A NEW COMPUTATIONAL METHOD FOR SINGLE PHASE CLASSICAL 1-D STEFAN PROBLEM

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ABSTRACT: In this paper we present a new computational method to obtain approximate solution to one phase Stefan problems. In this method for a fixed space step, higher order accurate initial step sizes are obtained by using Green's theorem of vector calculus. Subsequent step sizes are obtained, one by one, by an iterative process with assured convergence to the Neumann form of the Stefan problem.

KEY WORDS: Moving boundary problem, Starting solutions, Green's theorem, Crank-Nicolson scheme, Interface, Finite difference scheme.

1. INTRODUCTION:

Heat-diffusion moving boundary problems have numerous applications in fields such as the freezing and thawing of foods, production of ice, thawing or formation of ice around pipes, solidification of steel and diffusion limited chemical reactions, where either a moving freezing, moving melting or moving reaction front is present. Mathematically these problems involve solving the heat-diffusion equation in an unknown region, which has to be determined as part of the problem. Exact solutions to moving boundary problems are limited in number and for heat-diffusion problems the only physically relevant exact solutions occur when the position of the moving boundary (or boundaries) varies as the square root of time (that is, similarity solutions). This paper is mainly concerned with the development of numerical methodology with less or no emphasis of physical content of the problems.

Several methods have been developed for obtaining approximate solutions to moving boundary problems. Some of them are heat balance boundary integral method and boundary immobilization method. These methods involve transforming the basic equations into another Mathematical problem followed by the solution using finite difference or finite element methods.

We are primarily concerned with the classical single phase Stefan Problem. In non-dimensional variables we may summarize this general problem in the general form by [6]

$$\left.\begin{array}{c} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, 0 < x < s(t), t > 0 \\ s(0) = 0; T(x,0) = 0, T(s(t),t) = 0 \\ \beta \frac{ds}{dt} = -\frac{\partial T}{\partial x}|_{x=s(t)},\ \frac{\partial T}{\partial x} = g(t),\ at\ x = 0 \end{array}\right\} \quad (1)$$

Where $T(x,t), x, S(t)\ and\ t$ denote the dimensionless temperature of the solid, position, moving boundary position and time, respectively. The constant β called the Stefan number, is the ratio of latent heat of fusion to sensible heat of the solid and is therefore strictly positive. Douglas and Gallie [1], Gupta and Kumar [2], Kutluay et al [4] and Marshall [5] also developed approximate methods for solving this type of problems.

The present work develops a front tracking finite difference method. We assume the Problem has a solution and that it is unique. We do not consider the theoretical problem of establishing the convergence of the numerical solution to that of mathematical problem as the step sizes go to zero. However, we establish the accuracy of solution working with varying step sizes in space and time.

We choose for fixed space step as h and find k_1, k_2, k_3 ..., the intervals of time for the interface to move a distance of h.

If $T_{i,n}$ is the temperature at$x_i = ih$, $t_n = \sum_{l=1}^{n} k_l$. $T_{i,n} = 0, i \geq n$and$i = n$ gives a point on the interface.

Crank-Nicholson scheme for the diffusion equation is

$$\frac{T_{i,n+1} - T_{i,n}}{k_{n+1}} = \frac{1}{2h^2}\left[\left(T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}\right) + \left(T_{i-1,n} - 2T_{i,n} + T_{i+1,n}\right)\right] \quad (2)$$

The finite difference scheme is of second order in space and time and computationally stable. Knowing$k_1, k_2, k_3 \ldots k_n$ and $(g(t_n) =)T_{0,n}, T_{1,n}, T_{2,n} \ldots T_{n-1,n}, T_{n,n}(= 0)$, we need to obtain k_{n+1} and $T_{1,n+!}, T_{2,n+1}, \ldots T_{n,n+1}$.

To initiate this scheme, we need to know $T_{(0,2)}, T_{(1,2)}\ and\ T_{(2,2)}$. $T_{(2,2)} = 0, T_{(0,2)}, T_{(1,2)}$ are unknown. In this problem we incorporate the condition into the difference scheme at (0, 1), (0, 2). To know these starting ingredients, we need to find $k_1$and k_2. In section 2, we derive equations to find $k_1$and k_2. In section 3 we develop an iterative procedure to find $k_n, for\ n \geq 3$. in section 4 convergence of the iterative method is given and in section 5 two examples are given.

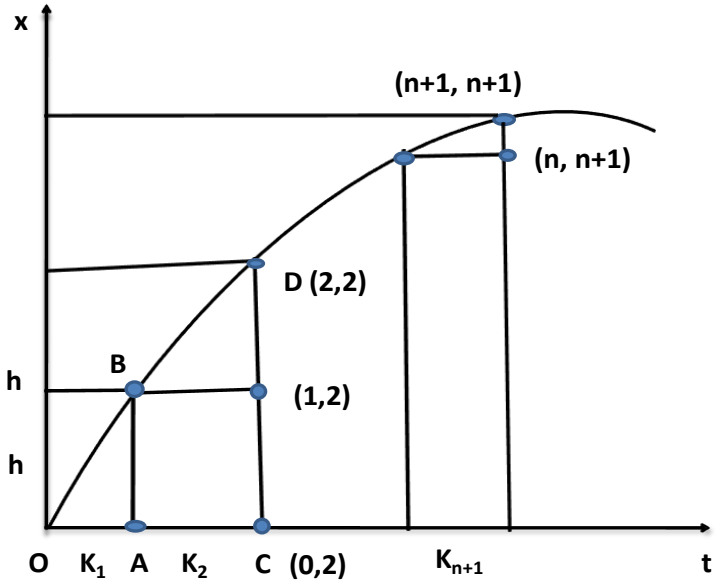

Figure 1

MOVING BOUNDARY PROBLEM

2. FINDING k_1 AND k_2:

Our search for better approximation culminated in the application of **Green's Theorem** covering the region in the first cell. We need in the process, the second degree polynomial as an approximation for the interface through $(0,0)$, (k_1,h) and $(k_1+k_2,2h)$ as

$$s(t)=\frac{th}{k_1}+t(t-k_1)\frac{(k_1-k_2)}{k_1k_2(k_1+k_2)}$$ (Newton divided difference polynomial)

$$\frac{ds}{dt}_{t=0}=\dot{s}(0)=h\frac{[k_2^2-k_1^2+2k_1k_2]}{k_1k_2(k_1+k_2)}=-\frac{1}{\beta}T_{x\,(0,0)}$$

$$\frac{ds}{dt}_{t=t_1}=\dot{s}(t_1)=h\frac{[k_2^2+k_1^2]}{k_1k_2(k_1+k_2)}=-\frac{1}{\beta}T_{x\,(1,1)}$$

$$\frac{ds}{dt}_{t=t_2}=\dot{s}(t_2)=h\frac{[k_1^2-k_2^2+2k_1k_2]}{k_1k_2(k_1+k_2)}=-\frac{1}{\beta}T_{x\,(2,2)}$$

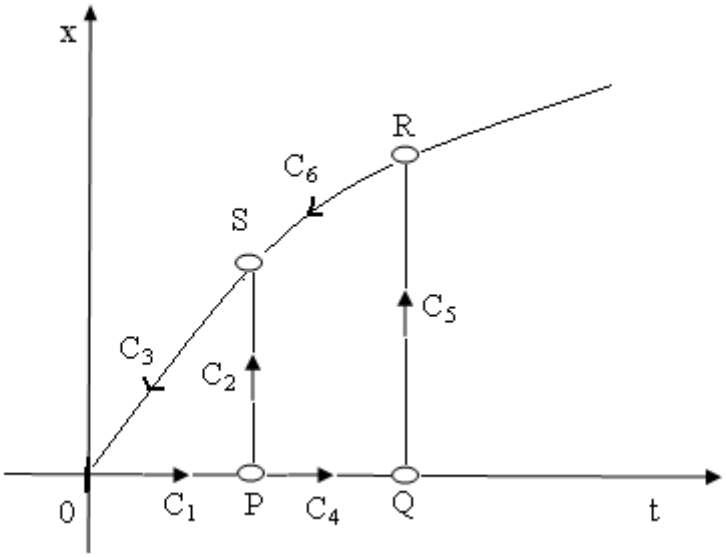

Fig.2

To find the two relations for $k_1$and k_2 we need approximations for T along AB and CD.

At A: $(x, T_x) = \big(0, g(t_1)\big)$and B:$(x, T_x) = \big(h, -\beta\dot{s}(t_1)\big)$

Straight line through A and B is: $T_x = g(t_1) - \frac{x}{h}[\beta\dot{s}(t_1) + g(t_1)]$

Hence $T = g(t_1)x - \frac{x^2}{2h}[\beta\dot{s}(t_1) + g(t_1)] + \frac{h}{2}[\beta\dot{s}(t_1) - g(t_1)]$
[Constant of integration is obtained, imposing $T(h) = 0$ at B]

Similarly using C: $(x, T_x) = \big(0,\ g(t_2)\big)$, D: $(x, T_x) = \big(2h, -\beta\dot{s}(t_2)\big)$& T(2h)=0 at D

We obtain the approximations for CD as $T_x = g(t_2) - \frac{x}{h}[\beta\dot{s}(t_2) + g(t_2)]$

Hence $T = g(t_2)x - \frac{x^2}{4h}[\beta\dot{s}(t_2) + g(t_2)] + h[\beta\dot{s}(t_2) - g(t_2)]$

$T(h) = \frac{h}{4}[3\beta\dot{s}(t_2) - g(t_2)]$ and $T(0) = h[\beta\dot{s}(t_2) - g(t_2)]$

Now considering the region OAB, We know that by Green's Theorem
$\iint_R [T_{xx} - T_t]dxdt = 0 \Rightarrow \int_C [T_x dt + T dx] = 0$, where C is the boundary and $C = OA \cup AB \cup BO$

$$\int_0^{k_1} g(t)dt + \int_0^h \left[g(t_1)x - \frac{x^2}{2h}\{\beta\dot{s}(t_1) + g(t_1)\} + \frac{h}{2}\{\beta\dot{s}(t_1) - g(t_1)\}\right]dx + \int_{k_1}^0 (-\beta)\frac{ds}{dt}dt = 0$$

This simplifies to

$k_1k_2(k_1+k_2)[3k_1g(0)+(3k_1-h^2)g(t_1)+6\beta h]+2\beta h^3(k_1^2+k_2^2)=0$ (3)

Consider the region ACDB, $\int_C [T_x dt + T dx] = 0, C: AC \cup CD \cup DB \cup BA$

$$\int_{t_1}^{t_2} g(t)dt + \int_0^{2h}\left[g(t_2)x - \frac{x^2}{2h}\{\beta\dot{s}(t_2)+g(t_2)\}+h\{\beta\dot{s}(t_2)-g(t_2)\}\right]dx +$$
$$\int_{t_2}^{t_1}(-\beta)\frac{ds}{dt}dt + \int_h^0\left[g(t_1)x - \frac{x^2}{2h}\{\beta\dot{s}(t_1)+g(t_1)\}+h\{\beta\dot{s}(t_1)-g(t_1)\}\right]dx = 0$$

This simplifies to

$k_1k_2(k_1+k_2)[(3k_1+4h^2)g(t_1)+(3k_2-8h^2)g(t_2)+6\beta h]+2\beta h^3(3k_1^2-5k_2^2+8k_1k_2)=0$ (4)

Here we have used the expressions for $\dot{s}(0), \dot{s}(t_1)$ and $\dot{s}(t_2)$.

We can solve the equations (3) and (4) for k_1 and k_2. In equation (2), i=0,1,2,…,n, $T_{0,i}$ is not known. To start the computation, we need, $T_{0,2}, T_{1,2}, (T_{2,2}=0)$

$T_{0,2}=T(0)$ from the equation to CD and $T_{1,2}=T(h)$. Further (2) for i=0, changes as follows, using $\frac{T_{1,n+1}-T_{-1,n+1}}{2h}=g(t_{n+1})$

$$T_{0,n+1}\left[\frac{2}{k_{n+1}}+\frac{2}{h^2}\right]-\frac{2}{h^2}T_{1,n+1}=T_{0,n}\left[\frac{2}{k_{n+1}}-\frac{2}{h^2}\right]+\frac{2}{h^2}T_{1,n}-\frac{2}{h}[g(t_n)+g(t_{n+1})]$$

Rests of the equations remain same.

3. MAIN ALGOTIRHM FOR THE SOLUTION OF THE PROBLEM:

We have n equations in (n+1) unknowns $T_1, T_2, T_3, \dots, T_n$ (at t_{n+1}) and k_{n+1}. Much needed another relation comes from Stefan condition at (n+1, n+1).

$$-\beta\frac{h}{k_{n+1}}=\frac{(T_{n-1,n+1}-4T_{n,n+1}+3T_{n+1,n+1})}{2h}$$

From which we obtain

$4T_{n,n+1}-T_{n-1,n+1}=2\beta\frac{h^2}{k_{n+1}}$ (5)

With i= n, in the system we have only implicit part

$\frac{T_{n,n+1}-T_{n,n}}{k_{n+1}}=\frac{(T_{n+1,n+1}-2T_{n,n+1}+T_{n-1,n+1})}{h^2}$

simplifying to $T_{n,n+1}=\frac{k_{n+1}}{(h^2+2k_{n+!})}T_{n-1,n+1}$

This, when substituted in (5), we get

$T_{n-1,n+1}=\frac{2\beta h^2(2k_{n+1}+h^2)}{k_{n+1}(2k_{n+1}-h^2)}$ (6)

and

$T_{n,n+1}=\frac{2\beta h^2}{(2k_{n+1}-h^2)}$ (7)

(6) is a quadratic in k_{n+1} whose positive root is

$$k_{n+1} = \frac{h^2}{4T_{n-1,n+1}}\left[T_{n-1,n+1} + 4\beta + \sqrt{\left(T_{n-1,n+1} + 4\beta\right)^2 + 16\beta T_{n-1,n+1}}\right] \qquad (8)$$

and one equation (i=n) is reduced in (2). This has been used to obtain (6),(7) and (8). This round about looking manipulation is done to ensure the convergence of the following iterative process to obtain k_{n+1} and T values.

4. CONVERGENCE OF ITERATIVE METHOD:

We have (n-1) equations in (2) and another is (8) for the n unknowns $T_1, T_2, T_3, \ldots, T_{n-1}$ (at t_{n+1}) and k_{n+1}. This arrangement is made to ensure convergence of the iterative process. This assurance comes from a theorem in [3]. We can view (8) as an (n-1) dimensional manifold in the space of n variables $T_1, T_2, T_3, \ldots, T_{n-1}$ (at t_{n+1}) and k_{n+1}.

Choose an initial approximation for k_{n+1} lies on the manifold in view of relations (6) and (7). This process is termed as implicit iteration in [3]. In our setup, the manifold is simply given by (8).

If (2) is solved for the n unknowns $(T_1 \ldots . T_n)$ assuming k_{n+1} and obtain k_{n+1} from (8), the initial guess may not be on the manifold given by (7) Theorem in [3] ensures convergence for a choice of initial approximation to k_{n+1} from (8) and carrying one iteration before refining k_{n+1}(by Jacobi, Gauss-Seidal). In practice we iterated (2) until convergence occurred (equivalent to solving the tri-diagonal system). As a test, we started with k_{n+1} equal to say 5 or even 10, iteration converged. Of course number of iterations increased from 2 or 3 to 5 or 6.

5. EXAMPLE AND DISCUSSION:

Method described in sections 2 and 3 is used to obtain solution of the following problem. The results (points on the interface) are given with varying step sizes. Our method gives results up to four significant digits. The purpose of the paper being primarily development of methodology.

Example :$T_x(0,t) = g(t) = t - e^t,\ \beta = 1.0$

X	h=0.1	h=0.05	h=0.025
0.1	0.1044	0.1015	0.1053
0.2	0.2221	0.2015	0.218
0.3	0.3387	0.3014	0.3359
0.4	0.4608	0.4013	0.4573
0.5	0.5842	0.5012	0.5805
1	1.1909	1.1909	1.1904
2	2.2883	2.291	2.2918
3	3.2914	3.2944	3.2953
4	4.2608	4.2638	4.2647
5	5.2209	5.2241	5.225

The accuracy achieved in the estimation of k_1 and k_2 for a given h depends on the approximation used for the integrands and the integration formulae while evaluating the line integrals. We have observed that it is at least of second order in our calculations. Higher order accuracy can perhaps be obtained by improving these approximations. The high accuracy achievable in finding k_1 and k_2 by application of Green's theorem may not be so important to obtain approximate solutions to the problems, However we hope this technique may be useful in application elsewhere. The iterative method for finding k_{n+1} of this paper may be useful in problems where one relation is different from rest of the relations. As a last remark, we want to observe that the algorithm developed in the paper is simple and easy to implement through computer programming.

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REFERENCES:

[1] Douglas Jr Jim and Jr Gallie T.M. On the numerical integration of parabolic differential equations subject to a moving boundary condition. Duke Math. J. 22 (1955), 557-571.
[2] Gupta P.S. and Kumar D. A modified variable time step method for one dimensional Stefan problem. Comp. Math. Appl. Mech. Engineering 23 (1980), 101-108.
[3] Koneru S.R. and Lalli B.S. On Convergence of iteration for fixed points of repulsive type. Canad. Math. Bulletin 14 (1971), 353-357.
[4] Kutluay S., Bahadir A.R. and Ozdes A. The numerical solution of one phase classical Stefan problem. J. Comput. Appl. Math 81 (1997), 135-144.
[5] Marshall Guillermo A front tracking method for one-dimensional moving boundary problems. SIAM J. Sci. Stat. Comput 7 (1986), 252-263.
[6] Mayer G.H. One dimensional parabolic free boundary problems, SIAM review. 119 (1977), 17-34.
[7] Mitchel S. L. and Vynnycky Finite difference method with increased accuracy and correct initialization for 1-dimensional Stefan problem. Applied Mathematics and Computation 215 (2009), 1609 – 1621.