

## ACCURATE SOLUTIONS OF MOVING BOUNDARY PROBLEMS USING THE ENTHALPY METHOD

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**Abstract** — After highlighting the problems associated with the conventional numerical implementations of Stefan problems using the enthalpy formulation, a simple development is described which leads to very accurate solutions. The extension of this technique to two dimensional problems is then demonstrated using a straightforward explicit method.

An implicit scheme for one dimensional problems, based upon the above development, is then described which can cope with any size phase change temperature range and the influence of internal heating, simultaneously. Finally, the utility of this scheme is demonstrated by its application to a welding problem.

### NOMENCLATURE

$C$ ,	specific heat;
$C_l$ ,	liquid specific heat;
$C_s$ ,	solid specific heat;
$H$ ,	enthalpy;
$J$ ,	Jacobian matrix;
$J_{ik}$ ,	Jacobian matrix elements;
$K$ ,	thermal conductivity;
$K_l$ ,	liquid thermal conductivity;
$K_s$ ,	solid thermal conductivity;
$L$ ,	latent heat of solidification;
$S$ ,	fraction of element which is solid;
$T$ ,	temperature;
$T_2$ ,	initial temperature of region;
$T_m$ ,	melting temperature;
$T_l$ ,	liquid temperature;
$T_s$ ,	solid temperature;
$X(t)$ ,	boundary between liquid–solid phases;
$\varepsilon$ ,	half phase change temperature interval;
$\kappa$ ,	thermal diffusivity;
$\kappa_l$ ,	liquid thermal diffusivity;
$\kappa_s$ ,	solid thermal diffusivity;
$\theta$ ,	weight in finite difference scheme;
$\lambda$ ,	constant;
$\omega$ ,	relaxation factor;
$\omega^*$ ,	relaxation factor;
$\phi$ ,	body heating term;
$\rho$ ,	density of region.

### 1. INTRODUCTION

HEAT flow and diffusion involving phase change occurs in many physical systems. Since there are relatively few analytical solutions [1, 2\*] to these so-called Stefan problems a large number of numerical techniques have been developed [2, 3], especially over the last 15 years. For problems involving a phase

change at a specified temperature, the continuously moving phase change boundary has to be tracked accurately throughout a region approximated by a finite number of points. A great many methods have been developed to overcome this difficulty [2, 3], including moving grid points and isotherm migration. Recently, Goodrich [4] has published a very accurate method for these kinds of problems in one-dimension. However, to obtain reasonable results all the above methods require starting solutions, some of which are complicated [5].

In many industrial problems the phase change occurs over a temperature range rather than at a specified temperature. For these problems, the single point phase change schemes are inapplicable and none appear to have been published which track the upper and lower boundaries of the phase change region. In fact, problems involving phase change over a temperature range usually employ so-called enthalpy methods which are based upon the method of weak solutions [6–9]. These methods appear to have great flexibility and are easily extended to multi dimensional problems [7, 10]. Although, stable solutions may be obtained from enthalpy methods when the phase change takes place over a temperature range [6, 7], this is not so if the range becomes relatively small or degenerates to a single temperature [11]. In such cases, two non-physical features are introduced [11], (i) the phase change boundary moves in an oscillatory fashion, and (ii) the temperature history of any point within the region contains, in addition to the physical temperature plateau at the phase change, a number of rogue plateaux.

Meyer [7] has developed an enthalpy method which claims to be essentially independent of the phase change temperature range and, thus, suitable for problems where the phase change occurs at a single temperature. Although this proved to be true for his example [7], it is by no means universally so [11]. As such, it would appear that at the present time enthalpy

\* This monograph [2] contains an excellent review of most of the relevant analytical and numerical techniques.

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methods cannot be generally used for Stefan problems involving a phase change at a specified temperature. This means, of course, there is no method which is general enough to cope accurately with problems where the phase change region either degenerates to a single plane or grows.

The objective of this work is to show how results from the basic explicit numerical implementation of the enthalpy method can be reinterpreted to provide, at least for one dimensional problems, accurate evaluations of the boundary movement and the temperature history of any point within the region of interest. This interpretation is made in such a way that problems with phase change either at a point or across a temperature range can be solved with equal ease. The successful extension of this scheme to two-dimensions is also demonstrated and some factors which limit its application to all such problems are highlighted.

The simple one-dimensional scheme is then used to provide the basis for the development of a comprehensive implicit numerical scheme which requires no starting solution and is able to cope with any size phase change range plus the influence of internal heating sources or sinks.

2. BACKGROUND

2.1. The Stefan problem

The classical problem of heat flow involving a change of state, is the one-dimensional freezing problem first posed by Stefan in 1889 [1]. A material which can exist in two phases (liquid and solid) fills the half space  $x \geq 0$ . For times  $t \leq 0$  the material is in the liquid phase at a constant temperature  $T(x, 0) = T_2 > T_m$ , where  $T_m$  is the phase change temperature. At time  $t = 0$  the temperature of the surface  $x = 0$  is instantaneously lowered and maintained at  $T(0, t) = T_1 < T_m$ . This will cause a layer of solid to be formed adjacent to the surface  $x = 0$  and as time increases this layer will expand into the liquid. Assuming that the heat transfer is only due to conduction the problem can be described by a pair of Fourier heat conduction equations; one for the solid,

$$\frac{\partial}{\partial x} \left( K_s \frac{\partial T_s}{\partial x} \right) = \rho C_s \frac{\partial T_s}{\partial t}, \quad 0 \leq x < X(t) \tag{2.1a}$$

and the other for the liquid

$$\frac{\partial}{\partial x} \left( K_l \frac{\partial T_l}{\partial x} \right) = \rho C_l \frac{\partial T_l}{\partial t}, \quad X(t) \leq x, \tag{2.1b}$$

where the subscripts  $s$  and  $l$  refer to the solid and liquid phases respectively. At the phase change boundary, (i.e. the solid-liquid interface) the following conditions hold:

$$T_l = T_s = T_m \tag{2.2}$$

and

$$K_s \frac{\partial T_s}{\partial x} \Big|_{x=X(t)} - K_l \frac{\partial T_l}{\partial x} \Big|_{x=X(t)} = \rho_s L \frac{dX(t)}{dt} \tag{2.3}$$

where  $L$  is the latent heat released on solidification. Equation (2.3) is known as the Stefan condition and represents the heat balance across the phase change boundary  $x = X(t)$ . The Stefan problem is to follow the solid/liquid interface  $x = X(t)$  as it moves through the liquid. The analytic solution of this one-dimensional Stefan freezing problem is well known and given by [1]

$$X(t) = 2\lambda (\kappa_s t)^{1/2} \tag{2.4}$$

where  $\kappa_s = K_s/\rho_s C_s$  and  $\lambda$  is a constant which may be evaluated from the following equation

$$\frac{e^{-\lambda^2}}{\text{erf } \lambda} - \frac{K_l}{K_s} \frac{\kappa_s^{1/2} [T(x, 0) - T_m] e^{-\kappa_s \lambda^2}}{\kappa_l^{1/2} [T_m - T(0, t)] \text{erfc}[\lambda(\kappa_s/\kappa_l)^{1/2}]} = \frac{\lambda L \pi^{1/2}}{C_s [T_m - T(0, t)]} \tag{2.5}$$

The temperature at any point is then

$$T = \begin{cases} \frac{T_m - T(0, t)}{\text{erf } \lambda} \text{erf} \left( \frac{x}{2(\kappa_s t)^{1/2}} \right) + T(0, t), & x < X(t) \\ T_m & x = X(t) \\ T(x, 0) - \frac{[T(x, 0) - T_m]}{\text{erfc}[\lambda(\kappa_s/\kappa_l)^{1/2}]} \text{erfc} \left( \frac{x}{2(\kappa_l t)^{1/2}} \right), & x > X(t). \end{cases} \tag{2.6}$$

Throughout this work the one-dimensional freezing problem defined by equations (2.1)–(2.3) will be used as the main test problem, together with the data in S.I. units applied by Goodrich [4]:

$$\begin{aligned} T_m &= 0; \quad T(\infty, t) = 2; \quad T(x, 0) = 2(x \geq 0); \\ T(0, t) &= -4 \quad \text{or} \quad -10; \quad K_s = K_l = 2; \tag{2.7} \\ C_s = C_l &= 2.5 \cdot 10^6; \quad \rho_l = \rho_s = 1; \quad L = 100 \cdot 10^6. \end{aligned}$$

The temperature history of a point 25 cm from the surface is shown in Fig. 1. The characteristic ‘‘knee’’ as the temperature passes through the phase change point is clearly shown.

2.2. The enthalpy method

The class of Stefan problems for which analytic solutions exist is small [1, 2]. Numerical schemes based on the equations (2.1)–(2.3) require the phase change boundary,  $x = X(t)$ , to be accurately traced. This necessity renders a large proportion of the available numerical schemes difficult to implement. One way to overcome this problem is to reformulate

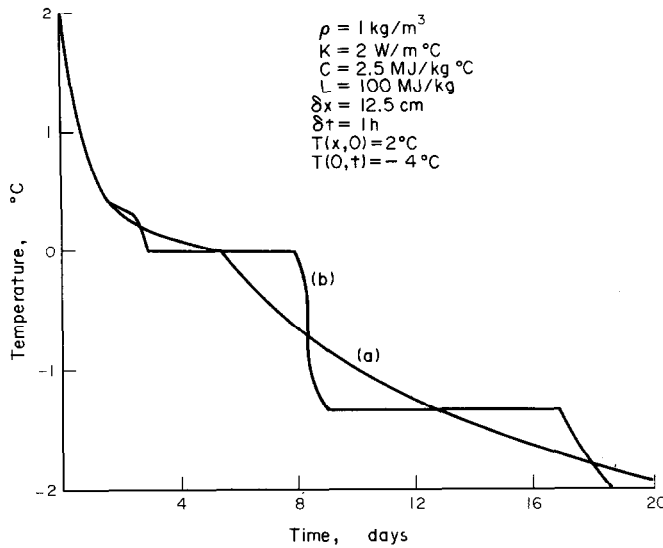


FIG. 1. Comparison of analytic [curve (a)] and enthalpy [curve (b)] solutions for the temperature history at  $z = 25$  cm.

the equation in terms of the enthalpy  $H$  [6–9], the sum of sensible and latent heats. In this case, the Stefan equations reduce to a single equation

$$\frac{\partial}{\partial x} \left( K \frac{\partial T}{\partial x} \right) = \rho \frac{\partial H}{\partial t}, \quad x \geq 0 \quad (2.8)$$

where the conductivity  $K$  and density  $\rho$  are functions of temperature and the temperature is related to the enthalpy via

$$T = \begin{cases} H/C, & H \leq CT_m \\ T_m, & CT_m \leq H \leq CT_m + L \\ (H - L)/C, & H > CT_m + L. \end{cases} \quad (2.9)$$

Equivalently equation (2.9) can be written as [9]

$$H(T) = \begin{cases} CT & T < T_m \\ CT + L, & T > T_m. \end{cases} \quad (2.9a)$$

The advantages of this approach are:

- (i) there are no conditions to be satisfied at  $x = X(t)$ , the phase change boundary;
- (ii) there is no need to accurately track the phase change boundary;
- (iii) there is no need to consider the regions on either side of  $x = X(t)$  separately, and
- (iv) it is easy to introduce a “mushy” region, i.e. where the phase change occurs over a temperature range rather than at a single point.

The explicit finite difference representation of enthalpy formulation is very straightforward [8, 9]

$$H_i^{t+1} = H_i^t + \frac{K}{\rho} \eta (T_{i+1}^t - 2T_i^t + T_{i-1}^t) \quad (2.10)$$

which when combined with equation (2.9) provides a simple algorithm to calculate the temperature history

of a one-dimensional region. Further, the condition needed to ensure convergence is simply

$$\eta = \frac{\delta t}{\delta x^2} < \frac{\rho C}{2K}.$$

The test problem described in Section 2.1 has been solved using the above approach. When  $\delta t = 3600$  s and  $\delta x = 12.5$  cm, the predicted temperature history for  $x = 25$  cm is shown as curve (b) in Fig. 1. Clearly the results of this method are inaccurate. The reason for the behaviour in the predicted temperature history curves has been fully examined elsewhere [11].

In many physical problems the phase change takes place over a temperature range rather than at a single value. In this case the enthalpy  $H(t)$  of equation (2.9a) is replaced by a smooth continuous function [6] or a piecewise continuous function [7], e.g.

$$H(T) = \begin{cases} CT & T \leq T_m - \varepsilon \\ H(T_m - \varepsilon) + L(T - T_m + \varepsilon)/2\varepsilon & T_m - \varepsilon < T < T_m + \varepsilon \\ H(T_m + \varepsilon) + C(T - T_m - \varepsilon) & T_m + \varepsilon \leq T \end{cases} \quad (2.11)$$

where  $\varepsilon$  is the half temperature range of phase change. It has been shown [11] that when  $H(t)$  is defined in this way smooth (i.e. non-oscillatory) temperatures histories will only be predicted when at least two nodal temperatures lie in the phase change range at all time steps. As such, the efficacy of the scheme is critically dependent upon the size of  $\varepsilon$  for any problem. This conclusion is in direct conflict with Meyer’s [7] assertion that this scheme is essentially independent of  $\varepsilon$ .

3. A NEW INTERPRETATION OF THE ENTHALPY METHOD

3.1. Interpretation of the enthalpy

Comparing the two curves in Fig. 1 it may be observed that the curve predicted by the explicit scheme of the enthalpy method oscillates about the true solution. If the points of agreement of these two curves could be predicted, then an accurate algorithm for the classical Stefan problem may be devised. As a first step towards obtaining such an algorithm, the enthalpy in a discretized region, which is being frozen, needs to be interpreted. Let  $i$  be a node point in such a discretized region and let  $e_i$  be the element associated with that node point. The total heat in the element  $e_i$  at any time is approximated as  $H_i \delta x$  where  $H_i$  is the nodal enthalpy and  $\delta x$  is the length of the element (cf. Fig. 2). If at time  $t$  the freezing front is in element  $e_i$  and moving towards element  $e_{i+1}$  the total heat in the element may be approximated as the sum of the heat in the solid and liquid parts of the elements, that is

$$H_i \delta x = \{CT_i S + (CT_i + L)(1 - S)\} \delta x \quad (3.1)$$

where  $S$  is the fraction of the element which is solid. When the freezing front reaches the node  $i$  then  $S = \frac{1}{2}$ ,  $T_i = T_m$  and equation (3.1) yields

$$H_i = CT_m + L/2. \quad (3.2)$$

Hence whenever the nodal enthalpy  $H_i$  in a discretized region, is the sum of the sensible heat of the phase change and half the latent heat associated with the phase change, the phase change boundary should be approximately on the node  $i$ . In essence any element can be thought of as a bucket of "volume"  $L$  which is filled (thawing) or emptied (freezing) as the phase change boundary moves through it.

3.2. A new algorithm

From the interpretation of the enthalpy given above, the following algorithm for solution of Stefan problems is proposed. The enthalpy and a "working" temperature is calculated at each time step from the explicit finite difference scheme (2.10) and equation (2.9).

Whenever the enthalpy at a node point is such that

at time level  $j + 1$ ,  $H_i^j > CT_m + L/2$  and  $H_i^{j+1} < CT_m + L/2$  (for a freezing problem) the phase change boundary has passed through the point  $i \delta x$  in the preceding time interval  $\delta t$ . Furthermore, assuming that the enthalpy changes linearly in any time interval the time at which the phase change is on the point  $i \delta x$  (i.e. when  $H_i = L/2 + CT_m$ ), is given by

$$t_i = (j + X) \delta t \quad (3.3)$$

where  $X < 1$  is estimated via linear interpolation, in time, viz.

$$X = \frac{(L/2 + CT_m - H_i^j)}{(H_i^{j+1} - H_i^j)} \quad (3.4)$$

At time  $t_i$  the temperature at node  $i$  is  $T_m$ . The temperature at the other node points are easily estimated by using a linear interpolation i.e.

$$T_k^{i+X} = X(T_k^{i+1} - T_k^i) + T_k, \quad (k \neq i). \quad (3.5)$$

In a case where the thermal properties differ between the solid and liquid the algorithm is modified by using the following finite difference scheme

$$H_i^{j+1} = H_i^j + \rho \frac{\delta t}{\delta x^2} \{K_{i-1}(T_{i-1}^j - T_i^j) - K_{i+1}(T_i^j - T_{i+1}^j)\} \quad (3.6)$$

in place of equation (2.10).

The test problem (2.7) has been solved with  $T(0, t) = -10^\circ\text{C}$  using an  $x$ -step of 12.5 cm and a time step of 1 h. Figure 3(a) compares the analytic movement of the boundary  $X(t)$  with that predicted by the algorithm, over 1200 time steps. Away from the freezing plane  $x = 0$  the relative error between the predicted and analytic results is of order 0.1%. This error is compatible with the error found in a typical finite difference solution of a heat conduction problem involving no phase change. The predicted temperature history for  $x = 50$  cm is compared with the analytic history in Fig. 3(b). The predicted history is never more than  $0.1^\circ\text{C}$  away from the true history. Similar results are shown for a problem with differing thermal properties between the solid and the liquid phases, in Figs. 4(a) and 4(b). Once again the predicted results are accurate. Hence the results given by the explicit finite difference

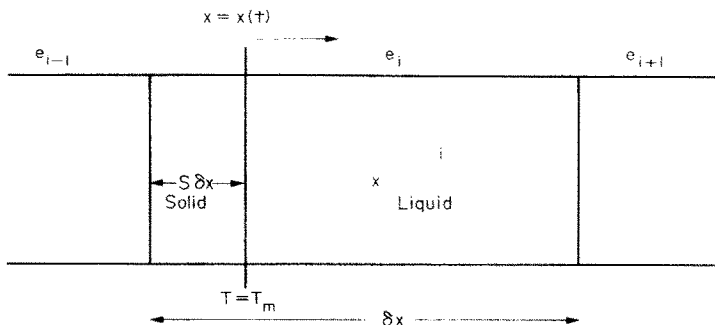


FIG. 2. The element  $e_i$ .

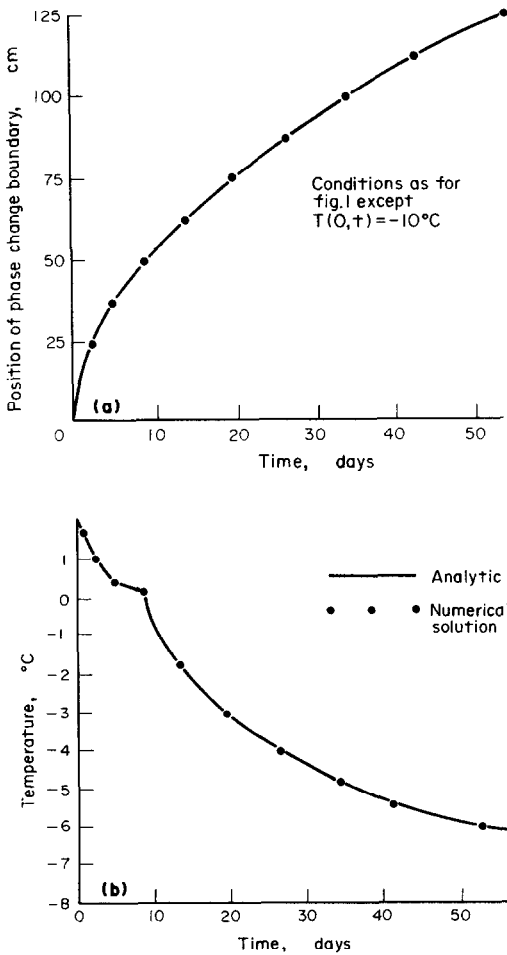


FIG. 3. Comparison of analytic and explicit enthalpy solutions for phase change at a single temperature with constant thermal properties, showing (a) the movement of the boundary, with time and (b) the temperature history at 50 cm.

scheme [equations (2.10) and (3.6)] may be reinterpreted to give accurate solutions for freezing–thawing problems in one-dimension.

Furthermore, smooth predictions may also be made of the movement of the liquidus and solidus boundaries for problems where the phase change occurs over a temperature range. The test problem was run using a phase change temperature range of 1°C and the movement of the boundaries is plotted in Fig. 5. Notice that the 0°C isotherm is nearest to the -5°C isotherm and is to be expected since the heat flow rates are steeper on the solid side of the phase change for the last problem.

3.3. A two-dimensional problem

With modifications to the above scheme accurate predictions for movement of the freezing plane in some two-dimensional problems can be made. One such problem is examined below.

In two-dimensions the enthalpy formulation for a problem with constant thermal properties becomes

$$\frac{\partial}{\partial x} \left( K \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( K \frac{\partial T}{\partial y} \right) = \rho \frac{\partial H}{\partial t} \quad (3.7)$$

combined with equation (2.9). The “working” temperature for the algorithm may be calculated by the explicit finite difference scheme

$$H_{i,k}^{j+1} = H_{i,k}^j + \lambda_x R (T_{i-1,k}^j - 2T_{i,k}^j + T_{i+1,k}^j) + \lambda_y R (T_{i,k-1}^j - 2T_{i,k}^j + T_{i,k+1}^j) \quad (3.8)$$

where  $\lambda_x = \delta t / (\delta x)^2$ ,  $\lambda_y = \delta t / (\delta y)^2$  and  $R = k / \rho C$ . In a freezing problem the phase change boundary is placed at the grid point (i, k) in the usual way [equations (3.3) and (3.4)] whenever  $H_{i,k}^{j+1} < L/2 + CT_m$  where  $H_{i,k}^j > L/2 + CT_m$ . The current method employed to find the temperature history of a point 0 is of an ad-hoc nature and is outlined below. The phase change front is plotted along a line parallel to one of the coordinate directions and whenever the phase change falls on a node on this line the temperature at point 0 is noted.

The two-dimensional enthalpy algorithm has been

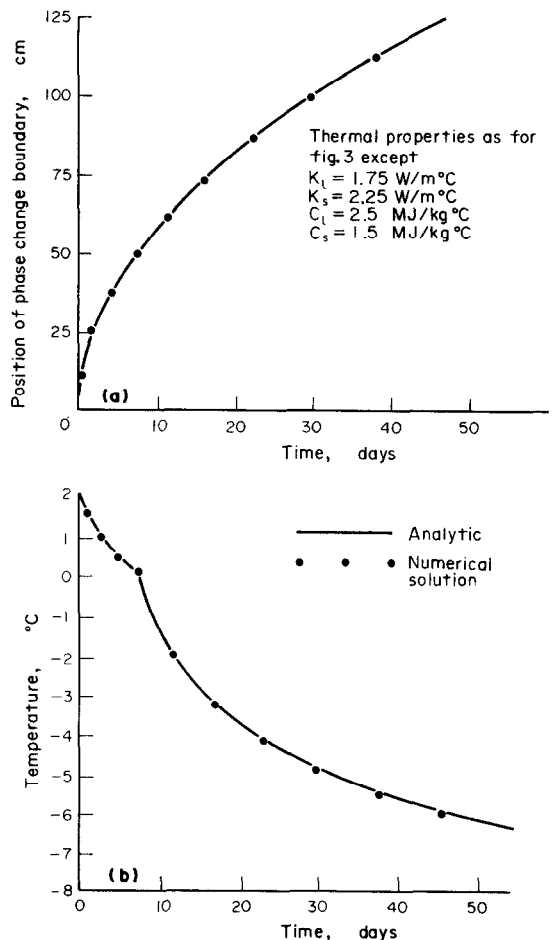


FIG. 4. Comparison of analytic and explicit enthalpy solutions for phase change at a single temperature with non-constant thermal properties showing (a) the movement of the boundary, with time and (b) the temperature history at 50 cm.

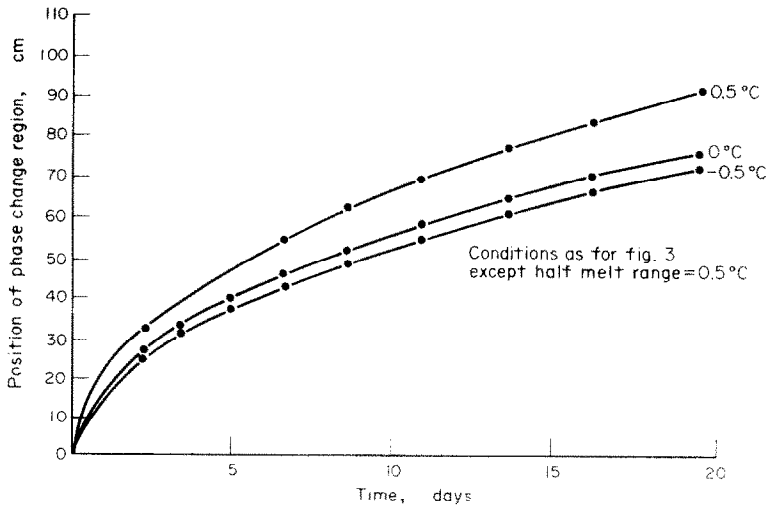


FIG. 5. Movement of mushy region with time.

used to solve a problem similar to that treated by Crowley [10] involving freezing in a square channel. However, it should be noted that the initial temperature in this problem is greater than the phase change temperature. In the problem devised by Crowley [10] the initial temperature was assumed equal to the phase change temperature, a feature which considerably simplifies the numerical problems [11]. An infinitely long square channel is filled with liquid at 2°C. At time  $t = 0$  the temperature on the walls of the channel is lowered and held fixed at  $-10^\circ\text{C}$ . The cross sectional area of the channel is  $1\text{ m}^2$  and the thermal properties of the liquid are as in the test problem. The predictions of the two-dimensional algorithm with  $\delta x = \delta y = 10\text{ cm}$  and  $\delta t = 1\text{ h}$  are illustrated in Fig. 6. The progression of the freezing point with time is shown in Fig. 6(a) whilst Fig. 6(b) plots the movement of the  $x$ -coordinate of the freezing front. From Fig. 6(b) it is observed that the rate of advance of the freezing front increases near the centre of the channel, when there is less liquid to freeze. The predicted temperature history of the grid point (1, 3) [i.e. point 0 in Fig. 5(a)] is plotted in Fig. 6(c) and exhibits the features expected in a temperature history. This temperature history is found by following the freezing front along the line  $x = \delta x$ .

#### 4. AN IMPLICIT ALGORITHM

##### 4.1. The basis of an implicit algorithm

The draw back to the algorithms outlined in Section 3 is that the position of the freezing front and the temperature of a grid point can only be calculated at specific time steps. In this section an algorithm is described that calculates the freezing front at every time step. The objective of the algorithm is to choose a time step  $\delta t$  such that the phase change boundary moves one and only one grid point for each choice of  $\delta t$ , i.e. force the phase change boundary to move from

node to node on successive time steps.

The method of choosing a time step has also been used in conjunction with the full Stefan formulation for one phase problems by Douglas and Gallie [12]. Using this approach (i) the position of the phase change will be known at each time step, and (ii) the nodal temperature distribution will be correct at each time step. With these constraints problems which include temperature dependent function, e.g. body heating terms, can be solved. In order to satisfy the above constraints an implicit scheme for the solution of the enthalpy equation is required. In the next section the general form of the explicit scheme devised by Longworth [13] is outlined.

##### 4.2. An implicit scheme for solution of the enthalpy equations [13]

When equation (2.9) is written as

$$T = F^*(H) \quad (4.1)$$

a finite difference representation of the enthalpy equation (2.8) is

$$\mathbf{H}^{j+1} = \mathbf{H}^j + \delta t(1 - \theta)\mathbf{F}(\mathbf{H}^j) + \theta\delta t\mathbf{F}(\mathbf{H}^{j+1}) \quad (4.2)$$

where  $0 \leq \theta \leq 1$ ,  $\mathbf{H}$  is a vector whose components are the nodal enthalpies  $H_i$  and  $\mathbf{F}$  is a non-linear function with  $i$ th component

$$F_i(\mathbf{H}) = K/(\rho\delta x^2)[F^*(H_{i-1}) - 2F^*(H_i) + F^*(H_{i+1})]. \quad (4.3)$$

If  $\theta \geq \frac{1}{2}$  then equation (4.2) is unconditionally valid [14] and defined an implicit scheme for solution of the enthalpy equation. When  $\theta = \frac{1}{2}$  then equation (4.2) is the Crank-Nicolson type scheme proposed by Longworth [13], this is the scheme used in this paper.

As equation (4.2) is non-linear an iterative method is required to solve for  $\mathbf{H}^{j+1}$  and when  $\theta = \frac{1}{2}$  a non-linear successive over relaxation method may be used [13, 15]. An initial estimate for  $\mathbf{H}^{j+1}$  is given by

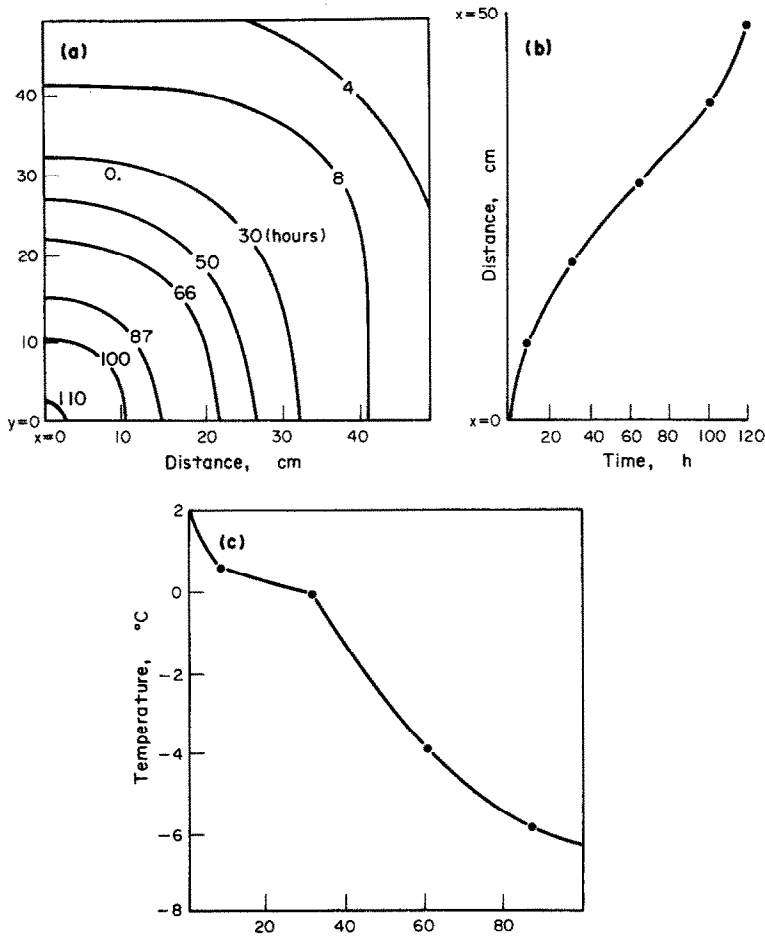


FIG. 6. Results of two-dimensional problem, showing: (a) movement of the freezing front with time, (b) movement of the freezing front along the x-axis and (c) the temperature history of point 0 ( $x = 10, y = 30$ ).

$$\mathbf{H}_0^{j+1} = \mathbf{H}^j + \delta t \mathbf{F}(\mathbf{H}^j). \tag{4.4}$$

This is improved upon by a sequence of corrections with components [13]

$$(\mathbf{c}_m)_i = \frac{\omega \{ \mathbf{H}^j + \frac{1}{2} \delta t \mathbf{F}(\mathbf{H}^j) - \mathbf{H}_m^{j+1} + \frac{1}{2} \delta t \mathbf{F}(\mathbf{H}_m^{j+1}) \}_i}{(1 - J_{ii})} \tag{4.5}$$

where  $\omega$  is the relaxation factor, the  $m$ th estimate of the enthalpy at time level  $(j + 1)$  is

$$\mathbf{H}_m^{j+1} = \mathbf{H}_0^{j+1} + \sum_{i=0}^{m-1} \mathbf{c}_i, \tag{4.6}$$

and  $J$  is the Jacobian matrix with components given by

$$J_{ik} = \frac{\delta t}{2} \frac{\partial F_i}{\partial H_k} \Big|_{\mathbf{H} = \mathbf{H}_m^{j+1}}. \tag{4.7}$$

A more detailed description of the above method can be found in reference 13.

In a physical problem the region of interest may contain body heating and if the material contains impurities the phase change may take place over a temperature range. In such an example, the enthalpy equation becomes [8]

$$\rho \frac{\partial H}{\partial t} = \frac{\partial}{\partial x} \left( K \frac{\partial T}{\partial x} \right) + \phi(T) \tag{4.8}$$

where  $\phi(T)$  is a body heating term. The finite difference approximation of equation (4.8) is as before, i.e. equation (4.3) except that

$$F_i(\mathbf{H}) = K/(\rho \delta x^2) \cdot [F^*(H_{i-1}) - 2F^*(H_i) + F^*(H_{i+1})] + \frac{1}{\rho} \phi[F^*(H_i)] \tag{4.9}$$

where

$$F^*(H) = \begin{cases} H/C & H < C(T_m - \varepsilon) \\ [H + L/2\varepsilon(T_m - \varepsilon)]/(C + L/2\varepsilon) & C(T_m - \varepsilon) \leq H \leq C(T_m + \varepsilon) + L \\ (H - L)/C & H > C(T_m + \varepsilon) + L \end{cases} \tag{4.10}$$

which is the inverse of equation (2.11) and  $\varepsilon$  is half the phase change range. With the equations (4.9) and (4.10) the solution may proceed as above.

4.3. The algorithm

The essential feature of the algorithm proposed above (Section 4.1) is to ensure that at each time step one and only one nodal enthalpy takes the value  $(CT_m + L/2)$ .

The algorithm is implemented in the following way. Assuming that at time  $t$  the phase change boundary is at node  $k$ , an initial guess for the time step  $\delta t_k$  is

$$\delta t_k^0 = \delta t_{k-1}. \tag{4.11}$$

The enthalpy distribution  $H^{t+\delta t_k^m}$  is found on solution of equations (4.4)–(4.7) where the  $m$ th time step is calculated from an iterative scheme e.g.

$$\delta t_k^{m+1} = \delta t_k^m + \omega^*(\delta c^m - \delta t_k^m) \tag{4.12}$$

$$\delta c^m = \delta t_k^m [H^{t+\delta t_k^m} / (CT_m + L/2)]$$

where  $\omega^*$  is the relaxation factor. When  $H_{k+1}^{t+\delta t_k^m}$  has converged to  $L/2 + CT_m$  the temperature distribution is found from equation (4.1).

The test freezing problems have been solved using the above methods with  $T(0, t) = -10^\circ\text{C}$  and  $\delta x = 12.5$  cm. The results for the problem with constant thermal properties are shown in Fig. 7.

The predicted position of the boundary is always within 0.5 cm of the analytic position whilst the predicted temperature history of  $x = 50$  cm is accurate within  $0.1^\circ\text{C}$ . Similar results have been obtained for the problem with differing thermal properties across the phase change, cf. Fig. 8. Hence the implicit node jumping solution of the Stefan problem is stable and accurate. Furthermore only 8 time steps are used to move the phase change 1 m ( $t = 36$  days). In the explicit algorithm Section 3 around 1000 time steps would have been required, whilst the method derived by Goodrich [4] uses 36 time steps.

4.4. A welding problem

The spot welding problem examined by Atthey [8], can be slightly modified to include all the features highlighted above that are associated with physical problems, i.e. body heating and phase change range.

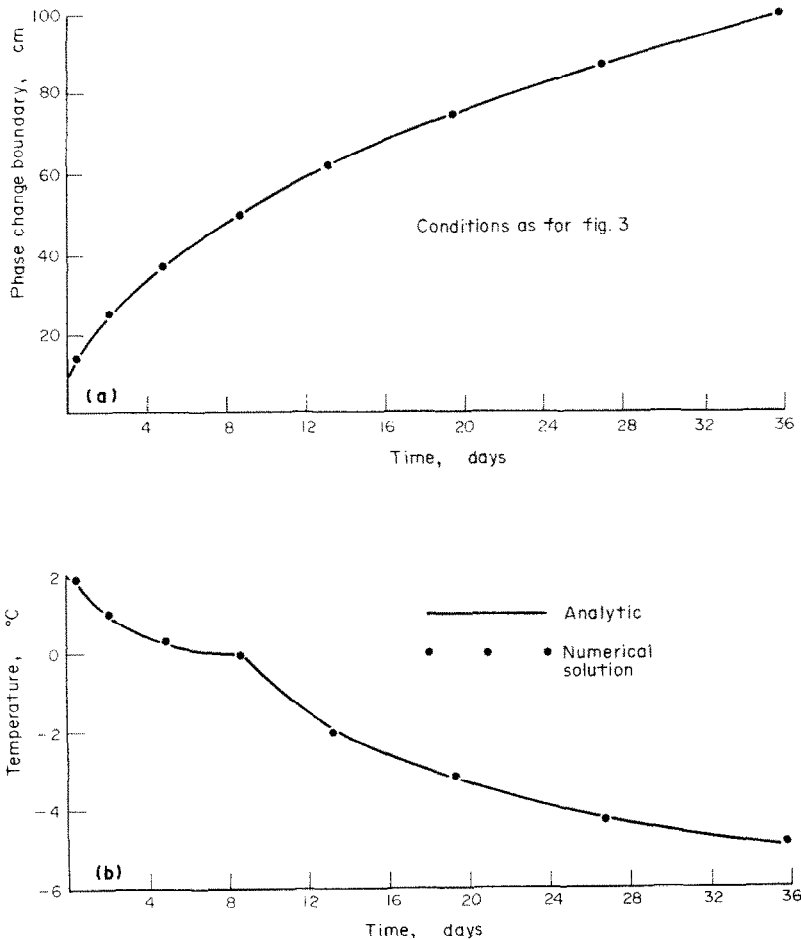


FIG. 7. Comparison of analytic and implicit enthalpy solutions for phase change at a single temperature with constant thermal properties, showing (a) the movement of the boundary with time and (b) the temperature at 50 cm.



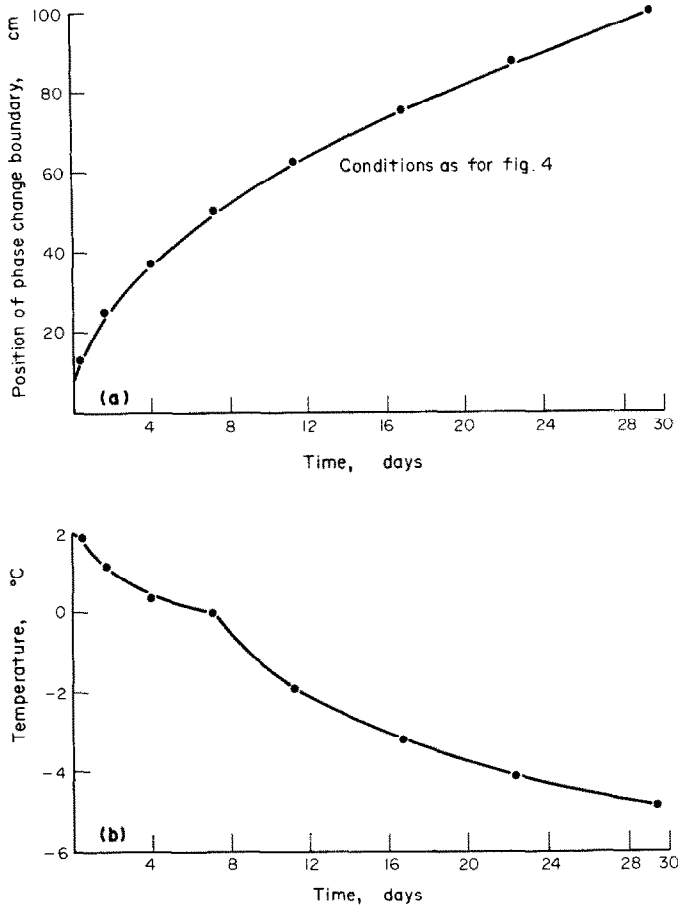


FIG. 8. Comparison of analytic and implicit enthalpy solutions for phase change at single point with non-constant thermal properties showing (a) the movement of the boundary with time and (b) the temperature at  $x = 50$  cm.

Two large plates of steel of thickness  $l$  ( $2.2 \times 10^{-3}$  m) are contained between  $x = 0$  and  $x = 2l$ . At time  $t = 0$  a body heating term defined by the piecewise continuous function

$$\phi(T) = \begin{cases} (19T/48 + 50)10^8 & T < 800 \\ [(T - 800)/16 + 1100/3]10^8 & T > 800 \end{cases} \quad [\text{W/m}^3] \quad (4.13)$$

is introduced between  $x = 0$  and  $2l$ . By symmetry only the top plate need be considered. This plate is subject to the conditions

$$\begin{aligned} dT/dx &= 0 & \text{at } x &= l \\ dT/dx &= T/2 & \text{at } x &= 0 \\ T &= 0 & \text{at } t &= 0. \end{aligned} \quad (4.14)$$

The thermal properties of steel may be summarised as specific heat  $C = 620$  J/kg °C conductivity  $K = 24$  W/m °C, density  $\rho = 7800$  kg/m<sup>3</sup> latent heat of melt  $L = 271 \cdot 10^3$  J/kg melt-temperature  $T_m = 1530$ °C and melt range  $2\varepsilon = 20$ °C. The chosen melt range is quite typical for steel. From equation (4.14) it is clear that melting will begin at  $x = l$  where the plates join and move outwards to  $x = 0$ . The presence of the

body heating term and the melt range of the steel will mean that at any time an area of the plate will be undergoing melting rather than a point. This area of melting is referred to as the 'mushy' region and is bounded by a solidus and liquidus boundary. This welding problem is essentially described by equations (4.8) and (4.10) and may be solved by the method outlined above i.e. the phase change isotherm  $T = T_m$  is forced to move  $\delta x$  for each choice of the time step  $\delta t$ . The extent of the 'mushy' region at any time will be of interest. This can be found by an interpolation on the temperature distribution, e.g. the position of solidus boundary at time  $t = j\delta t$  can be calculated from

$$\text{Solidus} = [S + (T_S^j - T_{m+\varepsilon})/(T_S^j - T_{S+1}^j)]\delta x \quad (4.15)$$

where  $S$  is the last node in the solid between  $x = 0$  and  $x = l$ .

The spot welding problem outlined above has been solved with  $\delta x = 10^{-4}$  m and whilst  $H(l, t) \leq C(T_m - \varepsilon)$  (i.e. the steel is all solid) a fixed time step of  $\delta t = 2 \times 10^{-2}$  s. After melting commenced the extent of the mushy region at each time step was found on use of the linear interpolation equation (4.15). This result is shown in Fig. 9. The movement of both the

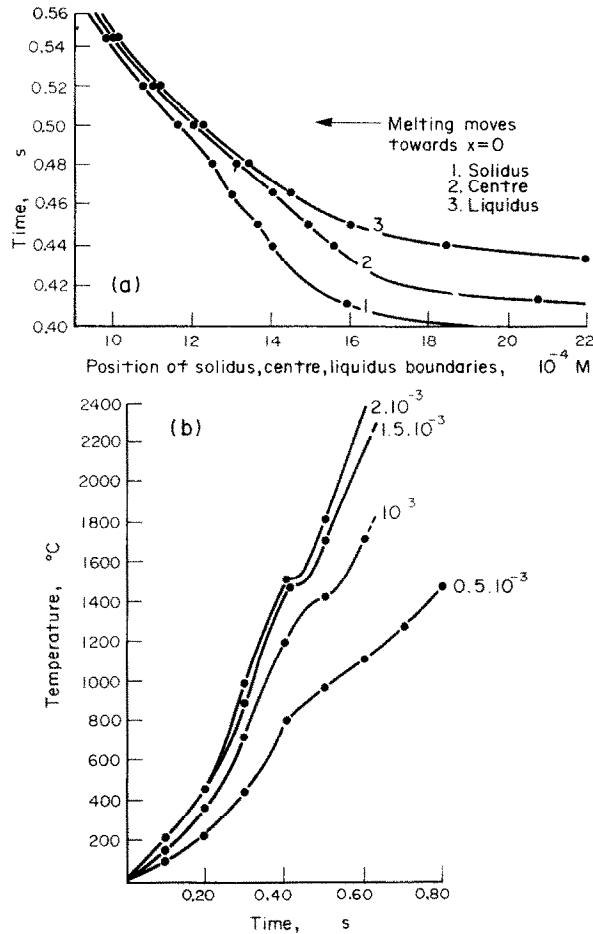


FIG. 9. The welding problem showing (a) the extent of the mushy region as the melting front moves towards  $x = 0$  and (b) the temperature histories at points  $x = 0.5, 1, 1.5, 2 \times 10^{-3} m$ .

solidus and liquidus boundaries is very rapid near to  $x = l$  and the mushy region is large ( $\gg \delta x$ ). However, as the melting advances towards  $x = 0$  the solidus and liquidus boundaries converge and the extent of the 'mushy' region becomes very small ( $\ll \delta x$ ). During this phase of the problem the melt range almost degenerates to phase change at a single point. Even though this significant change in the size of the melt range takes place the only sign of instability is in the predicted movement of the solidus boundary where some slight oscillations occur.

However, even these oscillations may be ascribed to the crude linear interpolation used to position the solidus boundary. The predicted temperature histories at various depths, shown in Fig. 9, have no oscillations. The interesting feature in these results is that the characteristic "knee" in the temperature histories does not occur at the phase change temperature for the nodes near to  $x = 0$ . The flattening of the history curves appears to take place when the extent of the "mushy" region is large, this suggests that the "mushy" region acts as a heat "block" utilizing all the heat being created to undergo the phase change.

## 5. CONCLUSION

A simple extension to the explicit finite difference solution to the enthalpy formulation has been described which provides accurate solutions to Stefan problems, whether the phase change occurs at a specific temperature or across a range. The non-physical features usually associated with enthalpy methods are eliminated, the resulting algorithm is extremely simple to implement and solutions with a relative accuracy of 0.1% have been obtained.

The explicit algorithm has been extended to two dimensional regions and a problem solved which produces stable, physically reasonable results which compare well with those of other authors [10, 12, 16].

The principle used in the simple one-dimensional method has also been exploited to develop an implicit algorithm which is both accurate and fast. For example, it took only eight time steps to trace the phase change boundary 1 m, compared to 1000 using the explicit method and 36 by Goodrich's method. Furthermore, this implicit method is capable of producing stable solutions to problems where the phase change region varies from a point to a temperature range

during its solution and internal heating both occur simultaneously. This flexibility is demonstrated in solving a welding problem similar to that originally posed by Atthey [8].

Finally, by carefully reinterpreting the numerical results from the standard enthalpy method powerful numerical tools have been developed to solve complex Stefan problems. The main advantages of the modified explicit enthalpy method and the implicit "node jumping" scheme may be summarized as: (i) simple in concept and easy to program, (ii) no starting solution required, (iii) accurately tracks the phase change boundary and the temperature history curves at any point, (iv) copes easily with non-constant thermal properties, (v) deals with problems involving any size phase change temperature range (including a single point) and body heating, simultaneously, and (vi) extends easily to multi-dimensional problems.

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#### SOLUTIONS PRECISES DES PROBLEMES DE FRONTIERE MOBILE EN UTILISANT LA METHODE DE L'ENTHALPIE

**Résumé** — Après avoir examiné les problèmes associés aux développements numériques des problèmes de Stefan utilisant la formulation enthalpique, on décrit un développement simple qui conduit à des solutions très précises. L'extension de cette technique à deux problèmes dimensionnels utilise une méthode explicite directe.

Un schéma implicite pour des problèmes à une dimension basé sur le développement précédent est ensuite décrit qui peut concerner simultanément une étendue quelconque de température de changement de phase et l'influence d'un chauffage interne. Finalement, l'utilité de ce schéma est démontré par son application à un problème de soudure.

#### GENAUE LÖSUNGEN VON PROBLEMEN MIT BEWEGLICHEN RANDBEDINGUNGEN UNTER VERWENDUNG DER ENTHALPIEMETHODE

**Zusammenfassung** — Nach der Beschreibung von Problemen, die mit den gewöhnlichen numerischen Behandlungen von Stefan-Problemen bei Gebrauch der Enthalpieformulierung verbunden sind, wird eine einfache Methode beschrieben, die zu sehr genauen Lösungen führt. Die Erweiterung dieser Technik auf zweidimensionale Probleme wird anschließend an einer direkten expliziten Methode demonstriert. Weiterhin wird ein implizites Verfahren für eindimensionale Probleme auf der gleichen Grundlage beschrieben. Es kann jeden Temperaturbereich beim Phasenwechsel und gleichzeitig den Einfluß von inneren Wärmequellen beschreiben. Schließlich wird die Brauchbarkeit dieses Verfahrens bei der Anwendung auf ein Problem der Schweißtechnik gezeigt.

### ИСПОЛЬЗОВАНИЕ МЕТОДА ЭНТАЛЬПИЙ ДЛЯ ТОЧНОГО РЕШЕНИЯ ЗАДАЧ С ПЕРЕМЕЩАЮЩИМИСЯ ГРАНИЦАМИ

**Аннотация** — Дан обзор проблем, связанных с обычными численными решениями задач Стефана на основе энтальпийных формулировок, и предложена простая методика, позволяющая получать точные решения. Распространение предложенной техники на двумерные задачи демонстрируется с использованием прямого явного метода. Затем приведено описание неявной схемы для одномерных задач, которая позволяет получать решения для любого диапазона температур фазовых превращений при одновременном действии внутренних источников тепла. Наконец, показана применимость схемы к проблемам сварки.