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Computer simulation of moving-interface, convective, phase-change processes

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Abstract—The paper presents a numerical study of phase-change problems, using finite-volume procedures of the 'enthalpy' formulation. A mathematical model is developed, and is applied to predict the transient behaviour of internal solidification in a cooled pipe, for flows at laminar Reynolds numbers. Work is directed towards predicting the production of solid crust when both diffusion and convection effects are important. Results are presented, and they are compared with available experimental measurements. It is concluded that the procedure is robust and flexible and that the results are promising.

1. INTRODUCTION

THE PURPOSE of this work is the development and application of mathematical models for simulating phase-change engineering problems, under the effects of both convection and diffusion. Such problems are encountered, for example, in the metallurgical and environmental industries.

The complexity of the phase-change process depends on both the structure of the material and the type of conditions imposed on it.

Previous analytical work is limited to the one-dimensional diffusion case, generally classified as a 'moving boundary' problem. The theory is idealized to instantaneous irreversible molecule immobilization, presenting a sharp planar surface moving through the medium (the 'Stefan problems' [1], of isothermal phase change). Many approximate analytical techniques such as the heat-balance integral [2], and the variational technique [3] have been developed and used to acquire approximate solutions in diffusion type problems. Numerical methods, both finite difference [4] and finite element [5] appear more powerful in solving such 'moving-boundary' problems, especially in the presence of strong convection [6–9]. Under isothermal conditions, most work to date has been concerned with the prediction of the position and shape of the solid/liquid interface, using either time-variant or fixed mesh systems. The time-variant mesh systems [10–12] tend to be restricted to simple problems and geometries. The fixed-mesh studies tend to use empirical relationships for the convective heat transfer in the liquid phase [13–16], a more general approach being to take account of such effects in the governing equations [17–20]. A different modelling approach is to remove the dependence on the position of the phase-change front by employing an enthalpy function. This technique appears successful in natural convection type problems [21–23] as well as in pure diffusion problems. A comprehensive review of the most recent pure conduction/diffusion methods may be found in the recent paper by Hsiao [24], in which a simple algorithm for determining the physical state (liquid, molten or solid phase) at each computational node is presented. The problem for analytical work is the diffusion coefficient discontinuities at the phase-change front, that limit the analysis to semi-infinite media. Attempts to overcome the problem have been reported by Danckwerts [25] and by Crank [26], the latter being the nearest solution to the flat plate problem. In all cases, however, the strength, accuracy and practical usefulness of Stefan-type formulations may be considered as limited. Thus, in metallurgical solidification we are often dealing with a non-planar front due to poor control of the imposed temperature gradient. Dendrites form, instead of the assumed cellular formation, and large uncontrolled temperature gradients may cause instability at the front, leading to protruberances or 'facets' forming on the cell face. The latter becomes undulatory, causing irregular solidification. Furthermore, natural convection makes the real fronts nonvertical, causing intermittent solidification and melting. A detailed summary of recent work in this area may be found in ref. [26].

Most numerical solutions to date are still restricted to Stefan-type problems (i.e. 'plane front/diffusion only') and concentrate on front shape and position tracking. Therefore, a numerical method is still required to account for forced convection effects and for latent heat evolution. For this purpose, an enthalpy formulation has been developed which, although it does not offer information on the precise position within a computational cell of the solid/liquid

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interface, is found to be attractive in terms of accuracy, simplicity and practicality. The technique is applied to model solidification of an isomorphous fluid, flowing through a cooling pipe, with a view to predicting the build-up of solid crust, the likelihood of laminar flow blockage, and the detailed enthalpy and flow fields during solid development. The predictions are obtained using a fully-implicit, iterative, finite-volume procedure embodied in a general computer program called PHOENICS [27], and are compared with available experimental data.

2. THE MATHEMATICAL MODEL

2.1. *The equations and solution procedure*

The conservation equations applicable to the flow and heat/mass transfer problems considered here are of the following general form:

$$\frac{\partial}{\partial t}(r\rho\phi)+\nabla(r\rho\phi\mathbf{v}-r\Gamma_\phi\nabla\phi)=\dot{m}\Phi+rS_\phi \quad (1)$$

where ϕ is the general conserved property of phase under consideration, Γ_ϕ the exchange coefficient of ϕ, S_ϕ the source rate of ϕ per unit volume, r the volume fraction of phase, ρ the phase density, $\mathbf{v}$ the velocity vector of phase, Φ the ϕ-content of material crossing the phase boundary, and $\dot{m}$ the mass per unit volume entering the phase, from all sources per unit time.

The three momentum equations for each phase are generated by setting $\phi = u$, v or w, e.g. the phase velocity components in three space directions, and the exchange coefficient, Γ_ϕ, equal to viscosity; S_ϕ are forces (e.g. pressure gradient, gravitational, frictional forces, etc.). For the energy equation, $\phi = h$, the sensible heat, and $\Gamma_\phi = K/C$, where K is the thermal conductivity and C the specific heat. In a phase-change problem the source S_h will depend on the nature of the latent heat evolution and will require careful definition.

Finally, mass continuity dictates that

$$\frac{\partial}{\partial t}(r\rho)+\mathrm{div}\,(r\rho\mathbf{v})=\dot{m}. \quad (2)$$

The above equations can be solved by a general program called PHOENICS [27]. This program solves for the relevant variable ϕ_P at finite-difference node P, using a finite-volume form of the conservation equation

$$a_P\phi_P=\Sigma a_i\phi_i+S_\phi \quad (3)$$

where ϕ_P is the value of ϕ at node P, at the centre of its control volume, ϕ_i the value of ϕ at the relevant neighbouring point at the centre of its control volume (including the 'old' time value ϕ_τ), a_P the coefficient for node P which, in the absence of sources and boundary conditions, is the sum of the a_i's, and a_i the coefficients for relevant neighbouring nodes consisting of convection and diffusion, added together.

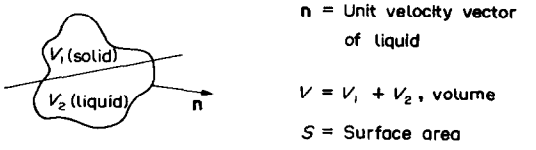

FIG. 1. An arbitrary control volume.

The source term in the finite-difference equation, S_ϕ, is linearized for stability, and the convection contribution is upwinded.

The solution procedure in PHOENICS is a variant of the SIMPLE solution algorithm called SIMPLEST (cf. Patankar [6], and Rosten and Spalding [27].

2.2. *The enthalpy formulation*

The essential feature of the proposed enthalpy technique for convection/diffusion phase change is the latent-heat source term treatment, in the energy equation. In a system which is undergoing a change of phase under heat transfer the total enthalpy, H, may be expressed as

$$H=h+\Delta H \quad (4)$$

i.e. the sum of sensible enthalpy h and latent heat ΔH. The latter is some function of temperature, $F(T)$, with form depending on the problem. For isothermal solidification

$$F(T)=\begin{cases}L, & T>T_m\\ 0, & T_m>T\end{cases}$$

where T_m is the melting temperature for a pure substance.

With the definition of enthalpy provided by equation (4) it is possible to develop the energy conservation equation for a region undergoing a phase change. When this equation is cast into the form of equation (1) the form of the latent heat source, S_h, is derived. An energy balance over an arbitrary control volume V, with phase change occurring within it (Fig. 1), gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_V\rho H\,\mathrm{d}V=\int_S K\nabla T\cdot\mathbf{n}\,\mathrm{d}S-\int_S\rho H\mathbf{v}\cdot\mathbf{n}\,\mathrm{d}S \quad (5)$$

where $V=V_1+V_2$, $\mathbf{n}$ the unit vector and S the surface area. The term on the left-hand side represents the overall rate of heat change, and the terms on the right-hand side are the diffusional and convective heat transfer through the surface, respectively. The vector functions $\rho H\mathbf{v}$ and $K\nabla T$ have continuous first derivatives (because in the solid $\mathbf{v}=0$), and application of the divergence theorem to equation (5) gives

$$\int_V\left[\rho\frac{\partial H}{\partial t}+\nabla\cdot(\rho H\mathbf{v})-\nabla\cdot(K\nabla T)\right]\mathrm{d}V=0$$

or, since V is arbitrary

$$\rho\frac{\partial H}{\partial t}+\nabla\cdot(\rho H\mathbf{v})-\nabla\cdot(K\nabla T)=0. \quad (6)$$

Using definition (4) for H, invoking the conservation of mass, and recalling that the solid interface velocity is zero we have

$$\frac{\partial}{\partial t}(\rho h)+\nabla\left(\rho h\mathbf{v}-\frac{K}{C}\nabla h\right)=S_h=-\rho\frac{\partial\Delta H}{\partial t} \quad (7)$$

which is in the standard form of the conservation equation (1), with the latent-heat source term defined as the rate of change of volumetric latent heat.

Therefore, to model phase change in the presence of convection, a standard program like PHOENICS can be used with appropriate source-term modifications, to implement the latent heat behaviour and the solid velocity behaviour. These are described below.

2.3. *Latent heat behaviour*

Suppose that phase change is taking place at $T = 0$°C. Then for $h > 0$, heat can be extracted from h. When heat extraction causes h to become less than 0 one must account for the phase-change behaviour. The amount of heat extracted at $T = 0$°C must be taken from the latent heat and h must be set to zero. This process should continue until all the latent heat has been extracted; then, any further heat exchange is from the sensible amount. This may be summarized as follows, where subscript j denotes the time step and L the latent heat.

Phase change not started yet		
$h_j > 0$	$\Delta H = L$	heat extracted from h.
Phase change occurring		
$h_{j+1} < 0$	$\Delta H = L$	heat extracted from H, h set to zero.
Phase change occurring		
$h_{j+2} < h_{j+1}$	$0 < \Delta H < L$	heat extracted from H if possible. h corrected to zero if possible. If this is not possible, heat is taken from H until it becomes zero and rest is taken from h.
Phase change complete		
$h_{j+3} < 0$	$\Delta H = 0$	heat extracted from h.

(8)

The methodology for dealing with the above scheme during SIMPLEST iterations is as follows. Essentially if a control volume is changing phase on convergence the nodal latent heat ΔH_P must be consistent with the predicted value of the enthalpy, h_P, according to the relationship given by the $\Delta H = F(T)$ expression. Therefore, at each time step, the sensible-enthalpy values at the control volumes are computed by the standard solution procedure, and they are then corrected and set back as values of h_P for the next time-step calculation. The correction stage involves the following operations. The computed sensible-enthalpy value for the control volume is added to the latent heat value, which is initialized to L. When the outcome of this summation exceeds the value L, i.e. $h_P > 0$, the phase change has not commenced in this control volume and the latent heat is left unmodified, the source for h_P being zero. When the summation leads to a negative result, the phase change has occurred in one time step. Then all the latent heat is extracted and an equal amount is added to the sensible heat, which may or may not set it to zero (in the latter case, the cell has gone through the phase change and further in one time step). The latent heat is set equal to the enthalpy value at this time step, and therefore all heat extraction will be from h_P at the following time steps, the source for h_P being again zero.

For cells requiring more than one time step to solidify, and for cells just starting to do so, the latent heat is corrected as follows. Subtraction from the old latent heat value (which is equal to L if solidification starts in the current time step) gives the amount of heat extracted from ΔH to the sensible enthalpy in the source. In the next time steps when less heat has been extracted than the latent heat, this process continues until all ΔH has been used up. When an insufficient amount of latent heat is left, h_P at the current time step has a negative source (equal to the difference of the heat extraction and the remaining latent heat), and no source for the subsequent time steps. The above procedure ensures that a control volume is in the liquid state if $(h_P)_j > 0$ and $(\Delta H_P)_j = L$, whereas if a control volume is in the solid state $(h_P)_j < 0$ and $(\Delta H_P)_j = 0$. On convergence the enthalpies in control volumes changing state will be zero with an appropriate latent heat in the range $0 < \Delta H_P < L$.

2.4. *Solid velocity treatment*

Since a fixed grid is used, the velocities at its nodes must be monitored and possibly altered, in accordance with the principle that liquid above its melt temperature should possess the velocity dictated by the momentum equations, and solid material must have zero velocity. Since at the solid/liquid interface the velocities must go to zero, the momentum equations must reflect this behaviour. Various techniques of modelling the behaviour of the velocities in the vicinity of the phase change have been investigated. It was found that the most accurate of those was a gradual 'slow down' technique rather than a complete solid-velocity switch off at some arbitrary point over the phase change (e.g. start, middle or end).

Gradual slow-down techniques have been successfully applied to cases of natural convection in square cavities. Gartling [28] suggested a slow-down technique based on a variable viscosity function, which is inversely proportional to the amount of latent heat contained in a cell. This method has proved to be inadequate because it reduces artificially the liquid velocities as well as those of the solidifying material, and therefore overestimates the solidified domain. Furthermore, it is difficult to devise an accurate function for the viscosity term.

For modelling purposes, the solidification process

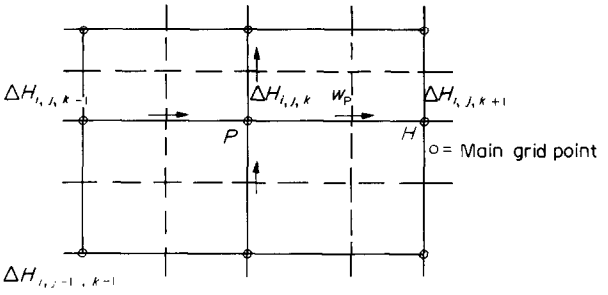

FIG. 2. Grid system and notation.

can be envisaged as a case of elements of the numerical discretization forming grains in a complex and irregular pattern. This process gradually reduces the fluid flow through the element, by decreasing the cell 'porosity' or 'voidage', ε (which is defined as the ratio of unblocked volume over the nominal cell volume). This concept leads naturally to the model of a porous medium with the liquid fraction flowing through a solid matrix. This model has physical significance in a mushy phase change, whereas for an isothermal phase change the model is the result of the numerical discretization.

Notable work on fluid flow through a porous medium of constant porosity has been carried out by Ergun [29]. However, the constant porosity assumption is obviously not applicable to the solidification process; and the Ergun terms for estimating the pressure drop through a cell are unnecessarily complex for this application, containing too many assumptions in evaluating a representative size and distribution of forming grains. A simpler method can be derived from Darcy's law which states that the velocity of flow in a porous medium is proportional to the pressure gradient, e.g.

$$\frac{k}{\varepsilon}u = -\frac{\partial p}{\partial x} \tag{9}$$

where u is the interstitial velocity, ε the porosity and k an empirical constant. Hence the flow in a porous medium can be accounted for by momentum equations (1) where $S_x = -ku/\varepsilon$ and $S_y = -kv/\varepsilon$.

For the above porous-medium model the porosity ε will be a function of the representative latent heat content of a cell. As $\Delta H \to 0$ the porosity $\varepsilon \to 0$, and the source term will dominate the momentum equation and force the related velocities u_P and v_P close to zero; and as the latent heat content of a cell tends to its maximum, the porosity $\varepsilon \to 1.0$.

The task is now to construct the appropriate function to operate between these limits. The simplest one, e.g. direct proportionality between latent heat and porosity, was discarded for two main reasons. Firstly, it is known that the 'grain formation' occurs much faster near the end of the solidification region than near its start. Secondly, implementation of such a function demonstrated that velocity changes were sudden unlike the real behaviour. For these reasons an exponential function was chosen, and implemented as follows. Consider flow in the z-direction (Fig. 2). The velocities are staggered ahead of the cell centres, at which all other variables are stored, and the latent-heat content at the velocity locations is calculated by arithmetic averaging, e.g. for the w-velocity node (Fig. 2)

$$\Delta H_w = \frac{H_{(i,j,k)} + H_{(i,j,k+1)}}{2}. \tag{10}$$

The porosity in a velocity control volume will be a function of the latent heat ΔH_w, satisfying the above-mentioned conditions. Thus, as $\Delta H_w \to 0$, $\varepsilon \to 0$ and the source term added to the momentum equation must dominate it and force the velocity w_P to values close to zero. A suitable choice for the source term is

$$S_w = -B[\exp(L - \Delta H_w) - 1]w_P \tag{11}$$

where B is a constant discussed below and the -1 is used to ensure zero source when a cell is still in the fully liquid state. This source is rearranged

$$S_w = B[\exp(L - \Delta H_w) - 1](0 - w_P) \tag{12}$$

and upon addition to the discrete momentum equation (3) yields for w_P

$$(a_P + B([\exp(L - \Delta H_w) - 1])w_P = \Sigma a_i w_i + (p_P - p_H)A_H = G$$

or

$$w_P = \frac{G}{a_P + B[\exp(L - \Delta H_w) - 1]} = \frac{G}{a_P + S}. \tag{13}$$

Hence, w_P is gradually set to a smaller and smaller number, as solidification proceeds, its ultimate value depending on the situation modelled (i.e. value of G) and on the value of the constant B in equation (13). In the extreme case when the cell is fully solid, S is very large and $w_P \to 0$. The constant B is chosen with regard to the following factors: it should be large enough to produce velocities in solidified regions at least three orders of magnitude less than the velocities in the liquid regions; it should not be so large as to cause very rapid changes in velocity, especially in the case of forced convection with large initial velocities, as this would cause high pressure corrections and possible convergence failure; finally, it should react fast enough to produce small velocities immediately upon a phase change. Tuning of this constant was carried out by monitor observations, and its final

value was of the order of 10^{-1}% of the mean stream velocity.

3. RESULTS AND DISCUSSION

The problem chosen for demonstrating the present technique is that of forced convection through a cylinder with the wall maintained at a temperature below the freezing point of liquid material entering at uniform temperature and velocity. The liquid was assumed incompressible, Newtonian, with constant properties. Radiation and free convection effects were neglected.

This problem having never been successfully modelled to the authors' best knowledge, is considered of prime interest in the metal casting field. In metal pouring, care must be taken to ensure that fluid does not start solidifying until it has entered the mould, and that its forced momentum is not unnecessarily large, resulting in undesirable solidification and microstructure because of possible flow separation in the sprue. However, its inlet flow should be large enough to avoid metal–air contact, that would lead to oxidization. The quantity used to gauge the flow is fluidity (i.e. reciprocal of viscosity) or the length from the inlet to the beginning of solidification, claimed to be independent of the fluid flow but significantly dependent on the temperature difference $(T_{wall} - T_{in})$ applied, the latent heat and the thermal resistance of the pipe wall.

3.1. *Pipe blockage literature*

It is conceivable that as fluid flows through a pipe with its wall maintained at a sub-freezing temperature two possible final conditions may arise. Firstly, if the heat extracted is in excess of that contained by the fluid at its supply, the system may reach a steady state at which crust formation ceases and flow continues. Secondly, the crust may develop until it blocks fully the pipe and stops the flow. This problem is of major concern to metallurgists and has previously been studied using various approaches. A general numerical approach, suggested by Szekely and Di Nivo [30], and a Nusselt number formulation by Thomason *et al.* [31] lead to poor solutions. Another approach presented by Sellors *et al.* [32], and more recently by Sleider *et al.* [33], solves the steady-state radial conduction and axial convection heat equations, and describes the growth of the crust to inhibiting conditions, but fails near a pipe blockage, especially at large Stefan numbers. Various variations on ref. [33] were proposed by Shibani and Ozisik [34] but they assume a large Peclet number, i.e. 'fast' fluid flow reducing buoyancy and axial heat-transfer effects negligible. This is not suitable for a liquid metal in laminar flow ($Pe < 1$). The most developed method to date was proposed by Sampson and Gibson [35, 36], who supply a variable pressure drop across the pipe in order to obtain blockage. Their method is applicable to cases where for a given discharge end pressure, the inlet pressure is allowed to decrease, but not to cases where fluid is supplied at an approximately constant rate. That work also encounters problems on nearing blockage, but it predicts that the crust growth rate decreases nearing the blocked condition, and provides a useful relationship for the blockage.

A good summary of other methods for particular problems is given in ref. [37].

3.2. *Convergence and parametric studies*

Initial convergence difficulties were overcome by using a simultaneous solver for the pressure-correction equation, and false-time-step relaxation on enthalpy and velocities. Many runs were performed in order to optimize the required number of sweeps per time step, and the grid and time-step sizes, as shown in Table 1.

The change in solution with time-step refinement was found to be important in this transient, and it was monitored carefully by plotting the solutions at various times and positions in the pipe, as illustrated for enthalpy in Fig. 3. It was found that the time-step effect was more pronounced near the inlet. As indicated in the table, the final run was one with 40 sweeps per time step, a 20×40 grid and 40 time steps over a period of 1 s.

3.3. *Discussion of results*

Sample results are presented in Figs. 4–6 in the form of velocity vectors and solid and liquid enthalpy contours. The results are presented at four times, e.g. $t = 0.25$, 0.50, 0.75 and 1.0 s. The enthalpy plots are actually isotherm plots, as the specific heat was taken as unity for both solid and liquid.

Continuation of the transient to a time of 2.0 s revealed insignificant changes, indicating that the system reached steady state after 1.0 s. The greatest rate of change of crust thickness occurred in the last quarter of a second. The predicted behaviour during the transient is summarized below.

3.3.1. *Crust development and solid enthalpy.*

(1) $0 < t < 0.5$ s. The rate of crust development is greatest over the initial 0.25 s of this period. Solidification proceeds from the outlet end of the wall, developing into a solid layer of approximately constant thickness along the pipe, except for its curvature at the start of wall heat extraction. The solidification band (i.e. the flow region between the $T = 0$ and 1°C isotherms) is very narrow near the inlet, widening to a width greater than the crust thickness at outlet. The relative thinness near the inlet is an indication of the high 'bulk enthalpy' of the fluid there. It is of interest to observe that in approaching a steady state, solid only forms up to the $T = 1$°C isotherm, which is almost constantly positioned for this period.

The relative change in isotherm spacing is also of interest. The expected trends of tighter isotherms in the centre of the solid layer, and of highest temperature gradients occurring adjacent to the fluid and wall, are clearly observed.

Table 1.

Run No.	Number of sweeps per time step	Grid	Time steps	Comments
1	20	10 × 20	40	No significant change from 40 to 80 sweeps per time step, therefore choose 40
2	40			
3	80			
4	40	20 × 40	40	No significant change in accuracy
5		40 × 80		
6	40	20 × 40	80	Small change in accuracy from run 4
7			160	Insignificant change in accuracy from run 6

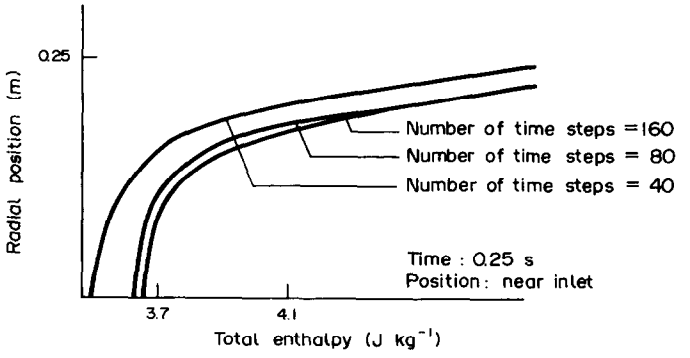

FIG. 3. Time-step refinement (transient run for 2.0 s).

(2) $0.5 < t < 1.05$ s. In this time period, steady state is reached very rapidly and the isotherm characteristics are most dissimilar to earlier transient states. For instance, the 'solidifying band' has narrowed considerably and inspection of the velocity vectors indicates a molten region here, as velocities are high and therefore there is no sign of full solidification. The minimum temperature of the crust has reached a value 0.3°C less than in the previous times, and the region of tight bulk isotherms has moved upstream. The outlet temperature gradient across the solid is nearly constant, the isotherms having curved to match the more complex sloping profile of the crust surface. Extrapolation of this inference to the case of pipe blockage would imply that the axial blockage thickness would only be a small percentage of the pipe length.

3.3.2. *Liquid enthalpy plots.*

(1) $0 < t < 0.5$ s. Inspection of the relevant plots reveals that the isotherms for times up to 0.5 s are, with little approximation, similar in pattern showing the bulk of the flow to be between 1 and 2°C above the phase-change temperature. Axial heat conduction at the inlet close to the wall, accompanied by effects of the flow convergence and development has brought the bulk of the fluid to 2°C. Possibly due to small velocity vectors in the fluid 'impacting' on, or diverging from the start of the solid crust, this region of fluid is seen to reach freezing temperature faster, explaining the strong curvature of the $H = 2.0$ J kg^{-1} K^{-1} isoenthalpy near the wall, which eventually flattens out across the fluid core, where approximately constant velocities are found.

(2) $0.5 < t < 2.0$ s. Once the steady state is reached, the isotherms elongate indicating a constant radial conduction state for the fluid that accelerates because of the negative axial area differential. In other words, the heat extraction from the fluid is less, due to the reduced 'residence time'. This has effectively inverted the $T = 4$°C isotherm, while the central core only reaches the temperature of 2°C (cf. isotherm position in earlier time) at approximately three-quarters along the pipe length. The curvature is as would be expected for flow near the crust, the isotherms converging towards the pipe inlet. The effects of axial conduction on fluid 'impacting' on the upstream end of the crust are more pronounced in this state, as demonstrated by the inversion of the $T = 4$°C isotherm between 0.5 and 1.0 s. The plot at $t = 1.0$ s reveals also that fluid retains its initial temperature (all fluid to the left of the $T = 5.0$°C isotherm is at its initial temperature) for a considerable time in the steady state, being retained the longest by the accelerated core well into the crust zone. This is very different to the transient development. Extrapolation of this behaviour would confirm that pipe blockage would occur very rapidly in agreement with experimental behaviour. It has to be mentioned that the setting of equal thermal conductivities for solid and liquid has simplified the isotherm considerations.

3.3.3. *Velocity vectors.*

(1) $0 < t < 0.5$ s. During this time, the profile of the

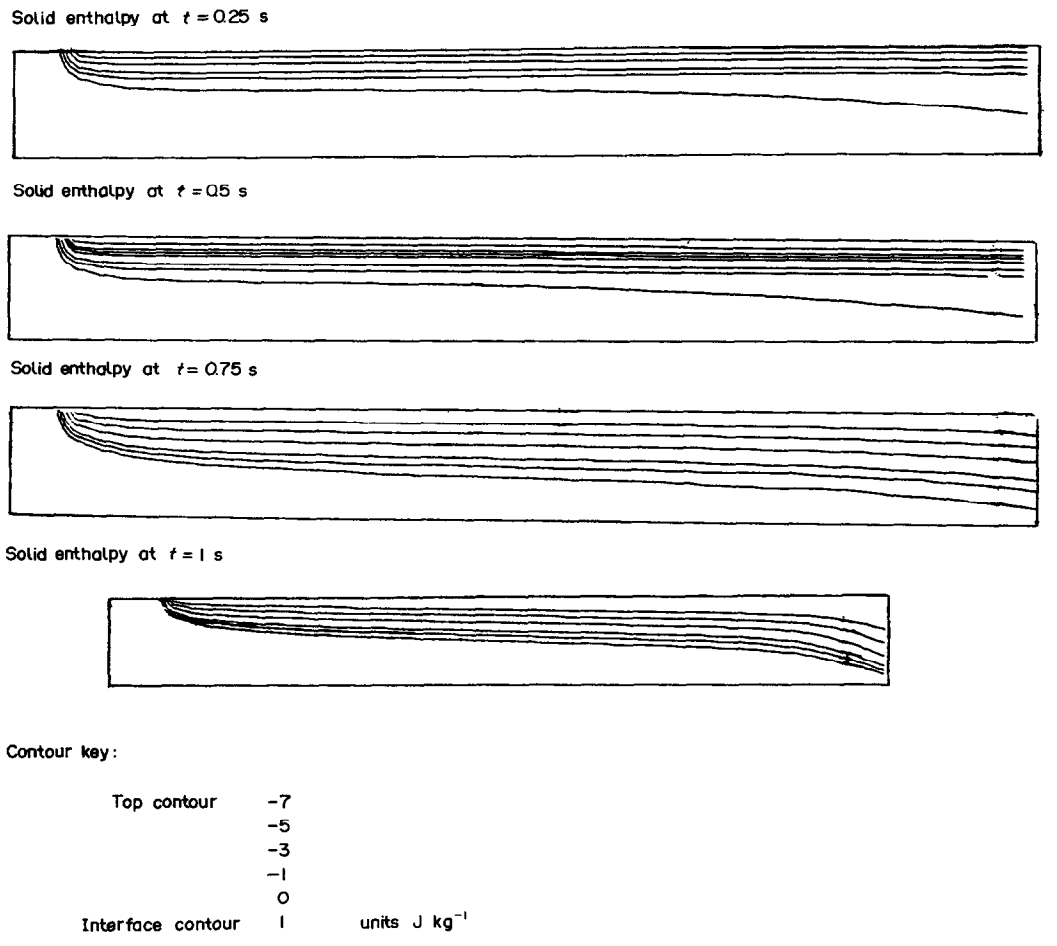

FIG. 4. Solid enthalpy history.

solid crust is approximately flat. The effect is that the velocity vectors adjusted by the initial flow area convergence of about 30%, become approximately parallel and their profile 'develops' after half the pipe length. There is retardation and solidification occurring in the proximity of the crust surface. The resulting 'fully developed' flow profile is not of the parabolic laminar shape but it is flatter along the core. This may be the result of the thickening of the solidification band near the outlet, i.e. the phase-change effects near the outlet are strong even in the core, where a mushy region exists. The resultant drag is of a purely viscous nature in the boundary layer, which is quite in keeping with a hydraulically smooth flow attributed laminar friction.

(2) $0.5 < t < 1.0$ s. During this time, the high negative axial flow area gradient dominates the flow leading to a more parabolic velocity profile at the exit, the core acceleration being comparatively unaffected by the phase-change band, due to its relative thinness. The core flow has accelerated to roughly six times its initial axial velocity value. In this case, an obvious two-dimensional profile is present with considerable negative radial components. These facts would suggest that the rate at which the crust thickness increases with time at the outlet, would decrease on nearing blockage due to high convection there. Looking along constant radial values, vectors near the solid at entry are very small and are hence easily absorbed into the crust. This process takes longer further downstream, and at the outlet vectors in the solidifying band are very high in comparison, indicating a thick, steady-state mushy region.

4. COMPARISON WITH EXPERIMENTS

The ultimate test for any mathematical model is to compare its predictions with results from accurate physical experiments. In this case the model was run until steady state was reached for the laminar, isothermal flow of water, in order to compare predictions with data found in Lazaridis [4].

In these experiments (for which a schematic view of the apparatus is given in Fig. 7) thermocouples were used to measure the temperature of the fluid at the pipe wall 1.5 in. downstream from the test section inlet and 3 in. before the outlet. Acetone was pumped at a high rate through the cooling wall keeping this

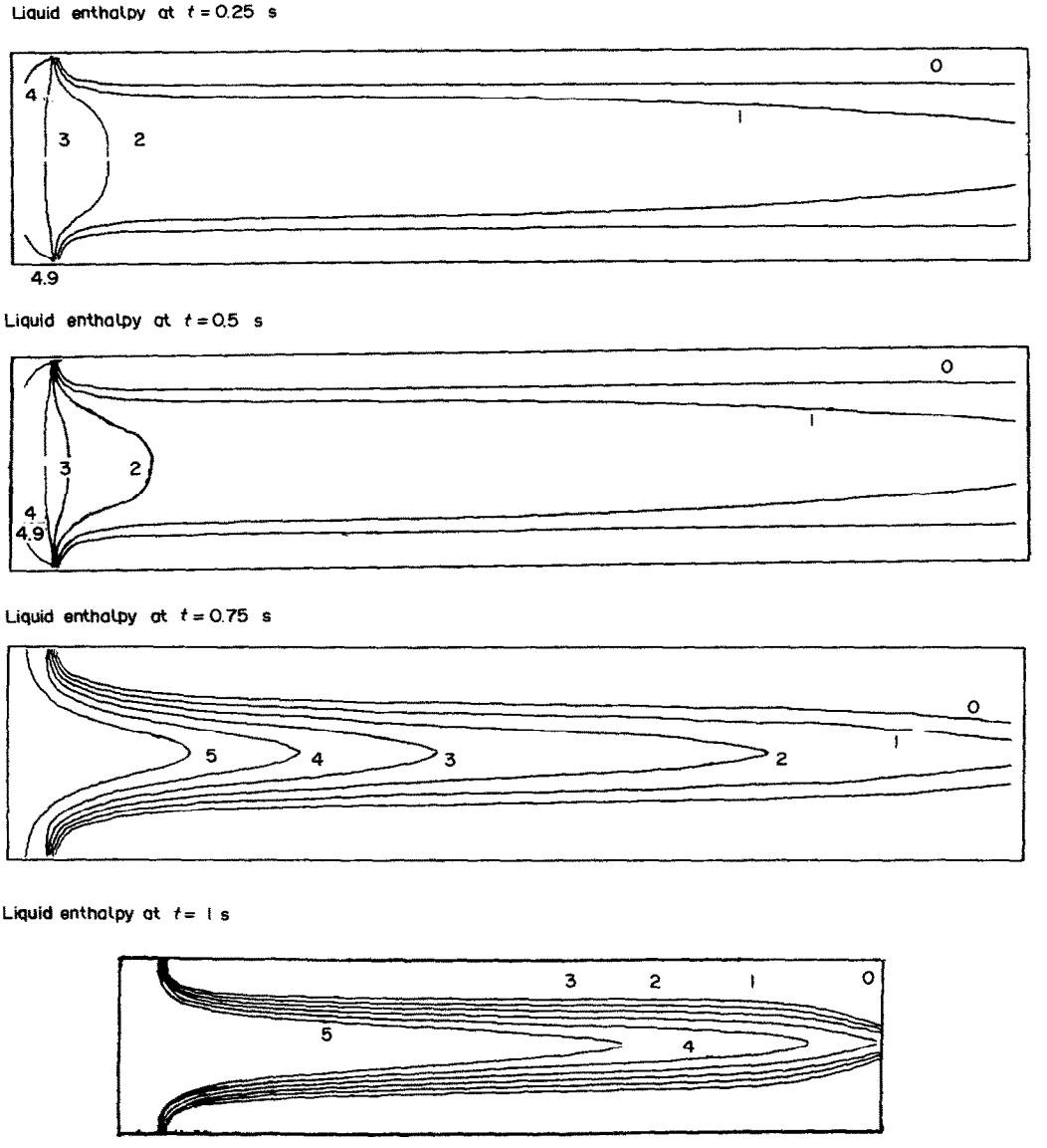

FIG. 5. Fluid enthalpy history.

section at approximately constant temperature. The mass flow rate used for the computations was set to that of the experimental steady-state value (which might lead to overprediction of temperatures) and no account was taken of dissolved air (which might help correct the afore-mentioned deviation). The predicted results were compared with the experimental results, for the conditions as stated in Table 2. Numerical results were obtained using a 10×20 grid, requiring 15 min CPU time on a PRIME 750 mini-computer.

The experimental water outlet temperature represents a bulk reading; and in the presence of model crust build up the predicted outlet fluid temperature values were suitably averaged. The properties used are given below

$$\mu = 6.4 \times 10^{-4}\,\mathrm{kg\,m^{-1}\,s^{-1}}$$

$$K = 6.18 \times 10^{-4}\,\mathrm{kW\,m^{-1}\,K^{-1}}$$

$$C_p = 4.2\,\mathrm{kJ\,kg^{-1}}$$

$$LAT = 335\ \mathrm{kJ\ kg^{-1}}$$

$$\text{Test length} = 0.95\,\mathrm{m}$$

$$\text{Test diameter} = 0.05\,\mathrm{m}.$$

Five experimental points do not allow a conclusive comparison to be derived, but it may be seen that even with significant freezing for both low and high Reynolds numbers ($Re_d = 585$ and 1617) the present method slightly overpredicts outlet temperatures. The agreement is, however, very fair for any practical application.

For the five test runs performed, blockage data may

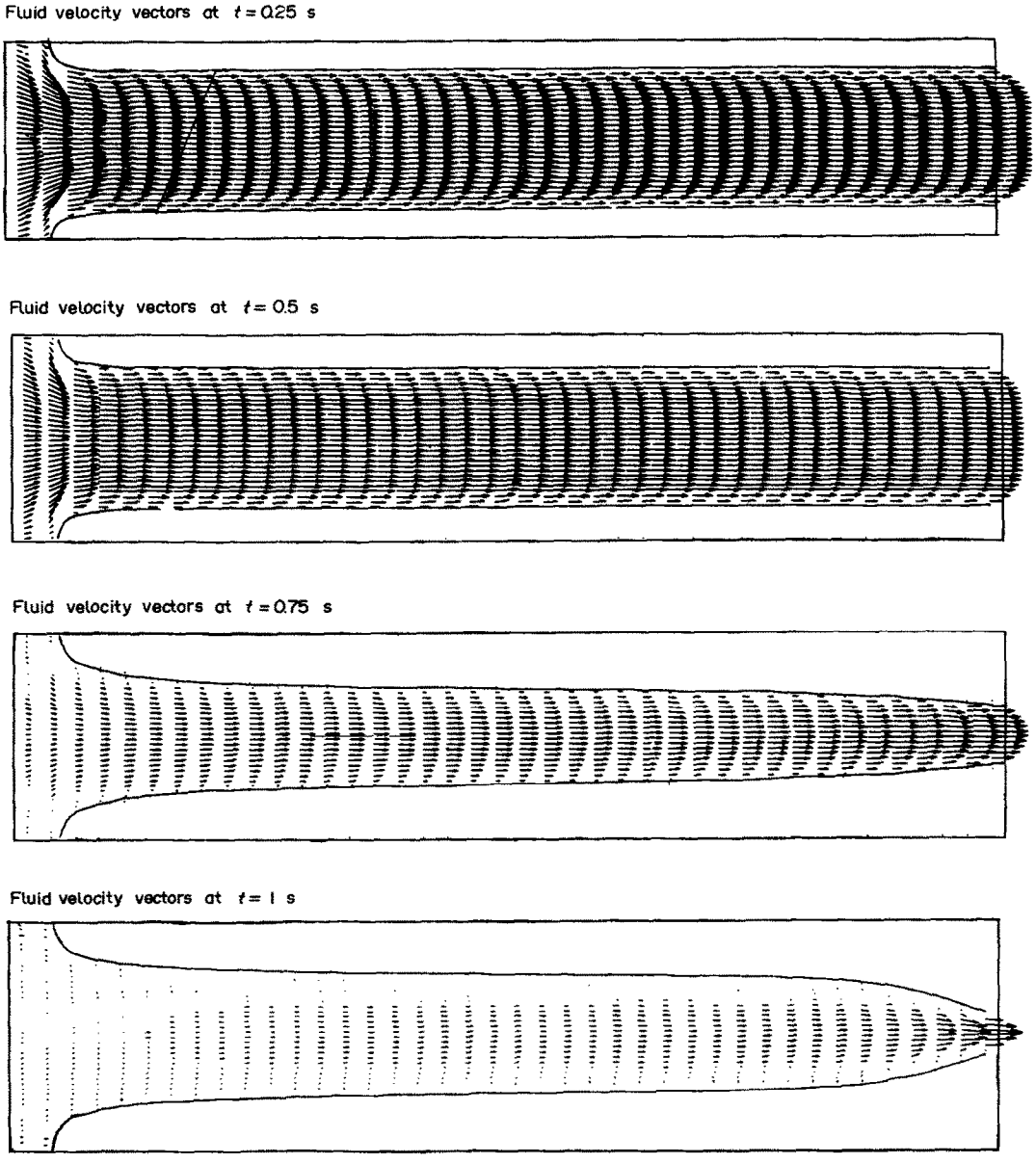

FIG. 6. Fluid velocity history.

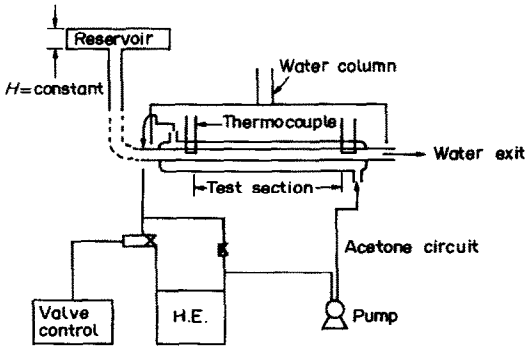

FIG. 7. Schematic view of experimental apparatus.

be compared with the predictions by Sampson and Gibson [35]. They proposed an equation as a criterion for the likelihood of complete laminar flow blockage: complete blockage will result if

$$\log_{10}\beta > \tfrac{3}{4} - \tfrac{7}{20}\log_{10}\alpha \text{ in which:}$$

$$\beta = \frac{K_f(T_m - T_w)}{K_s(T_0 - T_m)}$$

$$\alpha = \frac{4}{Pe}\frac{k_f}{\left(\frac{T_0}{2}\right)^4}. \tag{14}$$

Applied to the test runs, both models show complete agreement with the experimental behaviour.

Table 2.

m (g s^{-1})	Re_d (unblocked)	T_m (K)	T_w (K) (av)	T_{out} (K) Experimental	T_{out} (K) Model
1.45	585	302.0	204.6	282.1	283.2†
1.87	725	300.7	266.7	291.6	292.3
2.55	1040	301.9	274.3	296.3	298.1
3.93	1560	301.7	274.3	297.8	301.7
4.02	1617	305.0	265.2	274.5	275.2†

† Cases with significant freezing.

5. CONCLUSIONS AND FURTHER WORK

A general mathematical model has been developed for predicting solidification/melting processes, applicable to any geometrical or heat and mass flow conditions. It appears that the enthalpy method is general and conforms well with general control-volume techniques for fluid-flow and heat/mass transfer simulations. As such it can be readily incorporated into large-scale models of heat/mass transfer processes. Dealing with the moving interface, the exponential 'Darcy-like', slow-down method appears flexible and robust, and its implementation does not involve detailed interpolations.

Future refinements could include:

(a) more complex property relationships for larger temperature variations (e.g. density, viscosity, etc.);

(b) the introduction of turbulence quantities;

(c) introduction of more complex microstructures as would be required for accurate metal processing work (this phenomenon in itself is an undesirable process);

(d) for much lower flow rates buoyancy effects might be introduced to encompass the effects of free convection.

Perhaps the most useful applications of this work might be made in designing less separating sprue and funnel devices used in the casting industry and for reduction of heating/cooling requirements for long distance fluid transportation or controlled forging.

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SIMULATION NUMERIQUE DE MECANISME CONVECTIF D'INTERFACE MOBILE ET CHANGEMENT DE PHASE

Résumé—On présente une étude numérique des problèmes de changement de phase en appliquant des procédures de volume fini à la formulation "enthalpique". On développe un modèle mathématique et on l'applique à la prédiction du comportement variable de solidification interne dans un tube refroidi, pour des écoulements laminaires. L'étude est dirigée vers la prédiction de la production de la croûte solide quand les effets de la diffusion et de la convection sont ensemble importants. Des résultats sont présentés et ils sont comparés avec des mesures expérimentales. On conclut que la procédure est robuste et flexible et que les résultats sont prometteurs.

RECHNER-SIMULATION VON KONVEKTIVEN PHASENÄNDERUNGSPROZESSEN MIT WANDERNDER GRENZFLÄCHE

Zusammenfassung—Es werden Phasenänderungs-Vorgänge aufgrund von Enthalpie-Bilanzen mit Hilfe eines "Finite-Volume"-Verfahrens numerisch untersucht. Mit einem mathematischen Modell wird das transiente Verhalten der Vorgänge bei der Verfestigung in einem gekühlten Rohr berechnet, das bei Reynolds-Zahlen im laminaren Bereich durchströmt wird. Die Arbeit konzentriert sich auf die Berechnung der Entstehung einer festen Kruste, und zwar für den Fall, daß sowohl Leitung als auch Konvektion von Bedeutung sind. Die Ergebnisse werden dargestellt und mit den zur Verfügung stehenden Meßdaten verglichen. Es wird der Schluß gezogen, daß das Verfahren unempfindlich und flexibel ist und daß die Ergebnisse ermutigend sind.

МОДЕЛИРОВАНИЕ НА ЭВМ ДВИЖУЩЕЙСЯ МЕЖФАЗНОЙ ГРАНИЦЫ И ПРОЦЕССОВ ФАЗОВОГО ПРЕВРАЩЕНИЯ ПРИ НАЛИЧИИ КОНВЕКЦИИ

Аннотация—Представлено численное исследование задач фазового превращения с использованием метода конечного объема для формулировки энтальпии. Разработанная математическая модель применяется для расчета неустановившегося режима внутреннего затвердевания в охлажденной трубе с течением при ламинарных числах Рейнольдса. Цель работы—рассчитать образование твердой корки в условиях, когда эффекты диффузии и конвекции являются существенными. Представленные результаты сравниваются с имеющимися данными экспериментальных измерений. Сделаны выводы, что метод является надежным и гибким, а результаты—обнадеживающими.