1 INTRODUCTION

The essential numerical difficulty in dealing with phase change problems rests in the requirement to account for nonlinear phenomena that change in time and space. In the basic case of solidification of a pure material (the Stefan problem [1]) this involves the tracking of a sharp, moving phase change boundary at which latent heat is evolved. More general cases involve not only the evolution of latent heat but also the evolution of structure and the coupling of thermal and solutal fields [2].

The aim of this article is to provide an overview of the numerical methods that can be used to deal with the nonlinear phenomena associated with solidification phase change processes. In the first instance, the focus is on fixed and deforming grid solutions of Stefan problems. Later, this discussion is expanded to include fixed grid methods directed at more general phase change systems.

The numerical solutions presented are based on full domain discretizations (i.e., finite elements, control volumes, or finite differences). Solutions based on boundary element methods [3-5], in which only the domain surface is discretized, are not covered.

Throughout, the focus is on the mechanics of the various phase change numerical schemes. Although performance comparisons are made, specific comparisons based on pure CPU efficiency are avoided. The author feels that the efficiency of any given scheme is a vague concept dependent on the implementation.

This work is dedicated to my former student and colleague C.R. (Swami) Swaminathan, who passed away on June 5 1995. In his short time with us he made many significant contributions to the numerical solutions of phase change problems.
of the method, its accuracy, the problem to be modeled, the convergence criteria, the computer architecture, and the choice of space and time steps. In general, an efficient phase change solution requires a numerical scheme with the correct balance of robustness, flexibility and accuracy to solve the given problem within the available resources. In this context, all of the methods presented in this article can be deemed to be efficient.

2 NUMERICAL DISCRETIZATION SCHEMES

The first stage in a numerical solution of a phase change problem involves covering the solution domain by a grid of node points on which appropriate equations relating nodal values of the unknowns are obtained. There is a wide range of discretization approaches that can be used. In this article, a general approach, independent of a particular discretization will be adopted. Nevertheless, to provide an explicit context for discussion and exploration of various phase change methods, two particular discretization schemes will be used in detail, (1) one-dimensional finite difference control volumes [6]; and (2) two-dimensional finite element control volumes on an unstructured grid of linear elements [7, 8]. The operation of each of these schemes in discretizing the transient heat condition equation

\[
\rho c \frac{\partial T}{\partial t} = \nabla \cdot (K \nabla T)
\]

where \( \rho \) is the density, \( c \) is the specific heat, \( K \) is the conductivity and \( T \) is the temperature, is examined below.

2.1 One-dimensional Control Volumes

Using a linear approximation for the heat flux between nodes, the heat balance on the control volume \( P \) shown in Fig. 1 can be written as

\[
[p\rho] \frac{T_P - T_P^0}{\Delta t} = \frac{K_w}{\Delta x^2} (T_w - T_p) + \frac{K_e}{\Delta x^2} (T_E - T_p)
\]

where a fully implicit (backward Euler) time integration has been applied. The superscript ‘o’ refers to values at the old time level, the lowercase subscripts refer to the interfaces between control volumes, the uppercase subscripts refer to the nodal points, \( \Delta t \) is the time step and \( \Delta x \) is the space step.

2.2 Two-Dimensional Finite Element Control Volumes

The domain is covered with a grid of finite elements (linear triangles are used in Fig. 2) and on this grid control volumes are created by joining mid points of elements to the mid points of element sides. The heat balance on a given volume can then be
Figure 1 A control volume finite difference grid.

written as

\[
\rho c A_p \frac{T_p - T_p^o}{\Delta t} = \sum_j \left[ K \frac{\partial T}{\partial x_j} \Delta y_j - K \frac{\partial T}{\partial y_j} \Delta x_j \right]
\]  \tag{3}

where \(A_p\) is the area of the control volume associated with node \(P\), the summation is over the sides of the control volume, and \(\Delta x_j\) and \(\Delta y_j\) are the length components (measured counter clockwise around node \(P\)) along the \(j\)-th control volume side. When the gradient terms in Eq. (3) are approximated using the finite element shape functions in each element, a discretized equation relating the nodal temperature at point \(P\) to the surrounding (neighboring) nodal temperatures is obtained.

2.3 The General Form

Regardless of the discretization method used (including Galerkin finite elements with nodal lumping) the discretized equation for a given node point takes the general form

\[
([\rho c]_P a_P^o + a_P) T_P = \rho c a_P^o T_P^o + \sum_{nb} a_{nb} T_{nb}
\]

\]  \tag{4}

where the \(a\)'s are coefficients, the subscript \(\text{nb}\) refers to the nodes that are neighbors to node \(P\) and the nodal temperatures under the summation can, in general, be evaluated at both the old and current time levels.

Figure 2 Control volume finite elements.
3 THE STEFAN PROBLEM

3.1 The Governing Equations

The Stefan problem involves the solidification or melting of a pure material and is characterized by a distinct moving phase change boundary at which a heat balance condition has to be met. A detailed derivation of the governing equations can be found in Crank's book [1]. In a heat-conduction-controlled Stefan problem, the domain of interest consists of a solid region and a liquid region, separated by a sharp, moving interface, $\Gamma(t)$, which coincides with the phase change temperature isotherm $T = T_m$. The governing equations are:

Heat Transfer in the solid (s):

$$\rho c_s \frac{\partial T_s}{\partial t} = \nabla \cdot (K_s \nabla T_s)$$

(5)

Heat Transfer in the liquid (l):

$$\rho c_l \frac{\partial T_l}{\partial t} = \nabla \cdot (K_l \nabla T_l)$$

(6)

Heat Balance at the solid/liquid moving interface, $\Gamma(t)$, (the Stefan Condition):

$$K_s \nabla T_s \cdot n - K_l \nabla T_l \cdot n = \rho L v \cdot n$$

(7)

where $n$ is the unit normal on the phase interface (pointing into the liquid), $v$ is the velocity of the interface and $L$ is the latent heat per unit mass of solid. For a number of simple geometries and conditions analytical and approximate solutions to the Stefan problem, Eqs. (5)-(7), can be constructed. The important solutions can be found in Crank [1] and Carslew and Jaeger [9]. Note that in the above equations the specific heat is constant in each phase and the density is set constant throughout the domain. Problems that involve a density difference across the phase change require an additional advection term in the heat transfer equations to account for shrinkage driven flows [1].

3.2 A Conserved Formulation: The Enthalpy

An alternative, conserved formulation of solid/liquid phase change is based on an enthalpy variable, heat per unit mass, defined by

$$H = \begin{cases} c_s T & ; \quad T < T_m \\ c_l T + (c_s - c_l) T_m + L & ; \quad T \geq T_m \end{cases}$$

(8)
where the use of an upper case symbol is common in the literature. In more compact form

\[
H = [g c_1 + (1-g)c_\infty] T + g(c_\infty-c_p)T_m + gL
\]  

where the step function, \( g \), is the liquid volume fraction. In terms of the enthalpy, the Stefan formulation, Eqs. (5)-(7), involving two heat conduction equations and a heat balance condition, can be reduced to a single equation

\[
\rho \frac{\partial H}{\partial t} = \nabla \cdot (K \nabla T)
\]

This is a conserved formulation that holds in both the solid and liquid phases and as shown by Shamsundar and Sparrow [10], implicitly includes the Stefan heat balance condition, Eq. (7). In a numerical context, the main advantage of the enthalpy formulation is that a solution does not require an explicit tracking of the phase interface \( \Gamma \). Note also, on appropriate definition of the enthalpy, general phase change situations, not characterized by a single sharp interface, can be modeled.

3.3 An Overview of Numerical Schemes

The majority of numerical schemes for dealing with the Stefan problem can be broadly separated into two classes:

1. Fixed grid schemes: These approaches are based on the enthalpy formulation, Eq. (10), and employ a fixed space grid. The movement of the phase change interface is tracked on the specification of a nodal liquid fraction \( 0 \leq g_p \leq 1 \).

2. Deforming grid, front tracking schemes: These approaches are based on the complete Stefan formulation, Eqs. (5)-(7), and employ deforming space grids that ensure that a line of node points always lie on the phase interface, \( \Gamma \).

In the next two sections, fixed and deforming grid schemes for Stefan problems are discussed in detail.

4 FIXED GRID SCHEMES

4.1 An Explicit Fixed Grid Scheme

As noted above, fixed grid solutions are based on solutions of the conserved enthalpy formulation, Eq. (10). The numerical discretization of this equation, using explicit (Euler) time integration has the form

\[
\rho a_p^o H_p = \rho a_p^o H_p^o \sum_{nb} a_{nb} T_{nb}^o - a_p T_p^o
\]  

for Stefan problems are discussed in detail.
where

\[ T_p = \begin{cases} 
  \frac{H_p}{c_s T_m}, & H_p < c_s T_m \\
  ; & c_s T_m \leq H_p < c_s T_m + L \\
  \frac{H_p (c_s - c_l) T_m}{c_l} L, & H_p \geq c_s T_m + L 
\end{cases} \tag{12} \]

In a one dimensional control volume, discretization Eq. (11) is

\[ \rho H_p = \rho H_p^o + \frac{\Delta t K_w}{\Delta x^2} (T_w^o - T_p^o) + \frac{\Delta t K_c}{\Delta x^2} (T_E^o - T_p^o) \tag{13} \]

where, for stability, the time step and space steps need to be chosen such that

\[ \max \left| \frac{\Delta t K_s}{\rho c_s \Delta x^2}, \frac{\Delta t K_l}{\rho c_l \Delta x^2} \right| \leq \frac{1}{2} \tag{14} \]

After selection of space and time steps and appropriate treatment of boundary conditions the numerical solution is very straightforward. At each time step, Eq. (11) is explicitly solved for the nodal enthalpy field, \( H \). Calculations in a time step are completed on updating the nodal temperature field, \( T \), via Eq. (12). In addition, if desired, the nodal liquid fractions can be calculated from

\[ g_p = \begin{cases} 
  0, & T_p < T_m \\
  \frac{H_p - c_s T_m}{L}, & T_m = 0 \\
  1, & T_p > T_m 
\end{cases} \tag{15} \]

and the phase front position estimated on interpolating for the \( g = 0.5 \) contour. The solution can then proceed to the next time step.

Important features of the above enthalpy scheme, which are also valid for implicit time integration enthalpy schemes (see below) are:

1. When a control volume associated with a given node point \( P \) is undergoing the phase change, the nodal temperature remains fixed at \( T_p = T_m \), a condition that can be maintained for a number of time steps.
2. The nodal liquid fraction at a phase change node will have a value \(0 \leq g_p \leq 1\); i.e., even though the continuous liquid fraction is a step function, the nodal discretized values can take intermediate values between 0 and 1.

3. In one-dimensional Stefan problems, one and only one control volume in the domain can be undergoing the phase change in any given time step.

In one dimensional problems, this last feature allows for a more exact placement of the phase front, \(s(x, t) = 1\). If the node point is in the center of the control volume, then during solidification,

\[ s = x_w + (1 - g_p) \Delta x \]  \hspace{1cm} (16)

where it is assumed that the solidification front is moving west to east and \(x_w\) is the location of the west face of the phase change volume. If melting is occurring the position is given by

\[ s = x_w + g_p \Delta x \]  \hspace{1cm} (17)

When \(g_p = 0.5\) in Eqs. (16) or (17) the phase front will be on the node P. Furthermore, on appropriate modification to account for radial changes in geometry, similar equations can be obtained for axi-symmetric problems [11].

4.1.1 Performance. The performance of the explicit fixed grid enthalpy scheme is evaluated on solving a one-dimensional solidification Stefan problem. Material with a phase change temperature \(T_m = 0\) and thermal properties \(\rho = c = K = 1\) is contained in the half space, \(x \geq 0\). At time \(t < 0\) the material is at a temperature of \(T_i = 1\). At time \(t = 0\) the temperature of the surface at \(x = 0\) is lowered and fixed at \(T = T_s = -1\) so that, as time increases, a solid phase attaches to \(x = 0\) and grows. Predictions of front movement and temperature history at \(x = 0.4\) are compared with the Neumann analytical solution [1, 9] in Figs. 3-5. In these calculations, a space grid of 50 steps \((\Delta x = 0.1)\) and a time step of \(\Delta t = 0.002\) are used, and three different cases corresponding to latent heat values of \(L = 0.1\) (Stefan Number = \(c(T_m - T_s)/L = 10\)), \(L = 1\) (St = 1) and \(L = 10\) (St = 0.1) are investigated. At the low Stefan number, St = 0.1 (Fig. 3), where the latent is larger than the sensible heat, the front movement is relatively slow and the numerical prediction for the front movement given by Eq. (16) is in very close agreement with the analytical solution \(s = 0.378 \sqrt{t}\). On the other hand, the prediction of the temperature history exhibits large oscillations involving plateaux followed by sharp drops. This is a characteristic of the enthalpy method [12] and is caused by the temporary trapping of nodes in the pseudo steady state region bounded by the surface \(x = 0\) and the current nodal position of the phase change.

At intermediate Stefan number, St = 1 (Fig. 4), the plateaux in the temperature history are still present, but reduced. The front movement is faster \((s = 0.755 \sqrt{t})\) and although the numerical predictions of the front movement are still reasonably good there are clear signs of oscillations.

The behavior at large Stefan number, St = 10 (Fig. 5), when latent heat
Figure 3 Temperature History at $x = 0.4$ and front movement for $St = 0.1$

Figure 4 Temperature history at $x = 0.4$ and front movement for $St = 1$. 

Figure 5 Temperature history at $x = 0.4$ and front movement for $St = 10$. 
effects are small, is almost the reverse of the small Stefan number case. Due to the relatively rapid movement of the phase front \((s = 0.926 \sqrt{t})\) the plateaux in the temperature history are effectively eliminated. On the other hand, the front tracking approach given by Eq. (16) exhibits clear oscillations.

4.2 A Remedial Scheme

There is no doubt that the explicit enthalpy method is an effective solution approach for the Stefan problem. The method is easy to implement, and although some solutions show oscillations, their behavior is stable, i.e., the oscillations do not grow with time. Problems with oscillations are reduced in (1) multidimensional problems, since it may not be possible to completely trap nodes in long term pseudo steady state regions; and (2) in cases where Neumann as opposed to Dirichlet boundary conditions are applied. Furthermore, in the one-dimensional case Voller and Cross [13], based on an original suggestion by Price and Slack [14], have proposed a remedial scheme that can recover accurate results from enthalpy solutions.

Price and Slack [14] observed that in one-dimensional solutions of the Stefan problem with Dirichlet boundary conditions, when a nodal liquid fraction was \(g_p = 0.5\) the predicted front position (viz., the position of node P) and the nodal temperature field agreed closely with the analytical solution. Voller and Cross [13] utilized this observation in devising a remedial enthalpy scheme that interrogates the enthalpy predictions and only reports predictions when a nodal liquid fraction becomes 0.5, usually requiring iteration across a time step. The effect of the remedial scheme on the explicit enthalpy solution of the current test problem is shown in Fig. 6. In this figure it is observed that the oscillations associated with the temperature history when \(St = 0.1\) and the front movement when \(St = 10\) are removed. The remedial scheme is also effective in removing oscillations in implicit time integration enthalpy schemes and has been successfully implemented in a variable time step node jumping scheme [15].

4.3 Implicit Fixed Grid Schemes.

Although the explicit fixed grid scheme is very easy to apply, a small time step is required to ensure stability. In some cases this restriction requires a time step that is too small for an effective computation. The alternative is to use an implicit time integration, e.g., a backward Euler finite difference

\[
p_a \rho_0 H_p = \rho_0 a^o T_p^n + \sum_{nb} a_{nb} T_{nb} - a_T T_p
\]  

which is free of any stability restrictions on the time step. This discretized equation, however, is nonlinear and developing an appropriate solution that outperforms an explicit scheme is a numerical challenge. A basic approach is to employ a linearization and adopt an iterative solution of Eq. (18). There are many potential ways of achieving this, and some key schemes are outlined below.
4.3.1 Source update methods. Substitution of the enthalpy, defined in Eq. (9), into Eq. (18) leads to the basic heat equation

$$\rho c \frac{\partial T}{\partial t} = \nabla(K \nabla T)$$

which has the fully implicit discretized form

$$(\rho c a_p^* + a_p) T_p^n = \rho c a_p^* T_p^{n-1} + \sum_{nb} a_{nb} T_{nb}^{n-1} + \rho L a_p^* (g_p^* - g_p^{n-1})$$

where the specific heat term is volume averaged between the phases. This equation isolates the nonlinear behavior associated with the phase change into a source term. A possible iteration scheme, within a given time step, is outlined below:

1. At the start of the time step, the initial iterative fields are set to the previous time step values.

2. PREDICTION: From the known nodal temperature and liquid fraction fields at iteration n-1, the system of equations

$$\begin{align*}
(\rho c a_p^* + a_p) T_p^n &= \rho c a_p^* T_p^{n-1} + \sum_{nb} a_{nb} T_{nb}^{n-1} + \rho L a_p^* (g_p^* - g_p^{n-1})
\end{align*}$$

is solved for the temperature field at iteration level n.

3. CORRECTION: The nodal liquid fraction field, $g^n$, needs to be evaluated before
the next iteration can proceed. In the case of a Stefan problem with the phase change temperature scaled to be \( T_m = 0 \) a basic update scheme is constructed as follows. If the phase change is occurring at node P, it is recognized that the nodal temperature will be given by \( T_p = T_m = 0 \) and hence with the correct nodal liquid fraction, Eq. (21) becomes

\[
0 = \rho c a_p^o T_p^o + \sum_{nb} a_{nb} T_{nb}^n + \rho L a_p^o (g_p^o - g_p^n)
\]  

(22)

From which, after subtraction from Eq. (21), the update formula

\[
g_p^n = g_p^{n-1} + \frac{\lambda (\rho c a_p^o + a_p)}{a_p^o \rho L} T_p^n
\]  

(23)

is obtained, where \( \lambda \) is a relaxation factor. In practice, after the evaluation of the nodal temperature field, \( T^n \), the liquid fraction update is applied at every node point, followed by the correction

\[
g_p = \max[0, \min[g_p, 1]]
\]  

(24)

to account for nodes where the phase change is not occurring. The use of this last equation ensures "smooth" transitions between phase changing and non-phase changing nodes within a time step.

4. Steps 2 and 3 are repeated until convergence, which is declared when the residual of the discretized conserved enthalpy equation, Eq. (18), falls below a defined tolerance. In this way the scheme will conserve energy.

The above approach, which is similar to the fictitious heat source method developed for finite element phase change solutions [16, 17], is extremely robust and has been used to solve a variety of problems including those that involve fluid flow and mushy phase change regions [18]. The price of robustness, however, is lack of computational efficiency. The obvious place for improvement is in the liquid fraction update. In an efficient update scheme proposed by Voller [19], steps 2 and 3 in the above algorithm are modified as follows:

2. **PREDICTION:** When solving Eq. (21), at nodes where the phase change is occurring (identified by \( 0 < g_p^{n-1} < 1 \)) the coefficient \( a_p^* = [pc a_p^o + a_p] \) is replaced by \( a_p^* = [pc a_p^o + a_p] + \text{BIG} \) (a large value of \( 10^{20} \)). This step ensures that on solution the correct value of \( T_p = 0 \) is returned at all nodes where \( 0 < g_p^{n-1} < 1 \). Furthermore, if the liquid fraction field at iteration \( n-1 \) is correct, the entire nodal temperature field at level \( n \) will be correct.

3. **CORRECTION:** An appropriate evaluation for the liquid fraction can then be obtained on rearranging Eq. (21); i.e.,
\[ \rho L a_p^0 g_p^n = \rho L a_p^0 g_p^0 + \rho c a_p^0 T_p^0 + \sum_{nb} a_{nb} T_{nb}^n \quad (25) \]

or, as an alternative, following the derivation used in the previous CORRECTION step, the update

\[ g_p^n = g_p^{n-1} + a_p^* T_p^n \quad (26) \]

can be used. Note that, in Eq. (25) it is assumed that the nodal temperature \( T_p = 0 \) and Eq. (25) or (26) are applied at all nodes followed by the under/over shoot correction, Eq. (24).

In matrix form the nonlinear set of equations to be solved in the prediction step, Eq. (21), can be written as

\[ C T = C T^{old} + K T + F \quad (27) \]

where, assuming nodal lumping, \( C \) is a diagonal matrix containing the term \((\rho c a_p^0 + a_p)\), \( K \) is a "stiffness matrix" representing the discretization of the Laplacian, and \( F \) is a vector containing the liquid fraction source terms. When solving this equation in the modified source approach, the elements in \( C \) corresponding to a node changing phase \((0 < g_p < 1)\) are replaced by the value BIG. This has the desired effect of returning a value of \( T_p = 0 \). An alternative, but completely equivalent, approach recently suggested by Gong and Mujumdar [20] is to set the columns in the stiffness matrix, corresponding to the phase change nodes to zero.

Note that the basic source update can be readily modified to deal with cases where \( T_m \neq 0 \). In the modified updates, however, to avoid problems with round off, a temperate scaling such that \( T_m = 0 \) is recommended.

4.3.2 Enthalpy linearization. A general method that incorporates the above source based method is the enthalpy linearization proposed by Swaminathan and Voller [21]. The key feature in this method is to assume that the phase change occurs over an arbitrarily thin temperature range. In this way the enthalpy can be related to the temperature by a piecewise continuous function; e.g., assuming constant specific heats in each phase, the enthalpy can be approximated as

\[ H = \begin{cases} c_s T ; & T \leq T_m - \epsilon \\ c_s (T_m - \epsilon) + \frac{c_s + c_l}{2} \left( T - T_m + \epsilon \right) ; & T_m - \epsilon < T < T_m + \epsilon \\ c_l T + (c_s - c_l) T_m + L ; & T \geq T_m + \epsilon \end{cases} \quad (28) \]

where \( \epsilon \) is an arbitrarily small value representing half the phase change temperature
interval. The approximate definition of $H(T)$ can be readily differentiated with respect to temperature to obtain

$$C_A = \frac{dH}{dT} = \begin{cases} 
c_s ; & T \leq T_m - \epsilon \\
c_s + \frac{c_1}{2} + \frac{L}{2\epsilon} ; & T_m - \epsilon < T < T_m + \epsilon \\
c_1 ; & T \geq T_m + \epsilon
\end{cases} \tag{29}$$

a quantity referred to as the apparent specific heat. In these equations the temperature interval, $\epsilon$, can be arbitrarily small. The efficiency and accuracy of the resulting method are in no way affected by the size of this interval.

The definitions of $H(T)$ and $C_A$ can be used to linearize the discretized enthalpy equation. In iterative form:

$$\rho a_p H_p^n + a_p T_p^n = \rho a_p H_p^o + \sum_{nb} a_{nb} T_{nb}^n \tag{30}$$

which on using the Taylor series expansion

$$H_p^n = H_p^{n-1} + \left. \frac{dH}{dT} \right|_{T_p^{n-1}} [T_p^n - T_p^{n-1}] \tag{31}$$

can be linearized as

$$(a_p + \rho C_A a_p^o) T_p^n = \rho C_A a_p^o T_p^{n-1} + \sum_{nb} a_{nb} T_{nb}^n + \rho a_p^o [H_p^o - H_p^{n-1}] \tag{32}$$

In a time step the solution of Eq. (32) proceeds as follows:

1. At the start of the time step, the initial iterative fields are set to the previous time step values.

2. PREDICTION: From the known temperature and enthalpy fields at iteration $n-1$, the term $C_A$, Eq. (29), is calculated, and the nodal temperature field at iteration level $n$, $T^n$, is obtained on solving Eq. (32).

3. CORRECTION: The nodal enthalpy field at level $n$ is updated using the Taylor series expansion in Eq. (30), and, in order to ensure consistency with the enthalpy, the temperature field is corrected; e.g., if $H$ is defined by Eq. (28),
This last step — correcting the nth iterate of the temperature — is of key importance.

4. Steps 2 and 3 are repeated to convergence, which is declared when the residual of the discretized conserved enthalpy equation, Eq. (18), falls below a defined tolerance. In this way the scheme conserves energy.

Features of the enthalpy linearization:

1. The scheme is closely related to the improved source based method proposed by Voller [19]. In particular, in the phase change range, assuming a small value of \( \varepsilon \), the value of \( \frac{dH}{dT} \) will take a large value and the prediction step will return a temperature value close to \( T_p = 0 \) in cells that are changing phase. As with the improved source based scheme, the scaling of the temperature so that \( T_m = 0 \) is recommended.

2. In most times steps, assuming a direct solution of Eq. (32), the linearized enthalpy scheme only requires one iteration to converge. The only time that additional iterations are required is when the phase front moves from one control volume to another within a time step. In these cases the source term in Eq. (32) takes the role of ensuring a smooth transition of the phase front (no oscillations in the iterations) and the additional iterations ensure satisfaction of the local heat balance. The scheme could be run in a mode where only a single iteration was imposed at each time step. Such a scheme would not conserve heat at every time step, but if the time steps are small enough, the error invoked by the failure to completely conserve heat may be smaller than the numerical errors inherent in the numerical discretization as a whole. This is essentially the idea behind the apparent heat capacity scheme with post iterative correction that will be discussed next.
4.3.3 The apparent heat capacity. One of the most widely used enthalpy schemes involves the reformulation of the governing equation in terms of the apparent heat capacity. On noting that
\[
\frac{\partial H}{\partial t} = C^A \frac{\partial T}{\partial t}
\]
the governing enthalpy equation becomes
\[
\rho C^A \frac{\partial T}{\partial t} = \nabla \cdot (K \nabla T)
\]
with the discretized form
\[
(p C^A a_p^o + a_p) T_p = \rho C^A a_p^o T_p^o + \sum_{nb} a_{nb} T_{nb}
\]
In this approach, the nonlinear behavior associated with the phase change has been absorbed into the definition of \( C^A \). The advantage of this approach is that the governing equation and the associated discretized equation have the general form of a heat conduction equation with a nonlinear specific heat. As a result, with appropriate numerical treatment of the apparent heat capacity, \( C^A \), the Stefan problem can be solved using a standard heat transfer code. The key to using this approach effectively is to identify an appropriate approximation for the apparent heat capacity, \( C^A \). A simple approach based directly on the definition of \( C^A \) given by Eq. (29) may not work, because if the half phase change range \( \epsilon \) is too small, it is possible to “skip” the latent heat contribution. A wide number of schemes have been suggested [22-25] to overcome this drawback. One of the most effective is the temperature correction scheme pioneered by Pham [26] and Comini et al. [27]. In this approach, after calculation of the current nodal temperature field, a “post iterative” correction is applied to ensure that all of the latent heat effects are accounted for. Pham [28] has suggests that in using this approach the apparent heat capacity is best approximated across time, e.g., the approximation proposed by Morgan et al. [29]

\[
C^A = \frac{H^o - H^\infty}{T^o - T^\infty}
\]

where the superscript ‘oo’ implies evaluation at the time step two steps behind the current time step. The post iterative temperature correction scheme, however, will also work with the direct definition of \( C^A \) given in Eq. (29).

In a time step the calculations used in this scheme are as follows:

1. At the start of the time step, the initial fields are set to the previous time step values.
2. **PREDICTION**: An appropriate approximation for $C^A$ is made from the known temperature and enthalpy fields (e.g., Eq. (37) or Eq. (29)) and the nodal temperature field, $T^o$, is obtained on solving Eq. (36).

3. **CORRECTION**: The nodal enthalpy field at level $n$ is updated by using the expression

$$H^n_p = H^o_p + C^A [T^n_p - T^o_p]$$

(38)

and, in order to ensure consistency with the enthalpy, the temperature field is corrected, e.g., see Eq. (33). This last step — correcting the temperature — is of key importance.

4. Steps 2 and 3 are carried out only once, i.e., no iteration in time is employed. Hence, unlike the source based and enthalpy linearization schemes, there is no guarantee of conservation; i.e., the predicted enthalpy and temperature are not guaranteed to satisfy the enthalpy equation, Eq. (18), at every time step.

4.3.4 **Performance.** The performance of the various implicit schemes outlined above are tested on the one-dimensional Stefan test problem. Using a fixed grid with 50 volumes ($\Delta x = 0.1$) the various schemes are used to predict the time taken, $tsol^{pre}$, for the phase front to reach the position $s = 1.0$. The performance of each scheme is tested across a range of time steps, starting with $\Delta t = 0.05$ (the explicit stability limit) and terminating with $\Delta t = 10$ (20 times the explicit limit). Convergence in iterative schemes is declared when the maximum nodal imbalance (based on Eq. (18)) falls below $10^{-2}$% of the current nodal enthalpy value. Performance is reported in terms of the error between the predicted and analytical solutions, i.e.,

$$\% Error = 100 \left(1 - \frac{tsol^{pre}}{tsol^{ana}}\right)$$

(39)

and the number of iterations required. Note that in the non-conserved one step schemes iterations = time steps. In performance evaluations it is found that:

1. The predictions from schemes that conserve energy are essentially identical.

2. The iterations required by the modified source scheme match those required by the linearized enthalpy scheme. In all cases, however, the basic source scheme requires under relaxation of Eq. (23) and the iteration count is significantly more.

3. The performance of the one step, non-iterative version of the linearized enthalpy is identical to the apparent heat capacity scheme based on the direct approximation of $C^A$. 
For all cases tested, the apparent heat capacity scheme based on the direct approximation was more accurate than the apparent heat capacity scheme based on the Morgan approximation, Eq. (37).

In light of the above, the critical comparison in performance should be between the conserved enthalpy linearization (LINH) and the apparent heat capacity (AHC) based on the direct approximation, Eq. (29). Figures 7 and 8 compare the performance of these two schemes with Stefan numbers of 0.2 and 2 respectively. There are some important conclusions to be made.

1. The extra work involved in using the LINH is small. Most time steps only require one iteration (equivalent to one step of the AHC). Additional iterations are only required when the phase front crosses between control volumes.

2. The LINH scheme is more accurate at large time steps and small Stefan numbers, Fig. 7. At large Stefan numbers and small time steps, however, there is little difference between the schemes.
There is little to choose between the LINH and AHC schemes, it is a question of “trading off” the benefits of accuracy improvement over effort required. On balance, the present author favors the conserved LINH scheme for the following reasons:

1. The user buys the peace of mind that the scheme locally conserves heat at every point in time and space, for the price of a small amount of additional work. Further on defaulting the iteration count to 1, the linearized enthalpy will mimic the apparent heat capacity scheme.

2. As reported by Pham [28], in some problems, at early time steps, large oscillations in the temperature profile are predicted by the AHC scheme.

3. In solving real problems other nonlinear terms may be present and an iterative solution required. Furthermore, in solving large scale multidimensional linear problems an iterative solver is often preferred. In such cases there is no disadvantage in using the linearized enthalpy scheme.

The AHC scheme, however, is a viable alternative. The post iterative correction scheme proposed by Pham [26] and Comini et al. [27], is a key contribution, that negates the endless discussions in the literature comparing the performance of differing heat capacity approximations. The current author feels that almost any approximation of the heat capacity (including a direct evaluation) will work with the post iterative correction.

The above discussion does not cover all of the implicit fixed grid schemes in the literature. For example, the recently proposed conserved apparent heat capacity scheme suggested by Yao and Chait [30]. In terms of the Stefan problem, however it is hard to imagine an alternative basic scheme that will have performance characteristics better than those exhibited by the AHC and LINH schemes.

4.4 A Two Dimensional Fixed Grid Solution.

The mechanics in the fixed grid schemes presented above are independent of the dimension, and the application to multidimensional problems is straightforward. As

Figure 9 Cartesian grid for pipe freeze problem
an example, consider the growth of a freeze-layer on a cooled half-pipe, \( T_{\text{pipe}} = -1 \), of radius \( R_{\text{pp}} = 1 \), placed in a liquid at the phase change temperature. This problem is axi-symmetric and can be solved as a one-dimensional problem in cylindrical polar coordinates. In Cartesian coordinates, however, the problem is two-dimensional and can be used as an effective test problem for the multi-dimensionality of a given approach. This test problem, with all thermo-physical properties set to unity, is solved on the fixed Cartesian linear finite element grid shown in Fig. 9. A control volume finite element method is used with a time step of \( \Delta t = 0.01 \) and the latent heat evolution is handled using the LINH scheme, see section 4.3.2. In Fig. 10 the predicted growth of the freeze-layer (radial position with time) is compared with the predictions from a one-dimensional axi-symmetric solution (employing a fine grid of 100 elements in the domain \( 1 < r < 3 \)). The comparison is excellent clearly indicating the worth of fixed grid methods in the solution of two-dimensional problems.

5 DEFORMING GRID SOLUTIONS

The basic principle in a deforming grid solution of a Stefan problem is to continuously deform the space grid to always ensure that a line of specified node points lies on the phase change front. In this way, the Stefan heat balance condition, Eq. (7), can be easily satisfied and the movement of the front readily tracked.

Deforming grid solutions of phase change problems are common in the finite element literature [31-35]. In this article a closely related Deforming Control Volume Finite Element (DCVFE) scheme for the Stefan problem will be presented [36].

5.1 A Deforming Control Volume Finite Element Solution of the Stefan Problem

The DCVFE scheme is based on a grid of continuously deforming finite elements on which deforming control volumes, centered around node points, are defined. The morphology of the grid is identical to that shown in Fig. 9. In this case, however, the node points and the associated control volumes are continuously deforming.

![Figure 10 Two-dimensional fixed grid solution.](image)
Following the work of Demirdzic and Peric [37], in a heat-conduction-controlled problem, the heat balance on this volume can be written as

\[ \frac{\partial}{\partial t} \int_{A_0} \rho H dV = \int_{S_0} \left[ \rho v H + K \nabla T \right] n \]

where \( A(t) \) is the area of the 2-D volume, \( v \) the velocity of the volume surface \( S(t) \) and \( n \) is the unit outward normal to this surface. To demonstrate how this equation can be reduced to an appropriate discretization and used in a deforming grid solution, we will consider the problem of freeze-layer growth onto a uniformly cooled half-pipe introduced in section 4.4 and Fig. 10. The deforming grid solution of this problem is illustrated by the time “snapshots” shown in Fig. 11. At internal node points of this two-dimensional grid (which are always in the frozen state), Eq. (40) can be written as

\[ \rho c \frac{A_p T_p - A_p^* T_p^*}{\Delta t} = \sum_j \left[ \rho c (v T)_j + K \frac{\partial T}{\partial x} \right] \Delta y_j - \left[ \rho c (v T)_j + K \frac{\partial T}{\partial y} \right] \Delta x_j \]

where \( j \) is summed over the sides of the control volume and the velocities and temperatures are evaluated at the mid sides. This equation is very similar to the basic
control volume equation, Eq. (3), with the important modifications that the control volume area $A_p$ changes with time, and the movement of the grid introduces an additional advection term under the summation sign.

In the first instance, in order to clearly see how Eq. (41) is used in a deforming grid solution of a Stefan problem, we will restrict discussion to solidification problems in which the initial condition is a liquid at the phase change temperature, $T_m = 0$. In these problems, one of the deforming domain boundaries will coincide with the phase change interface, $\Gamma$, and the nodes on this interface will always take the value $T = 0$. At these nodes the balance equation over the associated control volume, see Fig. 12, takes the form

$$
\Delta t \sum_{\text{INT}} \left[ \rho c(vT)_j + K \frac{\partial T}{\partial x} \Delta y_j \right] \Delta x_j + \rho L (\Delta y^\Gamma - \Delta x^\Gamma)[\delta x_i + \delta y_i] = 0
$$

(42)

where \text{INT} indicates the summation over interior control volume faces and the values, $\Delta x^\Gamma$ and $\Delta y^\Gamma$ are as indicated in Fig. 12. In Eq. (42) the velocity at the phase change interface has been approximated by

$$
\mathbf{v}^\Gamma = \left[ \frac{\delta x_i}{\Delta t}, \frac{\delta y_i}{\Delta t} \right]
$$

(43)

where $\delta x_i$ and $\delta y_i$ are, respectively, the x and y movements of boundary node $I$ over the time step. Equation (42) can be used to determine how the interface nodes need to be moved to satisfy the Stefan Condition. This equation, however, is under-specified, providing two unknowns ($\delta x_i$ and $\delta y_i$) at each node. In order to fully specify the problem, the nodes on the interface need to be constrained to move along specified paths, (e.g., spines [38]) such that

$$
\delta x_i = f_i(x,y) \delta y_i
$$

(44)

where $f_i(x,y)$ is a prescribed known function associated with node $I$. In theory, the choice of spine directions is arbitrary, since, through Eq. (42), the satisfaction of the heat balance at the interface is assured. In practice, however, the spine directions affect the grid deformation and a poor choice will lead to large grid distortions causing error and non-convergence. In some problems it is possible to use global spine directions that hold throughout the calculation; e.g., in the case of the freeze-layer growing on a pipe, Figs 11, a global choice would be to use the radial lines, i.e.,

$$
f(x,y) = \cotan(\theta)
$$

(45)

where $\theta$ is the corresponding angle of the radial line. In more general cases, with reference to Fig. 12, a local spine direction can be calculated for each node at each time step,
where \( n_w = (n_{wx}, n_{wy}) \) and \( n_e = (n_{ex}, n_{ey}) \) are the unit outward normals, at the old time step, on the phase front segments that meet at node \( I \).

Equations (41)-(44) are the central equations in the DCVFE approach. In order to provide more detail on the mechanics involved, consider a one-dimensional problem. In this case a spine condition is not needed, and assuming a uniform grid (see Fig. 1) and constant thermal properties, the balance at internal nodes, becomes

\[
\rho c \Delta x + \Delta t \left( K \frac{2K}{\Delta x} + v_w \rho c + v_e \rho c \right) T_p = \rho c \Delta x \Delta \theta T^o_p
\]

\[
+ \Delta t \left( K \frac{K}{\Delta x} - v_w \rho c \right) T_w + \Delta t \left( K \frac{K}{\Delta x} + v_e \rho c \right) T_e
\]

where \( v_e \) and \( v_w \) are the velocities of the control volume interfaces. In evaluating the temperature at these interfaces a central difference has been used, i.e.,

\[
T_e = \frac{T_E + T_P}{2} = \frac{T_W + T_P}{2}
\]

On the phase boundary, node \( N \), the general balance reduces to
\[ K_w \frac{T_{N-1}}{\Delta x} - \frac{\nu_w \rho c T_{N-1}}{2} = -\rho L \frac{ds}{dt} \]  (49)

where \( ds/dt \) is the velocity of the phase interface.

The iterative steps in the DCVFE algorithm, over one time step, can be constructed as follows:

1. The coefficients in Eq. (41) — Eq. (47) in the one-dimensional case — are evaluated. On the first iteration in the time step the previous grid locations are used. This means that the first time step requires an initial starting solution. In a one-phase freezing problem, simply assuming the initial existence of a thin frozen layer at the freezing temperature is often sufficient. More sophisticated starting solutions could involve the use of local one-dimensional analytical solutions of the Stefan problem.

2. After solution of Eq. (41) — Eq. (47) in the one-dimensional case — the predicted nodal temperature field is used in Eq. (42) — Eq. (49) in the one-dimensional case — which along with the spine constraints (e.g., Eq. (44) or Eq. (46)) can be used to calculate the phase boundary nodal displacements (\( \delta x_i \) and \( \delta y_i \)), over the time step.

3. Following this step, the entire grid is updated. This can be achieved on solving "pseudo elastic" equations in the grid displacements, i.e.,

\[
\nabla^2 \delta x_i = 0, \quad \nabla^2 \delta y_i = 0
\]  (50)

where on the phase boundary, \( \Gamma \), the displacements are fixed to be those calculated in the previous step. The advantages of using Eq. (50) are that the coefficients can be directly obtained from the existing diffusion coefficients used in the solution of Eq. (41), and a reasonably uniform grid is maintained. Note also that additional grid management can be undertaken on providing non-zero right-hand sides in Eq. (50).

4. After calculation of the nodal displacements, the grid locations and velocities can be updated for use in the next iteration.

5. Iterations continue until convergence, usually when the maximum difference in the grid adjustment values between subsequent iterations falls below a given tolerance.

Possible modifications to this algorithm include:

1. The introduction of a second deforming grid for the solution of two phase Stefan problems.
2. Replacing the fully implicit update of the phase front with a Crank Nicolson update. That is, after the first time step, use the update scheme

$$\delta x^* = \frac{2}{3} \frac{\delta x}{\Delta t} + \frac{2}{3} \frac{x^{\infty} - x_1^{\infty}}{\Delta t}$$

(51)

where the second term on the right-hand side arises from the product of the time step and the average velocity in the previous time step, and $x_1^{\infty}$ is the nodal position two time steps back.

The aim of the above discussion of the DCVFE scheme has been to highlight typical steps in a deforming grid solution of the Stefan problem. As noted above, there are many alternative approaches, particularly in the Finite Element literature [31-35]. There is also some significant current research aimed at improved schemes for updating the grid during deforming grid calculations.

### 5.2 Examples

The first example of the DCVFE is directed at the two phase, one dimensional Stefan problem studied above in the discussion on the implicit schemes. Oscillation free predictions for the temperature history at $x = 0.4$ when $St = 0.2$ and the front movement when $St = 2$, are compared with the analytical solutions in Fig. 13.

The second example is freezing on a uniformly cooled half-pipe emersed in a liquid at the phase change temperature (see Section 4.4 for details). The DCVFE solution is started by assuming a thin frozen region $1 < r < 1.05$ at a uniform temperature of $T = 0$. The grid used and its deformation in time is indicated in Fig. 11. A time step of $\Delta t = 0.01$ and global spines along radial lines are used. The predictions for the radial growth of the frozen layer are very close to the one-dimensional fine fixed grid solution, Fig. 14.
The last example is freezing onto a non-uniformly cooled half-pipe placed in a liquid at the phase change temperature. The prediction for the freeze-layer at time \( t = 1 \), when the surface temperature

\[
T = 2.8 \left( \frac{\theta}{\pi} - 1 \right)
\]

and the other conditions are identical to the previous test problem, is compared with a fixed grid solution in Fig. 15.

5.3 Front Fixing Methods

Front fixing is often presented as an alternative to deforming grid methods for solving phase change problems. This approach involves a coordinate transformation such that the position of the phase front in the transformed coordinates remains fixed. Both one-dimensional [41] and multidimensional [42-46] fixed grid solutions of Stefan problems are found in the literature.
In one-dimension the Landau transformation \([41]\)

\[
\eta = \frac{x}{s(t)}
\]  

(53)

is used as the transformation variable. In the transformed space, the governing equation for the solidification of a pure material at the phase change temperature becomes

\[
\rho c \frac{\partial (sT)}{\partial t} = \frac{K}{s} \frac{\partial^2 T}{\partial \eta^2} + \frac{\partial}{\partial \eta} \left( \eta \frac{ds}{dt} \rho c T \right) \quad 0 \leq \eta \leq 1
\]  

(54)

After suitable discretization, the effect of the transformation is to introduce an additional grid convection term. Furthermore, if reasonable and appropriate discretization choices are made, the resulting discretized equations can be made identical to the deforming grid discretized equations presented in Eqs. (47) and (49). A result that has also been shown to hold in multidimensional problems by Lynch \([33]\). The bottom line is that, in the strict sense, a transformed grid is not a true alternative to a deforming grid scheme, but just an alternate route to the discretized equations.

6 HYBRID SOLUTIONS

Whereas, in general, deforming grid approaches are more accurate than fixed grid approaches the improved predictive performance is at the cost of increased computations. As a result, there have been a number of hybrid solutions suggested in the literature that combine fixed and deforming grid approaches. The objective is to improve the accuracy of fixed grid schemes without the cost of adopting a fully deforming grid solution. The class of hybrid schemes includes:

1. Node jumping. A well-known hybrid approach suitable for one-dimensional problems uses a fixed space grid but employs a variable time step so that the phase front moves from one node to the next within the time step. This method was first presented by Douglas and Gallie \([47]\) and a recent version, based on an enthalpy formulation, has been presented by Voller \([11, 15]\).

2. Local tracking. These methods only employ a deforming grid in the local region of the phase front. In one-dimensional problems \([48-50]\) the typical approach is to employ local interpolation in the phase change region to improve the accuracy of temperature gradient terms. A prime objective of these methods is to improve the accuracy in treating Stefan problems with discontinuous thermal properties (see discussion in Section 7). Extension to multi dimensions is possible \([49-50]\) but often overburdened with interpolations rules. In the finite element literature,
however, a practical multidimensional local front tracking method has been proposed by Crivelli and Idelson [51]. In this approach the oscillations in the basic enthalpy method are removed on splitting of the finite elements that are changing phase into solid and liquid components. This approach has recently been extended by Celentano et al. [52] to deal with mushy phase change.

3. Deforming enthalpy methods. There is no reason why the enthalpy formulation, Eq. (10), should be discretized on a fixed grid and computational advantages may be obtained on implementing the enthalpy on a deforming grid. For example, due to the conserved nature of the enthalpy scheme, an approximate front tracking scheme that only needs to locate the phase front in specified volumes, as opposed to specified node points, can be devised. Voller and Peng [36] demonstrate that this hybrid approach can lead to predictions, in both one and two dimensional problems, that have the accuracy of a deforming grid approach but the computational efficiency of a fixed grid approach.

7 DISCONTINUOUS THERMAL PROPERTIES

In all the test problems presented above the thermal properties take single constant values. In general, this is not the case and some care needs to be taken in problems that have variable thermal properties. In particular, problems where the thermal properties are discontinuous across the phase change.

In deforming grid approaches, since an element always remains in one phase throughout the calculation discontinuous thermal properties are readily dealt with by specifying the thermal properties of each element in the computational grid.

In fixed grid calculations, the treatment of discontinuous thermal properties requires some special procedures. If a nodal lumping approach is used, discontinuities in the specific heat and density can be calculated in terms of nodal averaged values, e.g.,

$$c_p = g_p c_l + (1 - g_p) c_s$$  \hspace{1cm} (55)

where $g_p$ is the liquid fraction of the control volume around node $P$. The difficulty comes in dealing with discontinuities in the thermal conductivity, $K$. In constructing coefficients, the values of $K$ need to be calculated at integration points (e.g., mid sides of control volume faces), which generally do not coincide with the node points. A naive approach, not recommended by this author, is to assign conductivities based on nodal averaged values, i.e.,

$$K_p = g_p K_l + (1 - g_p) K_s$$  \hspace{1cm} (56)

and then to take appropriate interpolations for integration point values. Although this approach is conservative, it leads to poor predictions, particularly when the change in conductivity across the phase change is large. One recommended approach [53] is to use a Kirchhoff transformation [1]
Figure 16. Front predictions for discontinuous conductivity.

\[ \phi = \int_0^T K(\alpha) d\alpha \]  \hspace{1cm} (57)

where a phase change temperature of \( T_m = 0 \) has been assumed. With the Kirchhoff transformation

\[ \frac{\partial \phi}{\partial x} = K \frac{\partial T}{\partial x}, \quad \frac{\partial \phi}{\partial y} = K \frac{\partial T}{\partial y} \]  \hspace{1cm} (58)

and the diffusion term in the heat transport equation can be written as

\[ \nabla \cdot (K \nabla T) = \frac{\partial}{\partial x} \left( K_x \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( K_y \frac{\partial T}{\partial y} \right) \]  \hspace{1cm} (59)

where

\[ K_x = \frac{[\partial \phi/\partial x]}{[\partial T/\partial x]}, \quad K_y = \frac{[\partial \phi/\partial y]}{[\partial T/\partial y]} \]  \hspace{1cm} (60)

In effect, this approach uses a Kirchhoff transformation, but through the definition
of the nonlinear, non-isotropic conductivity in Eq. (60), it retains temperature as the only dependent variable. The use of Eq. (59) and Eq. (60) simply requires the calculation of the Kirchhoff variable at each node point, similar to calculating a nodal conductivity. After appropriate element approximations of the terms $\partial \phi / \partial x$, etc., the values of $K_x$ and $K_y$ can be calculated at the integration points. Note that these values will be constant in linear triangular elements.

To illustrated the Kirchhoff approach consider the standard one-dimensional two phase test problem with $St = 0.2$ but with $K_1 = 1$ and $K_2 = 10$. The Kirchhoff predictions for the front movement are shown in Fig. 16 and compared with the analytical solution ($s = 1.725 \sqrt{T}$) and predictions obtained using the averaging approach defined by Eq. (56). These results clearly show the effectiveness of the Kirchhoff approach and highlight the much poorer performance of the averaging approach.

8 PROBLEMS WITH FLUID FLOW

The Stefan problems investigated above have been controlled by heat conduction alone. In an important class of Stefan problems, however, fluid flow and advective heat transfer are important. References [42-46] document front fixing solutions for Stefan problems with flow, and an extensive review of general numerical solutions has been made by Samarskii et al. [54]. In this article, we will explore fixed grid techniques for Stefan problems with flow in some detail.

As an example problem, consider the case of melting a rectangular ($H \times 2H$) solid block (insulated on three sides and initially at temperature $T_i \leq T_m = 0$) by maintaining an isothermally hot wall ($T_o > 0$) along $x = 0$. In this problem, a melted layer will form along the heated wall and will progress into the solid. If the solid is a pure material, there is a distinct liquid/solid interface and due to natural convection the melting rate at the top of the cavity ($y = H$) is enhanced. With a view to using a fixed grid solution, the governing equations for this two dimensional problem can be written in dimensionless form [55]

$$\nabla u = 0$$  \hspace{1cm} (61)

$$\frac{\partial T}{\partial t} + u \nabla T = \nabla^2 T - \frac{1}{St} \frac{\partial g}{\partial t}$$  \hspace{1cm} (62)

$$\frac{\partial u}{\partial t} + u \nabla u = Pr \nabla^2 u - \frac{\partial P}{\partial x} + S_u$$  \hspace{1cm} (63)
\[
\frac{\partial \nu}{\partial t} + u \nabla \nu = \Pr \nabla^2 \nu - \frac{\partial p}{\partial y} + S_{\nu} + Ra \Pr T
\]  

(64)

where \( P \) is pressure, \( \Pr \) is the Prandtl number, \( Ra \) the Raleigh number (based on cavity height \( H \)) and \( St \) is the Stefan number introduced above.

There are two central problems involved in solving the above equations:

1. **The treatment of the evolution of latent heat.** The heat transfer equation, Eq. (62), is the liquid fraction source form of the enthalpy equation (cf. Eq. (19)) and, after appropriate discretization with implicit time integration, the treatment of the phase change can follow the source-based algorithms outlined in Section 4.3.1. Alternatively, on rewriting Eq. (62), a linearized enthalpy (Section 4.3.2) or apparent heat capacity (Section 4.3.3) scheme can be used.

2. **Velocity switch off.** The momentum equations in the component velocities \( u \) and \( v \) are solved throughout the domain. This approach requires that the velocities are switched off as the solid is formed. In a numerical treatment a given computational cell will take a number of time steps to complete solidification,

\[
\mu_{\text{eff}} = \mu + (1 - \gamma)B \Gamma G
\]  

(65)

Hence as the computational cell solidifies, the material becomes increasingly "stiffer" and the flow at full solidification is suppressed. The alternative approach, preferred by this author [55, 57, 58], is to model the phase change cells as "pseudo porous" media and introduce a Darcy-like term such that the source terms, \( S_u \) and \( S_v \) in Eqs. (63) and (64) become

\[
S_u = -(1 - \gamma)B \Gamma G u, \quad S_v = -(1 - \gamma)B \Gamma G v
\]  

(66)

As a cell solidifies, these source terms will dominate the discretized momentum equations and return velocity values close to zero.

Solutions (phase front movement and shape and flow field) of the given problem for the case \( T_i = 0, T_o = 1, St = 0.042, Ra = 2.2 \times 10^5, Pr = 0.021 \) (corresponding to the melting of gallium [59]), are shown in Fig. 17. In these calculations, as detailed in refs [55, 57], the SIMPLE algorithm with upwinding [6] is used to solve the fluid flow equations, the modified source update is used to deal with the phase change, and the pseudo porous approach, Eq. (66), with \( B \Gamma G = 10^3 \), is used to deal with the velocity switch off. The grid size used is 20x40, and the time step is (in dimensional time) \( t = 5s \). The simulation to real time \( t = 12 \text{ min} \) required an average of 28
iterations per time step, with the weak point, in terms of convergence, in the fluid flow solver. An interesting point to note is that the flow calculations, Fig. 17, only show a single flow cell in the melt region. In an alternative finite element analysis Dantzig [60] observes, when the cavity is thin, a number of flow cells. This is attributed to the fact that the upwinding used in the SIMPLE algorithm tends to smear out the detailed flow fields. Nevertheless, as documented elsewhere [57], the approach presented here produces predictions in reasonable agreement with experiments and in close agreement with alternative approaches, e.g., transformed coordinates [55].

9 GENERAL PHASE CHANGE PROBLEMS

Up to now, all of the problems investigated have been Stefan problems characterized by a sharp phase front. Although the investigation of such problems is useful in terms of developing robust algorithms that can deal with latent heat evolution and boundary tracking they are somewhat removed from many practical phase change problems. In general, phase change processes involve multi-component material, and the phase change occurs over a mushy region in which a distinct solid/liquid interface cannot be identified on the scale of the process. The common and natural numerical approach to use on such problems is a fixed grid scheme based on an enthalpy function.

9.1 Mushy Problems

In the most straightforward cases, the extent of the mushy region can be defined by a solidus $T_s$ and liquidus $T_l$ temperatures that remain fixed throughout the process. The mushy region can be characterized by a known liquid fraction temperature
relationship, \( g(T) \), which immediately implies a known enthalpy temperature relationship, \( H(T) \). A simple linear relationship, e.g.,

\[
H = cT + \frac{T - T_s}{T_1 - T_s} L
\]

in the mushy region is often used as a first cut model. In many systems, however, the form of \( g(T) \) and \( H(T) \) is controlled by the local scale segregation of the solute phases, and more complex nonlinear relationships between the enthalpy and temperature result \[61, 62\]. For example, in a binary dendritic alloy, if at the local scale of the dendrite arm space the mass diffusion in the liquid and solid phase is rapid, the lever rule \[61\] can be applied and the enthalpy temperature relationship is

\[
H(T) = cT + \left[ 1 - \frac{1}{k-1} \left( \frac{T_1 - T}{T_m - T} \right) \right] L
\]

where \( k \) is the partition coefficient for the alloy and \( T_m \) is the phase change temperature of the pure solvent. Regardless of the exact enthalpy temperature relationship, if \( H(T) \) is well defined, any of the fixed grid techniques (both explicit \[63\] and implicit \[21, 64, 65\]) recommended above can be readily applied.

9.2 Mushy Problems with Fluid Flow

The previous situation is made more complex when fluid flow is present. As an illustration, consider the advection term, which, on combining the two phase equations presented by Ni and Beckermann \[2\], has the general form

\[
\text{TERM} = \nabla \cdot (\rho u_s (1-g) H_s + \rho u_l g H_l)
\]

where \( u \) is a velocity, the subscripts \( s \) and \( l \) refer to the solid and liquid respectively and

\[
H_1 = cT + L, \quad H_s = cT \quad (70)
\]

The final form of Eq. (69) will depend on the nature of the mushy region. Two extreme cases can be readily investigated.

1. The mushy region consists of a fixed solid phase such that \( u_s = 0 \). Here Eq. (69) will have the form

\[
\text{TERM} = (\rho u_l g H_l)
\]

which on using Eq. (70), can be expanded as

\[
\text{TERM} = (\rho u_l g c T) + \nabla \cdot (\rho u_l g L)
\]

\[72\]
The last term can be dropped by using the continuity of liquid to arrive at

\[ \text{TERM} = \rho u_g c \nabla T \] (73)

Hence in the fixed solid mushy region there is no convection of latent heat.

2. The mushy region consists of a fine dispersed solid phase such that \( u_s = u_i = u \).

Here Eq. (69) will, after expanding using Eq. (70), have the form

\[ \text{TERM} = (\rho u c T) + \nabla (\rho u g L) \] (74)

In this case the second term cannot be dropped. Hence, in a dispersed mushy region, latent heat will be transported. Voller et al. [66] demonstrate that the effect of the mushy region morphology on the advection or non-advection of latent heat has a dramatic influence on heat transfer and mushy region shape.

In a dispersed mushy region, some additional analysis can be carried out. Applying mass continuity the advection term in Eq. (74) can be written as

\[ \text{TERM} = \rho u c \nabla T + \rho u g \nabla T \] (75)

which, on noting that \( \nabla g = (dg/dT) \nabla T \), can be rewritten as

\[ \text{TERM} = \rho u [c + L \frac{dg}{dT}] \nabla T \] (76)

or with reference to Eq. (29),

\[ \text{TERM} = \] (77)

where \( C^A \) is the apparent heat capacity. Equation (77) is exactly the form of the advection term that would be used in an apparent heat capacity treatment of a fluid flow controlled phase change [60, 67]. This suggests that the choice of an apparent heat capacity scheme in the modeling of a fluid flow phase change with a mushy region implicitly assumes that the mushy region is dispersed and that latent heat is advected. In general, this may not be the case, e.g., in a dendritic binary alloy. Hence care needs to be taken in using the apparent heat capacity method for fluid flow phase change problems.

9.3 Solute Transport

The above discussion on mushy region problems has assumed that the limits of the region are defined by fixed temperatures. If the segregation (solute transport) is controlled by local scale mass diffusion alone, then such a treatment is valid. In general, however, it would be expected that advective transport of the solute, driven by forced and natural convection flows, will be present. This solute transport will
occur over a much larger scale, and the assumption of fixed temperature boundaries on the mushy region will no longer be valid. The treatment of the phase change in this case involves the coupled solution of solute and heat transport equations. Typically, in a binary alloy calculation, the computations involve the calculation of nodal temperature, concentration and liquid fraction fields that satisfy the transport equations constrained by the requirement, in the mushy region, that the temperature and solute concentration fields lie on the liquidus line of the phase diagram. A number of schemes for dealing with this coupled problem have been suggested in the literature [68-80] and an initial attempt has been made to review them [81].

10 CONCLUSIONS

Dealing with the evolution of latent heat is a central requirement in the numerical modeling of phase change problems. This review article has outlined the mechanics of various schemes for modeling the Stefan problem. If a robust scheme can be found to deal with this problem, it will be a suitable base for developing a more general phase change scheme. The objective has been to provide the reader with basic information on the construction and performance of various schemes so that s/he is able to develop more specific schemes. There has not been room to include all the important references in the area of numerical methods for phase change problems. The reader is directed toward additional reviews and discussions [1, 22-25, 54, 81-86] for a more complete picture.

In closing a few highlights are worth emphasizing.

1. The author would like to think we are close to the final word on implicit time integration fixed grid schemes based on the enthalpy equation. The apparent heat capacity method with post iterative correction is an excellent scheme [26, 27]. It's only drawback, the lack of local heat conservation at every time step, is, with a minimal amount of additional computational effort, taken care of with the linearized enthalpy scheme [21].

2. Although the fixed grid schemes are easy to apply, solutions can be subjected to oscillations that may be undesirable. The obvious way around this is to employ a front tracking approach based on a deforming mesh. An effective deforming mesh solution for the Stefan problem has been demonstrated in this article.

3. The central problem with using a deforming grid is in the grid management. If it is poorly implemented, the grid will distort and error and lack of convergence will result. This can be avoided by using hybrid schemes that combine fixed grid approaches with local [48-52] or approximate [36] front tracking. A well-implemented hybrid scheme will have the flexibility and efficiency of a fixed grid scheme with the accuracy and smoothness of a pure deforming grid scheme. There is an opportunity for further research in the area of developing efficient hybrid schemes.
4. A common application of hybrid schemes deals with discontinuous thermal properties, in particular conductivity. When poor approximations are used in pure fixed grid schemes, errors can result. A recently proposed method based on a Kirchhoff transformation [53] has been outlined in this article. This approach, which is relatively easy to apply, leads to predictions with the same quality as those seen in problems with constant thermal properties.

5. The physics in Stefan phase change problems is very straightforward, and for the most part the best computational solution approaches are well established. In more general phase change problems, however, the physics is much more complex. Questions related to such things as the morphology of the mushy region, the enthalpy temperature relationship, and the coupling of thermal and solute fields, must be considered. Best computational practice for general phase change problems is not established, and it is in this area that the most relevant and exciting research is currently taking place.

11 REFERENCES


