ONE DIMENSIONAL ONE PHASE STEFAN PROBLEM

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Abstract

In this paper we developed a front tracking finite difference method to solve one dimensional one phase moving boundary problem with Neumann condition. We present the basic difficulty, apart from the need to find the moving boundary, is that there is no domain for the first phase at initial time. This difficulty is handled by the age old principle of basic mathematics. Naturally, giving symbolic names to the unknowns develop equations using the conditions of the problem. Methodology developed here sets the tone for solving the two phase problem.

1. Introduction

If thin rod of a solid material is melted by suppling heat, at one end, melting takes and the interface keeps moving. When we ignore the heat diffusion in the solid phase, mathematical problem (non dimensional form and melting temperature normalized to zero) is [5]

$$\frac{\partial T}{\partial t}=\frac{\partial^2 T}{\partial x^2}, 0<x<s(t), t>0 \quad (1.1)$$

$$s(0)=0; T(x,0)=0, T(s(t),t)=0 \quad (1.2)$$

$$\frac{\partial T}{\partial x}=g(t), at\ x=0 \quad (1.3)$$

$$\frac{\partial T}{\partial x} \vee ¿_{x=s(t)} \quad (1.4)$$

$$\beta \frac{ds}{dt}=-¿$$

Starting with any standard numerical method is not possible as the initial domain for x does not exist. An extensive interest was shown by a large number of researchers to develop approximate methods for solving these problems. Reference is made to the excellent book by J. Crank [1] among others, describing these efforts. Only one method proposed by Douglas and Ghallie [2] is relevant to us in the context of the method to be developed. For a fixed space step, they are the first to use variable time step sizes to track the front. Gupta and Kumar [7] have subsequently improved the iterative procedure of [2] for finding the time step. The method in [2] will be taken up after developing our finite difference front tracking method. Gupta and Kumar [7] and Marshall [4] have subsequently improved the iterative procedure of [2] for finding the

time step. Kutluay et al. [3] obtained numerical solution of a specific problem with variable space grid. Even these front tracking methods have made certain transformations of the original problem before writing down the finite difference method. We keep the problem as it occurred in formulation and use the finite difference method applicable to any parabolic problem. One dimensional Stefan problem related methodology available in [9-12].By a theorem of Koneru and Lalli [8] for every iteration of the finite difference equations, convergence is assured.

Another approach relevant to us is the well known method of lines developed by [6]. He discretized the mathematical problem with respect to time resulting in a system of ordinary differential equations with respect to space variable. He obtained at each time level, the position of the interface by solving the boundary conditions followed by the solution of the system using Euler's method. We can interpret the present work as discretization of space first and solving the ordinary differential equations in time by modified Euler's method i.e. Crank Nicholson scheme while finding the points on the interface. The method of lines is, of course, possible only for finite domain of the space variable.

2. Preliminary Setup Of The Method

Let h be a fixed given discrete step size in space. Let $k_1, k_2, \ldots$ be the time intervals needed for the front (interface) to move this specified distance of h. If $T_{i,n}$ is the temperature at $x_i = ih, \quad t_n = \sum_{l=1}^{n} k_l ; T_{i,n} = 0, i \geq n \;\; ; \;\; i = n$ gives a point on the interface.

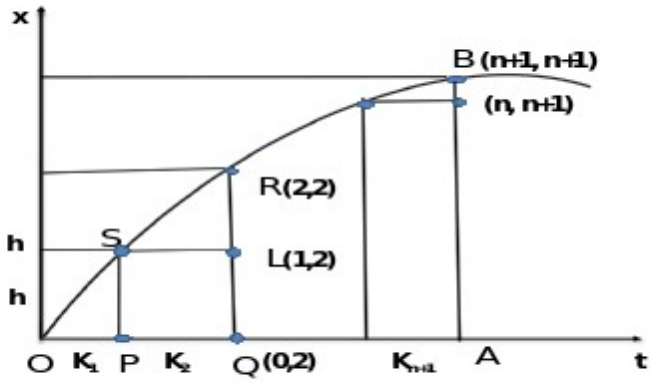

Fig. 1. Moving boundary with fixed space step and variable time step.

Crank-Nicholson scheme for the diffusion equation (1.1) is

$$\frac{T_{i,n+1} - T_{i,n}}{k_{n+1}} = \frac{1}{2h^2}\left[\left(T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}\right) + \left(T_{i-1,n} - 2T_{i,n} + T_{i+1,n}\right)\right] \quad (2.1)$$

Sometimes we need the fully implicit scheme (for manipulations at a later stage)

$$\frac{T_{i,n+1}-T_{i,n}}{k_{n+1}}=\frac{1}{h^2}\left(T_{i-1,n+1}-2T_{i,n+1}+T_{i+1,n+1}\right)(2.2)$$

The finite difference scheme (2.1) is of second order in space and time and is computationally stable. To enable us using this scheme, we need to know T at three points, (0,2), (1,2) and (2,2) (see figure1) . Of these three; $T_{2,2}=0,$ $T_{0,2}$ and $T_{1,2}$ are not known. In this problem of Neumann condition, 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 . The method developed in this article hinges on ones ability to find k_1 and k_2 . Once we do this, we can find $T_{0,3}, T_{1,3}, T_{2,3}$ provided k_3 , the time needed for the interface to move a distance of h is known. We can continue to solve the diffusion equation for n=3, 4, 5… number of points along the line parallel to x-axis increasing by one. In section 3, we derive equations to find k_1 and k_2 . In section 4, we develop an iterative procedure to find k_n , for $n\geq 3$ and give the computational procedure as an algorithm in this section. In section 5, examples are given. The example originally considered in [2] is interpreted in terms of our method and their algorithm is analyzed.

3. Finding k_1 and k_2

For a given h, we need to find $k_1, k_2, T_{0,1}, T_{0,2} \wedge T_{1,2}$. Hence we need to develop sufficient number of equations to obtain these five ingredients. To our knowledge there are three ways, other than series expansion, one can generate these equations.

(i) Application of Green's theorem of vector calculus to a closed region over which the problem is defined. We have several choices in choosing this region.
(ii) Collocation at one or more points of the front.
(iii) Finite difference equivalents of the parabolic equation at chosen points of the lines $t=t_1 \vee t=t_2$.

These choices may vary from problem to problem depending on the available data and is also a matter of convenience for solving these equations. Neither we can collocate nor can we use the basic equation at $'O'$. Greens theorem comes handy in this situation. Using this theorem

$$\iint_{OPSO} \left(T_{xx}-T_t\right)dxdt=0=\oint_C \left(T_x\,dt+T dx\right)$$

where 'C' is the boundary of the closed region under consideration.

$$\int_0^{k_1} T_x\,dt+\int_0^{h} T dx+\int_S^{O} T_x\,dt=0 \; as \; T=0 \; along \; SO$$

We use Trapezoidal rule for the first two integrals and noting that $T_x=\frac{-dS}{dt}$ $along\, SO\,;$

$$\oint_S^O T_x\,dt=\beta\int_h^0(-ds)=\beta h.$$

The above relation reduces to

$$\frac{k_1}{2}\left(g(0)+g(k_1)\right)+\frac{h}{2}T_{(0,1)}+\beta h=0 \quad (3.1)$$

We obtain another relation by finite difference equivalent to the basic equation (1.1) at P.

$$\frac{T_{0,1}-0}{k_1}=\frac{1}{h^2}\left[T_{1,1}-2T_{0,1}+T_{-1,1}\right]$$

and $T_{-1,1}$ is evaluated using $T_x=g(t).$ That is, $\frac{T_{1,1}-T_{-1,1}}{2h}=g(k_1)$

Giving $T_{-1,1}=-2h\,g(k_1)$.

Thus, the equation reduces to $T_{0,1}=\frac{-2hk_1}{h^2+2k_1}g(k_1) \quad (3.2)$

We obtain from (3.1)

$$k_1\left(h^2+2k_1\right)\left[g(0)+g(k_1)\right]-2h^2k_1g(k_1)+2\beta h\left(h^2+2k_1\right)=0 \quad (3.3)$$

This equation can be solved for k_1 and followed by $T_{0,1}$ using (3.2).

Now we consider the region PQRS for the application of Green's theorem and collocation at R and finite difference form of the basic equation at L. Thus

$$\int_P^Q T_x\,dt+\int_Q^R T\,dx+\oint_R^S T_x\,dt+\int_S^P T\,dx=0$$

Giving us

$$\frac{k_2}{2}\left[g(k_1)+g(k_1+k_2)\right]+\frac{h}{3}\left[T_{0,2}+4T_{1,2}\right]+\beta h-\frac{h}{2}\left[0+T_{0,1}\right]=0 \quad (3.4)$$

By collocation at R, that is, $\frac{\partial T}{\partial x}=-\beta\frac{dS}{dt},\left(T_{22}=0\right)$

$$\frac{1}{2h}\left(T_{0,2}-4T_{1,2}\right)=-\beta\frac{h}{k_2} \quad (3.5)$$

At L, we have $\frac{T_{1,2}-T_{1,1}}{k_2}=\frac{1}{h^2}\left[T_{2,2}-2T_{1,2}+T_{0,2}\right]$, simplifying to $T_{1,2}=\frac{k_2T_{0,2}}{h^2+2k_2}$

From (3.5) and this last relation, we can obtain

$$T_{0,2}=\frac{2\beta h^2\left(h^2+2k_2\right)}{k_2\left(2k_2-h^2\right)}\wedge T_{1,2}=\frac{2\beta h^2}{\left(2k_2-h^2\right)}(3.6)$$

$$T_{0,2}+4T_{1,2}=\frac{2\beta h^2\left(h^2+6k_2\right)}{k_2\left(2k_2-h^2\right)}$$

With this last relation and (3.4), we have the equation for k_2 as

$$3k_2\left(2k_2-h^2\right)\left\{k_2\left[g\left(k_1\right)+g\left(k_1+k_2\right)\right]+2\beta h-hT_{0,1}\right\}+4\beta h^3\left(h^2+6k_2\right)=0(3.7)$$

Knowing k_1, we can solve this equation for k_2 .

NOTE: One can choose the region SLRS for the application of Green's theorem. In place of collocation at R, we can use finite difference equivalent at Q, as well. It is ultimately the ease of obtaining $k_2, T_{(0,1)}\wedge T_{(0,2)}$ that decided the issue. These choices are considered later.

4. Algorithm For Continuing The Solution For Subsequent Time Step

We have (n+1) unknowns $T_1, T_2, T_3, \ldots, T_n$, $k_{n+1} at\, t=t_{n+1}$ with n equations coming from the Crank Nicholson scheme. Much needed another equation comes from the Stefan condition (1.4). Using one sided three point finite difference approximations

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

This can be put as: $4T_{n,n+1}-T_{n-1,n+1}=2\beta h^2/k_{n+1}(4.1)$

With $i=n$ in the system (2.2), we have

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

$$T_{n,n+1}=\frac{k_{n+1}}{\left(h^2+2k_{n+!}\right)}T_{n-1,n+1}(4.2)$$

(In fact, we cannot use Crank Nicolson scheme at (n, n+1), since point outside the domain occurs in the difference equation). This, when substituted in (4.1), we obtain

$$T_{n-1,n+1}=\frac{2\beta h^2\left(2k_{n+1}+h^2\right)}{k_{n+1}\left(2k_{n+1}-h^2\right)}(4.3)$$

and $T_{n,n+1}=\frac{2\beta h^2}{\left(2k_{n+1}-h^2\right)}(4.4)$

Considering (4.3) as a quadratic in k_{n+1}, the positive root can be obtained as:

$$k_{n+1}=\frac{h^2}{4T_{n-1,n+1}}\left[T_{n-1,n+1}+4\beta+\sqrt{\left(T_{n-1,n+1}+4\beta\right)^2+16\beta T_{n-1,n+1}}\right] \quad (4.5)$$

By considering the appendix, we have to choose k_{n+1} as a function of $T_{(i,n+1)}, i=1,2,\ldots,n.$ For physical consideration of the problem, we have to incorporate the Stefan condition (4.1) into this functional development. This is achieved, in what follows, by aligning the discrete equivalent of the parabolic equation with the discrete equivalent of the Stefan condition. We can choose any initial approximation to $k_{n+1}(¿0)$, solve the fully implicit scheme and obtain k_{n+1} from the resultant value of $T_{(n,n+1)}$ of (4.4) as

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

By the manner in which the relations (4.2) and (4.3) are derived, any choice of k_{n+1}, satisfies the requirements for convergence. With this new value of k_{n+1}, repeat the process until convergence which is ensured. But Crank-Nicholoson scheme is more accurate than the fully implicit scheme; therefore we decided to use this scheme as follows:

Choose an initial approximation for k_{n+1}; calculate $T_{n,n+1}$ using (4.4). Solve the finite difference equations for i = 1, 2… n-1 with $T_{n,n+1}$ as a boundary condition. From the resultant value for $T_{n-1,n+1}$, obtain k_{n+1} from the relation (4.5). Calculate $T_{n,n+1}$ using (4.4) and solve the difference equations as earlier. Repeat the process until desired degree of accuracy obtained.

4.1 Algorithm

STEP1: Obtain k_1 from (3.3) followed by k_2 from (3.7). We obtain $T_{0,1}$ from (3.2) and $T_{0,2}$ and $T_{1,2}$ from (3.6).

STEP2: Assume k_{n+1} (possibly, as $2k_n-k_{n-1}$)

STEP3: Obtain $T_{n,n+1}$ from (4.4)

STEP4: Solve the tri-diagonal system (2.1) for i = 1, 2, 3… n-1 using $T_{n,n+1}$ as a boundary condition.

STEP5: Knowing $T_{n-1,n+1}$, obtain k_{n+1} from (4.5). Repeat the steps (3), (4), (5) until convergence occurs.

5. Examples

EXAMPLE.1: The problem considered by Douglas and Gallie [2] later improved by Gupta and Kumar [3].The results are summarized in the following table1.

Table 1. Points on the front: $g(t)=-1;\beta=1$

x	Our Result		Results of Gupta & Kumar	
	h=0.02	h=0.01	h=0.1	h=0.01
0.2	0.2194	0.2188	0.2091	0.2172
0.6	0.7464	0.7447	0.7186	0.7406
1	1.3697	1.3672	1.3285	1.3604
1.6	2.4584	2.455	2.3944	2.4413
2	3.2762	3.2723	3.1993	3.2522
2.6	4.6294	4.0249	3.534	4.5916
3	5.6108	5.606	5.5004	5.5399
5	11.384	11.3787	--------	--------

5.1 Discussion on the paper by innovators of variable time step method

Douglas and Gallie [2], the first to introduce the variable time step for a fixed space step, wrote down the finite difference scheme by replacing the Stefan condition with

$$x(t)=t-\int_0^{x(t)} u(x,t)dx \quad (5.1)$$

Their iterative scheme for finding the time step is

$$k_{n+1}^{(r+1)}=\left(n+1+\sum_{\square}^{\square} T_{i,n+1}^{(r)}\right)h-t_n \quad (5.2)$$

along with $T_{0,n+1}^{(r)}-T_{1,n+1}^{(r)}=h$ and using the fully implicit scheme for parabolic equation. They started with assumption $k_1=h$ and $T_{0,1}=h$.

This algorithm had a problem of convergence while trying iteratively to find the time step as the solution progressed. Gupta and Kumar [3] used the Stefan condition and their iteration is defined by $k_{n+1}^{(r+1)}=h^2/T_{n,n+1}^{(r)}$ which can be obtained from the first order discrete equivalent of the Stefan condition.

$$\frac{\partial T}{\partial x}=\frac{-dS}{dt} \quad \text{as} \quad \frac{T_{n+1,n+1}-T_{n,n+1}}{h}=-h/k_{n+1}$$

Giving the iteration $k_{n+1}=h^2/T_{n,n+1}\left(T_{n+1,n+1}=0\right)$

Later authors reported difficulties for large x with their layout $[1;p170]$. Indeed, the authors did not establish the convergence of their iterative method for finding k_{n+1}. But we have established that our iteration necessarily converges. In fact, iteration for k_{n+1} (which is of the order of 10^{-1}) converged when we started with 1, 5 or 10 or even higher. Of course, the number of iterations increased from 7 or 8 to 12 or 13. This is the power of our algorithm as established in appendix.

We want to note that the finite difference analogue of the problem for finding k_{n+1} as appeared in [2] can be obtained by the application of Green's theorem for the region OABO.

Thus

$$T_x\,dt+\int_0^{(n+1)h} Tdx+\int_{(n+1)h}^{O} T_x\,dt=¿0$$

$$\int_0^{t_{n+1}} ¿$$

For this problem $T_x=-1\,along\,OA\wedge\beta=1$

Evaluating the first two integrals by Composite Trapezoidal rule,

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

Giving us

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

This is same as given in their paper; except that $\frac{1}{2}T_{0,n+1}$ is missing.

For comparison, from (3.3), when $T_x=-1\wedge\beta=1,$

$$k_1\approx h+\frac{h^2}{2}(by\,expansion\,of\,the\,positive\,square\,root\,of\,the\,quadratic\in k_1)$$

and $T_{0,1}\approx h-\frac{h^2}{2}\,as\,against\,h\,for\,both\,k_1\wedge T_{0,1}\,of\,[2].$

Further, if we apply Green's theorem to the region R: OQRO (as was indirectly done in [2]), then $R=R_1\cup R_2$ where R_1 is the region OPS and R_2 is the region PQRS. As R_1 is used to find k_1, it seems redundant to include this region to find k_2. The authors in [2] have precisely done this for all time steps.

Example.2: $T_x(0,t)=g(t)=-e^t,\beta=1$

This problem has a closed form solution, $s(t)=t$ and $u(x,t)=e^{t-x}-1$ as noted by Mitchel and Vynnycky [6]. Noting that $g'(t)$ is needed while solving k_1 and k_2 by Newton's method, our method gives results up to four significant digits with h=0.0125.

Example.3:

We present an example for illustration. The results (points on the interface) are given with varying step sizes.

Table 3.$T(0, t) = g(t) = 1- 0.5.\sin(\pi t/2), \beta = 1.0$

x	h=0.1	h=0.05	h=0.025	h=0.0125
0.1	0.0187	0.0118	0.0087	0.0074
0.2	0.082	0.03	0.03	0.0278
0.3	0.0889	0.0719	0.0648	0.0618
0.4	0.1455	0.1233	0.1141	0.1102
0.5	0.2191	0.1907	0.1791	0.1741
1	0.9759	0.8845	0.8453	0.8279
3	6.456	6.3269	6.2528	6.2214
5	16.8887	16.7472	16.6835	16.6557

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