Modelling Simul. Mater. Sci. Eng. **4** (1996) 371–396. Printed in the UK

Mathematical modelling of solidification and melting: a review

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Received 14 March 1996, accepted for publication 28 May 1996

Abstract. The major methods of mathematical modelling of solidification and melting problems are reviewed in this paper. Different analytical methods, nowadays still used as standard references to validate numerical models, are presented. Various mathematical formulations to numerically solve solidification and melting problems are categorized. Relative merits and disadvantages of each formulation are analysed. Recent advances in modelling solidification and melting problems associated with convective motion of liquid phase are discussed. Based on this comprehensive survey, basic guidelines are outlined to choose a correct mathematical formulation for solving solidification and melting problems.

Nomenclature

a	coefficient in discretized equations
b	source term in discretized equations
C_A	concentration
C_s, C_l, C_{in}	heat capacities at constant pressure for solid, liquid and liquid-solid interface
D_A	diffusion coefficient
g	gravitational acceleration
h	enthalpy
H_f	latent heat
i_b	interface node index
k	thermal conductivity
p	pressure
r	cylindrical coordinate direction
S	source term
St	Stefan number
t	time
T	temperature
ΔT_r	fictitious temperature rise
u	velocity in the x direction
V	volume
$\boldsymbol{V}$	velocity vector
v	velocity in the y direction
w	velocity in the z direction
x	Cartesian coordinate direction
$X(t)$	position of liquid–solid interface
y	Cartesian coordinate direction
z	Cartesian coordinate direction

0965-0393/96/040371+26$19.50

Greek symbols

α	thermal diffusivity
Γ_μ, Γ_α, Γ_D,	dimensionless diffusion coefficients for the momentum, energy and diffusion equations
δ	thickness of boundary layer
η	dimensionless number used in derivations as a temporary substitution
ϕ	arbitrary dependent variable
λ	dimensionless number in solution to Neumann problem, liquid fraction
ν	kinematic viscosity
θ	Kirchhoff temperature
ρ	density
μ	dynamic viscosity
ω	vorticity
Ψ	stream function
ζ	coefficient of thermal expansion

Subscripts

app	apparent
b	bottom control volume face
c	concentration
e	east control volume face
eff	effective
h	enthalpy
i	pertaining to any coordinate value
in	liquid–solid interface
l	liquid
m	melting
n	north control volume face
nb	general neighbour grid point
n	old value (at time t) of the dependent variable
$n+1$	new value (at time $t + \Delta t$) of the dependent variable
o	initial
P	present nodal point
p	location of moving interface
s	solid, south control volume face
t	top control volume face, thermal
v	velocity
w	west control volume face
x	Cartesian coordinate direction
y	Cartesian coordinate direction
z	Cartesian coordinate direction

Superscripts

o	at the previous time step

1. Introduction

The phenomena of solidification and melting are associated with many practical applications. They occur in a diverse range of industrial processes, such as metal processing, solidification of castings, environmental engineering and thermal energy storage system in a space station. In these processes, matter is subject to a phase change. Consequently, a boundary separating two different phases develops and moves in the matter during the process. Transport properties vary considerably between phases, which result in totally different rates of energy, mass and momentum transport from one phase to another. In these problems, the position of the moving boundary cannot be identified in advance, but has to be determined as an important constituent of the solution. The term 'moving boundary problems' is associated with time-dependent boundary problems, where the position of the moving boundary must be determined as a function of time and space. Moving boundary problems, also referred to as Stefan problems, were studied as early as 1831 by Lame and Clapeyron [1]. However, the sequence of articles [2, 3] written by Stefan has given his name to this family of problems, which resulted from his study of the melting of the polar ice cap around 1890.

In early years, analytical methods were the only means available to render mathematically an understanding of physical processes involving the moving boundary. Although analytical methods offer an exact solution and are mathematically elegant, due to their limitations, analytical solutions are mainly for the one-dimensional cases of an infinite or semi-infinite region with simple initial and boundary conditions and constant thermal properties [4]. Practical solidification and melting problems are rarely one dimensional, initial and boundary conditions are always complex, thermophysical properties can vary with phases, temperatures and concentration, and various transport mechanisms (for example, convection, conduction, diffusion and radiation) can happen simultaneously. With the rise of high-speed digital computers, mathematical modelling and computer simulation often become the most economical and fastest approaches to provide a broad understanding of the practical processes involving the moving boundary problems. Nowadays in most engineering applications, recourse for solving the moving boundary problems has been made to numerical analyses that utilize either finite difference, finite element of boundary element methods. The success of finite element and boundary element methods lies in their ability to handle complex geometries, but they are acknowledged to be more time consuming in terms of computing and programming. Because of their simplicity in formulation and programming, finite difference techniques are still the most popular at the present.

Hence, the evolution of mathematical analyses on solidification and melting problems has undergone three distinct eras. Most of the earlier investigations were confined to one-dimensional diffusion-controlled problems with very simple geometries due to constraints in the tools available to scientists and engineers at that time. The analytical solutions developed during this first era serve as a cornerstone of this discipline and are still used today as standard references to validate the numerical models. The advent of computers, a couple of decades ago, enabled the consideration of multidimensional problems with more complex geometries. A new era of analysis in the solidification and melting problems commenced with the birth of numerical methods. Perhaps owing to the limited power of the earlier computers, the numerical models in the second era that were developed were based on one equation (e.g., and energy or diffusion equation) and omission of convection. With the help of the more advanced and powerful computers which have been developed in the past decade, mathematical modelling has proceeded into a modern era. More sophisticated numerical models have been developed

to handle multidimensional phenomena involving convection as well as the presence of the moving boundary in complex geometries. The succeeding review will summarize the major developments in mathematical analyses of the phase change problems involved in melting and solidification phenomena. The intention of this review is to present and compare some of the well known and novel numerical methods available to solve phase change problems since it is impossible to review all the existing methods within one article.

2. Analytical methods

2.1. Neumann's method

The simplest phase change problem is the one-phase problem first solved analytically by Stefan [2]. The term 'one phase' designates only one of the phases (liquid) being 'active', the other phase staying at its melting temperature. Stefan's solution with constant thermophysical properties shows that the rate of melting or solidification in a semi-infinite region is governed by a dimensionless number, known as the Stefan number (St),

$$\mathrm{St} = [C_\mathrm{l}(T_\mathrm{l} - T_\mathrm{m})]/H_\mathrm{f} \tag{1}$$

where C_l is the heat capacity of the liquid, H_f is the latent heat of fusion, and T_l and T_m are the temperatures of the surrounding and melting point, respectively.

Neumann [5] extended the Stefan's solution to the two-phase problem. In this more realistic scenario, the initial state of the phase change material is assumed to be solid, for a melting process, but its initial temperature is not equal to the phase change temperature, and its temperature during the melting is not maintained at a constant value. If melting of a semi-infinite slab ($0 < x < \infty$) is considered, initially solid at a uniform temperature $T_\mathrm{s} \leqslant T_\mathrm{m}$, and a constant temperature is imposed on the face $x = 0$, with assumptions of constant thermophysical properties, the problem can be mathematically expressed as follows:

Heat conduction in liquid region

$$\frac{\partial T_\mathrm{l}}{\partial t} = \alpha_\mathrm{l}\frac{\partial^2 T_\mathrm{l}}{\partial x^2} \qquad \text{for } 0 < x < X(t),\ t > 0 \tag{2}$$

Heat conduction in solid region

$$\frac{\partial T_\mathrm{s}}{\partial t} = \alpha_\mathrm{s}\frac{\partial^2 T_\mathrm{s}}{\partial x^2} \qquad \text{for } X(t) < x,\ t > 0 \tag{3}$$

Interface temperature

$$T(X(t), t) = T_\mathrm{m} \qquad t > 0 \tag{4}$$

Stefan condition

$$k_\mathrm{s}\frac{\partial T_\mathrm{s}}{\partial x} - k_\mathrm{l}\frac{\partial T_\mathrm{l}}{\partial x} = H_\mathrm{f}\rho\frac{\mathrm{d}X}{\mathrm{d}t} \qquad \text{for } x = X(t),\ t > 0 \tag{5}$$

Initial conditions

$$T(x, 0) = T_\mathrm{s} < T_\mathrm{m} \qquad \text{for } x > 0,\ X(0) = 0 \tag{6}$$

Boundary conditions

$$T(0, t) = T_\mathrm{l} > T_\mathrm{m} \qquad \text{for } t > 0 \tag{7}$$

$$T(x, t) = T_\mathrm{s} \qquad \text{for } x \to \infty,\ t > 0 \tag{8}$$

where $X(t)$ is the position of the melting interface (moving boundary). Figure 1 illustrates this problem more clearly.

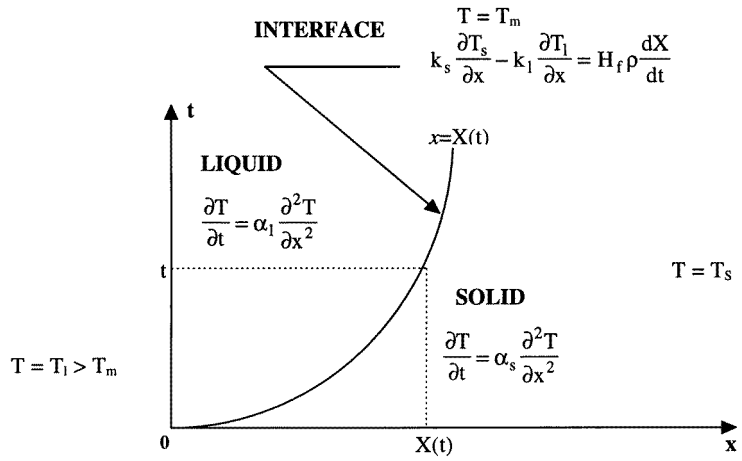

Figure 1. Schematic illustration of spacetime for the two-phase Stefan problem.

And analytical solution to such a problem was obtained by Neumann in terms of a similarity variable

$$\eta = \frac{x}{2\sqrt{\alpha_l}}. \tag{9}$$

The final Neumann's solution can be written as:

Interface position

$$X(t) = 2\lambda\sqrt{\alpha_l t} \tag{10}$$

Temperature in the liquid phase

$$T(x,t) = T_l - (T_l - T_m)\frac{\operatorname{erf}\left(x/2\sqrt{\alpha_l t}\right)}{\operatorname{erf}\lambda} \tag{11}$$

Temperature in the solid phase

$$T(x,t) = T_s + (T_m - T_s)\frac{\operatorname{erfc}\left(x/2\sqrt{\alpha_s t}\right)}{\operatorname{erfc}\left(\lambda\sqrt{\alpha_l/\alpha_s}\right)}. \tag{12}$$

The λ in equations (10)–(12) is the solution to the transcendental equation

$$\frac{\mathrm{St_l}}{\exp(\lambda^2)\operatorname{erf}(\lambda)} - \frac{\mathrm{St_s}\sqrt{\alpha_s}}{\sqrt{\alpha_l}\exp(\alpha_l\lambda^2/\alpha_s)\operatorname{erfc}\left(\lambda\sqrt{\alpha_l/\alpha_s}\right)} = \lambda\sqrt{\pi} \tag{13}$$

where

$$\mathrm{St_l} = \frac{C_l(T_l - T_m)}{H_f} \qquad \mathrm{St_s} = \frac{C_s(T_m - T_s)}{H_f}. \tag{14}$$

However, the Neumannn's solution is available only for moving boundary problems in the rectangular coordinate system.

For phase change problems in the cylindrical coordinate, fortunately, Paterson [6] has shown that the exact solution is obtained if the solution is chosen as an exponential integral function in the form $\mathrm{Ei}(-r^2/4\alpha t)$. Consider the case where the surface of separation between the solid and liquid phases is at radius $X(t) = r(t)$. The liquid and solid regions exist for $r > X(t)$ and $r < X(t)$, respectively. Both phases have

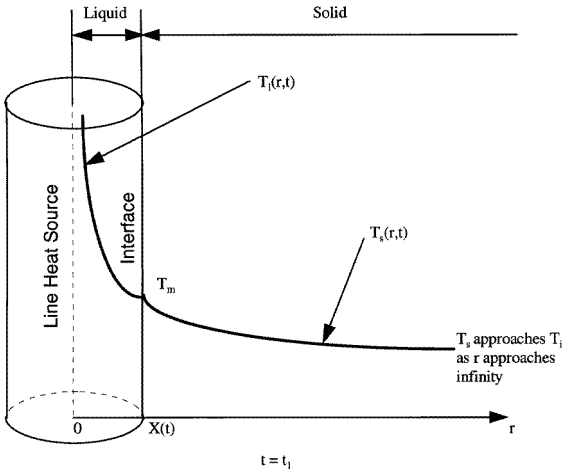

Figure 2. Schematic illustration of melting by a line-heat source in an infinite medium with cylindrical symmetry.

constant thermophysical properties. A line heat source of strength Q (W m^{-1}) is located at $r = 0$ in an infinite fusible solid at a uniform temperature T_i lower than melting temperature T_m of the material. The heat source is activated at time $t = 0$ to release heat continuously for time $t > 0$. Consequently, the melting commences at the origin $r = 0$ and the solid–liquid interface moves in the positive r direction. Figure 2 illustrates schematically this case. The energy balance around the line-heat source is expressed as

$$\lim_{r\to 0}\left[-2\pi r k_\mathrm{l}\frac{\partial T_\mathrm{l}}{\partial r}\right] = Q. \tag{15}$$

The solutions for the temperatures in the solid and liquid phases are given by

$$T_\mathrm{s} = T_\mathrm{m} - \frac{Q}{4\pi k_\mathrm{s}}\left[\mathrm{Ei}\left(-\frac{r^2}{4\alpha_\mathrm{s}t}\right) - \mathrm{Ei}(-\lambda^2)\right] \tag{16}$$

$$T_\mathrm{l}(r,t) = T_i - \frac{T_i - T_\mathrm{m}}{\mathrm{Ei}(-\lambda^2\alpha_\mathrm{s}/\alpha_\mathrm{l})}\mathrm{Ei}\left(-\frac{r^2}{4\alpha_\mathrm{l}t}\right). \tag{17}$$

The constant λ is determined from the following transcendental equation:

$$-\frac{Q}{4\pi}\mathrm{e}^{-\lambda^2} + \frac{k_\mathrm{l}(T_i - T_\mathrm{m})}{\mathrm{Ei}(-\lambda^2\alpha_\mathrm{s}/\alpha_\mathrm{l})}\mathrm{e}^{-\lambda^2\alpha_\mathrm{s}/\alpha_\mathrm{l}} = \lambda^2\alpha_\mathrm{s}\rho H_\mathrm{f}. \tag{18}$$

The solid–liquid interface can be located by the following equation:

$$X(t) = 2\lambda(\alpha_\mathrm{s}t)^{1/2}. \tag{19}$$

2.2. Heat balance integral method

Since the exact analytical solutions as discussed in the preceding section exist only for semi-infinite problems with parameters constant in each phase and constant initial and imposed temperatures, they are not applicable to problems with constant imposed

flux. Clearly then, for most realistic cases, one is forced to seek approximate solutions. In this section, one of them introduced by Goodman [7] is presented. Based on the Karman–Pohlhausen's method of the momentum integral [8] in the boundary-layer theory, Goodman developed an integral equation which expresses the overall heat balance of the system by integrating the one-dimensional heat conduction equation with respect to the spatial variable x and inserting boundary conditions. The method is outlined below:

(a) assume that the temperature distribution depends on the spatial variable in a particular form which is consistent with the boundary conditions, e.g. a polynomial relationship;

(b) integrate the heat conduction equation with respect to the spatial variable over the appropriate interval and substitute the assumed form of the temperature distribution to attain the heat balance integral;

(c) solve the integral equation to obtain the time dependence of the temperature distribution and of moving boundaries.

The method was used to solve the single-phase melting-ice problem with various boundary conditions [7]. Goodman and Shea [9] also applied the method to the two-phase problems of melting of a finite slab. In such problems, as illustrated in figure 3, a constant heat flux is applied at one face of a finite slab which is initially at a uniform temperature below the melting point; the other face of the slab is either insulated or kept at its initial temperature. They determined how the melting propagates and how the temperature is distributed in the melted and unmelted portions of the slab.

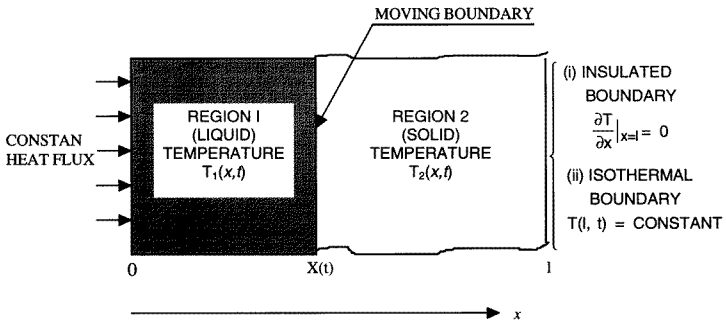

Figure 3. Schematic representation of melting of an infinite slab.

The heat balance integral method has been extensively applied to different problems, and has often been modified with the intention of improving and easing the mathematical analysis. The mathematical manipulations required for the heat balance integral method, for anything other than relatively simple problems, can be very complicated and cumbersome. Besides, selecting a satisfactory approximation to the temperature distribution is a major difficulty with this method. For instance, the use of a high-order polynomial makes this approach highly complicated, and even does not necessarily improve the accuracy of the solution.

In an effort to improve the accuracy of the heat balance integral method, Noble [10] proposed a spatial subdivision scheme in which quadratic profiles are used in each subregion. Bell [11] later modified Noble's scheme to solve a single-phase melting problem.

3. Numerical methods for solving the pure heat conduction equation with a phase change involved

3.1. Fixed grid methods

In this method, the heat flow equation is approximated by finite difference replacements for the derivatives in order to calculate values of temperature $T_{i,n}$, at $x_i = i\Delta x$ and time $t_n = n\Delta t$ on a fixed grid in the (x, t) plane. At any time $t_n = n\Delta t$, the moving boundary will be located between two adjacent grid points; for instance, between $i_b\Delta x$ and $(i_b+1)\Delta x$, as illustrated in figure 4.

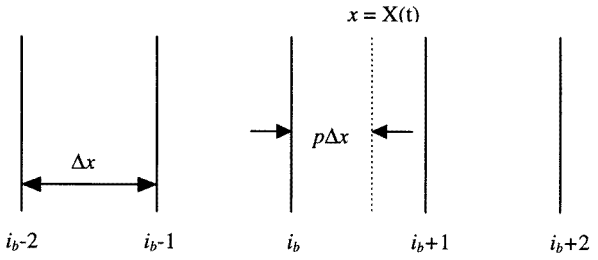

Figure 4. Position of the moving boundary in a fixed grid.

The numerical solution of the one-phase ice-melting problem, defined by equations (2) and (4)–(8), offer a simple illustration of this method. The new temperature is calculated from temperatures of the previous step on the basis of the following formulation:

$$T_{i,n+1} = T_{i,n} + \left(\frac{\Delta t}{\Delta x^2}\right)\{T_{i-1,n} - 2T_{i,n} + T_{i+1,n}\} \qquad i = 0, i_b - 1. \tag{20}$$

In terms of three-point Lagrange interpolation [12] instead of (20), the temperature at $x = i_b\Delta x$ is computed,

$$T_{i_b,n+1} = T_{i_b,n} + \left(\frac{2\Delta t}{\Delta x^2}\right)\left\{\frac{1}{p_n+1}T_{i_b-1,n} - \frac{1}{p_n}T_{i_b,n}\right\}. \tag{21}$$

The variation of the location of the moving boundary is

$$p_{n+1} = p_n - \left(\frac{\Delta t}{\rho H_f \Delta x^2}\right)\left\{\frac{p_n}{p_n+1}T_{i_b-1,n} - \frac{1}{p_n}T_{i_b,n}\right\}. \tag{22}$$

As seen, the numerical solution of the method is carried out on a space grid that remains fixed throughout the calculation.

Various schemes have been proposed for approximating both the Stefan conditions on the moving boundary and the partial differential equation at the adjacent grid points. For example, in a grid space containing the moving boundary at any time, Murray and Landis [13] introduced two fictitious temperatures, one achieved by quadratic extrapolation from temperatures in the solid region and the other from temperatures in the liquid region. The fusion temperature and the current position of the moving interface are incorporated in the fictitious temperatures, which are then substituted into a standard approximate, such as equation (20), to calculate the temperature near the interface instead of using special formulae like equation (21). For the motion of the interface, an expression similar to equation (22) is used according to the Taylor extrapolation formula. Ciment and Guenther

[14] developed a method of spatial mesh refinement on both sides of the moving boundary, previously analysed by Ciment and Sweet [15]. With this method, Lazaridis [16] applied explicit finite difference approximations to solve two-phase solidification problems in both two and three space dimensions. Some numerical schemes have been developed based on an auxiliary set of differential equations, which express the fact that the moving boundary is an isotherm. Close to the boundary, formulae for unequal intervals were incorporated into the auxiliary equations. Standard finite difference approximations to the heat flow equation were used at grid points far enough from the moving boundary. To avoid loss of accuracy associated with singularities, which can arise when the moving boundary is too near a grid point, localized quadratic temperature profiles were applied. The mathematical manipulations are very lengthy and complex indeed.

The major advantage of fixed grid methods is that these methods can handle multidimensional problems efficiently without much difficulty. Thus, the numerical treatment of the moving boundary can be achieved through simple modifications of existing heat transfer codes. As such, they have come into common use for modelling a variety of complex moving boundary problems. Two excellent surveys of the fixed grid methods can be found in [17] and [18].

3.2. Variable grid methods

The fixed grid methods sometimes break down as the boundary moves a distance larger than a space increment in a time step. This constraint, that depends on the velocity of the moving boundary, may largely increase the array size (i.e. memory) and the cpu-time if computations are to be performed for extended times. The problems associated with the fixed grid method can be avoided by using the variable grid methods. In the variable grid methods, the exact location of the moving boundary is evaluated on a grid at each step. The grid can be either interface fitting or dynamic.

The interface-fitting grids (also referred to as the variable time step methods), where a uniform spatial grid but a non-uniform time step are used, has been repeatedly employed to solve two-phase and one-dimensional problems. Instead of applying a fixed time step and searching for the location of the moving boundary, Douglas and Gallie [19] intended to determine a variable time step, as part of the solution, such that the moving boundary coincides with a grid line in space. The fully implicit finite difference equations were used. Gupta and Kumar [20] formulated the same set of finite difference equation as Douglas and Gallie but they used the Stefan condition to update the time step. The instability, that develops as the depth of the moving boundary increases, was avoided with Gupta and Kumar's method. Goodling and Khader [21] gave another variable time step method in which the finite difference form of the Stefan condition was incorporated into the system of the equations to be solved. The system is solved for an arbitrary value of the temperature of the node adjacent to the moving boundary, which is then updated from the Stefan condition. However, Gupta and Kumar [22], in a study of a convective boundary condition at the fixed end, found that Goodling and Khader's method does not converge as the computation progresses in time. They showed a satisfactory agreement between their results and those obtained by using other variable time step methods and the Goodman's integral method [7]. Gupta and Kumar [23] also modified the Douglas and Gallie's method to solve the oxygen diffusion problem due to the absence of an explicit relationship between the velocity of the moving boundary and mass flux. Their results are very close to those obtained by Hansen and Hougaard [24] and by Dahmardah and Mayers [25]. However, this approach is not applicable for multidimensional problems.

The other variable methods are based on variable space grids, also known as the dynamic grids, where the number of spatial intervals are kept constant and the spatial intervals are adjusted in such a manner so that the moving boundary lies on a particular grid point. Thus, in these methods the spatial intervals are a function of time. The substantial temperature derivative of each grid point is

$$\left.\frac{\mathrm{d}T}{\mathrm{d}t}\right|_i = \left.\frac{\partial T}{\partial x}\right|_t \left.\frac{\mathrm{d}x}{\mathrm{d}t}\right|_i + \left.\frac{\partial T}{\partial t}\right|_x \tag{23}$$

where the moving rate of each grid point is related to the moving boundary by

$$\left.\frac{\mathrm{d}x}{\mathrm{d}t}\right|_i = \frac{x}{X(t)}\frac{\mathrm{d}X}{\mathrm{d}t}. \tag{24}$$

By substituting equations (24) and (2) into (23), the governing equation for one-dimensional problems becomes

$$\left.\frac{\mathrm{d}T}{\mathrm{d}t}\right|_i = \frac{x}{X(t)}\frac{\mathrm{d}X}{\mathrm{d}t}\frac{\partial T}{\partial x} + \frac{\partial^2 T}{\partial x^2}. \tag{25}$$

The position of the moving boundary $X(t)$ is updated at each step by using a finite difference form of the Stefan condition on the moving boundary.

Murray and Landis [13] used these formulations to solve a freezing problem by the explicit method. This method was applied by Heitz and Westwater [26] to solve a one-dimensional problem of solidification with the liquid initially at saturated temperature. They incorporated the volume change and a higher value of liquid thermal conductivity to simulate the effect of fluid flow. Tien and Churchill [27] extended them to cylindrical coordinates. Although multidimensional problems are more complex, with this method Rathjen and Jiji [28] and Tien and Wilkes [29] have obtained solutions of several two-dimensional problems. The complications due to the non-uniform grid size around the moving boundary were avoided by the methods of Crank and Gupta [30], in which the entire uniform grid system moves with the velocity of the moving boundary. They presented two schemes of obtaining the interpolated values of temperatures at the new grid points, to be used for the next step, in terms of cubic spline or polynomials. Instead of the interpolations, Gupta [31] used a Taylor expansion of space and time variables and derived an equation which is actually a particular case of the Murray and Landis equation (25). Detailed discussions of various variable time step methods can be found in [4, 17, 32].

3.3. Methods of latent-heat evolution

The focus of numerical methods described in the preceding subsections is on applying finite difference techniques to the strong formulation of the process, locating moving boundaries and finding temperature profiles at each time step. These methods are called strong numerical solutions and are applicable to the problems involving one or two phases in one space dimension. For two-dimensional cases, the complicated schemes must be used. Hence, with the strong solution, much more computational time is required. It is very difficult to apply the strong solution to a problem with fluid flow involved and in three-dimensional cases.

The alternative is to reformulate the problem in such a way that the Stefan condition is implicitly incorporated in a new form of equations, which applies over the entire region of a fixed domain. These methods are referred to as weak numerical solutions, in which explicit attention to the nature of the moving boundary is avoided. They are the apparent capacity method, the effective capacity method, the heat integration method, the source

based method, the enthalpy method, and so on. Since a large number of superb papers in this area have been published, it is impossible to make a fully comprehensive review. In this subsection, several prevalent methods will be discussed.

3.3.1. Apparent heat capacity methods. In this method, the latent heat is accounted for by increasing the heat capacity of the material in the phase change temperature range. For instance, if the latent heat is released uniformly in the phase change temperature range, the apparent heat capacity can be defined as

$$C_{\text{app}} = \begin{cases} C_{\text{s}} & T < T_{\text{s}} \quad \text{solid phase} \\ C_{\text{in}} & T_{\text{s}} < T < T_{\text{l}} \quad \text{solid/liquid phase} \\ C_{\text{l}} & T > T_{\text{l}} \quad \text{liquid phase} \end{cases} \tag{26}$$

where

$$C_{\text{in}} = \frac{\left\{\int_{T_{\text{s}}}^{T_{\text{l}}} C(T)\,\mathrm{d}T + H_{\text{f}}\right\}}{(T_{\text{l}} - T_{\text{s}})}. \tag{27}$$

In terms of the definition of the apparent heat capacity, the energy equation in one dimension becomes

$$\rho C_{\text{app}} \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right). \tag{28}$$

Equation (28) can easily be discretized and solved numerically. The procedure for calculating the apparent heat capacity is as follows. (i) in the explicit finite difference formulation, C_{app} is determined using the temperatures at the grid points from the previous time step; (ii) in the implicit formulation, two ways are available, the first is to evaluate C_{app} based on the previous time step temperatures (as in the explicit case) and the second is according to the present time step temperatures by an iterative scheme.

The apparent heat capacity method was first presented by Hashemi and Sliepcevich [33] using a finite difference formulation based on the Crank–Nicolson scheme. They applied this method to one-dimensional problems where the phase change occurs in a finite temperature interval (i.e. a mushy range). Later Comini *et al* [34] extended the method to the finite element formulation in a generally applicable approach to one- and two-dimensional problems with both moving boundary and temperature-dependent physical properties.

Although the apparent heat capacity method is conceptually simple, it is apparent that the method does not perform well as compared with other methods [35]. The reason for such a drawback is that if, for a melting case, the temperature of a control volume rises from below the solidus to above the liquidus temperature in one time step, the absorption of the latent heat for that control volume is not accounted for. A similar flaw exists as the method is applied to solidification problems. As a result, very small time steps have to be used in this method in order to overcome its shortcoming. The consequence is poor computational efficiency. Moreover, for pure materials, an artificial phase change temperature range must be used to avoid making equation (27) undefined. Over this artificial phase change temperature range, the latent heat is assumed to be released or absorbed. The introduction of an artificial phase change temperature range would result in computational errors and simulation distortion of the real problem.

3.3.2. Effective capacity method. This method was proposed by Poirier and Salcudean [35] in an effort to improve the apparent capacity method. In this technique, a temperature

profile is assumed between the nodes; rather than determining an apparent capacity in terms of the nodal temperature, an effective capacity is calculated based on the integration through the control volume. The integration needed to obtain the effective capacity over the control volume is

$$C_{\text{eff}} = \frac{(\int C_{\text{app}} \mathrm{d}V)}{V} \tag{29}$$

where C_{eff}, C_{app} and V are effective heat capacity, apparent heat capacity and control volume, respectively.

This technique has been applied to one- and two-dimensional problems. Its implicit and explicit finite difference, and implicit finite element formulations have been studied. It has been seen that the method performs significantly better than the apparent heat capacity method. By evaluating equation (29) at each step, it is ensured that the method correctly accounts for the latent heat effect and the solution is independent of the artificial phase change temperature range. An assumption of a large artificial phase change temperature range is not required. The results were relatively insensitive to the time step and generally precise both on the entire domain and near the moving boundary.

In spite of its accuracy, the effective capacity method is very troublesome to implement. The numerical integration is substantially expensive, especially if the thermal gradients are steep in the phase change temperature range. Further details can be found in [36].

3.3.3. Heat integration method. This method, also known as the post-iterative method, is probably the simplest one of all the techniques reviewed in this subsection. In this method, the temperatures of all control volumes are monitored. For the melting case, if the temperature of any control volume rises above the melting temperature, the material in that control volume is assumed to undergo a phase change. The temperature of that control volume is set back to the melting temperature and the equivalent amount of heat due to setting the temperature back is added to an enthalpy account only for that control volume. Once the enthalpy in the account is equal to the latent heat, the temperature is allowed to rise based on the energy equation. The procedure can be expressed mathematically

$$\Delta T_{\text{r}} C_{\text{in}} = H_{\text{f}} \tag{30}$$

where the fictitious temperature rise ΔT_{r} is the sum of temperature differences between the temperature calculated by the energy equation at each time step and the melting temperature.

Early studies on the heat integration method were performed by Dusinberre [37]. Later Rolph and Bathe [38] applied this technique to the finite element method for transient thermal problems including a moving boundary in both a pure substance and an alloy. More recently, it was further extended to the explicit finite difference methods by Argyropoulos and co-workers [39–42] to simulate the steel shell growth and meltback around an exothermic addition when it is introduced into liquid steel. They reported that the numerical model can predict such a complex moving boundary problem in one dimension and the computer output is in good agreement with experimental results. Nevertheless, the model simplified the problem and considered it only from the energy contribution without solving the momentum equations simultaneously in the liquid bath.

The heat integration method can be easily applied for multidimensional problems with isothermal or non-isothermal phase change involved. The method is computationally economical. However, the accuracy of the solution strongly depends on the time step and the prediction in the region of the moving boundary is often inaccurate [35]. In addition, a somewhat exhaustive routine of accounting and indexing must be maintained for each control volume.

3.3.4. Source based method. This method allows any additional heat from either a heat source (e.g. latent heat during the solidification, and exothermic heat of mixing during the melting) or a heat sink (e.g. latent heat during the melting) to be introduced into the general form of the energy equation as an extra term, that is, the source term. For the illustration of this method, a general source based method recently developed by Voller and Swaminathan [43] will be presented as follows. In this general source based method derived from a standard enthalpy formulation, the sensible heat (defined as the product of the specific heat and temperature) and latent heat are separated in the transient term of the energy

$$\rho \frac{\partial (CT + H_{\mathrm{f}})}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right). \tag{31}$$

Recasting equation (30), the energy equation in the source formulation becomes

$$\rho C \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right) + S \tag{32}$$

where the latent heat is now included in the source term S as

$$S = -\rho \frac{\partial H_{\mathrm{f}}}{\partial t}. \tag{33}$$

The fully implicit discretization of equation (31) is

$$a_{\mathrm{P}} T_{\mathrm{P}} = \sum a_{\mathrm{nb}} T_{\mathrm{nb}} + b \tag{34}$$

where

$$b = a_{\mathrm{P}}^{\mathrm{o}} T_{\mathrm{P}}^{\mathrm{o}} + V_{\mathrm{P}}(h_{\mathrm{P}}^{\mathrm{o}} - h_{\mathrm{P}}) \tag{35}$$

where V_{P} is the volume associated with the grid point P, 'a' is the coupling coefficient, the superscript 'o' as well as the subscripts 'P' and 'nb' refer to the value at the previous time step, the grid point under consideration and the neighbouring grid points, respectively. The coefficients of equations (34) considered as a general discretization form can be obtained using either finite difference methods [44] or finite element methods [45].

The source based method has become more and more popular over the years [18, 43, 46]. The reason for this is that the algorithms handling the heat source or heat sink can be easily adapted to the existing numerical codes which have been widely used in the public domain, such as TEACH, PHEONICS etc. The overall accuracy of this method is fairly good, especially for non-isothermal phase change problems, since the latent heat content is directly joined to the temperature of the grid point. Also, the method is computationally efficient. Although the method may introduce unreasonable predictions around the moving boundary for isothermal phase change problems without using excessive underrelaxation for convergence, the solution oscillation can be eliminated with Voller's approach, that is the linearization of the discretized source term [43].

3.3.5. Enthalpy method. The essential feature of the basic enthalpy methods is that the evolution of the latent heat is accounted for by the enthalpy as well as the relationship between the enthalpy and temperature. The method can be illustrated by considering a one-dimensional heat conduction-controlled phase problem. An appropriate equation for such a case can be expressed as

$$\rho \frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(k \frac{\partial T}{\partial x}\right). \tag{36}$$

The relationship between the enthalpy and temperature can be defined in terms of the latent heat release characteristics of the phase change material. This relationship is usually

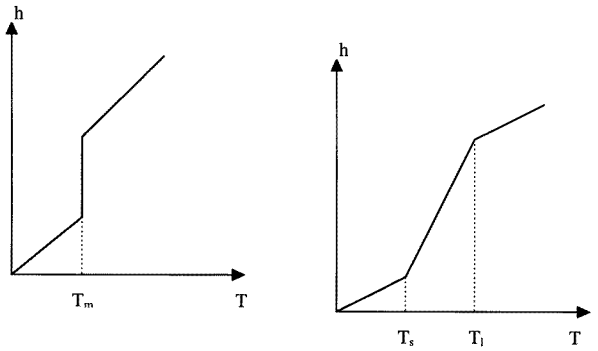

Figure 5. Enthalpy as a function of temperature for (*a*) isothermal phase change; (*b*) non-isothermal phase change.

assumed to be a step function for isothermal phase change problems and a linear function for non-isothermal phase change cases. Figure 5 shows the enthalpy–temperature curves for both cases. The enthalpy as a function of temperature for both cases is given by

$$h = \left\{ \begin{array}{lll} C_{\mathrm{s}}T & T \leqslant T_{\mathrm{m}} & \text{solid phase} \\ C_{\mathrm{l}}T + H_{\mathrm{f}} & T > T_{\mathrm{m}} & \text{liquid phase} \end{array} \right\} \text{ for isothermal phase change} \qquad (37)$$

$$h = \left\{ \begin{array}{lll} C_{\mathrm{s}}T & T < T_{\mathrm{s}} & \text{solid phase} \\ C_{\mathrm{in}}T + \dfrac{H_{\mathrm{f}}(T - T_{\mathrm{s}})}{(T_{\mathrm{l}} - T_{\mathrm{s}})} & T_{\mathrm{s}} \leqslant T \leqslant T_{\mathrm{l}} & \text{solid/liquid phase} \\ C_{\mathrm{l}}T + H_{\mathrm{f}} + C_{\mathrm{in}}(T_{\mathrm{l}} - T_{\mathrm{s}}) & T \geqslant T_{\mathrm{l}} & \text{liquid phase} \end{array} \right\} \text{ for}$$

non-isothermal phase change. (38)

The enthalpy approach was proposed as early as 1946 by Eyres *et al* [47] to avoid nonlinearity in a heat conduction problem. The earliest application of an enthalpy formulation to a finite difference scheme appears to be Rose [48]. Shamsunder and Sparrow [49] employed the enthalpy method in conjunction with a fully-implicit finite difference scheme to solve for solidification in a square geometry with convective boundary conditions. Their predictions were verified by the results from an enthalpy formulation used with the Crank–Nicholson scheme. Bell and Wood [50] evaluated the performance of the enthalpy method by using a simple, one-dimensional Stefan problem of melting a semi-infinite solid, initially at melting point, by exposure of one end to a hot temperature. A trigonometric series approximation of the temperature was used for the grid points near the moving boundary. Good agreement was obtained with the analytical solution given by Carslaw and Jaeger [51]. It was found that their formulation of treating the moving boundary performed better than the standard finite difference representation but the computational cost was higher. Poirier and Salcudean [35] reported that the enthalpy method is somewhat more complex and expensive than other methods. The computational cost increases with mesh refinement. The solution oscillation appears in the phase change case with large ratio of latent heat to sensible heat. However, the enthalpy method gives accurate solutions, especially for solidification of metal in which a phase change temperature range exists. Furthermore, the solution is independent of the time step and phase change temperature range. Tacke [52] proposed a discretization technique of the enthalpy method based on an assumption

of a linearized temperature distribution between the moving boundary and its adjacent grid points. As a result of the assumption of the linear profiles, the position of the moving boundary is calculated by

$$h_i = H_f\lambda + C_l(T_e - T_m)\lambda - C_s(T_m - T_w)(1 - \lambda) \tag{39}$$

where λ is the liquid fraction in the control volume. His formulation of the enthalpy method removes numerical oscillations in both temperature and moving boundary position, and produces a marked improvement in the accuracy of the results, particularly for cases with a large ratio of the latent heat to sensible heat.

Discussion of the enthalpy method has also been comprehensively covered by Voller and co-workers [18, 43, 53–55]. It has been known that the basic enthalpy method does not perform very well for modelling isothermal phase change problems. Voller proposed a technique to improve the accuracy of the prediction. He assumed that, as the moving boundary is in the control volume, the enthalpy change rate is proportional to the state change rate of the control volume, that is

$$\frac{dH_i}{dt} = \pm H_f \frac{d\lambda}{dt} \tag{40}$$

where λ is the liquid fraction in the control volume; the negative sign in equation (40) is for melting and the positive sign is for solidification. While the material in the control volume undergoes phase change, the enthalpy of the control volume must follow

$$CT_m \leqslant h_i \leqslant CT_m + H_f. \tag{41}$$

Based on equation (40), the following equations can be obtained:

$$\lambda = \frac{h_i - CT_m}{H_f} \qquad \text{for solidification} \tag{42}$$

$$\lambda = \frac{H_f + CT_m - h_i}{H_f} \qquad \text{for melting.} \tag{43}$$

For the Cartesian coordinate system, when the moving boundary reaches the grid point, the liquid fraction (λ) in the control volume is equal to 0.5. Substitution of this value into equations (42) and (43) yields

$$h_i = CT_m + 0.5H_f \tag{44}$$

for both solidification and melting. Analogous expressions may also be derived for other coordinate systems. For a melting problem, for instance, as the moving boundary crosses a grid point, the newly computed value of the enthalpy (h_i) at that point becomes greater than ($CT_m + 0.5H_f$). With the assumption that the enthalpy change is linear at each time step, a time can be determined at which the moving boundary is exactly at the grid point. At that time, the temperature at the grid point can be imposed as the melting point. This algorithm has been extended to track the moving boundary at all times. The accuracy of the predictions has been greatly improved by this technique. Recently, another highly efficient algorithm [43, 55], that incorporated the source-based method with the enthalpy technique, was proposed. As a result, the enthalpy method has been generalized so that more general forms of the enthalpy–temperature function can be handled; for example, cases in which an explicit enthalpy–temperature relationship cannot be found, as shown in figure 6. The method has been extended to two-dimensional cases and its effectiveness has also been demonstrated.

As the conductivity of a material is dependent on the temperature, the techniques discussed above may cause difficulties of the numerical discretization [56]. A good

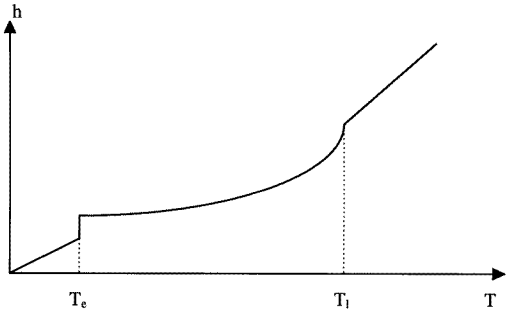

Figure 6. An implicit enthalpy–temperature relationship.

alternative is to employ the so-called 'Kirchoff transformation' [48] into the enthalpy method, to replace the temperature (T) by the 'Kirchoff temperature' (θ). The Kirchoff temperature is defined as

$$\theta = \int_{T_m}^{T} k(T)\,\mathrm{d}T. \tag{45}$$

With this definition,

$$\frac{\partial \theta}{\partial x} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) \tag{46}$$

and

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial t}\left(k\frac{\partial T}{\partial t}\right). \tag{47}$$

Substitution of the above equations into equation (32) results in the following governing equation:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial x}\left(\frac{k}{\rho C}\frac{\partial \theta}{\partial x}\right) + S. \tag{48}$$

Solomon *et al* [57] introduced the Kirchoff temperature into the enthalpy formulation to simulate the performance of a thermal energy storage system in a space station. An explicit finite difference scheme was used in an axisymmetric cylindrical coordinate system. Hunter and Kuttler [58] also incorporated the enthalpy with the Kirchoff transformation to put moving boundary problems in a particularly simple form. The simple form allows all nonlinearities in the thermophysical properties of the material to be concentrated in the functional temperature. More recently, Cao *et al* [59] developed an enthalpy model transformed by the Kirchoff temperature with the fixed grid methodology. In the model, the energy equation can be expressed only in terms of the enthalpy

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x}(\rho u h) + \frac{\partial}{\partial y}(\rho v h) + \frac{\partial}{\partial z}(\rho w h) = \frac{\partial^2}{\partial x^2}(\Psi h) + \frac{\partial^2}{\partial y^2}(\Psi h) + \frac{\partial^2}{\partial z^2}(\Psi h) + S_h \tag{49}$$

where $\Psi = k/C$. The model was tested by applying it to three-dimensional isothermal solidification and melting problems. Zeng and Faghri [60] have extended the model to two-dimensional non-isothermal phase change problems with the separation of the coupled effects of temperature and concentration on the latent heat evolution in the energy equation. The latent heat evolution due to temperature variation is accounted for by the definition of

an effective heat coefficient, while the evolution of the latent heat owing to the concentration variation is evaluated by a source term.

4. Numerical methods for solving convection/diffusion phase change problems

Understanding energy transport in phase change processes such as melting and solidification is important since heat transfer during the process can affect the overall efficiency and the evolution of the process. Meanwhile, the phase change process necessarily proceeds with temperature and/or concentration gradients in the liquid phase where convection arises under the action of buoyancy forces due to these gradients. Convection flow in the liquid phase has received less attention than conduction owing to the computer limitations in the past and considerable complexities entailed in the mathematical treatment. However, the convection flow can have a very significant influence on the phase change process. A number of researchers [61–67] have reported that the convection affects not only the rate of melting or solidification but also the resulting structure and distribution of the solutes in the liquid phase of a multicomponent system.

In order to determine quantitatively the convection in a Newtonian fluid, the set of mass and momentum conservation equations (the Navier–Stokes equations) must be solved. They can be written in vector notation as

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \boldsymbol{V}) = 0 \tag{50}$$

$$\rho \frac{\mathrm{D}\boldsymbol{V}}{\mathrm{D}t} = -\nabla p + \mu \nabla^2 \boldsymbol{V} + \rho g \tag{51}$$

where the operator

$$\frac{\mathrm{D}(\,)}{\mathrm{D}t} = \frac{\partial(\,)}{\partial t} + u\frac{\partial(\,)}{\partial x} + v\frac{\partial(\,)}{\partial y} + w\frac{\partial(\,)}{\partial z} \tag{52}$$

is the substantial derivative in Cartesian coordinates; the operator

$$\nabla = \frac{\partial}{\partial x} + \frac{\partial}{\partial y} + \frac{\partial}{\partial z} \tag{53}$$

and the operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \tag{54}$$

is the Laplacian operator.

Because of the nonlinearity of the Navier–Stokes equations, their analytical solutions relevant to the phase change problems are available only for a few simple cases. For example, Huang [68] has proposed an analytical solution to the one-dimensional momentum equation for the solution of the melting of a vertical semi-infinite region. Although analytical methods are mathematically attractive, they cannot be applied to complex cases. Fortunately, the development of numerical methods and the availability of more powerful computers in the last decade make the Navier–Stokes equations solvable. Two widely used numerical approaches, the stream-function–vorticity and the primitive variable formulations, will be discussed in the next section.

4.1. Stream-function–vorticity formulation

The stream-function–vorticity formulation is quite often applied in computational fluid dynamics for solving two-dimensional problems. For two-dimensional incompressible flow, the stream function (ψ) and vorticity (ω) are defined as

$$u = \frac{\partial \psi}{\partial y} \qquad v = -\frac{\partial \psi}{\partial x} \tag{55}$$

$$\omega = \frac{\partial v}{\partial x} - \frac{\partial u}{\partial y}. \tag{56}$$

With this definition, the continuity equation is automatically and implicitly satisfied, since

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = \frac{\partial^2 \psi}{\partial x \partial y} - \frac{\partial^2 \psi}{\partial y \partial x} = 0. \tag{57}$$

A drawback of the primitive variable formulation, discussed in the following subsection, is that the continuity equation must be satisfied separately from the solution of the Navier–Stokes equations. With the stream-function–vorticity formulation, this hindrance can be overcome.

With some simple algebra, the relationship between the stream function and the vorticity can be obtained:

$$\nabla^2 \psi = -\omega. \tag{58}$$

By substituting the stream function and the vorticity expressions into the primitive variable form of the differentiated momentum equations, the Navier–Stokes equations can be transformed to the vorticity transport equation

$$\frac{\mathrm{D}\omega}{\mathrm{D}t} = \nu \nabla^2 \omega. \tag{59}$$

Instead of dealing with equations (50) and (51) in the primitive variable form, the problem then becomes to solve equations (58) and (59). The technique eliminates the pressure term from the momentum equations. As a result, no iterations to correct the pressure field are required [44].

This formulation in conjunction with the alternating direction implicit (ADI) method [69] was used by Wilkes and Churchill [70] and Kublbeck *et al* [71] to solve the momentum and energy equations for natural convection in rectangular geometries. The ADI method provides economy of storage and speed of solution. Kee and Mckillop [72] also applied the same method to cylindrical geometries with asymmetric boundary conditions at the circumference. However, none of these works considered the moving boundary situation.

Ramachandran and Gupta [73] studied thermal and fluid flow effects during solidification in a rectangular enclosure with adiabatic top and bottom boundaries. The fluid flow was solved via the stream-function–vorticity formulation and the ADI method. The density variation causing the natural convection was handled by the Boussinesq approximation [74]. The velocity distribution, stream lines and isotherm patterns, that were obtained along with the interface movement with time, indicated that natural convection has a significant effect on the shape of the interface. Okada [75] incorporated this formulation with the variable transformation technique to solve two-dimensional melting from a vertical wall. This technique was also applied to simulate melting of ice around a horizontal cylinder by Ho and Chen [76]. The coupled, nonlinear, simultaneous equations were solved using the ADI finite difference scheme. The agreement between their predicted results and the existing experimental data appeared to be reasonably good. Guenigault and Poots [77] employed

the stream-function–vorticity formulation to study the inward solidification of spheres and cylinders with consideration of isothermal latent heat release and constant thermophysical properties. Lately, this formulation has also been utilized by Vabishchevich and Iliev [78] to predict metal solidification in a irregular mould.

Despite its attractive features, the stream-function–vorticity formulation has some major disadvantages. Implementation of the boundary conditions is less straightforward. The pressure, that has been eliminated, is often an important desired result or even an intermediate outcome required for determining thermophysical properties. Then, the effort of extracting pressure from vorticity offsets the computational efficiency obtained otherwise. Moreover, the major deficiency of the formulation is that it cannot easily be extended to three-dimensional scenarios, for which a stream function does not exist. Since most real situations are three dimensional, a method that is intrinsically constricted to two dimensions suffers from a serious limitation.

4.2. Primitive variable formulation

Instead of the stream function and vorticity, the dependent variables in this formulation are the velocities and pressure, which means that the Navier–Stokes equation will be solved in a primitive variable form. The focus of this subsection will be on two techniques available in this formulation.

The first one, known as the marker and cell (MAC) method, has been proposed and developed by Harlow and Welch [79] and Nichols *et al* [80]. In this technique, the nonlinear governing equations are discretized by finite difference methods based on a term by term Taylor series approximation. A staggered mesh is employed where the pressure is located at the cell centre and the velocities at the walls. The boundary conditions are imposed at a layer of fictitious cells adjacent to the computational domain. Every cell in the computational domain contains some massless marker particles that move at the local fluid velocity. The motion of the fluid can be followed by these particles. Since the technique is often used in the explicit form, the difference equations provide the time step values directly. At each time step, the discretized momentum equations calculate new velocities in terms of an estimated pressure field. Then, the pressure in each cell is iteratively adjusted and velocity changes induced by each pressure correction are added to the previous velocities. This iterative process is repeated until the continuity equation is satisfied under an imposed tolerance by the newly computed velocities. At this time, the marker particles are moved to their new positions and the time step is advanced.

Salcudean and Guthrie [81] utilized the MAC method to predict flow patterns during the filling of a cylindrical vessel from the top free surface. The MAC method has also been used by Stoher and Hwang [82] for the computation of the fluid flow during the filling of a rectangular mould from the side. In both studies, the computed output showed reasonable agreement with experimental results.

Although the explicit nature makes the implementation of the MAC method relatively easy, the method suffers from severe time step limitations [83]. The time step must be restricted in order to eliminate the possibility of the material movement and momentum transport through more than one cell in a time step. The limitations can become increasingly restrictive with the refinement of the mesh.

Another alternative available to solve the Navier–Stokes equations in the primitive variable form is the control volume method. As a representative in this category of the primitive variable formulation, the well known SIMPLE, and later the SIMPLER, algorithms were developed by Patankar [44]. In this technique, the equations of the mass, momentum,

energy and species conservation are expressed in a general differential equation of the form

$$\frac{\partial}{\partial t}(\rho\phi) + \nabla(\rho u\phi) = \nabla(\Gamma_\phi \nabla\phi) + S_\phi \tag{60}$$

where ϕ is a general variable, Γ_ϕ is the diffusion coefficient and S_ϕ is the source term. The four terms in equation (60) represent the unsteady term, the convection term, the diffusion term and the source term. The dependent variable ϕ can denote a variety of different quantities, such as the mass fraction of a chemical species, the enthalpy or the temperature, or a velocity component. Accordingly, for each of these variables, an appropriate meaning must be given to the diffusion coefficient and the source term, ϕ, Γ_ϕ and S_ϕ for the different equations are listed in table 1. The SIMPLER algorithm can solve the equations of the mass, momentum, energy and species conservation simultaneously.

Table 1. Diffusion coefficients and source terms for various dependent variables.

Equation	ϕ	Γ_ϕ	S_ϕ
Mass	1	0	0
Momentum	v_j	μ	$-\nabla_p + S^v$
Thermal energy	$h(T)$	$kC_\mathrm{p}(k)$	S_h
Chemical species	C_A	D	S_C

This technique has become more and more popular in recent years. Benard *et al* [84] applied this technique to the study of a melting process where heat convection in the liquid phase is non-negligible. Their numerical solution was validated by comparison with precise experimental results. Neilson and Incropera [85] investigated the solidification of a binary solution in a horizontal cylindrical annulus using the control volume technique with a finite difference scheme. The SIMPLER algorithm was employed by Kim and Kaviany [86] for solving a melting problem in a two-dimensional cavity driven by the coupling of heat conduction in the solid phase and natural convection in the liquid phase. Swaminathan and Voller [55] used the SIMPLER algorithm to simulate the melting of pure gallium in a cavity. Recently, with the use of the SIMPLER algorithm, Chabchoub *et al* [87] modelled and optimized the horizontal Ohno continuous casting process for pure tin. Trovant and Argyropoulos [88] also utilized the SIMPLER algorithm with the heat integration method to estimate the volumetric shrinkage in a cylindrical metal casting. Hu and Argyropoulos [89–92] integrated the enthalpy method in to the SIMPLER algorithm to simulate a unique melting phenomenon. This phenomenon quite often occurs in various materials processings, where a heat source, a heat sink and natural convection are coupled, as illustrated in figure 7. More details regarding the primitive variable formulation can be found in [93].

More recently, with the advent of the supercomputers, it appears that scientists and engineers are more interested in modelling of microstructure evolution occurring in solidification. The prediction of microstructure from macrotransport models that solve the mass, momentum, energy and species macroscopic conservation differential equations is very limited. In order to overcome this hurdle, a new generation of solidification models which integrate the transformation kinetics (TK) into the macrotransport models (MT), referred to as MT–TK models, is being developed [94, 95]. Various techniques which include the continuum (deterministic) approach [96, 97], the stochastic (probabilistic) approach [98] and a combined one [99] have been applied in MT–TK modelling to generate information on the microstructure evolution. Among them, the probabilistic approach is more popularized due to the advantages that individual grains can be identified and their shape and size can be illustrated graphically throughout the entire process of solidification. It has been attempted

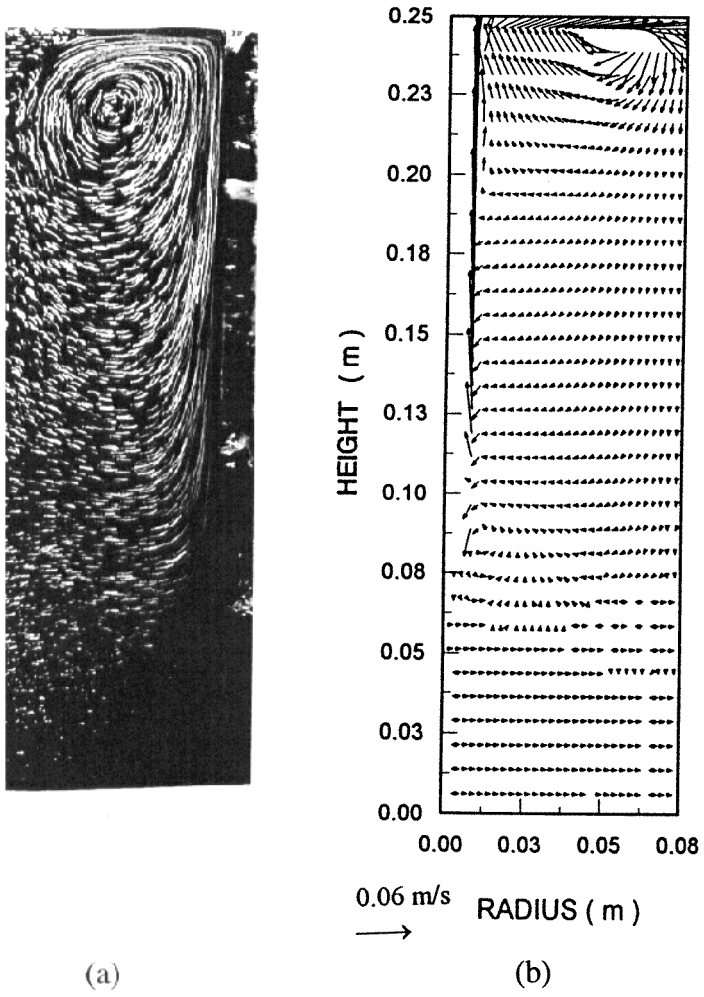

Figure 7. A solid exothermically melting in a liquid. (*a*) Visually observed fluid flow; computed results of (*b*) velocity field, (*c*) isotherm and (*d*) isoconcentrations.

by using the MT–TK analysis to predict various features of solidifying materials, such as dendritic structure, fraction of phases, structural transition, microsegregation and even mechanical properties. The impressive progress made in the past few years has resulted in a large number of publications and commercial software [100]. Despite increased efforts to verify the MT–TK models, however, their accuracy in predicting the characteristics of microstructure and mechanical properties resulting from the solidification condition is still in question.

5. Summary

The merits and disadvantages of various numerical methods for phase change problems which occur in solidification and melting have been surveyed in this paper. The choice

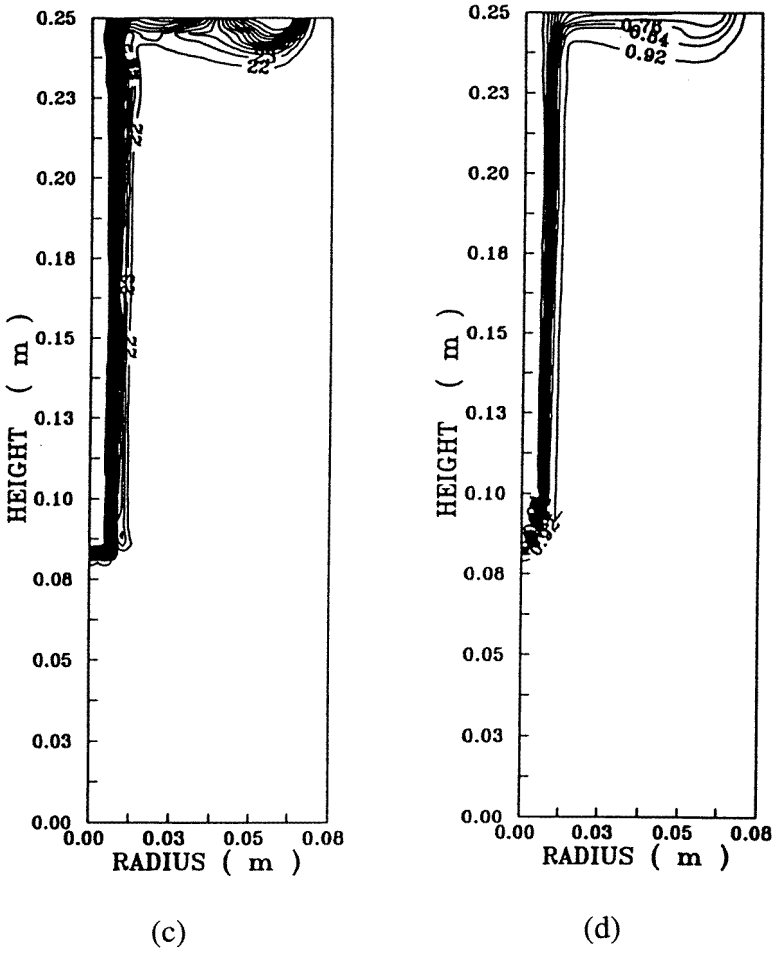

Figure 7. (Continued)

of the numerical method depends not only on the nature of the problem but also on the priorities set by the user for accuracy, computational efficiency and ease of programming. For pure substances, the variable grid methods often yield more accurate results than those based on the fixed grid method. However, the fixed grid method is very much easier to program. Moreover, the fixed grid method incorporated with the enthalpy technique can easily be extended to multidimensional problems for both pure and binary materials.

Due to the importance of convection in a large number of phase change problems, wide experience has been accumulated in the numerical simulation of convection/diffusion processes coupled with phase change. Numerical techniques for such complex phenomena are now being developed by scientists and engineers in different disciplines. The popularity of the primitive variable formulation is rising since it is capable of tackling three-dimensional problems which often occur in industrial processes. On the basis of experience gained so far, numerical methods based on the weak solution in conjunction with the control volume scheme in the fixed domain can be highly recommended for multidimensional melting and solidification problems.

With increasing interest in modelling of microstructure evolution occurring during solidification, a new generation of solidification models (MT–TK) is rising. However, their accuracy in predicting the peculiar characteristics of microstructure is still in question.

Acknowledgments

The authors would like to express their appreciation to the Natural Sciences and Engineering Research Council of Canada and the Institute of Magnesium Technology (ITM) for supporting this work.

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