T_1 &= T_v = T_m & \text{known} \\
    q_1 &= q_{sm} & q_2 = 0 & \text{known} \\
    s_2 &= x_l & T_2 = T_{sl} & \text{unknown}
\end{align*}
\]

This set of knowns and unknowns is identical to the one for Period 2 when \( t < t_{\text{melt}} \). Therefore the discretized BEM equations for vaporization of a solid domain would be given by Eqs. 3.17 - 3.18.

### 3.5 ITERATION SCHEME

In general, the unknown boundary values, at a given time step, \( \nu \) are heat fluxes, \( q \) or temperatures, \( T \). For a given phase, the 2 X 2 system of equations may be expressed as

\[
[A]_i[\Lambda]_i = [B]_i, \quad i = s, l \tag{3.27}
\]

where \([A]\) is the coefficient matrix, \([\Lambda]\) is the vector of unknown heat fluxes and/or temperatures, and \([B]\) is the matrix of known heat fluxes and temperatures at previous times. Equation 3.27 is easily solved using Cramer's Rule. For a Period 1 problem, the position of each boundary is fixed and Eq. 3.27 is solved without iterations. However, when phase change enters the problem, the position of a given phase change interface at \( \nu \) is also unknown and must be

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determined within a specified convergence criterion. Actually, a velocity $v_s$ is guessed and the position $s_x$ used in Eq. 3.27 is obtained from $\Delta s = v_s \Delta t$. The convergence criterion, $TOL$, is based upon the interface energy balance. For a Period 2 problem, where only one moving boundary, $s_m$, exists, the following condition, obtained from Eq. 2.7, must be met before moving on to the next time step:

$$q_{lm}^{pp} - q_{sm}^{pp} - \rho_s L_m v_{m,g}^{pp} \leq TOL$$ \hspace{1cm} [3.28]

where $v_{m,g}$ is the guessed melt front velocity at the current time step. If the condition is met, then the Period 2 solution obtained from Eq. 3.27 has converged and $v_m = v_{m,g}$, $s_m = s_{m,g}$. If the tolerance is not met, a new guess is made for the melt front velocity:

$$v_{m,g}^{pp} = \frac{q_{lm}^{pp} - q_{sm}^{pp}}{\rho_s L_m}$$ \hspace{1cm} [3.29]

and Eq. 3.27 is resolved with the improved value of $s_m$. The solution is iterated for Period 2 until the tolerance is met.

For a Period 3 problem with melting and vaporization, if the condition given by Eq. 3.28 is met, as well as the following condition (from Eq. 2.10),

$$q_{o}^{pp} - q_{lv}^{pp} - \rho_i L_v v_{v,g}^{pp} \leq TOL$$ \hspace{1cm} [3.30]

where $v_{v,g}$ is the guessed vapor front velocity, then the Period 3 solution obtained from Eq. 3.27 has converged and
\[ v_{m}^{pp} = v_{m,g}^{pp} , \quad s_{m}^{pp} = v_{m}^{pp} \Delta t \]

\[ v_{v}^{pp} = v_{v,g}^{pp} , \quad s_{v}^{pp} = v_{v}^{pp} \Delta t \]

If the tolerance is not met by both interface equations, a new guess is made for \( v_{m} \) from Eq. 3.29, and a new guess is made for \( v_{v} \) from

\[ v_{v,g}^{pp} = \frac{q_{o}^{pp} - q_{v}^{pp}}{\rho_{f} L_{v}} \]  \[3.31\]

and the same Period 3 iterative procedure is repeated.

For the first time step after a phase front is created, the initial guess for the velocity is expressed as

\[ v_{m,jg}^{pp} = \frac{q_{o}^{pp}}{\rho_{f} L_{m}} F , \quad v_{v,jg}^{pp} = \frac{q_{o}^{pp}}{\rho_{f} L_{v}} F , \quad 0 < F < 1 \]  \[3.32\]

where \( v_{m,jg} \) is used at the time step after \( t = t_{m} \) and \( v_{v,jg} \) is used at the time step after \( t = t_{v} \). Convergence problems occur when \( F = 1 \) or \( F = 0 \), so a suitable choice must be made for \( F \) by trial and error. For other time steps where an existing phase front velocity is established, the initial guesses for the velocity are:

\[ v_{m,jg}^{pp} = v_{m}^{pp} - 1 , \quad v_{v,jg}^{pp} = v_{v}^{pp} - 1 \]
The accuracy of the solution obtained from Eq. 3.27 as well as the CPU time required are both dependent on the convergence criterion, $TOL$ and the time step, $\Delta t$. 
This chapter consists of three major sets of results obtained from the BEM numerical solution. The chapter begins with a presentation of the numerical behavior of the BEM code. Following this, there is a presentation of the physical behavior of the phase change problem under consideration. These two sets of results are in terms of dimensionless variables. The chapter concludes with specific test cases of BEM results for the melting of metallic elements and also the pure vaporization of metallic elements.
4.1 NUMERICAL BEHAVIOR

4.1.1 Period 1

During the preheat stage of the phase change problem, the unknowns are the boundary temperatures, $\theta_{sm}$ and $\theta_{sl}$. For finite regions, BEM results are compared to an exact solution, derived from the integral transform technique (Appendix C). A specific case is given in Fig. 4. The unknown boundary temperatures are solved for initially using a crude time step of $\Delta \tau = 0.01$, and are successively solved for with more refined time steps. As the time step gets smaller, the BEM results for Period 1 approach the exact solution. Use of crude time steps in the BEM numerical scheme results in temperatures higher than those provided by the exact solution. Consequently, the time when melting begins, $\tau_m$, occurs earlier as the time step becomes more crude. The conclusion is that the BEM works well for finite one dimensional problems.

For semi-infinite regions, the only meaningful unknown during the preheat stage is the temperature at the origin, $\theta_{sm}$. Results obtained from the BEM are compared to an exact semi-infinite solution [70],

$$\theta_{sm} = \theta_s(0, \tau) = \theta_{IN} + 2Q_o(\tau/\pi)^{1/2}$$  \[4.1\]

A specific case is given in Fig. 5. The temperature at the origin is solved for using successively smaller time steps. Examination of the BEM solution for Period 1
Figure 4. Boundary temperatures during Period 1 for different time steps: (a) $X = S_m = 0$ (b) $X = X_L$. 

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$\theta_m = 0.8$
$Q_0 = 1$
$X_\infty \rightarrow \infty$
$\Delta \tau = 0.1$

Figure 5. Temperature of the heated boundary for a semi-infinite slab for different time steps.

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reveals that it is identical to the exact solution when using any time step, provided the domain is semi-infinite. Therefore, in this case, the free space Green's Function is the solution.

4.1.2 Periods 2 and 3

After the initial preheat stage, melting begins followed later by vaporization. Depending on the boundary conditions of the liquid and solid regions, the boundary temperatures and heat fluxes vary from being unknowns in some cases, to knowns in other cases. However, the position and velocities of the two phase fronts are generally unknown, thus causing the phase change problem to be non-linear. The numerical and physical results which will be presented for Periods 2 and 3 will be in terms of the behavior of the phase fronts.

In general, there is no independent analytical solution to compare to when phase change enters the problem. Therefore, in order to confirm that the BEM code converges to a very accurate solution for refined time steps, one alternative is to compare the BEM solution to itself. In Fig. 6, phase front behavior is given for a crude time step of $\Delta \tau = 0.01$ and for a refined time step of $\Delta \tau = 0.001$. It seems that when solving for the phase front position, there is close agreement among solutions given for different size time steps until the completion of melting. At that time vaporization occurs on a thin medium and as the time step becomes more refined, the BEM code produces a more accurate solution of $S_v$. The numerical behavior of velocity results is a little bit different. When melting occurs
Figure 6. Phase front behavior for different time steps: (a) Position (b) Velocity.
by itself or when vaporization occurs by itself (on an all-liquid domain), it is necessary to reduce the time step in order to achieve a more accurate solution for \( V_m \) or \( V_v \). However, when both melting and vaporization occur together, there is little difference between the velocities solved for by the crude time step and the velocities solved for by the more refined time steps. Since velocity is calculated as a difference in the numerically computed \( S \) values,

\[
V = \frac{S^p - S^p-1}{\Delta \tau}
\]

the velocity is expected to be less accurate than the position of the phase fronts.

For the special case of \( C_{ps} = C_{ps} \approx 0 \), there is an independent analytical solution (Appendix D) which is possible due to negligible sensible heat. In Fig. 7, results from the BEM solution are given first for a very crude time step, \( \Delta \tau = 50 \). In fact, when using this time step, only two time steps are necessary during Period 2. The BEM solution for Period 2 gives a constant velocity for the melt front. This velocity is \( V_m = Q_b \beta_m \) as a result of the energy balance Eq. 2.20 and is solved for exactly, regardless of the time step used. Once vaporization begins, there is disagreement between the BEM solution and the negligible sensible heat solution. However, as the time step becomes more refined, the BEM solution more closely resembles the negligible sensible heat solution. As is the case with a Period 1 type problem, a very accurate solution to the one dimensional phase change problem is possible.

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Figure 7. Phase front behavior for the case of negligible sensible heat for different time steps: (a) Position (b) Velocity
4.2 PHYSICAL BEHAVIOR

4.2.1 Semi-infinite medium

Physical behavior of the melt and vapor phase fronts is now presented for different melt temperatures and values of applied heat flux. Phase front behavior is exhibited initially for an applied heat flux of \( Q_o = 1 \), and then for \( Q_o = 5 \). Figures 8, 9 and 10 are for a semi-infinite medium with \( A = 1 \), \( K = 1 \), \( \beta_m = 2 \) and \( \beta_v = 2 \). In Fig. 8, the melt temperature is \( \theta_m = 0 \). Consequently, there is no preheat time and melting begins immediately. The temperature of the solid region remains constant at \( \theta_s(X, \tau) = 0 \). Also, the heat flux entering the solid region from the melt front remains constant at \( Q_{sm} = 0 \). At the onset of melting \( \tau_m \), the heat flux entering the melt front from the liquid region is \( Q_{lm} = Q_o \). As a result of energy balance Eq. 2.20, the initial velocity of the melt front is \( V_m = Q_o \beta_m \). This is only true when \( \theta_m = 0 \). When \( \theta_m > 0 \), the initial melt velocity is \( V_m = 0 \). This behavior is shown in Figures 8, 9 and 10. Obviously, the larger the applied heat flux, the larger the initial melt front velocity, holding everything else constant. Also, the vapor phase front always starts with a velocity of zero. At the beginning of Period 3, the melt front velocity steadily drops while the vapor front velocity steadily rises. When the melt temperature is greater than the initial temperature, as is the case in Fig. 9 and Fig. 10, some preheat time is necessary. Period 2 begins later for high melt temper-
Figure 8. Phase front behavior for a semi-infinite medium ($\theta_m = 0$): (a) Position (b) Velocity

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Figure 9. Phase front behavior for a semi-infinite medium ($\theta_m = 0.5$): (a) Position (b) Velocity
Figure 10. Phase front behavior for a semi-infinite medium \((\theta_m = 0.8)\): (a) Position (b) Velocity
atures and earlier for high applied heat fluxes. The behavior of the melt front is more irregular for cases where \( \theta_m > 0 \) and vaporization begins almost immediately after melting, as is the case for high heat fluxes like \( Q_s = 5 \). During Period 2, there is a sharp rise in the melt front velocity until vaporization begins, triggering a sharp drop. In the case of a high melt temperature, \( \theta_m = 0.8 \), this sharp rise and drop becomes less pronounced. For lower applied heat fluxes like \( Q_s = 1 \), changes in the melt and vapor phase front velocities are more gradual.

According to theory (Appendix A), for a semi-infinite medium, once melting and vaporization have continued for a long time, both phase fronts reach a quasi-steady state velocity and the distance separating both phase fronts remains constant. The higher the melt temperature, the earlier a quasi-steady state occurs and the smaller the separation distance between the phase fronts. Incidentally, while holding all thermal and physical properties constant, there is no effect on the value of the quasi-steady state velocity when changing the melt temperature. Also, the higher the applied heat flux, the higher the quasi-steady state velocity will be and the smaller the separation distance becomes. Thus for higher applied heat fluxes, neglecting the liquid layer and solving a pure vaporization problem would be accurate.

In Figures 11, 12 and 13, the magnitudes of Stefan numbers \( \beta_m \) and \( \beta_v \) for a semi-infinite medium are lowered by one tenth from their values in Figs. 8, 9 and 10. These parameters are basically the ratio between sensible heat and latent heat. For the case of \( \theta_m = 0 \), where the initial velocity of the melt front starts at

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Figure 11. Phase front behavior for a semi-infinite medium ($\theta_m = 0$): (a) Position (b) Velocity
Figure 12. Phase front behavior for a semi-infinite medium ($\beta_m = 0.5$): (a) Position (b) Velocity
Figure 13. Phase front behavior for a semi-infinite medium ($\theta_m = 0.8$): (a) Position (b) Velocity
\[ V_m = Q_0 \beta_m \] reducing \( \beta_m \) by a factor of 10 also reduces the initial value of \( V_m \) by a factor of 10. For different cases of \( \theta_m \), the time to initiate vaporization is later for the lower value of \( \beta_m \). For nonzero values of \( \theta_m \), the time to initiate melting is independent of \( \beta_m \) because the effects of latent heat aren't seen by the solid during Period 1. Lowering the values of \( \beta_m \) and \( \beta_v \) also affects the quasi-steady state behavior of the phase change problem. It takes longer for the problem to reach a quasi-steady state when the ratio of sensible heat to latent heat is reduced by a factor of 10. Also, the quasi-steady state velocity is lower for low values of \( \beta_m \) and \( \beta_v \).

Changing the magnitudes of the applied heat flux and the melt temperature has an effect on the time to initiate melting and the time to initiate vaporization. These times are summarized in Fig. 14 for the lowest possible melt temperature \( \theta_m = 0 \) and a high melt temperature \( \theta_m = 0.8 \). The thermal and physical parameters of the semi-infinite medium are: \( A = 1 \), \( K = 1 \), \( \beta_m = 2 \) and \( \beta_v = 2 \). No data points are shown for the time to initiate melting, \( \tau_m \) when \( \theta_m = 0 \) because melting occurs immediately for any applied heat flux. Naturally, some preheat time is necessary when \( \theta_m = 0.8 \) and for every order of magnitude that \( Q_o \) is raised, the time to initiate melting drops by approximately two orders of magnitude. The same trend also applies for the time to initiate vaporization, \( \tau_v \). When applying any value of heat flux on a semi-infinite medium, it always takes a bit longer to initiate vaporization for \( \theta_m = 0 \) than it does for \( \theta_m = 0.8 \).
Figure 14. Effect of applied heat flux and melt temp. on the time to initiate melting and time to initiate vaporization for a semi-infinite medium.
4.2.2 Finite medium

Similar analysis of phase front behavior is now made for a finite medium. As before, phase front behavior is exhibited initially for an applied heat flux of $Q_o = 1$, and then for $Q_o = 5$. Figures 15, 16 and 17 are for a medium of length $x_L = 1$ with $A = 1, K = 1, \beta_m = 2$ and $\beta_v = 2$. For a finite medium, both phase fronts eventually reach the back wall. Naturally, this doesn't happen for a semi-infinite medium. In Fig. 15, $\theta_m = 0$, so melting starts immediately, and initially $V_m = Q_o \beta_m$. In Fig. 16, $\theta_m = 0.5$ and in Fig. 17, $\theta_m = 0.8$. For these two cases, some preheat time is necessary and $V_m$ is initially zero.

Depending on the problem parameters, melting and vaporization may be occurring at the same time, or melting may be completed before vaporization even begins. For example, Fig. 15 shows that for a finite medium exposed to a constant heat flux $Q_o = 5$ and having a melt temperature $\theta_m = 0$, vaporization begins shortly after melting is initiated and both continue together for a distinct amount of time. On the other hand, if the same medium is exposed to a heat flux of $Q_o = 1$, melting begins immediately, continues for a while then ends before the initiation of vaporization.

If melting and vaporization occur at the same time, the exact behavior of the two velocities is a bit unpredictable, as it changes for different values of melt temperatures and Stefan numbers of melting and vaporization ($\beta_m, \beta_v$). In Figs. 15 - 17, $\beta_m = \beta_v = 2$. In Fig. 15 where $\theta_m = 0$ and $Q_o = 5$, $V_m$ and $V_v$ gradually converge.
Figure 15. Phase front behavior for a finite medium ($\theta_m = 0$): (a) Position (b) Velocity

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Figure 16. Phase front behavior for a finite medium ($\theta_m = 0.5$): (a) Position (b) Velocity
Figure 17. Phase front behavior for a finite medium ($\theta_m = 0.8$): (a) Position (b) Velocity
to the same value as melting nears completion. This convergence is reminiscent of the semi-infinite case. In Fig. 16 where $\theta_m = 0.5$ and $Q_o = 1$, the velocities of the two phase fronts seem to be on the way to converging to the same value, until melting is completed. However, for the case of $Q_o = 5$, the phase front velocities converge momentarily, then drift apart, then suddenly converge again as melting nears completion. In Fig. 17 where $\theta_m = 0.8$ and $Q_o = 5$, the two phase front velocities almost immediately converge to the same value, and increase together for a distinct amount of time before separating just a bit. As in Fig. 16, they suddenly converge again as melting nears completion. For $Q_o = 1$, the behavior of the velocities in Fig. 17 is a more gradual convergence to the same value.

In Figs. 18 - 20, $\beta_m = \beta_v = 0.2$. In Fig. 18, where $\theta_m = 0$ and $Q_o = 5$, the behavior of the velocities is very similar to the same case with $\beta_m = \beta_v = 2$, described above (Fig. 15). The major differences are in the initial value of $V_m$ and the final value of $V_v$. Similar behavior is exhibited by the phase front velocities in Fig. 19, where $\theta_m = 0.5$ and $Q_o = 5$, and in Fig. 20, where $\theta_m = 0.8$ and $Q_o = 5$. The velocities converge to a shared value, which stays relatively constant until the completion of melting. Contrast this with the less orderly behavior already described for higher $\beta_m$ and $\beta_v$ in Figs. 16 and 17. Similar convergence of the phase front velocities also occurs in Fig. 19 and Fig. 20 for the lower heat flux, $Q_o = 1$, although in Fig. 19, where $\theta_m = 0.5$, the velocities do not absolutely converge to the same value as melting nears completion.
Figure 18. Phase front behavior for a finite medium ($\theta_m = 0$): (a) Position (b) Velocity
Figure 19. Phase front behavior for a finite medium ($\theta_m = 0.5$): (a) Position (b) Velocity
Figure 20. Phase front behavior for a finite medium ($\theta_m = 0.8$): (a) Position (b) Velocity
In all cases described above, melting and vaporization occur simultaneously and when melting is completed, the velocity of the vapor front shoots up. As the vapor front reaches the back wall, the domain becomes extremely small and there is hardly any gradient in the temperature distribution of the liquid, causing the vapor front velocity to approach \( V_v = Q_o \beta_v \). There is almost no remaining sensible energy and consequently, the energy balance Eq. 2.23 at the vapor front dictates that the applied heat flux, \( Q_o \), is almost completely absorbed as latent energy.

Most cases of phase front behavior shown in Figs. 15 - 20 have melting and vaporization occurring together. It is also possible for melting to occur alone, with the initiation of vaporization coming after melting is completed. This occurs when \( \theta_m = 0 \) and \( Q_o = 1 \) for both the case of \( \beta_m = \beta_v = 2 \) (Fig. 15) and \( \beta_m = \beta_v = 0.2 \) (Fig. 18). In Fig. 15, \( V_m \) gradually drops as the melt front reaches the back wall, while in Fig. 18, \( V_m \cong \) constant. Vaporization begins with \( V_v \) increasing from zero to a value of \( V_v = Q_o \beta_v \). For \( \beta_m = \beta_v = 0.2 \), \( V_v \) reaches this terminal value early in Period 3 and remains constant. For \( \beta_m = \beta_v = 2 \), \( V_v \) gradually increases and reaches its terminal value.

Making changes in the thermal diffusivity and thermal conductivity has an interesting effect on the phase front behavior of a finite medium. In Fig. 21, for \( \beta_m = \beta_v = 1 \), \( \theta_m = 0.8 \), \( Q_o = 1 \) and \( X_t = 1 \), phase front behavior is first exhibited for \( A = 0.1, K = 0.1 \). In other words, the solid thermal conductivity is ten times the liquid thermal conductivity. The opposite extreme is also shown with \( A = 10, K = 10 \). For \( A = K = 0.1 \), melting and vaporization occur together and
Figure 21. Phase front behavior for different thermal properties: (a) Position (b) Velocity
there is a small distance between the two phase fronts. The two phase front velocities gradually converge to the same value and quasi-steady behavior holds until melting is completed. At this time, the velocity of the vapor front rises rapidly to a terminal value approaching \( V_v = Q_o \beta_v \). For \( A = K = 10 \), the phase front behavior is completely different. Melting begins at the same time it does for \( A = K = 0.1 \). However, melting is completed and conduction in the liquid occurs for a while before the onset of vaporization. The velocity of the vapor front immediately shoots up and then gradually approaches its terminal value. This terminal value of \( V_v \) is the same for both pairs of thermal properties and the time required to complete vaporization is also the same. However, it takes much longer to complete melting when \( A = K = 0.1 \).

Changing the magnitudes of the applied heat flux and the melt temperature has an effect on the time to initiate melting and the time to initiate vaporization. These times are summarized in Fig. 22 for the lowest possible melt temperature \( \theta_m = 0 \) and a high melt temperature \( \theta_m = 0.8 \). The thermal and physical parameters of the finite medium are: \( A = 1, K = 1, \beta_m = 2, \beta_v = 2 \) and \( X_L = 1 \). As shown previously in Fig. 14, \( \tau_m = 0 \) when \( \theta_m = 0 \), while some preheat time is necessary when \( \theta_m = 0.8 \). When \( Q_o \) is lowered by an order of magnitude, the corresponding rise in \( \tau_m \) and \( \tau_v \) is approximately one order of magnitude. However, for \( Q_o \geq 1 \), when \( Q_o \) is raised by an order of magnitude, the corresponding drop in \( \tau_m \) and \( \tau_v \) is approximately two orders of magnitude. As in Fig. 14, it always takes a bit longer to initiate vaporization for \( \theta_m = 0 \) than it does for

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Figure 22. Effect of applied heat flux and melt temperature on the time to initiate melting and time to initiate vaporization for a finite medium.
\( \theta_m = 0.8 \). However, for \( Q_o \leq 1 \), there is hardly any difference in \( \tau_v \) for different melt temperatures.

Changing the magnitudes of the applied heat flux and the melt temperature also has an effect on the time to complete melting and the time to complete vaporization for different size domains. These times are summarized in Fig. 23 for the lowest possible melt temperature \( \theta_m = 0 \), an intermediate melt temperature \( \theta_m = 0.5 \) and a high melt temperature \( \theta_m = 0.8 \). The thermal and physical properties of the finite medium are \( \alpha = 1, k = 1, \beta_m = 0.2, \beta_v = 0.2 \) and \( X_l = 1 \). The applied heat fluxes under consideration are \( Q_o = 1, Q_o = 10 \) and \( Q_o = 100 \). For each of the three values of \( Q_o \), the time to complete vaporization for a medium of length \( X_l \) has no dependence on the melt temperature. By performing an energy balance between the energy applied at the origin and the energy required to totally ablate the domain, an analytical expression can be found for the time to totally ablate the domain, both in real variables and in dimensionless variables:

\[
t_{abl} = \frac{x_l}{\rho o} \left[ \rho_s L_m + \rho_s C_{ps}(T_m - T_{IN}) + \rho_v L_v + \rho_v C_p(T_v - T_m) \right] \\
[4.3]
\]

\[
\tau_{abl} = \frac{x_l}{Q_o} \left[ \frac{1}{\beta_m} + \frac{1}{\beta_v} + \theta_m(1 - \frac{K}{A}) + \frac{K}{A} \right], \\
[4.4]
\]

The trend just described from Fig. 23 is confirmed in Eq. 4.4 for \( \alpha = K = 1 \). Again referring to Fig. 23, when increasing the domain length by one order of magnitude, \( \tau_{abl} \) increases by approximately one order of magnitude. This is true for each of the heat fluxes under consideration. These trends are also confirmed

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Figure 23. Effect of applied heat flux, melt temperature and length of medium on the time to complete melting and time to complete vaporization.

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in Eq. 4.4. For a low heat flux of \( Q_o = 1 \), the time to complete melting \( \tau_{melt} \) occurs much earlier than \( \tau_{abl} \) for \( X_L \leq 0.1 \) and there is little discrepancy between the values of \( \tau_{melt} \) obtained from the three melt temperatures. In general, the lower the melt temperature, the less time it takes to complete melting. For \( Q_o = 10 \) and \( Q_o = 100 \), close agreement in \( \tau_{melt} \) for different melt temperatures occurs for longer domains, \( X_L \geq 1 \). Also, for the larger values of \( Q_o = 10 \) and \( Q_o = 100 \), ablation of the domain is completed almost immediately after melting is completed, especially for \( Q_o = 100 \) and \( X_L > 0.1 \). For any value of \( Q_o \), it is apparent that as the domain length gets longer, the difference between \( \tau_{melt} \) and \( \tau_{abl} \) gets smaller.

4.2.3 Pulsed heat source

Physical behavior of the melt and vapor phase fronts is now presented for the case of a pulsed (on and off) heat flux. In Fig. 24, a finite medium with \( \theta_m = 0 \), \( A = K = 1 \), \( \beta_m = \beta_v = 1 \) and \( X_L = 1 \) is exposed to a heat flux \( Q_o = 1 \) which has an on time \( \tau_{on} = 0.9 \) and an off time \( \tau_{off} = 0.1 \). Melting begins immediately and is completed before vaporization begins. The melt front has an initial velocity of \( V_m = Q_o \beta_m \) and during the initial on period for \( Q_o \), the melt front velocity gradually drops. When the heat source is turned off for the first time, the melt front continues to move forward but its velocity drops at a faster rate than during the on time for \( Q_o \). The melt front velocity continues to drop at this faster rate even as the heat source is turned on again. As the heat applied at the origin propagates to the melt front, the net sensible energy at the melt front begins to

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Figure 24. Phase front behavior for a finite medium ($\theta_m = 0$): exposed to a pulsed heat source (a); (b) Position (c) Velocity
rise and so does the melt front velocity (see Eq. 2.7). Melting is completed a short while later and conduction of an all liquid domain occurs during the second on time for $Q_o$. Vaporization begins and the vapor front moves toward the back wall with an increasing velocity. When the heat source is turned off for a second time, the vapor front immediately becomes stationary for the duration of the off time. This is because there is no net sensible energy entering the vapor front. Once the heat source is turned on for the third time, the vapor front velocity initially shoots up then gradually increases again until the heat source is turned off, at which time there is no net sensible energy entering the vapor phase front and it becomes stationary. As before, once the heat source is turned on again, $V_v$ shoots up again, then gradually increases to a terminal value of $V_v = Q_o \beta_v$ as the melt front approaches the back wall.

In Fig. 25, a finite medium with the same thermal and physical properties is exposed to the same pulsed heat source as in Fig. 24. However, this medium has a high melt temperature $\theta_m = 0.9$ and melting does not occur immediately. Also melting and vaporization both begin during the initial on time for $Q_o$. Both phase front velocities increase from zero until the heat source is turned off. At this time, there is no net sensible energy entering the vapor front and it remains fixed, very close to the origin. The sensible energy entering the melt front from the liquid is less than the sensible energy leaving to the solid, causing the melt front to move in the opposite direction with a negative velocity. This phenomenon cannot occur for $\theta_m = 0$ because of the isothermal temperature distribution in the solid region.
Figure 25. Phase front behavior for a finite medium ($\theta_m = 0.9$) exposed to a pulsed heat source
(a), (b) Position (c) Velocity

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In other words, for $\theta_m = 0$, there is never any sensible energy leaving the melt front so the lowest $V_m$ can become is zero.

In Fig. 26, a finite medium with $\theta_m = 0$ and $A = 1$, $K = 1$, $\beta_m = 1$, $\beta_v = 1$, $X_L = 1$ is exposed to a pulsed heat source with an on time of $\tau_{on} = 0.1$ and an off time of $\tau_{off} = 0.9$. As is the case in Fig. 24, where $\tau_{on} = 0.9$ and $\tau_{off} = 0.1$, melting begins immediately and is completed before vaporization begins. The melt front moves forward in a stepwise fashion as the heat source is continually turned on and off.

This stepwise motion eventually degenerates into a crude linear motion as the effect of turning off the heat source at the origin isn’t felt as much by the melt front, which is further into the material. The melt front does not immediately stop moving once the heat source turns off because sensible energy is still supplied to the melt front. However, as the origin continues to be denied heat, the sensible energy supplied to the melt front dwindles until there is no net sensible energy left to drive the melt front forward. At the beginning of Period 2, the melt front is still very close to the origin, causing the melt front to be immobilized early in the off cycle. As the melt front moves further into the domain, the impact of turning the heat source off is less immediate on the halting of the melt front. In fact, on the final off cycle during during melting, the melt front slows down but does not reach a zero velocity. After melting is completed, the temperature of liquid at the origin, $\theta_L$, fluctuates because the heat source is turned on and off a number of times. Eventually, $\theta_L = 1$ and vaporization begins. The vapor front is imme-
Figure 26. Phase front behavior for a finite medium ($\theta_m = 0$): exposed to a pulsed heat source (a): (b) Position (c) Velocity.
diately denied any incoming sensible energy when the pulsed heat source is turned off, leading to a clear stepwise movement as long as vaporization occurs. The vapor front velocity immediately drops to zero once $Q_o$ is turned off, leading to a gradually increasing, pulsed $V_v$, whose terminal value approaches $V_v = Q_o \beta_v$.

In Fig. 27, the same material with $\theta_m = 0.9$ is again exposed to a pulsed heat source with $\tau_{on} = 0.1$ and $\tau_{off} = 0.9$. Preheat time is required before melting starts and vaporization begins shortly thereafter. Both the melt and vapor phase front are in existence, however each front is affected a little differently by turning off the heat source. During the early stages of melting, the melt front is still very close to the origin and more sensible energy is released from it than supplied into it, causing the melt front to back up to the origin with negative velocity. This happens twice during Period 2. Once vaporization begins, the vapor front is immediately immobilized whenever the heat source is turned off because there is no sensible energy entering the vapor front. The vapor front position evolves in a stepwise fashion and the vapor front velocity has a spiked appearance, which is more easily apparent in Fig. 27 once melting is completed. The melt front does not immediately become immobilized when $Q_o$ is turned off because in the beginning of the off time, it does receive more sensible energy than it loses. The net sensible energy entering the melt front continues to drop as $Q_o$ stays off and eventually during the off cycle, both phase fronts are immobilized. Once melting is completed, the vapor front approaches a final velocity of $V_v = Q_o \beta_v$.

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Figure 27. Phase front behavior for a finite medium ($\theta_m = 0.9$): exposed to a pulsed heat source.
(a): (b) Position (c) Velocity
In Figs. 24 and 25, where the melt temperatures are different but the type of heat source is the same, there is no difference in the time required to totally ablate the finite medium. For a pulsed heat source with a short on time and a long off time (Figs. 26 and 27), there is no difference in the time required to complete ablation for finite mediums with different melt temperatures. However, it takes approximately nine times longer to complete ablation when the on time is reduced by a factor of nine. The same amount of energy is required to completely melt, then completely ablate the material, however for short pulses of heat applied at the origin, less energy is supplied per pulse than for the longer pulses of heat.

In Fig. 28 a comparison of phase front behavior is made between a pulsed heat source and a constant heat source. The thermal and physical properties are $A = K = 1$, $\beta_m = \beta_v = 1$ for a domain length of $X_L = 1$ and $\theta_m = 0$. For the case of a constant applied heat flux, $Q_o = 1$, melting begins immediately, and is completed before the onset of vaporization. The melt front velocity gradually drops from its initial value of $V_m = Q_o \beta_m = 1$. The vapor front velocity gradually rises from zero to a final value approaching $V_v = Q_o \beta_v = 1$.

For the case of a pulsed heat flux, $Q_o = 10$ with $\tau_{on} = 0.1$ and $\tau_{off} = 0.9$, the total energy supplied to the medium over the entire cycle time $\tau = \tau_{on} + \tau_{off}$ is equivalent to the energy supplied by the constant heat flux $Q_o = 1$ over the same cycle time. The initial melt front velocity is $V_m = Q_o \beta_m = 10$ and the final vapor front velocity approaches $V_v = Q_o \beta_v = 10$. Melting and vaporization occur together and the vapor front reaches the back wall soon after the melt front. Because no en-
Figure 28. Comparison of phase front behavior for a finite medium ($\dot{\theta}_m = 0$): exposed to (a) a pulsed heat source versus a constant heat source (b) Position (c) Velocity
ergy is supplied at the vapor front during each off cycle, both phase fronts propagates in a stepwise fashion. During each on cycle the melt front velocity drops while the vapor front velocity rises. When the heat source is turned off, the vapor front immediately halts its propagation toward the back wall, while the melt front slows down until it eventually attains zero velocity.

The most interesting physical trend in Fig. 28 is that for this set of parameters, it takes less time to totally ablate the domain when using the pulsed heat source. Basically, it takes less time to supply the energy required to complete ablation for the case of a pulsed heat source as most of the energy supplied by the heat flux goes to latent heat. This effect allows the phase fronts to propagate with higher velocities than for the case of the constant heat flux.

### 4.2.4 Pure vaporization

An interesting special case occurs when $\theta_m = \theta_v = 1$. Vaporization occurs on the solid material and only the vapor phase front is in existence. Two specific cases are exhibited in Fig. 29, where $A = 1$, $K = 1$, $\beta_m = 2$, $\beta_v = 2$, and $X_r = 1$. For an applied heat flux of $Q_o = 5$, after a short amount of preheat time, the vapor phase front velocity jumps from an initial value of zero, then gradually rises for a while, then jumps again to a final value approaching $V_v = Q_o \beta_v$ as the vapor front gets very close to the back wall. For an applied heat flux of $Q_o = 1$, a much longer amount of preheat time is necessary and the increase in the vapor front velocity is more gradual. The terminal velocity of $S_v$ is naturally smaller than the previous
Figure 29. Phase front behavior for pure vaporization of a solid ($\theta_m = \theta_v = 1$): (a) Position, $S_m = S_v = S$ (b) Velocity, $V_m = V_s = V$
case because $Q_s$ is smaller. Also, it takes a longer time to complete ablation of a solid for smaller applied heat fluxes.

### 4.3 APPLICATION TO PURE METALS

Up to this point, dimensionless variables have been used exclusively in the presented results. This section contains results of the BEM code for two cases: 1) melting of a semi-infinite pure metal by a constant applied heat flux $q_o$ which is turned off once vaporization begins and 2) pure vaporization of a semi-infinite pure metal due to an intense, pulsed heat flux. For the melting problem, results of the BEM code are compared to a finite difference solution found in the literature. For the pure vaporization problem, results of the BEM code are compared to experimental data.

Considering melting of a semi-infinite pure metal, because the heat flux is turned off once melting starts, the left boundary of the liquid thus remains at the origin, $x = x_o$. The melt front continues to move away from the origin at decreasing velocity because of the diminishing sensible heat entering the melt front. The melt front finally attains a maximum distance away from the origin at $t = t_{\text{max}}$. At times after $t_{\text{max}}$, the melt front moves in the opposite direction, provided the applied heat flux remains off.
Three pure metals were considered, Aluminum, Iron and Nickel. Their thermal and physical properties [71] are presented in Table 4. For a pure metal exposed to an arbitrary heat flux which is turned off at the onset of vaporization, there are three significant times: the time at which melting starts, \( t_m \), the time at which vaporization starts, \( t_v \), and the time at which the melt front attains its maximum position, \( t_{\text{max}} \). Interestingly enough, for a given metal, the values of \( q_o \sqrt{t_m} \), \( q_o \sqrt{t_v} \), \( q_o \sqrt{t_{\text{max}}} \) remain constant regardless of the value of \( q_o \). For a semi-infinite medium, both the time to initiate melting and the time to initiate vaporization are inversely proportional to the square of the applied heat flux:

\[
q_o^2 \propto \frac{1}{t_m}, \quad q_o^2 \propto \frac{1}{t_v}
\]

This trend is confirmed in Fig. 14.

Table 5 provides the values of \( q_o \sqrt{t_m} \), \( q_o \sqrt{t_v} \), and \( q_o \sqrt{t_{\text{max}}} \) for Aluminum, Iron and Nickel. A comparison is made to the values obtained from a finite difference scheme implemented by Hsu et al. [71]. There is excellent agreement among the values given by the BEM and FD schemes, with a maximum difference of 3 percent.

The second application under consideration is pure vaporization of a semi-infinite metallic element due to an intense heat flux with on time \( t_{\text{on}} \), which is applied once and then turned off. Only a vapor front exists because \( T_m = T_v \). The vapor front continues to move away from the origin, as long as \( 0 < t < t_{\text{on}} \), but once \( t > t_{\text{on}} \), it reaches a maximum depth, defined as \( x(t_{\text{on}}) \). Such a physical model can be
Table 4. Thermal and physical properties of selected elements used for Table 5

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<td>1728</td>
<td>3005</td>
<td>74</td>
<td>43</td>
<td>1.5</td>
<td>0.83</td>
<td>2.99</td>
</tr>
</tbody>
</table>
Table 5. Comparison of characteristic time values for the BEM and FD

<table>
<thead>
<tr>
<th>Element</th>
<th>$q_n\sqrt{t_m}$ J m$^{-3}$ s$^{-1/2}$</th>
<th>$q_n\sqrt{t_s}$ J m$^{-3}$ s$^{-1/2}$</th>
<th>$q_n\sqrt{t_{max}}$ J m$^{-3}$ s$^{-1/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum (BEM)</td>
<td>$1.43 \times 10^7$</td>
<td>$4.24 \times 10^7$</td>
<td>$5.10 \times 10^7$</td>
</tr>
<tr>
<td>(FD)</td>
<td>$1.43 \times 10^7$</td>
<td>$4.21 \times 10^7$</td>
<td>$5.19 \times 10^7$</td>
</tr>
<tr>
<td>Iron (BEM)</td>
<td>$2.03 \times 10^7$</td>
<td>$4.16 \times 10^7$</td>
<td>$4.34 \times 10^7$</td>
</tr>
<tr>
<td>(FD)</td>
<td>$2.02 \times 10^7$</td>
<td>$4.07 \times 10^7$</td>
<td>$4.26 \times 10^7$</td>
</tr>
<tr>
<td>Nickel (BEM)</td>
<td>$2.42 \times 10^7$</td>
<td>$4.25 \times 10^7$</td>
<td>$4.39 \times 10^7$</td>
</tr>
<tr>
<td>(FD)</td>
<td>$2.43 \times 10^7$</td>
<td>$4.27 \times 10^7$</td>
<td>$4.41 \times 10^7$</td>
</tr>
</tbody>
</table>
applied to laser drilling, and experimental results documenting the measured final depth of a laser-drilled hole are provided from Bar-Isaac and Korn [72]. Considering three pure metals, Aluminum, Copper and Lead, whose properties [72] are given in Table 6, a comparison of BEM results to the experimental measurements is summarized in Table 7.

If a material is subjected to an extremely intense, pulsed heat flux for only an instant in time, vaporization begins early in the pulse on time and it is reasonable to assume negligible conduction in the solid material at the vicinity of the vapor phase front. Consequently, for a given \( t_{on} \), the final position of \( S_r \) i.e. the hole depth, can be calculated from Eq. 4.3. The BEM almost exactly returns the expected value of \( x(t_{on}) \). A comparison of the analytical and numerical values of hole depth for this limiting case are summarized in Table 7. An on time of \( t_{on} = 1 \) msec was used in the BEM code.

Comparison to experimental results was made using an time of \( t_{on} = 50 \) msec. The value of hole depth returned by the BEM is less than for the case of \( t_{on} = 1 \) msec because there is some conduction in the solid at the vicinity of the vapor front. The experimental apparatus used in [72] consists of a pulsed ruby laser with its focal plane on the surface of the metal and energies of 1.8 and 5.6 Joules. The authors measured the final hole depth microscopically. Generally, it is difficult to experimentally measure the depth of a laser-drilled hole because of lighting problems. The authors therefore took an average value of \( x(t_{on}) \) from three measured holes. The authors specified only that \( t_{on} > 1.0 \) msec so a value
Table 6. Thermal and physical properties of selected elements used for Table 7

<table>
<thead>
<tr>
<th>Element</th>
<th>( \rho_r ) ( \text{kg/m}^3 )</th>
<th>( T_{in} ) K</th>
<th>( T_{in} = T_r ) K</th>
<th>( k_r ) W m K^{-1}</th>
<th>( \alpha_r ) m^2 s^{-1} X10^{-5}</th>
<th>( L_r ) J kg X10^{-5}</th>
</tr>
</thead>
<tbody>
<tr>
<td>Aluminum</td>
<td>2700</td>
<td>298</td>
<td>2673</td>
<td>290</td>
<td>8.6</td>
<td>109.4</td>
</tr>
<tr>
<td>Copper</td>
<td>8940</td>
<td>298</td>
<td>2855</td>
<td>390</td>
<td>11.4</td>
<td>50.0</td>
</tr>
<tr>
<td>Lead</td>
<td>11340</td>
<td>298</td>
<td>2024</td>
<td>35.8</td>
<td>2.5</td>
<td>9.92</td>
</tr>
</tbody>
</table>
Table 7. Comparison of measured and calculated depths of laser-drilled holes

<table>
<thead>
<tr>
<th>Element</th>
<th>Energy</th>
<th>Measured depth $x(t_{on})$</th>
<th>Hole depth, $x(t_{on})$ from Eq. 4.3</th>
<th>$x(t_{on})$, (BEM) using $t_{on} = 1,\text{ms}$</th>
<th>$x(t_{on})$, (BEM) using $t_{on} = 50,\text{ms}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Al</td>
<td>1.8 J</td>
<td>1.86 mm</td>
<td>2.10 mm</td>
<td>2.10 mm</td>
<td>1.80 mm</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>2.98</td>
<td>3.17</td>
<td>3.18</td>
<td>3.03</td>
</tr>
<tr>
<td>Cu</td>
<td>1.8</td>
<td>1.43</td>
<td>1.75</td>
<td>1.75</td>
<td>1.50</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>2.25</td>
<td>2.53</td>
<td>2.54</td>
<td>2.12</td>
</tr>
<tr>
<td>Pb</td>
<td>1.8</td>
<td>2.87</td>
<td>2.93</td>
<td>2.95</td>
<td>2.64</td>
</tr>
<tr>
<td></td>
<td>5.0</td>
<td>4.27</td>
<td>4.30</td>
<td>4.31</td>
<td>3.81</td>
</tr>
</tbody>
</table>
of $t_{on} = 50$ msec was used in the BEM code. The experimentally measured hole depths are less than for the limiting case of no diffusion losses, calculated from Eq. 4.3. The measured depths are also generally less than the hole depths given by the BEM when $t_{on} = 50$ msec.

A variety of physical effects, not incorporated in the one-dimensional BEM formulation, cause the actual hole depths to deviate from the theoretical values. The major physical effect is the reflectivity of the metal which causes only a fraction of the laser energy to be absorbed at the metal surface. Another effect is the accumulation of vaporized material, or plasma, in the laser-drilled hole, which "shields" the hole from the incident laser energy. Also, while $0 < t < t_{on}$, the further the hole's bottom moves from the laser focal plane, the larger the laser spot size. Consequently, the heat supplied decreases and the velocity of the vapor front drops as the pulse on time nears its end. Another physical effect is the loss of heat to the sides of the hole.
5.0 SUMMARY, CONCLUSIONS AND RECOMMENDATIONS

5.1 SUMMARY

The objectives of this thesis were to formulate an efficient numerical method (BEM) to solve one-dimensional heat transfer problems involving combined melting and vaporization, and to investigate the numerical and physical behavior of the combined melting and vaporization process. Previous solution techniques, both analytical and numerical were reviewed. The physics of the problem under consideration—the combined melting and vaporization of a finite medium, initially in the solid phase, exposed to a time varying applied heat flux at its origin—were described in great detail for all the possible situations which could arise. A derivation of the BEM integral equations followed, and was immediately accompanied with a set of discretized equations defined at the boundaries of a given
domain. An iterative, implicit numerical scheme was introduced in order to solve the BEM integral equations.

Results of the numerical scheme were presented for the numerical and physical behavior of finite and semi-infinite domains, and were expressed in terms of dimensionless variables. It was shown that a continued reduction in the time step size improved the accuracy of the BEM solution, up to a minimum time step size, whereafter there was little change in the BEM solution. For semi-infinite domains, a quasi-steady state behavior was confirmed. Comparisons of the physical behavior of finite domains with different thermal properties and applied heat fluxes were also made. Both constant and pulsed applied heat fluxes were considered in the results. A test case of selected metals was also run and results compared very favorably to a previous numerical solution. Another test case was run comparing the BEM results to experimental measurements and up to 25 percent error was reported because of the lack of multidimensional and other effects in the BEM model.

5.2 CONCLUSIONS

Upon completion of the theoretical analysis of combined melting and vaporization using the BEM, the conclusions which have been made are listed:

5.0 SUMMARY, CONCLUSIONS AND RECOMMENDATIONS
• The BEM scheme accurately tracks the phase change interface and solves for boundary temperatures and heat fluxes, when using a sufficiently fine time step.

• Confirmed expected physical effects:
  
  Quasi-steady behavior for a semi-infinite medium

  Pure vaporization is a good assumption for high heat fluxes and high melt temperatures

  Stepwise motion of phase fronts if heat source is pulsed (on and off)

• Can model natural and industrial phenomena (melting of ice, laser drilling)

5.3 RECOMMENDATIONS

After the successful implementation of a BEM scheme for the solution of the one-dimensional phase change heat transfer problem, several recommendations are listed. These are merely suggestions, which can be adopted to improve the BEM scheme and expand the scope of phase change problems it can handle.

• Implement a BEM scheme for two-dimensional applications (laser cutting)
• Allow for a moving applied heat source

• Introduce convection effects at the phase front boundaries

• Account for temperature dependent properties

• Apply the BEM to alloys, which experience phase changes over a temperature range
REFERENCES


Appendix A. Quasi-Steady State Solution:

Half-Space with Constant Surface Heat Flux

Assume that melting and vaporization have been occurring for a long time in a half space with \( q_o(t) = q_o = \text{const.} \). If

\[
\frac{ds_m}{dt} = \text{const.}, \quad \frac{ds_v}{dt} = \text{const.}, \quad s_m - s_v = \text{const.},
\]

then we expect a quasi-steady state with respect to the moving phase fronts. Let

\[
\begin{cases}
  z = x - s_v(t) \\
  t = t
\end{cases}
\]  

[A.1]

Thus

\[
\frac{\partial^2}{\partial x^2} = \frac{\partial^2}{\partial z^2}
\]
\[
\frac{\partial}{\partial t} = \frac{\partial}{\partial z} \frac{\partial z}{\partial t} + \frac{\partial}{\partial t} \frac{\partial t}{\partial t} = -s_v'(t) \frac{\partial}{\partial z} + \frac{\partial}{\partial t}
\]

With \(x_v \to \infty\) and \(q_s(t) = q_o = \text{const.}\), the Period 3 \((t < t_{mel})\) solid region, liquid region and interface Eqs. 2.1, 2.3 - 2.5, 2.7 - 2.8 and 2.10 - 2.11 now become

**Solid**

\[
\frac{\partial^2 T_s}{\partial z^2} = \frac{1}{\alpha_s} \left[-s_v'(t) \frac{\partial T_s}{\partial z} + \frac{\partial T_s}{\partial t}\right], \quad s_m - s_v < z < \infty
\]  \([A.2]\)

\(T_s \to T_{IN}, \quad z \to \infty\)  \([A.3]\)

**Liquid**

\[
\frac{\partial^2 T_l}{\partial z^2} = \frac{1}{\alpha_l} \left[-s_v'(t) \frac{\partial T_l}{\partial z} + \frac{\partial T_l}{\partial t}\right], \quad 0 < z < s_m - s_v
\]  \([A.4]\)

\(q_o = -k_l \frac{\partial T_l}{\partial z} + \rho L_v s_v'(t), \quad z = 0\)  \([A.5]\)

\(T_l = T_v, \quad z = 0\)  \([A.6]\)

**Interface conditions**

\(T_s = T_l = T_m, \quad z = s_m - s_v\)  \([A.7]\)

\[-k_l \frac{\partial T_l}{\partial z} + k_s \frac{\partial T_s}{\partial z} = \rho L_m s_m'(t), \quad z = s_m - s_v\]  \([A.8]\)
Note that when considering long time solutions, initial conditions are not relevant. If a quasi-steady state exists with respect to \( z = x - s, \) then the problem becomes independent of time and \( \frac{\partial}{\partial t} = 0 \) and the distance between phase fronts remains constant and both phase fronts share a constant velocity:

\[
s'_v = s'_m = v = \text{const.}, \quad s_m - s_v = d = \text{const}.
\]

Consequently, Eqs. A.2 - A.8 now become

**Solid**

\[
\frac{d^2 T_s}{dz^2} = -\frac{v}{\alpha_s} \frac{dT_s}{dz}, \quad d < z < \infty \quad [A.9]
\]

\[
T_s \to T_{IN}, \quad z \to \infty \quad [A.10]
\]

**Liquid**

\[
\frac{d^2 T_l}{dz^2} = -\frac{v}{\alpha_l} \frac{dT_l}{dz}, \quad 0 < z < d \quad [A.11]
\]

\[
q_0 = -k_l \frac{dT_l}{dz} + \rho L_v v, \quad z = 0 \quad [A.12]
\]

\[
T_l = T_v, \quad z = 0 \quad [A.13]
\]

**Interface conditions**

\[
T_s = T_l = T_m, \quad z = d \quad [A.14]
\]
\[- k_l \frac{dT_l}{dz} + k_s \frac{dT_s}{dz} = \rho L_m v, \quad z = d \quad [A.15]\]

The solutions to the ordinary differential Eqs. A.9 and A.11 can be expressed as

\[T_s(z) = C_1 + C_2 \exp\left(- \frac{v}{\alpha_s} z\right) \quad [A.16]\]

\[T_l(z) = C_3 + C_4 \exp\left(- \frac{v}{\alpha_l} z\right) \quad [A.17]\]

There are six unknown constants \((C_1, C_2, C_3, C_4, v, d)\) and six boundary conditions (Eqs. A.10, A.12 - A.15). Two conditions are given in Eq. A.14. Applying the conditions given in Eqs. A.10, A.14 to Eq. A.16 yields

\[T_s(z) = T_{IN} + (T_m - T_{IN}) \exp\left[- \frac{v}{\alpha_s} (z - d)\right] \quad [A.18]\]

Applying the conditions given in Eqs. A.13, A.14 to Eq. A.17 yields

\[T_l(z) = T_v - (T_v - T_m) \left[ \frac{1 - \exp\left(- \frac{v}{\alpha_l} z\right)}{1 - \exp\left(- \frac{v}{\alpha_l} d\right)} \right] \quad [A.19]\]

Expanding the exponential terms in Eq. A.19 in terms of a Taylor series for small \(\frac{z}{d}\), the liquid region temperature distribution is simplified for small \(\frac{z}{d}\)

\[T_l(z) = T_v - (T_v - T_m) \frac{z}{d}\]

Appendix A. Quasi-Steady State Solution: Half-Space with Constant Surface Heat Flux
The temperature gradients become

\[
\frac{dT_s}{dz} = - (T_m - T_{1N}) \frac{v}{\alpha_s} e^{-\frac{v}{\alpha_s}(z - d)}
\]

\[
\frac{dT_l}{dz} = - \frac{T_v - T_m}{1 - e^{-\frac{v}{\alpha_l}d}} \frac{v}{\alpha_l} e^{-\frac{v}{\alpha_l}z}
\]

Eqs A.12 and A.15 are used to find expressions for \( v \) and \( d \)

\[
v = \frac{q_o}{\rho [L_m + L_v + C_{ps}(T_m - T_{1N}) + C_p(T_v - T_m)]} \quad [A.20]
\]

\[
d = \frac{\alpha_l}{v} \ln \left[ \frac{L_m + C_{ps}(T_m - T_{1N}) + C_p(T_v - T_m)}{L_m + C_{ps}(T_m - T_{1N})} \right] \quad [A.21]
\]

As the applied heat flux \( q_o \) increases in magnitude, the quasi-steady state velocity \( v \) also increases while the distance between the phase fronts \( d \) decreases in magnitude.

**Pure Vaporization Limit**

In this case, \( T_m = T_v \), and because no melting occurs, \( L_m \) drops out. Eqs. A.18 - A.21 become

\[
v = \frac{q_o}{\rho [L_v + C_p(T_v - T_{1N})]} \quad [A.22]
\]
\[ d = \frac{\alpha}{v} \ln \left[ \frac{T_v - T_{IN}}{T_m - T_{IN}} \right] \] [A.23]

\[ T_s(z) = T_{IN} + (T_v - T_{IN})e^{-\frac{v}{\alpha} z} \] [A.24]

\[ T_f(z) = T_{IN} + (T_v - T_{IN})e^{-\frac{v}{\alpha} z} \] [A.25]
Appendix B. Integrals of One-Dimensional, Full-Space Green’s Functions

Time integrals:

\[
\int_{t_1}^{t_2} G(x,t|x_0, t_0) dt_0 = \left[ \frac{x - x_0}{\sqrt{\pi} 2\alpha} \right] \left\{ -\frac{1}{z_2} \exp(-z_2^2) + \frac{1}{z_1} \exp(-z_1^2) \right\} - \sqrt{\pi} \left[ \text{erf}(z_2) - \text{erf}(z_1) \right] \]  

\[B.1\]

\[
\int_{t_1}^{t_2} \frac{\partial G}{\partial x_0} (x,t|x_0, t_0) dt_0 = \frac{1}{2\alpha} \left[ \text{erf}(z_2) - \text{erf}(z_1) \right] \]  

\[B.2\]

where

\[
z_1 = \frac{x - x_0}{\sqrt{4\alpha(t - t_1)}} \quad \text{and} \quad z_2 = \frac{x - x_0}{\sqrt{4\alpha(t - t_2)}}
\]
Spatial integral:

\[
\int_{x_1}^{x_2} G(x,t/x_0,\tau_0)dx_0 = \frac{1}{2} \left[ \text{erf}(y_1) - \text{erf}(y_2) \right]
\]

where

\[
y_1 = \frac{x - x_1}{\sqrt{4\alpha(t - t_0)}}, \quad y_2 = \frac{x - x_2}{\sqrt{4\alpha(t - t_0)}}
\]
Appendix C. Exact Solution for Period 1 with Constant Applied Heat Flux

Considering conduction of a solid without phase change, the governing equation, boundary conditions and initial condition given by Eqs. 2.1 - 2.4 are repeated:

\[
\frac{\partial^2 T_s}{\partial x^2} = \frac{1}{\beta_s} \frac{\partial T_s}{\partial t} \quad , \quad x_o \leq x \leq x_L
\]

\[-k_s \frac{\partial T_s}{\partial x} = q_o \quad , \quad x = x_o\]

\[\frac{\partial T_s}{\partial x} = 0 \quad , \quad x = x_L\]

\[T_s = T_{IN} \quad , \quad t = 0\]

Assume the following temperature distribution:

\[T_s(x,t) = T_{fr}(x,t) + \Phi(x) + \Gamma(t) , \quad [C.1]\]
where the first term is transient, homogeneous, and exponentially decaying, the second term is the shape function that accounts for \( q_o \), and the third term is an accumulation term. Substituting Eq. C.1 into Eqs. 2.1 - 2.3 yields

\[
\frac{\partial^2 T_{tr}}{\partial x^2} + \frac{d^2 \Phi}{dx^2} = \frac{1}{\alpha_s} \frac{\partial T_{tr}}{\partial t} + \frac{1}{\alpha_s} \frac{d\Gamma}{dt}
\]

\[-k_s \frac{\partial T_{tr}}{\partial x} - k_s \frac{d\Phi}{dx} = q_o , \quad x = x_o\]

\[
\frac{\partial T_{tr}}{\partial x} + \frac{d\Phi}{dx} = 0 , \quad x = x_L
\]

make the following choices for the \( \Phi \) and \( \Gamma \) functions:

\[
\frac{d^2 \Phi}{dx^2} = \frac{1}{\alpha_s} \frac{d\Gamma}{dt} = C
\]

\[-k_s \frac{d\Phi}{dx} = q_o , \quad x = x_o\]

\[
\frac{d\Phi}{dx} = 0 , \quad x = x_L
\]

\( \Gamma(0) = 0 \),

where \( C \) is an independent function of \( x \) and \( t \) and the initial condition of \( \Gamma \) is arbitrarily chosen to be zero. Integrating the shape function and the accumulation term then yields
\[ \Phi(x) = \frac{q_o x_L}{k_s} \left[ \frac{1}{2} \left( \frac{x}{x_L} \right)^2 - \left( \frac{x}{x_L} \right) \right] \]  

\[ \Gamma(t) = \frac{\alpha_s}{k_s} \frac{q_o}{x_L} t \]  

Solving the homogeneous portion by the integral transform method leads to the following expression:

\[ T_r(x,t) = T_{IN} + \frac{1}{3} \frac{q_o}{k_s} x_L + \sum_{m=1}^{\infty} C_m e^{-\alpha_s \beta_m^2 t} \cos(\beta_m x) \]  

\[ C_m = -2 \alpha_s \frac{q_o}{k_s} \frac{1}{\beta_m^2}, \quad \beta_m = \frac{m\pi}{x_L} \]

Putting the three portions together yields the final expression for the temperature distribution during Period 1:

\[ T_s(x,t) = T_{IN} + \frac{\alpha_s}{k_s} \frac{q_o x_L}{k_s} t + \frac{q_o x_L}{k_s} \left[ \frac{1}{2} \left( \frac{x}{x_L} \right)^2 - \left( \frac{x}{x_L} \right) + \frac{1}{3} \right] \]

\[ + \sum_{m=1}^{\infty} C_m e^{-\alpha_s \beta_m^2 t} \cos(\beta_m x) \]  

Appendix C. Exact Solution for Period 1 with Constant Applied Heat Flux
Appendix D. Negligible Sensible Heat Approximation

Following is a derivation of the solution to the phase change problem with $T_{IN} = T_m$ for the case of negligible sensible heat. Because no preheat time is necessary, the Period 2 solution is first considered.

**PERIOD 2**

**Solid region**

Assuming $C_{ps} \to 0$, yields $\alpha_s \to \infty$, which causes the right side of energy Eq. 2.1 to drop out:
\[
\frac{d^2 T_s}{dx^2} = 0 \quad [D.1]
\]

The solid region has the boundary conditions

\[
\frac{dT_s}{dx} = 0, \quad x = x_L \quad [D.2]
\]

\[
T_s = T_m, \quad x = s_m(t) \quad [D.3]
\]

Applying these boundary conditions to Eq. D.1 yields

\[
T_s(x,t) = T_m \quad [D.4]
\]

**Liquid region**

Assuming \( C_{pl} \to 0 \) similarly yields the following energy equation and boundary conditions for the liquid region,

\[
\frac{d^2 T_l}{dx^2} = 0 \quad [D.5]
\]

\[
-k_l \frac{dT_l}{dx} = q_o, \quad x = x_o \quad [D.6]
\]

\[
T_l = T_m, \quad x = s_m(t) \quad [D.7]
\]

A linear temperature distribution is obtained for the liquid region:
\[ T_i(x,t) = \frac{q_o}{k_i} (s_m(t) - x) + T_m \]  \[ [D.8] \]

An independent expression is now necessary for the melt front position, \( s_m(t) \). The melt interface condition, for the case of \( T_{IN} = T_m \) is

\[ q_o = \rho_s L_m \frac{ds_m}{dt} \]  \[ [D.9] \]

which when integrated over time yields

\[ s_m(t) = \frac{q_o}{\rho_s L_m} t \]  \[ [D.10] \]

The final form of the liquid region temperature distribution during Period 2 becomes

\[ T_i(x,t) = \frac{q_o}{k_i} \left( \frac{q_o}{\rho_s L_m} t - x \right) + T_m \]  \[ [D.11] \]
PERIOD 3

Solid region

Upon entering Period 3, the solid region retains the energy equation and boundary conditions given by Eqs. D.1 - D.3 and therefore still has a temperature distribution of \( T_s(x,t) = T_m \)

Liquid region

During Period 3, the liquid region retains energy Eq. D.5, but now has a new set of boundary conditions:

\[
q_v(t) + k_i \frac{dT_i}{dx} = \rho_i L_v \frac{ds_v}{dt}, \quad T_i(t) = T_v, \quad x = s_v(t) \quad \quad [D.12]
\]

\[
- k_i \frac{dT_i}{dx} = \rho_s L_m \frac{ds_m}{dt}, \quad T_i(t) = T_m, \quad x = s_m(t) \quad \quad [D.13]
\]

Applying these boundary conditions to Eq. D.5 yields a temperature distribution of:

\[
T_i(x) = (T_m - T_v) \frac{x - s_v}{s_m - s_v} + T_v \quad \quad [D.14]
\]
Equations D.12, D.13 can easily be expressed in terms of the two phase fronts, yielding coupled ordinary differential equations, which can be solved for numerically:

\[ q_o + k_l \frac{T_m - T_v}{s_m(t) - s_v(t)} = \rho_l L_v \frac{ds_v}{dt}, \quad x = s_v(t) \quad [D.15] \]

\[ -k_l \frac{T_m - T_v}{s_m(t) - s_v(t)} = \rho_s L_m \frac{ds_m}{dt}, \quad x = s_m(t) \quad [D.16] \]

These equations were solved using a fourth order Runge-Kutta method.
VITA

Christos Fotios Fulakis was born on August 13, 1968 in Athens, Greece. He and his family moved to Richmond, Virginia in 1970, when little Chris was just two years old. However, thanks to his parents, he never lost an ounce of his Greekness. Chris attended Virginia Tech for both his B. S. and M. S. in Mechanical Engineering and believes that is enough for now. Hoping to enter the "real world", Chris will seek employment as an engineer in Richmond or nearby.

Chris Fulakis