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A fixed grid numerical modelling methodology for convection–diffusion mushy region phase-change problems

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Abstract—An enthalpy formulation based fixed grid methodology is developed for the numerical solution of convection–diffusion controlled mushy region phase-change problems. The basic feature of the proposed method lies in the representation of the latent heat of evolution, and of the flow in the solid–liquid mushy zone, by suitably chosen sources. There is complete freedom within the methodology for the definition of such sources so that a variety of phase-change situations can be modelled. A test problem of freezing in a thermal cavity under natural convection is used to demonstrate an application of the method.

1. INTRODUCTION

A LARGE number of numerical techniques are available for the solution of moving boundary problems, a comprehensive review has been presented by Crank [1]. The majority of these techniques are concerned with phase change in which conduction is the principal mechanism of heat transfer. In physical systems which involve a liquid–solid phase change, however, convection effects may also be important. As such, the problem of freezing of a pure liquid in a thermal cavity under conduction and natural convection has received some attention in recent years. For example see Ramachandran *et al.* [2], Gadgil and Gobin [3] and Albert and O'Neill [4]. In these works, a temperature formulation is used, and in order to treat the moving liquid–solid interface, deforming grids have been employed. An alternative approach is to use an enthalpy formulation in which case no explicit conditions on the heat flow at the liquid–solid interface need to be accounted for and therefore the potential arises for a fixed grid solution. This will have advantages in terms of simplifying the numerical modelling requirements, particularly in systems for which the phase change may only be a component part. Examples of fixed grid solutions of convection–diffusion phase change can be found in Morgan [5], Gartling [6] and Voller *et al.* [7–9].

The major problem with fixed grids is in accounting for the zero velocity condition as the liquid region turns to solid. Morgan [5] employs the simple approach of fixing the velocities to zero in a computational cell whenever the mean latent heat content, ΔH, reaches some predetermined value between 0 (cell all solid) and L (cell all liquid), where L is the latent heat of the phase change. Gartling [6] employs a more subtle approach in making the viscosity a function of ΔH such that as ΔH decreases from L to 0 the value of the viscosity increases to a large value thus simulating the liquid–solid phase change.

Voller *et al.* [7–9] have investigated various ways of dealing with the zero solid velocities in fixed grid enthalpy solutions of freezing in a thermal cavity. At the same time they proposed an alternative but similar approach to that used by Gartling [6]. Computational cells in which phase change is occurring, i.e. $0 < \Delta H < L$, are modelled as pseudo porous media with the porosity, λ, decreasing from 1 to 0 as ΔH decreases from L to 0. In this way, on prescribing a 'Darcy' source term, velocities arising from the solution of the momentum equations are inhibited, reaching values close to zero on complete solid formation.

To the authors' knowledge all applications of convection–diffusion phase-change numerical methodologies have been to isothermal phase-change problems. These applications assume that the liquid–solid phase change occurs in a pure material. In many practical situations, however, the material under consideration is not pure (e.g. a metallurgical alloy). In such cases the phase change takes place over a temperature range, $\varepsilon \leqslant T \leqslant -\varepsilon$ say. That is, the evolution of latent heat has a functional relationship with temperature, e.g. $\Delta H = f(T)$, as opposed to the step change associated with an isothermal phase change. Problems of this type are often referred to as mushy region problems to indicate the solid plus liquid state of the material in the phase-change range.

NOMENCLATURE

A	porosity function
a's	coefficients in numerical scheme
C	porosity constant
c	specific heat
$f(T)$	enthalpy temperature function
F_l	local liquid fraction
F_s	local solid fraction
g	gravity
h	sensible heat
H	total enthalpy (sensible plus latent)
ΔH	latent heat
K	permeability
k	conductivity
L	latent heat of phase change
P	pressure
q	small constant to avoid division by zero
S_y, S_z	momentum source term
S_b	Boussinesq source term
S_h	enthalpy source term
T	temperature
t	time
u	velocity, (v, w)
u_l	liquid velocity
y, z	coordinate directions.

Greek symbols

α	thermal diffusivity
β	thermal coefficient of expansion
ε	half mushy range
λ	porosity
μ	viscosity
ρ	density.

Subscripts

H	high neighboring node
L	low neighboring node
l	liquid value
N	north neighboring node
P	node point
S	south neighboring node
s	solid value.

Other symbols

$(\ )^\circ$	old value
$\|[A, B]\|$	maximum value of A and B
$[\ ]_n$	nth iterative value.

In a numerical modelling analysis of a mushy region solidification the enthalpy is a sound starting point in that any functional relationship $\Delta H = f(T)$ may be readily incorporated into the enthalpy definition. Furthermore, in problems that involve convection in the melt, the Darcy source approach proposed by Voller *et al.* [7–9], something of a numerical 'fix' in the isothermal case, now has some physical significance. For example, in metallurgical problems, it is fairly standard practice to model the flow in the mushy region via a Darcy law, see Mehrabian *et al.* [10].

The purpose of this paper is to present an enthalpy formulation based fixed grid methodology for the numerical solution of convective–diffusion controlled mushy region phase-change problems. The method is general and can handle situations where phase changes occur at a distinct temperature (pure material) or over a temperature range (alloys). Further, the functional relationship $\Delta H = f(T)$ can be of any form, though a linear relationship is used in the current work. The Darcy source approach is used to simulate motion in the mushy region. The essence of the paper is to present the basic methodology; the test example chosen is primarily a vehicle to explain the details of the procedure.

2. A TEST PROBLEM

The configuration for the test problem employed in this paper is illustrated in Fig. 1. The basic features of the problem are the same as previous studies of freezing in a thermal cavity, see Voller *et al.* [7–9], Albert and O'Neill [4], and Morgan [5]. Initially the liquid in the cavity is above the freezing temperature. At time $t = 0$ the temperature at the surface $y = 0$ is lowered and fixed at a temperature below the freezing temperature so that as time proceeds a solid layer attaches to this surface. The essential and important difference in this work is the introduction of a mushy region, which is defined as follows. The enthalpy of the material (the total heat content) can be expressed as

$$H = h + \Delta H$$

i.e. the sum of sensible heat, $h = cT$, and latent heat ΔH. In order to establish a mushy phase change the latent heat contribution is specified as a function of temperature, T

$$\Delta H = f(T). \tag{1}$$

On recognizing that latent heat is associated with the liquid fraction in the mushy zone a general form for $f(T)$ can be written

$$f(T) = \begin{cases} L, & T \geqslant T_l \\ L(1-F_s), & T_l > T \geqslant T_s \\ 0, & T < T_s \end{cases} \tag{2}$$

where $F_s(T)$ is the local solid fraction, T_l the liquidus temperature at which solid formation commences and T_s is the temperature at which full solidification is achieved. The task of fully defining the nature of the

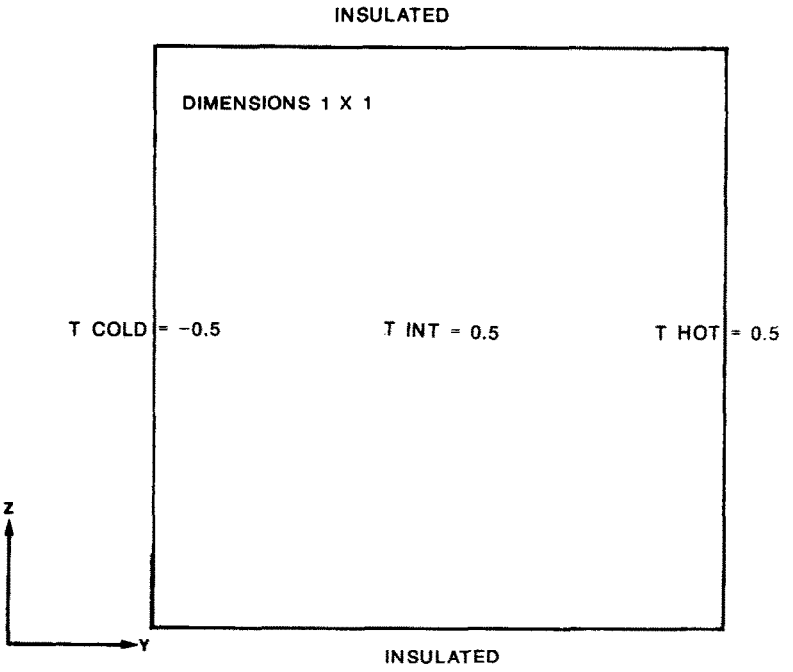

FIG. 1. The thermal cavity.

latent heat evolution in the mushy region is that of identifying the form of the local solid fraction–temperature relationship, i.e. $F_s(T)$. In the current work a simple linear form is chosen

$$F_s(T) = \begin{cases} 0, & T \geqslant \varepsilon \\ (\varepsilon - T)/2\varepsilon, & \varepsilon > T \geqslant -\varepsilon \\ 1, & T < -\varepsilon \end{cases} \quad (3)$$

where the temperature has been scaled such that $T = \varepsilon$ and $-\varepsilon$ are the liquidus and solidus temperatures, respectively. The quantity ε is referred to as the half temperature range of the mushy zone.

The method to be proposed is not restricted to the form for $F_s(T)$ given by equation (3) and it is recognized that in practical cases such a simple definition may not suffice. For example in metallurgical solidification of a binary alloy the function $F_s(T)$ will depend on the nature of the solute redistribution and the associated phase-change equilibrium diagram, see Flemings [11]. A treatment such as this, however, is outside the scope of this paper.

The current intention is to develop a basic methodology for the treatment of mushy solidification. In keeping with this approach the thermal properties used are assumed constant with temperature and phase. The values of the properties used along with the value of appropriate dimensionless numbers are given in Table 1.

3. THE GOVERNING EQUATIONS

The form of the governing equations for the test problem of Fig. 1 are similar to the equations for an isothermal phase change in a cavity derived by Voller *et al.* [7–9]. Important differences arise, however, in the definition of the source terms and in the treatment of the velocities.

For the purpose of the development of the methodology it is helpful to regard the entire cavity as a porous medium, where the porosity, λ, takes the values, $\lambda = 1$ in the liquid phase, $\lambda = 0$ in the solid phase, and $0 < \lambda < 1$ in the mushy zone. The governing equations can then be written in terms of the superficial velocity (i.e. the ensemble-average velocity) defined as

$$\mathbf{u} = \lambda \mathbf{u}_l$$

where $\mathbf{u}_l$ is the actual fluid velocity. On recognizing that the porosity $\lambda = 1 - F_s$ the above relationship can

Table 1. Test problem data

Initial temperature	$T_i = 0.5$
Hot wall temperature	$T_H = 0.5$
Cold wall temperature	$T_C = -0.5$
Reference temperature	$T_{ref} = 0.5$
Half mushy range	$\varepsilon = 0.1, 0.05, 0$
Cavity dimension	$l = 1$
Density	$\rho = 1$
Specific heat	$c = 1$
Viscosity	$\mu = 1$
Conductivity	$k = 0.001$
Coefficient of thermal expansion	$\beta = 0.01$
Gravity	$g = 1000$
Latent heat	$L = 5$
So that:	
Raleigh number	$Ra = \rho^2 g \beta c (T_H - T_C) l^3 / \mu k = 10^4$
Prandtl number	$Pr = \mu c / k = 10^3$
Stefan number	$Ste = L/c(T_H - T_C) = 5$

be expanded to give

$$\mathbf{u} = \begin{cases} \mathbf{u}_l, & \text{in the liquid phase} \\ (1-F_s)\mathbf{u}_l, & \text{in the mushy zone} \\ 0, & \text{in the solid phase.} \end{cases}$$

Using this definition along with the assumption of Newtonian, incompressible, laminar flow the governing equations are as follows.

Conservation of mass

$$\frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{4}$$

where w and v are the superficial velocities in the z- and y-directions, respectively.

Conservation of momentum

$$\frac{\partial(\rho v)}{\partial t} + \text{div}\,(\rho \mathbf{u} v) = \text{div}\,(\mu\ \text{grad}\ v) - \frac{\partial P}{\partial y} + S_y \tag{5a}$$

$$\frac{\partial(\rho w)}{\partial t} + \text{div}\,(\rho \mathbf{u} w) = \text{div}\,(\mu\ \text{grad}\ w) - \frac{\partial P}{\partial z} + S_z + S_b \tag{5b}$$

where P is pressure, ρ is density, μ is the liquid viscosity, $\mathbf{u} = (v, w)$, and S_y, S_z, and S_b are source terms which will be defined below.

The heat equation

$$\frac{\partial \rho h}{\partial t} + \text{div}\,(\rho \mathbf{u} h) = \text{div}\,(\alpha\ \text{grad}\ h) - S_h = 0 \tag{6}$$

where $\alpha = k/c$ is the thermal diffusivity and S_h is a phases related source term to be discussed below.

4. DEFINITION OF SOURCE TERMS

The above governing equations are in the general format suggested by Patankar [12] for the numerical solution of heat and fluid flow problems, i.e. a transient term plus a diffusive term plus a convective term plus sources. In this format a problem is driven by the definition of the source terms.

The S_y and S_z source terms are used to modify the momentum equations in the mushy region. If it is assumed that the flow in the mush is governed by the Darcy law, i.e.

$$\mathbf{u} = -(K/\mu)\ \text{grad}\ P \tag{7}$$

where K, the permeability, is a function of the porosity $\lambda (= 1 - F_s)$. As the porosity decreases the permeability and the superficial velocity also decrease, down to a limiting value of zero when the mush becomes completely solid. In a numerical model this behavior can be accounted for by defining

$$S_y = -Av \quad \text{and} \quad S_z = -Aw \tag{8}$$

where A increases from zero to a large value as the local solid fraction F_s increases from its liquid value of 0 to its solid value of 1. The effect of these sources is as follows. In the liquid region the sources take a zero value and the momentum equations are in terms of the actual fluid velocities. In the mushy region the value of A increases such that the value of the sources begin to dominate the transient, convective, and diffusive terms and the momentum equation approximates the Darcy law. As the local solid fraction approaches 1 the sources dominate all other terms in the momentum equation and force the predicted superficial velocities to values close to zero. In the case of an isothermal problem, where the porosity approach is a numerical fix, any increasing function for A would be suitable. For a mushy region phase change, however, where a porous region does exit, one can appeal to physics in order to derive a suitable form for the function 'A'. A well-known equation derived form the Darcy law is the Carman–Koseny equation [13]

$$\text{grad}\ P = -C(1-\lambda)^2/\lambda^3 \mathbf{u}. \tag{9}$$

This equation suggests the following form for the function A in equation (8)

$$A = -C(1-\lambda)^2/(\lambda^3 + q). \tag{10}$$

The value of C will depend on the morphology of the porous media. In the current study C is assumed constant and is set to 1.6×10^3. The constant q, introduced to avoid division by zero, is set at 0.001. With reference to the results, in Section 7, it may be observed that the chosen value of C is small enough to allow for significant flow in the mushy region at low local solid fraction whereas as the limiting value of A (i.e. $-C/q$) is large enough to suppress the fluid velocities in the solid. This is suitable behavior if the proposed methodology is to be fully tested.

The S_b source term, in the w momentum equation, is a buoyancy term used to induce natural convection in the cavity. Assuming the Boussinesq treatment to be valid, i.e. density is constant in all terms except a gravity source term, the buoyancy source term is given by

$$S_b = \rho g \beta (h - h_{ref})/c \tag{11}$$

where β is a thermal expansion coefficient and h_{ref} is a reference value of the sensible heat.

The form of the enthalpy source term S_h is derived from the enthalpy formulation of convection–diffusion phase change [9]

$$\frac{\partial \rho H}{\partial t} + \text{div}\,(H \rho \mathbf{u}) - \text{div}\,(k\ \text{grad}\ T) = 0. \tag{12}$$

This equation can be expanded on substitution of $H = cT + \Delta H$. Then on comparison with equation (6) and use of the continuity equation, equation (4), it is seen that

$$S_h = \frac{\partial \rho \Delta H}{\partial t} + \text{div}\,(\rho \mathbf{u} \Delta H). \tag{13}$$

In the isothermal case due to the step change in ΔH along with a zero velocity at the solid–liquid interface the convective part of this source term takes the value zero. In a mushy region case, however, the convective term needs to be included.

5. THE BASIC NUMERICAL SOLUTION

To numerically solve the governing equations along with the associated source terms a finite domain method is used. This is fully implicit in time and uses upwind differencing in space. As an example of the form the discretization takes consider the heat equation, equation (6). The finite domain discretization, following the notation in Patankar [12] and referring to Fig. 2, gives

$$a_P h_P = a_H h_H + a_L h_L + a_N h_N + a_S h_S + a_P^\circ h_P^\circ + b \quad (14)$$

where the subscripts indicate the appropriate nodal values, the a's are coefficients which depend on the diffusion and convective fluxes in to the pth control volume, $a_P^\circ = \rho\, \delta z\, \delta y/\delta t$ and $(\,)^\circ$ represents evaluation at the previous time step. The parameter b incorporates a discretized form of the source term S_h.

The discretized form of the momentum equations are very similar to equation (14). An important difference is that the grids used are 'staggered' over the enthalpy grid (see the dashed control volumes in Fig. 2). The reason for this is so that the pressure, which is the driving force for the velocities, can be correctly accounted for. For more details see Patankar [12]. A consequence of the staggered grid approach is that care has to be taken in numerically implementing momentum sources which depend on enthalpy.

The finite domain equations are solved by employing the PHOENICS code. This code uses a similar algorithm to the SIMPLE algorithm outlined by Patankar [12]. The numerical representation of various source terms is discussed in the Appendix. Of particular importance is the treatment of the latent heat source term S_h given by equation (13). Given a distribution of the ΔH field (and hence S_h), equation (6) can be solved to obtain the sensible heat h. To complete the computational cycle, ΔH needs to be iteratively updated from the predicted h field. The procedure for this iterative updating is seen as a main contribution of this paper, it is fully described in the Appendix. Details regarding the PHOENICS implementation may be found in ref. [14].

Table 2. Grid dependence

Size	Fraction of solid at $t = 250$
10×10	0.85
20×20	0.82
40×40	0.81

6. IMPLEMENTATION

The proposed test problem is solved on a 40×40 uniform square grid. A fixed time step of $\delta t = 10$ was used in all runs and the maximum simulation time was $t = 1000$. The grid size of 40×40 was reached after a grid refinement study. Essentially the total fraction of solid at $t = 250$ was recorded for uniform grid sizes 10×10, 20×20 and 40×40. The results of this study are summarized in Table 2. In each time step 50 iteration sweeps were used to solve the discretized equations. No under relaxation parameters were employed. The runs were performed on a Convex C1. The longest run (simulation to $t = 1000$) required of the order of 6 cpu hours.

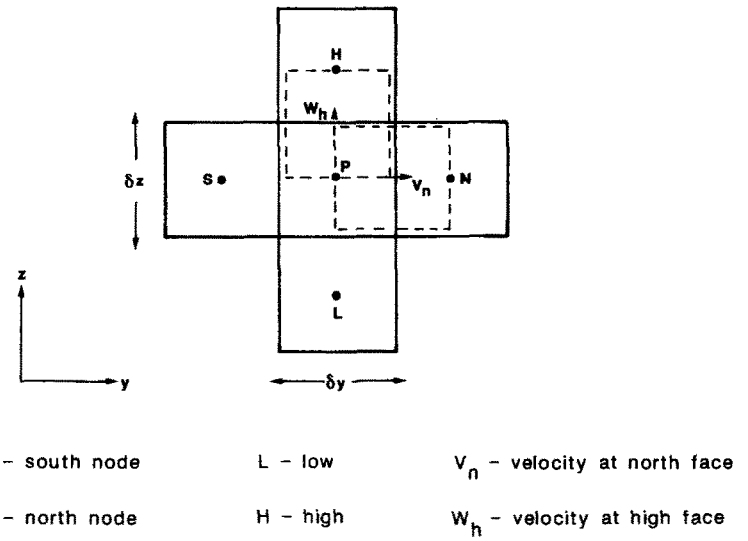

FIG. 2. The numerical control volumes.

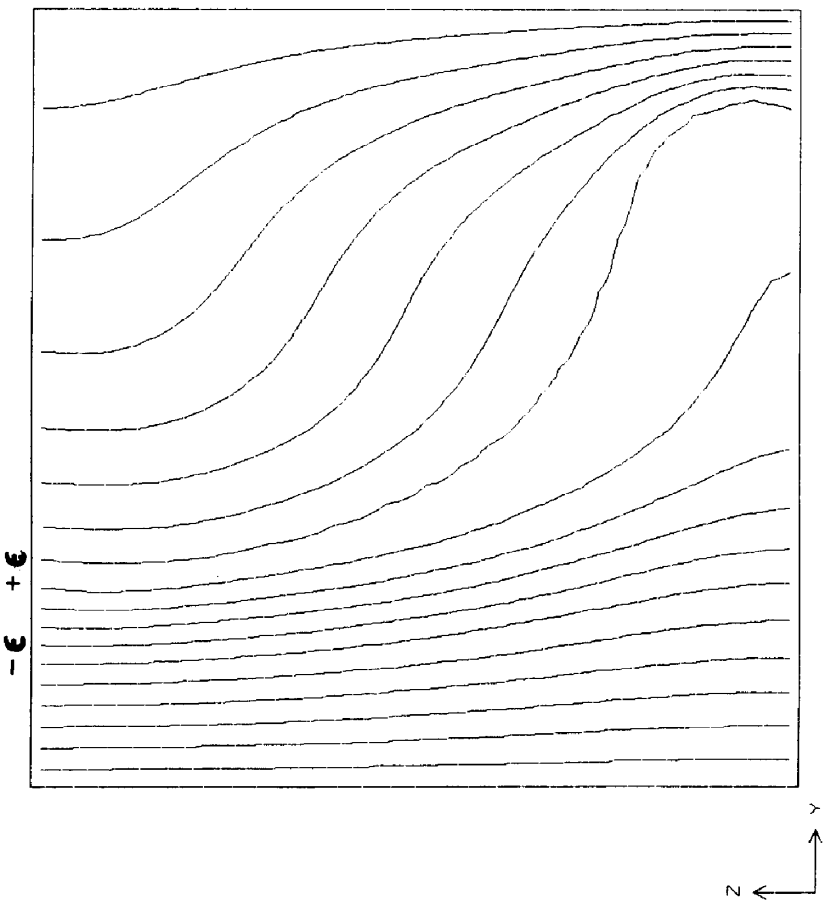

FIG. 4. Isotherms -0.45 to 0.45 ($\varepsilon = 0.1$), $t = 1000$.

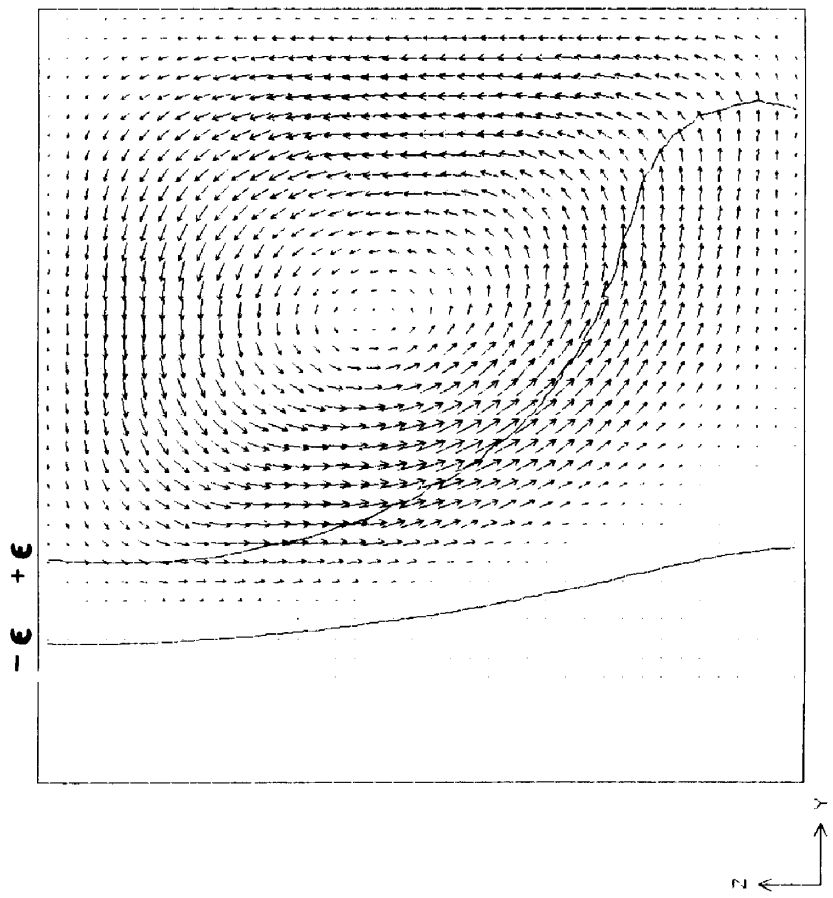

FIG. 3. Flow field and mushy region ($\varepsilon = 0.1$), $t = 1000$.

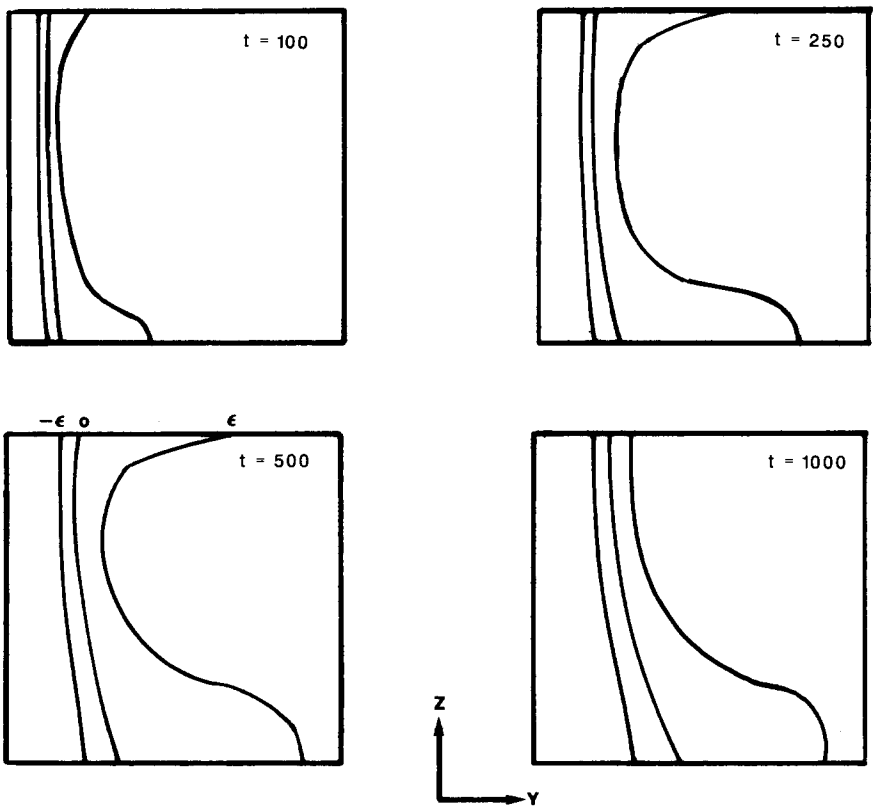

FIG. 5. Development of $\varepsilon = 0.1$ mushy region.

7. RESULTS

Figure 3 shows the position and shape of the mushy region ($\varepsilon = 0.1$) and the related flow field at time $t = 1000$. The solidus line, i.e. the temperature isotherm $T = -\varepsilon$, shows small deformation due to convection similar in shape to the deformation predicted in an isothermal phase-change case. The liquidus front, however, ($T = \varepsilon$) shows a pronounced 'bulge' along the lower wall ($z = 0$). This bulge is a direct effect of the convection in the mushy zone. The flow direction, away from the cold wall ($y = 0$), increases the heat loss in this area and hence extends the mushy region. At the same time the return flow, from the hot wall ($y = 1$), retards the growth of the mushy region at the top of the cavity making the bulge at the bottom more acute.

Figure 4 shows the isotherms at $t = 1000$. In the liquid portion of the cavity these isotherms are in qualitative agreement with other studies of natural convection in a thermal cavity, De Vahl Davis [15].

Figure 5 shows the development of the $\varepsilon = 0.1$ mushy region, along with the movement of the $T = 0$ isotherm, at time steps $t = 100$, 250, 500 and 1000. The bulge is noticeable at very early time steps. Furthermore, there appears to be some 'remelting' of the mushy region near the top of the cavity as a steady state is reached. Such remelting behavior can be explained in terms of the transient modification of the velocity field. At initial times the velocity near the top wall is small due to the no-slip condition. Hence significant solidification occurs in this area. At later times, the greater momentum of the fluid creates larger velocities near the top of the wall and remelting occurs.

Figure 6 shows the effect of reducing the size of the mushy region down to the isothermal case. When $\varepsilon = 0.05$ the deformation at $t = 1000$ is reduced. In the isothermal case there is no pronounced bulge and the position and shape of the phase-change front is consistent with that previously observed by Voller *et al.* [7–9].

The results in Fig. 6 suggest that the nature of the flow in the mushy region will influence its shape. The flow in the mushy region will be governed by the assumed nature of the porosity–permeability relationship, see equation (10). To demonstrate this a run was carried out with the parameters in equation (10) set at

$$C = 160 \times 10^3 \quad \text{and} \quad q = 0.1$$

With these choices the final value of the porosity source, at full solidification, will be the same, but the size of the source will increase more rapidly at commencement of the phase change. This will have the effect of reducing the flow in the mushy region.

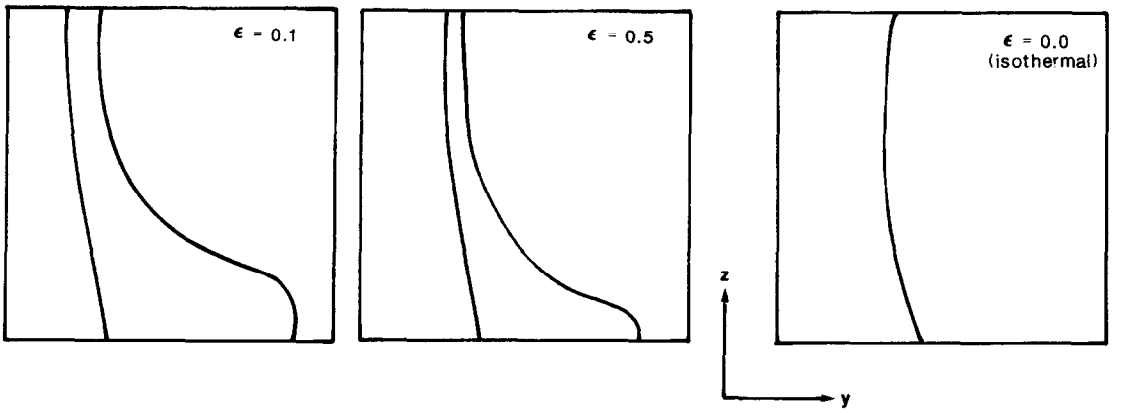

FIG. 6. Effect of mushy size at $t = 1000$.

Figure 7 shows results using the revised porosity source with all other conditions the same as in Fig. 3. These results clearly indicate the effect of a reduced flow in the mushy region with the liquidus deformation very much reduced. If the proposed methodology is to be used to investigate 'real' systems then clearly care has to be taken in defining the nature of the porosity source. In particular relationships between the morphology of the mushy region and the porosity source need to be investigated.

8. CONCLUSIONS AND DISCUSSION

The principal aim of this work has been to develop a generalized methodology for the modelling of mushy region phase change. This motivated the development

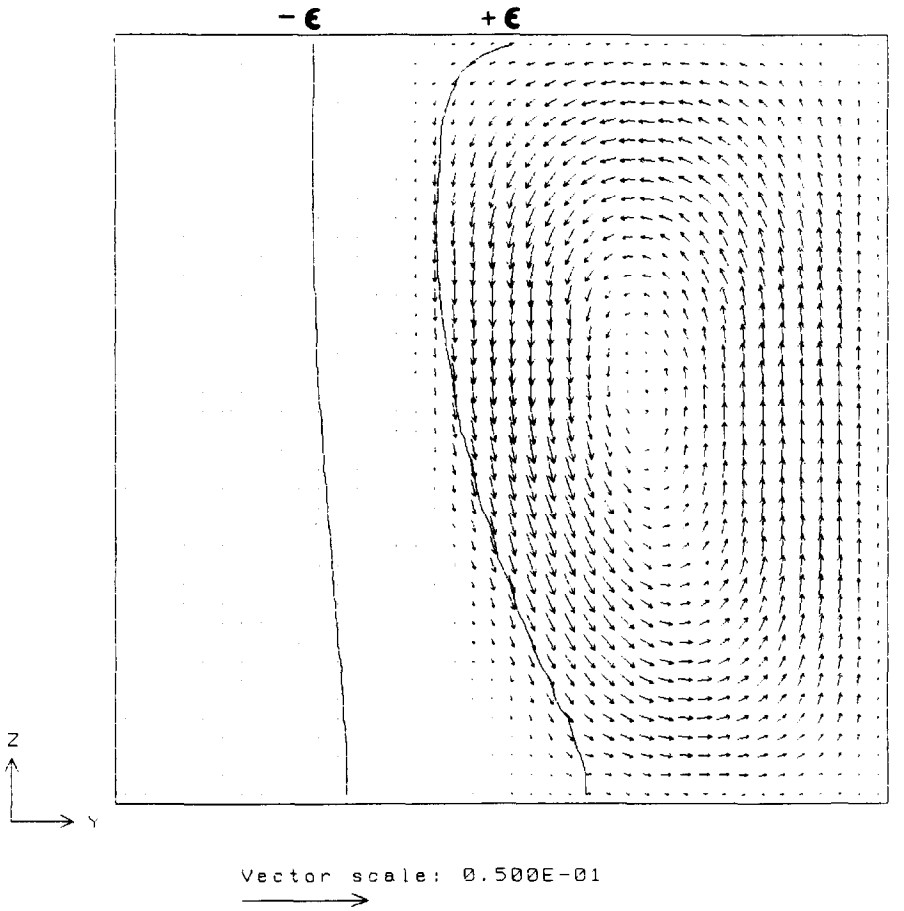

FIG. 7. Flow field and mushy region ($\varepsilon = 0.1$), $t = 1000$, for revised source.

of a fixed grid approach along with retaining the basic form of the hydromechanical equations. The phenomena associated with a particular phase change can be modelled on careful consideration and choice of source terms. The driving source terms are the 'Darcy' source and the latent heat source.

The Darcy source is used to model the effect of the nature of the porosity of the mushy region on the flow field. Preliminary results suggest that the nature of the porosity has a significant effect.

The latent heat source term is a function of the solid fraction which is a function of temperature. In this paper a linear change was assumed. In real systems the solid fraction–temperature relationship may not be such a simple form. In a binary alloy for example F_s will depend on the nature of the solute redistribution and may take a non-linear form possibly with a jump discontinuity at a eutectic front.

There is a need for further studies to be made. In particular:

(i) A comparison between the proposed fixed grid method and a deforming grid technique. Such a study would provide a mechanism by which the relative advantages and disadvantages of each approach could be analyzed.

(ii) An investigation into various approaches and models of flow in the mushy zone. Important questions in such a study will be; What is an appropriate form for the morphology–porosity relationship? and; Is the Darcy law appropriate? (i.e. should an alternative such as the Brinkman equation be used [16]). An investigation of this type could have particular relevance in applications of the proposed methodology to metal systems, where the flow in the mushy zone is significant.

(iii) Some experimental studies are required. The work presented in this paper lacks any validation. The authors concede that this is a major deficiency but are unaware of any suitable experimental studies of solidification in mushy systems. It is noted, however, that the isothermal case has been checked against limiting analytical solutions by Voller *et al.* [8, 9].

The questions raised on what is the appropriate form of the sources and the need for further studies does not detract from the proposed methodology. Indeed as it stands its framework nature makes it an ideal vehicle by which such studies can be carried out, thereby adding to the limited understanding of the mushy region solidification.

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APPENDIX: NUMERICAL TREATMENT OF SOURCES

Part A. The enthalpy source

The latent heat source, S_h, in equation (14) is considered to consist of two parts, a transient term and a convective term. The transient term has the discrete form

$$a_P^0(\Delta H_P^0 - \Delta H_P) \qquad \text{(A1)}$$

where ΔH is the nodal latent heat (i.e. the mean latent heat in control volume P). An obvious way of treating this source term during an iterative solution of equation (14) would be

to use the iterative update

$$(\Delta H_P)_{n+1} = f[(T_P)_n]$$

where $(\ )_n$ indicates evaluation at the nth iterative step and the function f is defined by equation (2). A drawback to this approach is that if the mushy range (ε) is small, (T_P) may oscillate between values greater than ε and values less than $-\varepsilon$, and hence $(\Delta H_P)_n$ will oscillate between 0 and L, and convergence will not be achieved. This problem will become acute as an isothermal phase change is approached. An alternative method which avoids this problem is as follows. At any point in the iterative solution, equation (14) may be rearranged as

$$[h_P]_n - h_P^\circ = [\text{TERMS}]_n + \Delta H_P^\circ - [\Delta H_P]_n \qquad \text{(A2)}$$

where

$$\text{TERMS} = [a_H h_H + a_L h_L + a_N h_N + a_S h_S - (a_H + a_L + a_N + a_S) h_P + \delta z \delta y \times \text{convective source}]/a_P^\circ$$

with the most current values of the nodal hs used. On convergence this equation becomes

$$h_P - h_P^\circ = \text{TERMS} + \Delta H_P^\circ - \Delta H_P. \qquad \text{(A3)}$$

Adding and subtracting appropriate terms to both sides equation (A3) may be rearranged as

$$[h_P]_n - h_P^\circ + h_P - [h_P]_n = [\text{TERMS}]_n + (\text{TERMS})c + (\Delta H_P^\circ - [\Delta H_P]_n) - (\Delta H_P - [\Delta H_P]_n)$$

where TERMS has been written as $[\text{TERMS}]_n + (\text{TERMS})c$ (i.e. the nth iterative value plus a correction). Subtraction of equation (A2) leads to the following expression for the latent heat content

$$\Delta H_P = [\Delta H_P]_n + [h_P]_n + (\text{TERMS})c - h_P.$$

An appropriate iterative scheme can now be developed. The value of $(\text{TERMS})c$ can be ignored (note its value will be zero on convergence) and the value of the nodal sensible heat can be approximated as

$$h_P = c \cdot f^{-1}([\Delta H_P]_n)$$

where f^{-1} is the inverse of the latent heat function given in equation (1). These approximations lead to the following updating scheme for calculating the nodal latent heat in the source term equation (A1)

$$[\Delta H_P]_{n+1} = [\Delta H_P]_n + [h_P]_n - c \cdot f^{-1}([\Delta H_P]_n). \qquad \text{(A4)}$$

Note that, this scheme will be consistent with the case of an isothermal phase change because f^{-1} is well defined, whereas f is multivalued at the phase-change temperature. In addition the scheme ensures that no serious oscillations occur in the predicted temperatures from one iteration to the next.

The convective part of the latent heat source, i.e.

$$-\text{div}\,(\rho \mathbf{u} \Delta H)$$

is treated via an upwinding discretization. The contribution to the source term may be written in the form

$$(\text{INFLOW}) - (\text{OUTFLOW}) \qquad \text{(A5)}$$

with

$$\text{INFLOW} = |[F_s, 0]|\Delta H_S - |[-F_s, 0]|\Delta H_P + |[F_1, 0]|\Delta H_L - |[-F_1, 0]|\Delta H_P$$

and

$$\text{OUTFLOW} = |[F_n, 0]|\Delta H_P - |[-F_n, 0]|\Delta H_N + |[F_h, 0]|\Delta H_P - |[-F_h, 0]|\Delta H_H$$

where $|[a, b]|$ means the maximum of a and b and

$$F_n = \rho v_n \delta z, \quad \text{etc.}$$

are evaluated at the cell faces of the enthalpy control volumes. Note the velocity v_n is the y-velocity on the north face of the pth enthalpy control volume, i.e. the nodal velocity of the pth 'v-velocity' control volume, see Fig. 2. In essence the formulation of the convective boundary condition states that the convective losses or gains in latent heat are governed by the direction of the flow field. It is noted that Prakash *et al.* [17] in a steady-state analysis of an arc welding model obtain a similar convective latent heat source which is also treated via an upwind differencing scheme.

Part B. The momentum source

The momentum source term corresponding to the Boussinesq approximation is added to the discretized w momentum equation in the form

$$\rho g \beta (h_P - h_{\text{ref}})/c\ \delta z \delta y.$$

The porosity of a control volume in the mushy phase is equal to the mean liquid fraction of that control volume. This value can be estimated as $\Delta H_P/L$ if the control volume is an enthalpy control volume. For velocity control volumes the liquid fraction can be estimated on averaging the latent heat contents of the enthalpy control volumes over which the velocity control volume is staggered. That is in the pth v-velocity control volume

$$[\Delta H_P]^v = (\Delta H_P + \Delta H_N)/2$$

and in the pth w-velocity control volume

$$[\Delta H_P]^w = (\Delta H_P + \Delta H_H)/2.$$

On dividing these values by the latent heat of the phase change L the appropriate control volume porosities can be calculated. These values can then be used in modifying the a_P coefficients of the discretized momentum equations via the use of the function A defined in equation (10).

MODELISATION NUMERIQUE A GRILLE FIXE POUR LA REGION TROUBLE DE CONVECTION DANS LES PROBLEMES DE CHANGEMENT DE PHASE

Résumé—Une formulation enthalpique basée sur une méthodologie à grille fixe est développée pour la résolution numérique des problèmes de changement de phase avec une région trouble contrôlée par la convection. La méthode proposée repose sur la représentation par des sources convenablement choisies de l'évolution des chaleurs latentes et de l'écoulement dans la zone trouble liquide–solide. Il y a une complète liberté dans la méthodologie pour la définition de telles sources de telle sorte qu'on peut modéliser une grande variété de situations. On étudie la congélation dans une cavité avec convection naturelle pour démontrer l'application de la méthode.

EINE NUMERISCHE FESTGITTERMETHODE FÜR ÜBERGANGSGEBIETE BEI PHASENWECHSELPROBLEMEN MIT KONVEKTION UND DIFFUSION

Zusammenfassung—Ein Festgitter-Verfahren, welches auf Enthalpiebilanzen basiert, wurde zur numerischen Lösung von Konvektions–Diffusionsgesteuerten Problemen des Phasenübergangs entwickelt. Der grundlegende Unterschied der vorgestellten Methode liegt in der Berücksichtigung der Entstehung der latenten Wärme und der Strömung in der Fest-flüssig-Übergangszone durch geeignet gewählte Wärmequellen. Für die Definition solcher Quellen hat man vollkommene Freiheit, sodaß eine Vielzahl von Phasenwechselvorgängen modelliert werden kann. Ein Testproblem des Gefriervorganges in einem thermischen Einschluß unter natürlicher Konvektion wird benutzt, um die Anwendung dieser Methode zu zeigen.

ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ ЗАДАЧ ФАЗОВОГО ПЕРЕХОДА С УЧЕТОМ КОНВЕКЦИИ И ДИФФУЗИИ

Аннотация—На основе энтальпийной формулировки используется метод неподвижной сетки для численного решения задач фазового перехода с учетом конвекции и диффузии. Характерной чертой предлагаемого метода является представление удельной теплоты фазового перехода и потока в зоне фазового перехода твердое тело–жидкость с помощью соответственно выбранных источников. Выбор этих источников предполагается таким, что позволяет моделировать различные случаи фазовых превращений. В качестве иллюстрации рассматривается задача о замерзании в полости при естественной конвекции.