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A fixed grid numerical methodology for phase change problems involving a moving heat source

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INTRODUCTION

MANY PROBLEMS arise in engineering in which heat transfer is accompanied by melting and solidification (phase change). The situation is particularly common in materials processing, e.g. welding, casting, heat treatment, crystal growth, etc. The work described in this note has been motivated by application to TIG (tungsten inert gas) or GTA (gas tungsten arc) welding processes [1]. The situation is described schematically in Fig. 1. A source of heat (arc) moves laterally over the surface of a plate to be welded. Due to intense heating, the material under the arc melts and, as the arc moves away, the material resolidifies resulting in a welded joint.

In this technical note a fixed grid numerical methodology is presented for solving phase change problems involving a moving heat source. The spirit of the paper is to emphasize only on the methodology and illustrate the procedure via a two-dimensional example; the solution for a complete three-dimensional TIG problem including the flow in the melt due to buoyancy, surface tension and electromagnetic forces, etc. is the subject of a separate paper [2] targeted for the material sciences community.

Viewed in the laboratory coordinates, the arc problem described in Fig. 1 is inherently unsteady. However, if one works with a coordinate system fixed to the arc, then the problem becomes steady, assuming the plate length to be infinite in the direction of arc motion. This note deals with such a steady state problem only; thus the arc and the melt under it are fixed in space while material enters and leaves the computational domain.

THE PROPOSED PHASE CHANGE METHODOLOGY

There are two approaches to solving phase change problems. The classical problem requires tracking of the phase change front by the satisfaction of the Stefan condition. This is often implemented computationally by deforming grid techniques. For steady state problems, this procedure would involve adjusting the grid 'iteratively' until the appropriate interface conditions have been satisfied.

Alternatively, the 'weak' or integral formulation of the Stefan problem leads to enthalpy methods which employ fixed grids. The technique proposed here falls into this second class. An important attribute of this method is its ease of implementation. The scheme has evolved from the recent work of Voller *et al.* [3, 4] and the concurrent work of Voller and Prakash [5].

The basic idea is to represent the total enthalpy as a sum of sensible and latent heats, i.e.

$$\underset{\text{total enthalpy}}{H} = \underset{\text{sensible enthalpy}}{h} + \underset{\text{latent heat}}{\Delta H} \tag{1}$$

where

$$h = c_p T \tag{2}$$

c_p being the specific heat and T the temperature. The latent heat, ΔH, is constrained by the limits

$$0 \leqslant \Delta H \leqslant L \tag{3}$$

where L represents the total latent heat of fusion. Thus, at any point, the value of ΔH has the following physical interpretation:

$$\text{liquid fraction} = \frac{\Delta H}{L} \tag{4}$$

$$\text{solid fraction} = 1 - \frac{\Delta H}{L}. \tag{5}$$

The energy conservation equation for steady situation can be written as

$$\nabla \cdot (\rho \mathbf{u} H) = \nabla \cdot \left(\frac{k}{c_p} \nabla h \right) \tag{6}$$

where ρ represents the density, $\mathbf{u}$ the material velocity and k and c_p are the thermal conductivity and specific heat of the material, respectively. Substituting equation (1) into equa-

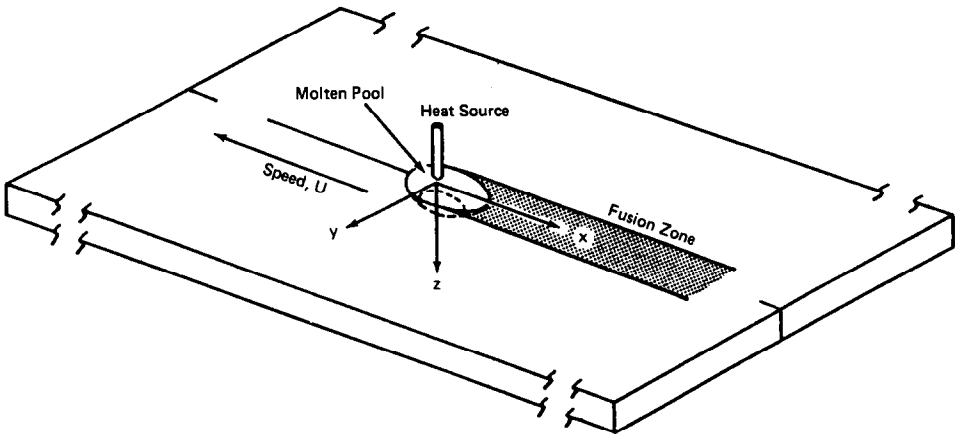

FIG. 1. Schematics of a TIG/GTA welding process.

tion (6) it follows:

$$\nabla\cdot(\rho\mathbf{u}h) = S+\nabla\cdot\left(\frac{k}{c_p}\nabla h\right) \tag{7}$$

where

$$S = -\nabla\cdot(\rho\mathbf{u}\Delta H). \tag{8}$$

Thus, the equation for the sensible enthalpy is the same as that for the no-phase change case, except for the source term S which accounts for the efflux of latent heat.

The discretization of the sensible enthalpy equation may now proceed in any manner as long as proper representation is made of the source term S. A popular methodology, which is quite widely used, is the control-volume finite-difference approach described by Patankar [6] and implemented in such general purpose codes as PHOENICS [7]. In such an approach, the discretization equations are obtained by applying conservation laws over finite size control volumes surrounding the grid nodes. Thus, for a typical two-dimensional control volume surrounding a node P (Fig. 2) what concerns us is the integral

$$\hat{S}_P = \iint_{\substack{\text{control}\\\text{volume}}} S\,dv = -\int_{\substack{\text{control}\\\text{surface}}} \{\rho\mathbf{u}\cdot\hat{n}\Delta H\}\,ds \tag{9}$$

which appears as a source term in the discretization equation for h at node P. This integral may be represented as

$$\hat{S}_P = (\rho u)_w\Delta y(\Delta H)_w + (\rho v)_s\Delta x(\Delta H)_s - (\rho u)_e\Delta y(\Delta H)_e - (\rho v)_n\Delta x(\Delta H)_n \tag{10}$$

where the subscripts w, e, n, s, etc. refer to the west, east, north and south faces of the control volume in Fig. 2. The interface values of (ΔH) can be related to the nodal value of ΔH by using the upwind methodology [6], thus

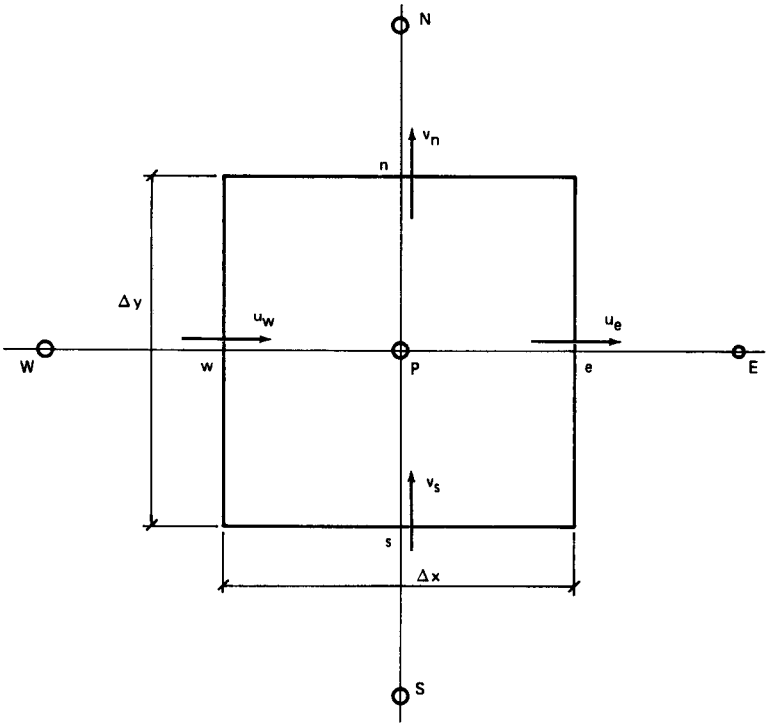

FIG. 2. Control volume around a grid node P.

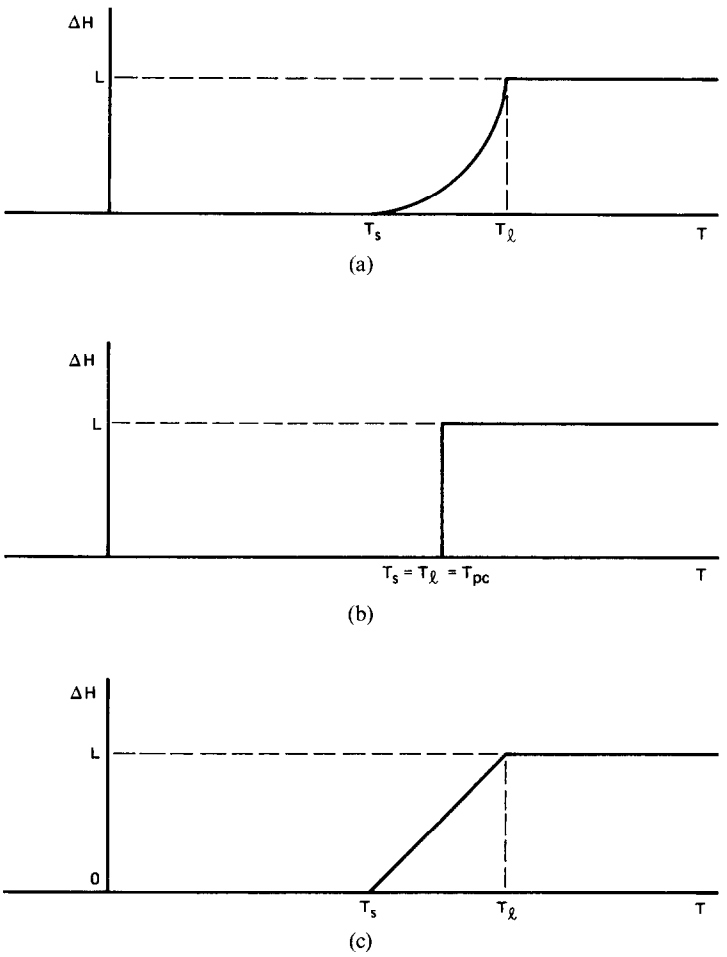

FIG. 3. Phase change processes: (a) general case; (b) isothermal phase change; (c) linear phase change.

$$(\Delta H)_w = (\Delta H)_W \quad \text{if} \quad u_w > 0$$
$$= (\Delta H)_P \quad \text{if} \quad u_w < 0 \tag{11}$$

and likewise for $(\Delta H)_s$, $(\Delta H)_e$, $(\Delta H)_n$, etc.

Given a ΔH field, the equation for h can now be solved. To complete the computational cycle, the next task is to relate ΔH and h through the constitutive equation for the phase change process. As shown in Fig. 3, the general relationship between ΔH and h may be represented by

$$\Delta H = f(h)$$

where

$$\begin{cases} f(h) = 0 & \text{for} \quad h < c_p T_s \\ 0 \leqslant f(h) \leqslant L & \text{for} \quad c_p T_s \leqslant h \leqslant c_p T_l \\ f(h) = L & \text{for} \quad h > c_p T_l. \end{cases} \tag{12}$$

Here T_s and T_l designate the solidus and the liquidus temperatures, respectively. Two special cases of the function f are also shown in Fig. 3 corresponding to an isothermal phase change and a linear phase change. Equation (12) may be appropriately inverted to read

$$h = f^{-1}(\Delta H). \tag{13}$$

The iterative solution for h and ΔH proceeds as follows:

(1) Let ΔH^k represent the ΔH field as it exists at the beginning of the kth iteration.

(2) Using ΔH^k to compute the source term S, solve equation (7) to obtain the sensible enthalpy h^k.

(3) Finally obtain ΔH^{k+1}, the ΔH field for the next iteration, using

$$\Delta H^{k+1} = \Delta H^k + h^k - f^{-1}(\Delta H^k) \tag{14}$$

with the imposed constraint

$$0 \leqslant \Delta H^{k+1} \leqslant L.$$

Once the iterative solution converges, equation (14) assures the satisfaction of the phase change relation (13).

The form of equation (14) for the two most common cases will now be presented.

Isothermal phase change (pure materials)

Isothermal phase change corresponds to phase change at a distinct temperature. Thus

$$T_s = T_l = T_{pc} \tag{15}$$

where T_{pc} defines the phase change temperature.

In the interval $0 \leqslant \Delta H \leqslant L$, h is a single valued function. Thus, from equation (13), $h = f^{-1}(\Delta H) = c_p T_{pc}$. Equation (14) then becomes

$$\Delta H^{k+1} = \Delta H^k + h^k - c_p T_{pc}$$
$$\Delta H^{k+1} = \max\,[0, \Delta H^{k+1}] \tag{16}$$
$$\Delta H^{k+1} = \min\,[L, \Delta H^{k+1}]$$

where max $[a, b]$ means the greater of a and b min $[a, b]$ means the smaller of a and b. The max, min statements are to enforce the constraint $0 \leqslant \Delta H^{k+1} \leqslant L$.

Linear phase change (alloys)

Linear phase change corresponds to the evolution of latent heat, ΔH, as a linear function of the temperature. Define

$$\text{phase change temperature,} \quad T_{pc} = \tfrac{1}{2}(T_s + T_l) \tag{17}$$

and

$$\text{phase change interval,} \quad \varepsilon = \tfrac{1}{2}(T_l - T_s). \tag{18}$$

The function f, equation (12), for the linear phase change case would read

$$\Delta H = f(h) = \frac{L}{2}\left[1 + \frac{1}{\varepsilon c_p}(h - c_p T_{pc})\right] \quad \text{for} \quad c_p T_s \leqslant h \leqslant c_p T_l$$
$$\Delta H = f(h) = 0 \quad \text{for} \quad h < c_p T_s \tag{19}$$
$$\Delta H = f(h) = L \quad \text{for} \quad h > c_p T_l.$$

Hence the equation for iteratively updating ΔH would be

$$\Delta H^{k+1} = \Delta H^k + h^k - \frac{c_p \varepsilon}{L}(2\Delta H^k - L) - c_p T_{pc} \tag{20}$$

$$\Delta H^{k+1} = \max\,[0, \Delta H^{k+1}]$$
$$\Delta H^{k+1} = \min\,[L, \Delta H^{k+1}].$$

Note that the linear case reduces to the isothermal when $\varepsilon = 0$. Hence, though the two cases have been presented separately for ease of understanding, the general linear case includes the isothermal phase change case.

CALCULATION OF THE FLOW FIELD

Phase change problems typically involve three distinct regions with regard to the flow field. These are: (i) the liquid region ($T > T_l$), (ii) the solid region ($T < T_s$), and (iii) the mushy zone ($T_s \leqslant T \leqslant T_l$) which exists between the liquid and the solid. A commonly used procedure for solving for the flow field is to prescribe a fluid viscosity which is equal to the liquid viscosity in the liquid region and which increases gradually over the mushy zone to a large value in the solid. This representation can be used quite conveniently because finite-difference procedures are in place [6, 8] which can properly handle large discontinuities in the diffusion coefficients. The central idea is to use the harmonic averaging of the nodal values of the diffusion coefficients (like viscosity) to compute the diffusional fluxes (like shear forces) at the faces of the control volume.

Another procedure for modeling the flow in the mushy region is to provide suitable sink terms in the momentum equations [3, 4]. Such a Darcy type flow representation, with the Carman–Koseny equation for the porosity [9], has recently been used by Voller and Prakash [5].

Since the focus of the present study is on the development of the numerical methodology for phase change, questions related to the modeling of the mushy region are not emphasized here; the proposed method can be used along with any representation of the mushy region.

APPLICATION OF THE PROCEDURE TO AN EXAMPLE PROBLEM

The proposed methodology has been applied to a two-dimensional example problem shown schematically in Fig. 4. The set of boundary conditions is also shown in Fig. 4. The heat source is at rest while material enters and leaves the computational domain. Only the buoyancy force has been considered in the melt, and the usual Boussinesq approximation is made. Phase change is assumed to occur linearly over a temperature range. The fluid viscosity is assumed to be equal to the liquid viscosity for $T > T_{pc}$ while it is taken to be a large value for $T < T_{pc}$. The standard Navier–Stokes equations apply for the flow in the melt. These equations were solved using the control-volume finite-difference approach of Patankar [6] with harmonic averaging of diffusion coefficient practice [8]. The velocity pressure coupling is handled using variants of the SIMPLE algorithm [6]. The example case corresponds to the following values of the dimensionless variables:

$$\frac{a}{t} = 0.2$$

$$Re = \rho \frac{u_{in}}{\mu} t = 100$$

$$Pr = \frac{\mu c_p}{k} = 0.01$$

$$Gr = g\beta \frac{(T_{pc} - T_{in})}{\nu^2} t^3 = 10^6$$

$$E = \frac{\varepsilon}{(T_{pc} - T_{in})} = 0.1$$

$$Ste = \frac{c_p (T_{pc} - T_{in})}{L} = 1$$

$$Q = \frac{q}{\rho c_p u_{in} (T_{pc} - T_{in})} = 20.$$

A 40×20 grid was used in the x–y plane. The grid was fine under the heat source and gradually expanded in the x-direction; the domain extended from $x/t = -7.9$ to 7.9. In the y-direction, the grid was uniform. The solution took about 40 iterations for the variables to converge up to four significant digits. Each of these iterations involved a cycle of the SIMPLE algorithm and the updating of the h and ΔH fields. No underrelaxation was found necessary for h or ΔH which reflects good stability of the proposed method.

Results of calculations are presented in Fig. 5. Attention is focused on a magnified portion of the computational domain under the source. The vectors represent the direction and magnitude of the velocity (normalized by u_{in}) while the con-

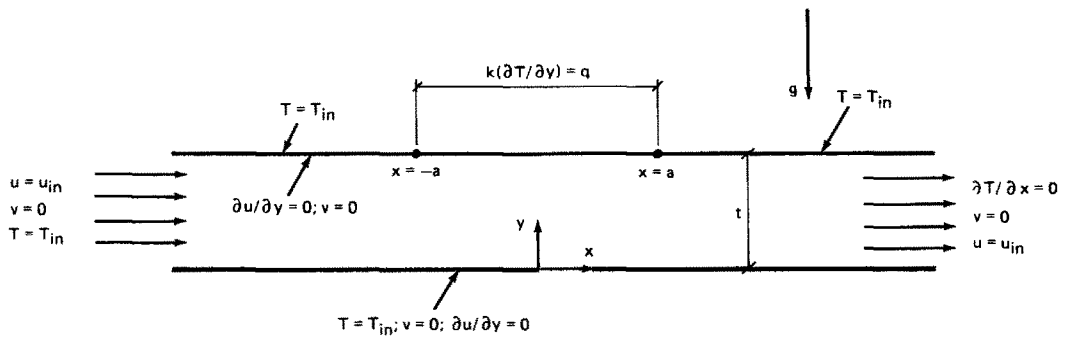

FIG. 4. Schematics and boundary conditions for the example problem.

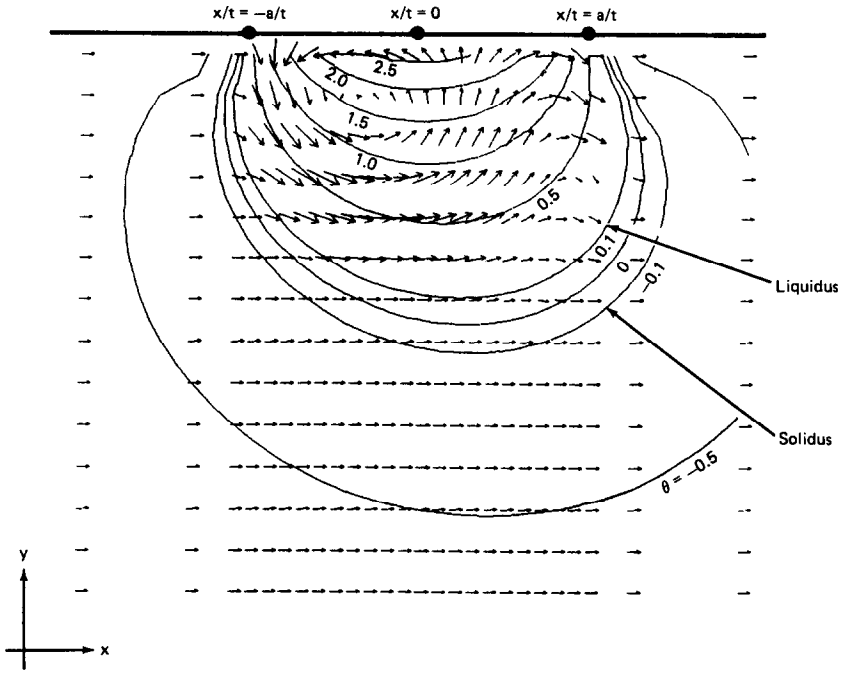

FIG. 5. Results for the example problem. Arrows correspond to the velocity vectors ($\mathbf{u}/u_{in}$) and contours are isotherms of $\theta = (T-T_{pc})/(T_{pc}-T_{in})$.

tours are isotherms of $(T-T_{pc})/(T_{pc}-T_{in})$. Thus the contours marked 0.1 and -0.1 correspond to the liquidus and solidus lines, respectively. As expected, buoyancy gives rise to an upward flow under the heat source and downward flow away from it.

CONCLUDING REMARKS

A numerical method is presented for the solution of phase change problems involving a moving heat source. The procedure works on a fixed grid and does not require the implementation of the Stefan condition at the solid–liquid interface. Hence, the procedure is easy to implement on fixed grid codes like PHOENICS. To illustrate the procedure, a two-dimensional problem involving natural convection flow in the melt is analyzed.

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