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A REFINEMENT OF THE HEAT BALANCE INTEGRAL METHOD APPLIED TO A MELTING PROBLEM

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Abstract—A mode of refinement of the heat balance integral method which is particularly suited to problems involving melting or freezing is presented. The dependent variable temperature is sub-divided into equal intervals and a system of first order, non-linear, differential equations is produced for a set of penetration variables. The penetration variables define the position of each isotherm created by the sub-division. The system of equations is then solved numerically. The improvement produced by this type of refinement is illustrated by results obtained for an idealised melting problem.

NOMENCLATURE

a_i, a coefficient in the profile u_i;
c, specific heat;
L, latent heat of fusion;
l_i, $X_i - X_{i+1}$, distance between adjacent isotherms;
n, number of sub-regions;
T, temperature;
T_0, melting temperature;
T_s, surface temperature;
T_i, value of ith isotherm;
u, approximation to temperature distribution $T(x, t)$;
u_i, assumed temperature profile in sub-region (X_{i+1}, X_i);
X_0, position of the melt line;
X_i, position of the ith isotherm, T_i;
y_i, coordinate defined in text.

Greek symbols

α, latent heat parameter $= L/c$;
β, γ, parameters defined in text;
κ, thermal diffusivity;
λ_i, penetration coefficient defined in text;
ρ, density.

INTRODUCTION

THE HEAT balance integral method as described by Goodman [1] has many pleasing features. It can be applied to a wide range of problems and the accuracy obtained is usually sufficient for most practical situations. In particular, it can be applied with relative ease to heat flow problems involving either temperature dependent thermal properties or a phase change. It is with the latter class of problem that this paper is concerned.

Conduction problems in which either melting or freezing takes place have received much attention in recent years and many numerical techniques have been devised to cater for this type of moving boundary. Reviews of some of these methods are given by both Crank [2] and Fox [3]. In connection with the heat balance integral method, Fox reports that the assumed temperature profile must be chosen with care. This sensitivity to the choice of profile is demonstrated in the results presented by Langford [4] for the simple case of plane flow in a semi-infinite medium. The result obtained from a cubic profile is less accurate than that produced by a quadratic one. Crank and Phahle [5] in a study of the isotherm migration method applied to the problem of melting of ice quote, for the purposes of comparison, results based on a quadratic profile given in [1]. For this particular example, it is easy to show that more accurate results can be obtained using a linear profile. It is therefore disappointing that the application of additional boundary conditions, in order to construct higher order approximations, can inhibit the accuracy of the method.

Noble [6] suggests that the most promising way of systematically improving the accuracy of the heat balance integral method is by repeated spacial sub-division, using quadratic profiles in each sub-region, as in a finite element approach. It is essentially this idea that is explored here together with the concept of penetration depth [1]. Instead of sub-division of the independent variable, space, in the usual way, the equal sub-division of the dependent variable, temperature, is considered. Using a suitable form of the heat balance integral, a system of first order, non-linear, differential equations is produced for a set of penetration variables. Each penetration variable is associated with an isotherm created by the sub-division. Therefore, the solution of the system of equations provides the position of each isotherm which automatically includes the location of the moving boundary, as in [5].

In the following section a suitable form of the heat balance integral is derived for a simple phase change problem. The equations obtained are also appropriate for a variety of other situations, under certain conditions. A discussion of the applicability of the method to be described appears in the final section.

THE HEAT BALANCE INTEGRAL

Consider the idealised problem of the melting of a semi-infinite solid, initially at its fusion temperature T_0, by raising its surface to temperature T_s. The equations describing the process are

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}, \quad 0 < x < X_0(t), \quad t > 0; \tag{1}$$

$$T(x,t) = T_0, \quad X_0(t) \leqslant x, \quad t \geqslant 0; \tag{2}$$

$$T(0,t) = T_s, \quad t > 0; \tag{3}$$

and

$$-\left(\frac{\partial T}{\partial x}\right)_{X_0} = \frac{\alpha}{\kappa}\dot{X}_0, \tag{4}$$

where T is temperature, X_0 is the position of the melt line, κ is the thermal diffusivity, assumed constant and α is the latent heat parameter defined by

$$\alpha = L/c,$$

again assumed constant.

Suppose a spacial sub-division is formed by sub-dividing the temperature range T_0 to T_s into n equal intervals, as illustrated in Fig. 1. Denote the depth of

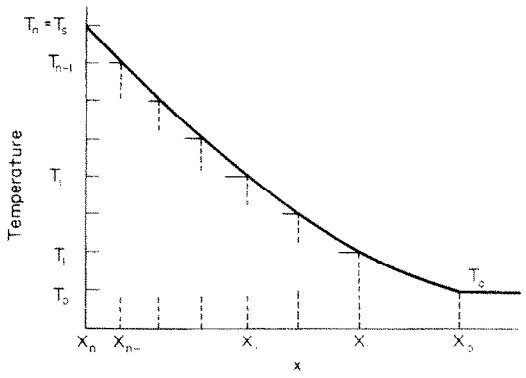

FIG. 1. Sub-division of the region.

penetration of the isotherm T_i, at time t, by $X_i(t)$ where

$$T_i = T_0 + \frac{i}{n}(T_s - T_0), \quad (i = 0, 1, \ldots, n),$$

and $T_n = T_s$.

Integrating equation (1) over the sub-region $X_{i+1}(t) \leqslant x \leqslant X_i(t)$ gives

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{X_{i+1}(t)}^{X_i(t)} T(\xi,t)\,\mathrm{d}\xi\right] - T_i\dot{X}_i + T_{i+1}\dot{X}_{i+1} = \kappa\left(\frac{\partial T}{\partial x}\right)_{X_i} - \kappa\left(\frac{\partial T}{\partial x}\right)_{X_{i+1}}$$

which is more conveniently written as

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{X_{i+1}(t)}^{X_i(t)} T(\xi,t)\,\mathrm{d}\xi + T_{i+1}X_{i+1} - T_iX_i\right] = -\kappa\left(\frac{\partial T}{\partial x}\right)_{X_{i+1}} + \kappa\left(\frac{\partial T}{\partial x}\right)_{X_i}, \tag{5}$$

expressing that the rate of change of the quantity of heat within the sub-region is equal to the difference between the flux entering the sub-region and emerging from it. Considering each sub-region (X_{i+1}, X_i), $i = 0, 1, \ldots, n-1$, in turn, n equations of the form (5) are produced in terms of the n unknowns X_i, $(i = 0, \ldots, n-1)$, (note $X_n = 0$) and the temperature distribution T. For the leading sub-region (X_1, X_0), condition (4) can be incorporated into (5) to give

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_{X_1(t)}^{X_0(t)} T(\xi,t)\,\mathrm{d}\xi + T_1X_1 - (T_0 - \alpha)X_0\right] = -\kappa\left(\frac{\partial T}{\partial x}\right)_A. \tag{6}$$

The heat-balance equation employed in [1] is simply the sum of these n equations, namely,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_0^{X_0(t)} T(\xi,t)\,\mathrm{d}\xi - (T_0 - \alpha)X_0\right] = -\kappa\left(\frac{\partial T}{\partial x}\right)_0. \tag{7}$$

The method is to approximate the temperature T by some function $u(x,t)$. The function u does not satisfy (1) but instead is required to satisfy (7) by simultaneously satisfying the n equations of the form (5). The details are given below.

THE APPROXIMATE SOLUTION

Let u consist of a series of profiles u_i where $u_i(x,t) \simeq T(x,t)$ in the sub-region $X_{i+1} \leqslant x \leqslant X_i$, $i = 0, 1, \ldots, n-1$. Clearly, the u_i must be such that

$$u_i(X_i) = T_i$$

and

$$u_i(X_{i+1}) = T_{i+1}.$$

These conditions alone are sufficient to determine the u_i when the profiles are taken to be linear functions of x. With a linear profile the flux is constant within each sub-region and has a discontinuity at X_i, $i = 1, \ldots, n-1$. However, for the purposes of this initial investigation it is desirable, though not essential, to choose an approximation $u(x,t)$ that is smooth.

If u_i is chosen to be a quadratic then one extra condition per sub-region is required. These are provided by the stipulation that the flux is to be continuous in $0 < x < X_0$ together with equation (4).

For convenience, the following notation is introduced. Let

$$x = X_{i+1} + y_i \quad \text{for} \quad X_{i+1} \leqslant x \leqslant X_i$$

and

$$l_i = X_i - X_{i+1}.$$

Therefore,

$$u_i(X_{i+1} + y_i) = T_{i-1} - \frac{y_i}{l_i}(T_{i+1} - T_i) + a_iy_i\left(1 - \frac{y_i}{l_i}\right), \tag{8}$$

where the coefficient a_i is determined from the "smoothing" condition

$$\left(\frac{\partial u_i}{\partial x}\right)_{X_i} = \left(\frac{\partial u_{i-1}}{\partial x}\right)_{X_i}, \quad (1 \leqslant i \leqslant n-1). \tag{9}$$

Substituting (8) into (9) gives the recurrence relation

$$a_i = \frac{(T_s - T_0)}{n}\left(\frac{1}{l_{i-1}} - \frac{1}{l_i}\right) - a_{i-1}, \quad (1 \leqslant i \leqslant n-1), \tag{10}$$

and once a_0 is determined from (4) the a_i can be generated.

The condition (4) can be reformulated, see [1], as

$$\alpha\left(\frac{\partial^2 T}{\partial x^2}\right)_{X_0} = \left(\frac{\partial T}{\partial x}\right)^2_{X_0} \tag{11}$$

which, upon applying (8) with $i = 0$, produces the result

$$a_0 = -\frac{(T_s - T_0)}{nl_0}[1 + \gamma \pm (\gamma^2 + 2\gamma)^{1/2}], \tag{12}$$

where

$$\gamma = \alpha n/(T_s - T_0). \tag{13}$$

As the latent heat becomes large the movement of the melt line becomes slower and the temperature distribution behind the melting front tends to a steady-state, therefore the property that

$$a_0 \to 0 \quad \text{as} \quad \alpha \to \infty$$

is required. This is achieved by choosing the negative sign in the expression for a_0.

Writing a_0 as

$$a_0 = -\frac{1}{l_0 n}(T_s - T_0)\beta, \tag{14}$$

where

$$\beta = 1 + \gamma - (\gamma^2 + 2\gamma)^{1/2}, \tag{15}$$

and substituting (8) into (6) gives the equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[(3 - \beta + 6\gamma)l_0 + 6(1+\gamma)\sum_{j=1}^{n-1} l_j\right] = \frac{6\kappa(1+\beta)}{l_0}. \tag{16}$$

Similarly, after generating the a_i's from (10) and substituting (8) into (5), the remaining $n-1$ equations are obtained,

$$\frac{\mathrm{d}}{\mathrm{d}t}\left\{l_i^2\left[2\sum_{j=1}^{i-1}\frac{(-1)^{i-j-1}}{l_j} + \frac{(-1)^{i-1}(1+\beta)}{l_0}\right] + 2l_i + 6\sum_{j=i+1}^{n-1} l_j\right\} = \frac{12\kappa}{l_i} - 12\kappa\left[2\sum_{j=1}^{i-1}\frac{(-1)^{i-j-1}}{l_j} + \frac{(-1)^{i-1}(1+\beta)}{l_0}\right], \quad (1 \leqslant i \leqslant n-1). \tag{17}$$

Equations (16) and (17) provide a system of n first order, non-linear, differential equations in the n penetration parameters $l(t)$.

METHOD OF SOLUTION AND RESULTS

To facilitate the solution of the system of equations in the form given in (16) and (17) a starting procedure is required as the equations are initially singular. This can be dealt with by the use of a small time series solution as derivated by Poots [7]. For melting problems where a boundary condition other than (3) is prescribed corresponding small time solutions can be derived. After the initial motion of the melt line has been determined, by means of a series solution, the system of equations, (16) and (17), can then be solved using standard numerical techniques.

However, in conduction controlled phase change problems of this type there often exists a similarity variable which simplifies the equations governing the process. Therefore, anticipating the analytic behaviour of the melt line to be proportional to $(\kappa t)^{1/2}$, a solution of the form

$$l_i = \lambda_i(\kappa t)^{1/2}, \quad \lambda_i > 0,$$

is sought. Upon substitution into (16) and (17), the system of differential equations reduces to a system of non-linear algebraic equations. These equations are

$$(3 - \beta + 6\gamma)\lambda_0^2 + 6(1+\gamma)\lambda_0\left(\sum_{j=1}^{n-1}\lambda_j\right) - 12(1+\beta) = 0 \tag{16a}$$

and

$$\lambda_i^3\left[\sum_{j=1}^{i-1}\frac{(-1)^{i-j-1}}{\lambda_j} + \frac{(-1)^{i-1}(1+\beta)}{2\lambda_0}\right] + \lambda_i^2 + 3\lambda_i\left[\sum_{j=i+1}^{n-1}\lambda_j + 8\sum_{j=1}^{i-1}\frac{(-1)^{i-j-1}}{\lambda_j} + \frac{4(-1)^{i-1}(1+\beta)}{\lambda_0}\right] - 12 = 0, \quad (1 \leqslant i \leqslant n-1). \tag{17a}$$

Again, for this example, anticipating that $\lambda_0 > \lambda_1 > \ldots > \lambda_{n-1}$ and also noting that $0 < \beta < 1$ and $\gamma > 0$, it is evident that each equation has a unique positive solution since the coefficients in the equations are positive.

As a similarity variable exists for the particular problem under consideration, the system of differential equations is solved in its reduced form given in (16a) and (17a). Had no such simplification been possible then the original system, (16) and (17), would have to be solved by the procedure outlined above.

The method adopted for solving the system of algebraic equations is firstly to solve (16a) for λ_0, given initial estimates of $\lambda_1, \ldots, \lambda_{n-1}$. These estimates can be obtained from Goodman's solution, given in [1], which corresponds to the case $n = 1$ in this present work. Then for the $n-1$ equations given in (17a), one iteration of Newton's method is performed on each of the cubic equations in turn providing an improved estimate of λ_i. As each improved estimate is obtained, it replaces its previous value in the remaining equations. After producing a new set of estimates for $\lambda_0, \ldots, \lambda_{n-1}$, the process is then repeated until consecutive estimates for each λ_i differ at most by some pre-assigned quantity. In the results that follow this value was taken as 0.5×10^{-6}. This particular procedure for solving the equations was employed be-

Table 1. Estimates of four isotherm positions $/(\kappa t)^{1/2}$ and incident flux for different sub-divisions

$(T-T_0)/(T_s-T_0)$	0.75	0.5	0.25	0	$-\left(\frac{\partial T}{\partial X}\right)_0 (\kappa t)^{1/2}/(T_s-T_0)$
$n=1$ [1]				1.32003	0.96055
2		0.56519		1.25452	0.91952
4	0.27657	0.56421	0.87746	1.24291	0.91255
8	0.27634	0.56375	0.87679	1.24070	0.91117
16	0.27626	0.56360	0.87658	1.24025	0.91087
32	0.27624	0.56356	0.87651	1.24015	0.91080
exact solution [8]	0.27624	0.56355	0.87650	1.24013	0.91078

cause it is easy to implement, requiring little programming effort, and is fairly efficient, as will be illustrated shortly. However, a more sophisticated approach can be used if rapid convergence of the iterations is considered essential.

The results presented in Table 1 correspond to the case $\alpha/(T_s-T_0)=1$. The results are quoted in the form of the position $/(\kappa t)^{1/2}$ of four selected isotherms for different sub-divisions. Also presented are estimates of the flux at $x=0$ for each sub-division considered. These results are compared with the exact solution of the problem given by Carslow and Jaeger [8]. The improvement due to sub-division can clearly be observed. The error is at most 2×10^{-5} in all computed values for the scheme with 32 sub-regions, the maximum number considered. Equally impressive is the improvement upon Goodman's solution ($n=1$) produced by using just two sub-regions. The percentage errors in the quantities melt line position $/(\kappa t)^{1/2}$ and dimensionless flux are about $6\frac{1}{2}$ and $5\frac{1}{2}\%$, respectively, for the case $n=1$. These errors are reduced to the order of 1% when the scheme is operated with just two sub-regions. Also, it is worth noting that when n is chosen to be two, the two equations to be solved, (16a) and (17a), simplify considerably and, with a revision of notation, can be recast as a pair of coupled equations for $X_0/(\kappa t)^{1/2}$ and $X_1/(\kappa t)^{1/2}$.

Table 2 presents results obtained when just two sub-regions are considered for a range of values of the dimensionless latent heat parameter $\alpha/(T_s-T_0)$. Such a simple refinement to the basic method [1] would appear to be adequate for a wide range of physical problems. The results in Table 1 emphasize the scope for obtaining further improvement, should higher order accuracy be required. Also, from a computational aspect, the technique described is surprisingly efficient. When two sub-regions are considered the C.P.U. time used on an I.B.M. 360/44 is under 2 s; eight iterations being performed. For the case with 32 sub-regions, only 8 s of processing time are required and 90 iterations are performed. Obviously, the number of iterations depends on the accuracy of the initial values used but these figures give an indication of the general performance of the method.

Table 2. Percentage error incurred by using the scheme with two sub-regions ($n=2$) for various values of $\alpha/(T_s-T_0)$

% error in:	$X_0/(\kappa t)^{1/2}$	$-\left(\frac{\partial T}{\partial X}\right)_0 (\kappa t)^{1/2}/(T_s-T_0)$
$\alpha/(T_s-T_0)=1$	+1.16	+0.96
10	+0.24	+0.23
50	+0.05	+0.05
100	+0.02	+0.03

CONCLUSION

A method has been described which effectively removes the sensitivity of the heat balance integral method to the choice of profile. Highly accurate results can be obtained by successive refinement as illustrated in the application to the phase-change problem considered in the preceding sections. The results presented indicate that the process converges and this is to be expected by the nature in which the approximations are constructed. However, no formal analysis of the process has been attempted.

The efficiency of the method has been aided by the existence of a similarity solution for the model problem under consideration. Its performance in a more general situation will be assessed in later work.

It would seem that provided the temperature distribution is a monotonic function, with regard to the space variable x, there is no inherent difficulty in applying this technique to other heat-transfer situations, such as those considered by Goodman [1]. The equation (5) remains unchanged and the construction of the profiles is as described earlier. The value of a_0, or alternatively a_{n-1}, is determined by the boundary conditions being inforced. For heat flow in a fixed, finite region the coefficient a_0 (or a_{n-1}) can remain as an unknown function to be determined from the system of differential equations, in a similar manner to the procedure described in [1].

However, this type of refinement is particularly suited to situations in which the concept of heat penetration is relevant, such as problems involving melting or freezing. The technique is even successful for the case of plane flow into a semi-infinite solid where the depth of penetration of the lowest isotherm is theoretically infinite. This is easily demonstrated by setting $\alpha=0$ (that is $\gamma=0$, $\beta=1$), in the equations (16a) and (17a) and proceeding as before. The formal

Table 3. A plane flow problem

$(T-T_0)/(T_s-T_0)$	0.5	0	$-\left(\frac{\partial T}{\partial x}\right)_0 (\kappa t)^{1/2}/(T_s-T_0)$
$n=2$	1.001	3.275	0.560
8	0.961	3.680	0.562
32	0.955	4.217	0.564
exact solution	0.954	∞	0.564

solution of the problem is

$$\frac{T-T_0}{T_s-T_0} = \text{erfc}[x/2(\kappa t)^{1/2}],$$

where T_0 is now the constant, initial temperature of the solid and T_s is the temperature to which the surface is raised. A selection of the results are given in Table 3. These again illustrate that successive sub-division improves the accuracy of the results, although the rate of improvement is not as rapid as observed earlier, which is to be expected.

In the numerical solution of the equations describing certain physical processes, the equal sub-division of the dependent variable can often be more appropriate than the equal sub-division of the independent one. For example, when a sudden change in temperature takes place over a small spacial region, this type of refinement automatically concentrates on the location of the change. The author has illustrated the success of such an approach combined with the heat balance integral method for solving melting or freezing problems. Further applications are at present under investigation.

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UNE AMELIORATION DE LA METHODE DU BILAN THERMIQUE INTEGRAL APPLIQUEE AU PROBLEME DE LA FUSION

Résumé—On présente une méthode améliorée du bilan thermique intégral particulièrement adaptée aux problèmes de fusion ou de solidification. La température variable dépendante est subdivisée en intervalles égaux et un système d'équations différentielles non linéaires du premier ordre est fourni pour un ensemble de variables de pénétration. Les variables de pénétration définissent la position de chaque isotherme créée par la subdivision. Le système d'équations est résolu numériquement. L'amélioration apportée est illustrée par les résultats obtenus pour un problème idéalisé de fusion.

VERBESSERUNG DER INTEGRALEN WÄRMEBILANZ-METHODE, ANGEWANDT AN EINEM SCHMELZVORGANG

Zusammenfassung—Eine Verbesserung der integralen Wärmebilanz-Methode, welche besonders für die Berechnung von Schmelz- und Gefriervorgängen geeignet ist, wird beschrieben. Die abhängige Variable, die Temperatur, wird in gleiche Intervalle unterteilt. Dadurch entsteht ein nicht-lineares Differential-Gleichungssystem erster Ordnung für einen Satz von Penetrations-Variablen. Diese bestimmen die Position jeder durch die Unterteilung erzeugten Isothermen. Das Gleichungssystem wird numerisch gelöst. Die mit dieser Methode erreichte Verbesserung wird durch Ergebnisse veranschaulicht, die für ein idealisiertes Schmelzproblem erhalten wurden.

УСОВЕРШЕНСТВОВАНИЕ ИНТЕГРАЛЬНОГО МЕТОДА ТЕПЛОВОГО БАЛАНСА ДЛЯ ЗАДАЧИ ПЛАВЛЕНИЯ

Аннотация — Предложен усовершенствованный интегральный метод теплового баланса, удобный для решения задач плавления или затвердевания. Для величин, зависящих от температуры, проведено разделение на равные интервалы; получена система нелинейных дифференциальных уравнений первого порядка в переменных, характеризующих процесс фазового перехода. Эти переменные определяют положение каждой изотермы, полученной в результате разбиения. Проведено численное решение системы уравнений. Преимущество предложенного метода иллюстрируется результатами, полученными для идеализированной задачи плавления.