COMPUTATION OF ONE DIMENSIONAL ONE PHASE STEFAN PROBLEMS

V.G. Naidu [1]*, P. Kanakadurga Devi[2]

[1]* Adama Science and Technology University, Ethiopia.
[2]Department of Mathematics, MLR Institute of Technology, Hyderabad, India
[1]Email: naidoovedam@gmail.com *(Corresponding author)
[2]Email: durga.thulasi@gmail.com

Abstract*:* To design an efficient device or to calculate the performance of existing device requires an accurate analysis of parameters involved in the system. In this work, an efficient front tracking finite difference method is developed to solve one dimensional single phase moving boundary problem with Neumann condition. The basic difficulty apart from the need to find the moving boundary presented, 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 by modelling the problem, governing equations are developed with the conditions of the Stefan type problem, solved it and compared the obtained solutions with existing results wherever possible.

Keywords: *Moving boundary problems, Interface, Green's theorem, One phase*

https://doi.org/10.47412/VGMP9196

1. Introduction

Stefan problems occur during the heat flow with phase change and dependent on time. The practical applications are melting of ice, solidification of steel, industrial metal processing and medical sciences, where particular cancer cells may be destroyed under extremely cold conditions (cryosurgery). Thus, the boundary separating two phases develop and moves. The position of moving boundary can be treated as the part of solution process. As two conditions are required on the moving boundary itself and the other to find the solution of differential equation. Let a thin rod of a solid material is melted by supplying heat at one end melting takes place and the interface keeps on moving. By modelling the physical problem a parabolic partial differential equation can be obtained, which is to be solved by an approximate computational method.

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 types of 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 reference [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 [9-11]. 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 Mayer [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. Formulation of the Method of Solution

2.1 Preliminary Setup of the Method

When we ignore the heat diffusion in the solid phase of the problem considered, mathematical modelling of the problem (non-dimensional form and melting temperature normalized to zero) gets reduced to the form given [1] as

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2}, 0 < x < s(t), t > 0 \tag{2.1}$$

$$s(0) = 0; T(x,0) = 0, T(s(t),t) = 0 \tag{2.2}$$

$$\frac{\partial T}{\partial x} = g(t), \ at\ x = 0 \tag{2.3}$$

$$\beta \frac{ds}{dt} = -\frac{\partial T}{\partial x}|_{x=s(t)} \tag{2.4}$$

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 $x_i = ih,\ t_n = \sum_{l=1}^{n} k_l$;

$T_{i,n} = 0, i \geq n;\ i = n$ gives a point on the interface.

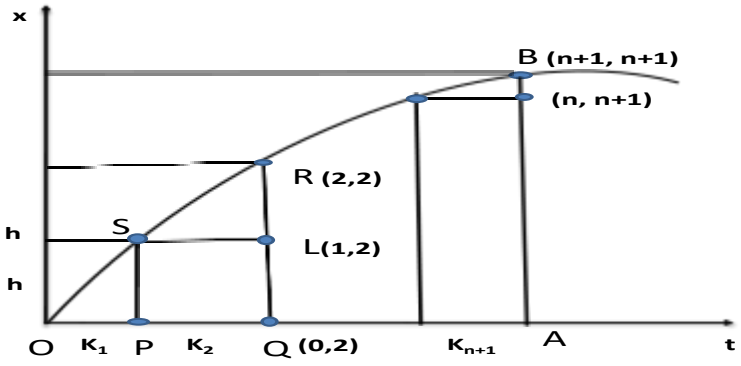

Fig.1 Moving boundary with fixed space step and variable time step.

Crank-Nicholson scheme for the diffusion Eq. (2.1) is

$$\frac{T_{i,n+1}-T_{i,n}}{k_{n+1}} = \frac{1}{2h^2}\left[\left(T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}\right) + \left(T_{i-1,n} - 2T_{i,n} + T_{i+1,n}\right)\right] \quad (2.5)$$

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

$$\frac{T_{i,n+1}-T_{i,n}}{k_{n+1}} = \frac{1}{h^2}\left(T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}\right) \quad (2.6)$$

The finite difference scheme Eq. (2.5) 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) as in Fig. 1. At these three points; $T_{2,2} = 0$, $T_{0,2}$ 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 one's 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 subsection 2.2, we derive equations to find k_1 and k_2. In subsection 2.3, we develop an iterative procedure to find k_n, for $n \geq 3$ and give the computational procedure as an algorithm, this subsubsection 2.3.1. In section 3, an example is given. The example originally considered in [2], which is interpreted in terms of our method and the algorithm developed is analysed.

2.2 Finding k_1 and k_2

For a given h, one needs to find $k_1, k_2, T_{0,1}, T_{0,2}\ and\ T_{1,2}$. 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 $t = t_1\ or\ t = t_2$.

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

$$\iint_{OPSO} (T_{xx} - T_t)dxdt = 0 = \oint_C (T_x dt + Tdx)$$

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

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

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

$\oint_S^O T_x dt = \beta\int_h^0(-ds) = \beta h$. 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 Eqn. (2.1) at P as

$$\frac{T_{0,1}-0}{k_1} = \frac{1}{h^2}\left[T_{1,1} - 2T_{0,1} + T_{-1,1}\right] \tag{3.2}$$

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

$T_{-1,1} = -2hg(k_1)$. Thus, the Eq. (3.2) reduces to

$$T_{0,1} = -\frac{2hk_1}{h^2+2k_1} g(k_1) \tag{3.3}$$

We obtain from Eq. (3.1) as

$$k_1(h^2 + 2k_1)[g(0) + g(k_1)] - 2h^2k_1g(k_1) + 2\beta h(h^2 + 2k_1) = 0 \tag{3.4}$$

This equation can be solved for k_1 and followed by $T_{0,1}$ using Eq. (3.3).

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, gives

$\frac{k_2}{2}[g(k_1) + g(k_1 + k_2)] + \frac{h}{3}\left[T_{0,2} + 4T_{1,2}\right] + \beta h - \frac{h}{2}\left[0 + T_{0,1}\right] = 0$. By collocation at R, $\frac{\partial T}{\partial x} = -\beta\frac{dS}{dt}$,

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

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 Eq. (3.5) and the last relation, we can obtain as $T_{0,2} = \frac{2\beta h^2(h^2+2k_2)}{k_2(2k_2-h^2)}$ *and* $T_{1,2} = \frac{2\beta h^2}{(2k_2-h^2)}$

$$T_{0,2} + 4\,T_{1,2} = \frac{2\beta h^2(h^2+6k_2)}{k_2(2k_2-h^2)} \tag{3.6}$$

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

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

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, $T_{(0,1)}$ *and* $T_{(0,2)}$ that decides the issue. These choices are considered later.

2.3 Continuing Solution for Subsequent Time Steps

We have (n+1) unknowns ($T_1, T_2, T_3, \dots, T_n, k_{n+1}$ at $t = t_{n+1}$) with n equations coming from the Crank Nicholson scheme. Much needed another equation comes from the Stefan condition Eq. (2.4), using one sided three point finite difference approximations gives

$$4T_{n,n+1} - T_{n-1,n+1} = 2\beta\, h^2/k_{n+1} \tag{4.1}$$

With $i = n$ in the system Eq. (2.6) simplifying, we have

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

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

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

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

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

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

By considering the appendix, we have to choose k_{n+1} as a function of $T_{(i,n+1)}, i = 1,2,\dots,n$. For physical consideration of the problem, we have to incorporate the Stefan condition Eq. (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 Eq. (4.4) as

$$k_{n+1} = \frac{h^2}{2T_{n,n+1}}\left(T_{n,n+1} + 2\beta\right) \tag{4.6}$$

By the manner in which the relations Eq. (4.2) and Eq. (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 Eq. (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 Eq. (4.5). Calculate $T_{n,n+1}$ using Eq. (4.4) and solve the difference equations as earlier. Repeat the process until desired degree of accuracy obtained.

2.3.1 Algorithm

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

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

Step 3: Obtain $T_{n,n+1}$ from Eq. (4.4)

Step 4: Solve the tri-diagonal system Eq. (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 Eq. (4.5). Repeat the steps 3, 4, 5, until convergence achieved.

3. Example

The problem considered by Douglas and Gallie [2] later improved by Gupta and Kumar [3] is considered here to compute and compare the results obtained using the method developed here. The results are summarized in the following table. 1.

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

x	Present Results		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	--------	--------

4. Observation and Analysis

This example considered by Douglas [2] and improved by Gupta and Kumar [7] and Marshall [4] is used in the development of the numerical method. The same problem is solved by our method developed in the paper and compared the solution with their solution. It is confirmed that working of our method is not affected by the value of β in reference [10]. 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 observed that it is at least of second order in our calculations. Higher order accuracy can perhaps be obtained by improving these approximations. We hope this technique of applying Green's Theorem may be useful in applications elsewhere. The iterative method for finding k_{n+1} may be useful in problems where one relation is different from rest of the relations. In fact we tried with various starting approximations for k_{n+1} (say 5 or even10), where convergence occurred smoothly. Of- course number of iterations increased from 1 or 2 to 5 or 6. As a last remark, we want to mention that the algorithm developed in the paper is simple and easy to implement through computer programming compared to other methods available in literature. We hope the methodology developed here sets the tone for solving the two phase problems also.

5. Conclusion

As a conclusion highlights of this work includes

- Use of Green's theorem to obtain starting parameters needed to develop the full algorithm.
- A powerful grinding machine (iterative process) is developed for finding the subsequent time steps;
- This method can be effectively used for finding the time steps while solving all moving boundary problems with the sign of the discrete form of the Stefan conditions.

References

[1] Crank. J, 1984. Free and moving boundary value problems. Oxford Science Publications.

[2] Douglas Jr Jim, Jr Gallie T. M. On the numerical integration of parabolic differential equations subject to a moving boundary condition. Duke Mathematics Journal 22**,** (1955) 557-571.

[3] Kutluay S., Bahadir A.R, Ozeds A. The numerical solution of one phase classical Stefan problem. Journal of Computer Applications 81, (1997) 135-144.

[4. Marshall Guillermo. A front tracking method for one-dimensional moving boundary problems. SIAM I.Sci.Stat. 7, (1986) 252-263.

[5] Mitchel S.L, Vynnycky. Finite difference method with increased accuracy and correct initialization for 1-dimensional Stefan problem. Applied Mathematics and Computation 215, (2009) 1609-1621.

[6] Mayer G.H. One -dimensional parabolic free boundary problems. SIAM Review 119, (1977) 17-34.

[7] Gupta P.S, Kumar D. A modified variable time step method for one dimensional Stefan problem**.** Comp. Math. Appl. Mech. Engineering no.23**, (**1980) 101-108.

[8] Koneru S.R, Lalli B.S. On convergence of iteration for fixed points of repulsive type. Canadian Maths Bulletin no.14 (1971) 353-357.

[9] Devi P.K, Naidu VG, A new finite difference front tracking method for Two phase 1-D moving boundary problems. Procedia Engineering (Elsevier) 127, (2015) 1034-1040.

[10] Kanaka durga Devi P. Front Tracking methods for one and two phase Stefan problems, Ph.D. dissertation S.V. University, Tirupati, India, 2016.

[11] Kanaka durga devi P, Naidu VG, Koneru S.R. Finite Difference method for 1-dimensional Stefan problems. Journal of Advanced Research in Dynamical and Control Systems no.3, (2018) 1245-1252.