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ONE-PHASE 1-D STEFAN PROBLEM USING BISECTION METHOD

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ABSTRACT The main purpose of this paper is to introduce a new method to obtain approximate solution to one phase Stefan problems. Several methods exist to solve these moving boundary problems. Each of them is mostly specific problem oriented and is not general enough to be applicable to a wide range of problems. The paper develops a front tracking finite difference method with variable time step. This variable time step method was suggested earlier, but without a well-defined complete methodology. For a fixed space step, first two time steps are obtained using collocation and/or Green's theorem of vector calculus. Subsequent step sizes are obtained by bisection of the discrete form of the Stefan condition. The method is general enough to be applicable to a broad class of moving boundary problems.

KEYWORDS : Moving boundary, Green's theorem, collocation, one phase problem, variable time step.

1. Introduction

The moving boundary problems occur mostly during the heat flows with phase changes. The phenomena of solidification and melting are associated with many practical applications. They take place in a diverse range of industrial processes, such as metal processing, solidification of castings, environmental engineering and thermal energy storage system in a space station. Material is subjected to a phase change in these processes. Thus, a boundary separating the two phases develops and moves. The position of the moving boundary cannot be identified in advance, but has to be determined as a part of the problem solution process. These problems are also referred to as Stefan problems.

1.1. Problem statement

At one end of a semi-infinite sheet of solid, initially at temperature zero (normalized), heat flux $g(t)$ is applied. The melting process starts and when the melting reaches a distance of $s(t)$, the diffusion of heat in the liquid phase is described by the moving boundary problem [1]

The heat equation having temperature T is:

$$\frac{\partial T}{\partial t}=\frac{\partial^2 T}{\partial x^2}, 0<x<s(t),\ \ t>0 \qquad (1)$$

$$s(0)=0;\ T(x,0)=0, T(s(t),t)=0 \qquad (2)$$

The Dirichlet condition:

$$T(x,t)=g(t),\ \text{at } x=0, \qquad (3)$$

Stefan condition:

$$\beta\frac{ds}{dt}=-\left.\frac{\partial T}{\partial x}\right|_{x=s(t)}. \qquad (4)$$

Diffusion coefficient is normalized to unity and diffusion of heat beyond $s(t)$ is assumed to be not taking place. Stefan number β is a constant depending on the density, specific heat and latent heat of the material. This is a one-phase problem. Two-phase problem considers the diffusion beyond $s(t)$ [2].

1.2. Theoretical background

Starting with any standard numerical method for Stefan problem 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 this problem. Reference is made in the books [3], [1] and [4] describing these efforts. Only one method [5] is relevant to us in the context of the method to be developed. For a fixed space step, they were the first to use variable time step sizes to track the front. Subsequently Douglas and Gallie improved iterative procedure in [6] for finding the time step. In [7] there were proposed applied level set and moving grid methods and phase field model to the classical problem of one and two phases with insulated ends over a finite interval. Finite difference method for Stefan problem was used in [8] and the Tau method used in [9]. Even these front tracking methods have made certain transformations of the original problem before writing down the finite difference method.

Another approach relevant to us is the well known method of lines developed in [10] where the mathematical problem was discretized with respect to time resulting in a system of ordinary differential equations with respect to space variable. In this paper, it was 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 [1], while finding the points on the interface. The method of lines is, of course, possible only for finite space domain.

We keep the problem as it occurred in formulation (1-4) and use the finite difference method applicable to *any parabolic problem*.

2. Preliminary setup of the method

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

If we know the T values along CD, it is easy to solve for the variable values along AB by any method applicable to a parabolic problem. We use Crank-Nicholson scheme. The question is how to find k_{n+1} and to start this procedure, how to obtain k_1 and k_2 along with T value at L. Obtaining k_1 and k_2 is presented in section 3, by application of Greens theorem and finite difference form of the parabolic equation. Finding k_{n+1} is presented in section 4 while simultaneously obtaining T values.

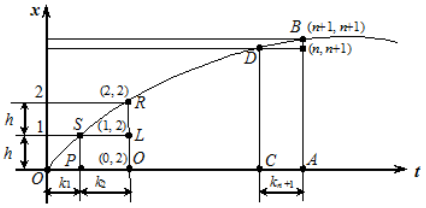

Fig. 1. Moving boundary with fixed space step and variable time step.

Crank-Nicholson scheme for the diffusion equation (1) is

$$\frac{T_{i,n+1}-T_{i,n}}{k_{n+1}}=\frac{1}{2h^2}\left[\left(T_{i-1,n+1}-2T_{i,n+1}+T_{i+1,n+1}\right)+\left(T_{i-1,n}-2T_{i,n}+T_{i+1,n}\right)\right] \quad (5)$$

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

$$\frac{T_{i,n+1}-T_{i,n}}{k_{n+1}}=\frac{1}{h^2}\left(T_{i-1,n+1}-2T_{i,n+1}+T_{i+1,n+1}\right) \quad (6)$$

The finite difference scheme (5) is of second order in space and time and is computationally stable [11]. To enable us using this scheme, we need to know a value of temperature *T* at three points: (0, 2), (1, 2) and (2, 2) (see Fig. 1). Of these three points $T_{2,2}=0$; $T_{0,2}$ and $T_{1,2}$ are not known. To know these starting values, we need to find time step sizes 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 $T_{0,3}$, $T_{1,3}$, $T_{2,3}$ at any value of 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 $n=3, 4, 5\ldots$ number of points along the line parallel to *x*-axis increasing by one. The example originally considered in [5] is interpreted in terms of our method and their algorithm is analyzed.

3. Finding time step sizes k_1 and k_2

For a given *h*, we need 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 components. 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*. Green's theorem comes handy in this situation. Using Green's theorem we get the expression at *O*. Green's theorem comes handy in this situation. Using Green's theorem we get the expression

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

where *c* is the boundary of the closed region under consideration.
As $T=0$ along segment *SO*, we have

$$\int_0^{k_1}T_x dt+\int_0^{h}T\,dx+\int_s^{o}T_x dt=0 \quad (7)$$

We use Trapezoidal rule for the first two integrals in (7) and, noting that $T_x=-\beta\frac{ds}{dt}$ along *SO*, we obtain

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

The relation (7) can be reduced to

$$\frac{k_1}{2}\left(g(0)+g(k_1)\right)+\frac{h}{2}T_{0,1}+\beta\,h=0 \quad (8)$$

To find $T_{0,1}$ we use finite difference which is equivalent to the basic equation (1) at point *P* (Fig. 1) and obtain

$$\frac{T_{0,1}-0}{k_1}=\frac{1}{h^2}\left[T_{1,1}-2T_{0,1}+T_{-1,1}\right] \quad (9)$$

The temperature $T_{-1,1}$ is evaluated using $T_x=g(t)$. That is, $\frac{T_{1,1}-T_{-1,1}}{2h}=g(k_1)$ giving the expression $T_{-1,1}=-2hg(k_1)$ Thus, the equation (9) is reduced to

$$T_{0,1}=-\frac{2hk_1}{h^2+2k_1}g(k_1) \quad (10)$$

We obtain from (8)

$$k_1\left(h^2+2k_1\right)\left[g(0)+g(k_1)\right]-2h^2k_1g(k_1)+2\beta h\left(h^2+2k_1\right) \quad (11)$$

The equation (11) can be solved for k_1 and followed by $T_{0,1}$ using (10).

Now we consider the region *PQRS* (Fig. 1) in order to apply Green's theorem, collocation at point *R* and finite difference form of the basic equation (1) at point *L*. Then we have

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

from where we obtain

$$\frac{k_2}{2}\left[g(k_1)+g(k_1+k_2)\right]+\frac{h}{3}\left[T_{0,2}+4T_{1,2}\right]+\beta h-\frac{h}{2}\left[0+T_{0,1}\right]=0 \quad (12)$$

By collocation at point *R*, that means that $\frac{\partial T}{\partial x}=-\beta\frac{ds}{dt}$ at $T_{2,2}=0$, we have

$$\frac{1}{2h}\left[T_{0,2}-4T_{1,2}\right]=-\beta\frac{h}{k_2} \quad (13)$$

At point L, in similar way we have $T_{1,2}=\frac{k_2T_{0,2}}{h^2+2k_2}$ from where and taking into account (13) we obtain formulas for temperatures

$$T_{0,2}=\frac{2\beta h^2\left(h^2+2k_2\right)}{k_2\left(2k_2-h^2\right)};\ T_{1,2}=\frac{2\beta h^2}{\left(2k_2-h^2\right)}\ \text{and}\ T_{0,2}+4T_{1,2}=\frac{2\beta h^2\left(h^2+6k_2\right)}{k_2\left(2k_2-h^2\right)} \quad (14)$$

From (12) and (14) we have the equation for k_2 as follows:

$$3k_2\left(2k_2-h^2\right)\left\{k_2\left[g(k_1)+g(k_1+k_2)\right]+2\beta h-hT_{0,1}\right\}+4\beta h^3\left(h^2+6k_2\right)=0. \quad (15)$$

Knowing k_1 we can solve this equation for k_2.

Notice that one can choose also the region *SLRS* for the application of Green's theorem. In place of collocation at point *R*, we can use finite difference equivalent at point *Q*, as well. It is ultimately the ease of obtaining k_2, $T_{0,1}$ and $T_{0,2}$ that decided the issue.

4. Finding time step k_{n+1}

We have $n+1$ unknowns $T_1, T_2, T_3, \ldots, T_n, T_{n+1}$ at $t=T_{n+1}$ with *n* equations coming from the Crank-Nicholson scheme. Much needed another equation comes from the Stefan condition (4). Using three point one sided finite difference approximations we have the following expression:

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

from which the following equation is derived:

$$4T_{n,n+1}-T_{n-1,n+1}=2\beta h^2/k_{n+1} \quad (16)$$

With $i=n$ in the expression (6), we have

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

from which we obtain

$$T_{n,n+1}=\frac{k_{n+1}}{\left(h^2+2k_{n+1}\right)}T_{n-1,n+1} \quad (17)$$

In fact, we cannot use Crank-Nicolson scheme at point (n, n+1), since this point occurs outside the domain in the difference equation). Substituting (17) in (16), we obtain

$$T_{n-1,n+1}=\frac{2\beta h^2\left(2k_{n+1}+h^2\right)}{k_{n+1}\left(2k_{n+1}-h^2\right)} \quad (18)$$

and then from (18) we have

$$k_{n+1}\left(2k_{n+1}-h^2\right)T_{n-1,\,n+1}-2\beta h^2\left(2k_{n+1}+h^2\right)=F \qquad (19)$$

From (17) and (18) it follows the equation

$$T_{n,\,n+1}=\frac{2\beta h^2}{\left(2k_{n+1}-h^2\right)} \qquad (20)$$

and temperature T1,2 can be taken from (14).

For any given time step $\Delta t\left(=k_{n+1}\right)$ obtain $T_{n,n+1}$ from (20) and solve the tri-diagonal system of equations (5) for $i = 1, 2, 3, \ldots, n-1$ (arising out of Crank-Nicholson scheme) using $T_{n,n+1}$ as a boundary condition. Knowing $T_{n-1,n+1}$ one can evaluate F using (19). Time step is found by bisection method with the sign of F.

5. Numerical example

Experimental investigations of the problem were conducted by Douglas and Gallie in [9] and later improved in [10]. They calculated points on the front at heat flux $g(t) = -1$ and Stefan number $= 1$ with step size $h = 0.1, 0.05, 0.025$ and 0.01. The results are summarized in Table 1 where are shown in cells with grey background. Method used in [10] was able to calculate time step sizes only for x varying from 0.2 through 3.

Results by our VTFS method implemented in FORTRAN 99 are presented up to $x = 20$ (it should be noticed that the method, by its nature, has no upper limit for x) with four different step sizes in an attempt to establish the accuracy of our results. For each time step the iteration was continued until accuracy of 10^{-10} is achieved.

For all values of x, number of iterations was the same and approximately equal to values reduced to Table 2.

Accuracy is less, for large x, in the results of [10]. Discretization error is more in the implicit scheme as compared to Crank-Nicholson scheme used in our VTFS method.

Table 1. Points on the front at heat flux $g(t) = -1$; Stefan number $\beta = 1$.

x	Step sizes			
	h = 0.1	**h = 0.05**	**h = 0.025**	**h = 0.01**
0.2	0.2186	0.2205	0.2196	0.2188
	−0.2091	−0.2141	−0.2161	−0.2172
0.4	0.4756	0.4727	0.4703	0.4685
	−0.4503	−0.4593	−0.4637	−0.4656
1	1.3868	1.3768	1.3709	1.3672
	−1.3265	−1.3465	−1.3569	−1.3604
1.4	2.099	2.0854	2.0779	2.0732
	−2.019	−2.0464	−2.0594	−2.0621
2	3.3058	3.2877	3.2781	3.2723
	−3.1993	−3.2373	−3.2531	−3.2522
2.4	4.1955	4.175	4.1642	4.1578
	−4.0727	−4.1172	−4.1346	−4.1295
3	5.6494	5.6255	5.6131	5.606
	−5.5035	−5.557	−5.5762	−5.5599
5	11.4363	11.4036	11.3868	11.3787
	*	*	*	*
10	31.3597	31.3118	31.2872	31.2809
	*	*	*	*
15	58.0377	57.9786	57.9461	57.9438
	*	*	*	*
20	90.7591	90.6901	90.6486	90.7011
	*	*	*	*

Symbol '*' indicates non availability of data in [10].

Table 2. Iteration numbers of VTFS method for different step sizes h

$h = 0.1$	$h = 0.05$	$h = 0.025$	h = 0.01
9	10	11	12

Table.2a: Example 2a: $T(0, t) = g(t) = 1, \beta = 2.0$

	0.1	0.05	0.025	0.0125		True Solution
0.1	0.0268	0.019	0.0149	0.0139	1.179	
0.2	0.0759	0.0595	0.0524	0.0491	1.108	
0.5	0.3536	0.319	0.3033	0.296	1.088	s(t)= 2α√t
1	1.2761	1.2133	1.1841	1.1703	1.082	
5	29.4635	29.1915	29.0606	29.0005	1.077	
6	42.2952	41.9723	41.8171	41.7479	1.077	
7	57.4412	57.0678	56.889	56.8139	1.077	
8	74.9017	74.4778	74.277	74.2008	1.077	

*The constant α depends on β in the true solution.

6. Accuracy of time step sizes calculation

Discontinuity in the initial and boundary conditions normally occur in the formulation of Stefan problems. Different techniques may give different values for these initial time steps. But as long as they are obtained by a consistent numerical method, the difference between two solutions with two different sets of k_1 and k_2 goes on reducing with time. This is what we observed in our computational experiments. This is supported by Pearson [17] while discussing the effect of impulsive condition for the standard heat equation defined over the unit length.

Consider (19) as a quadratic form in time step size k_{n+1} and obtain value of k_{n+1} as its positive root:

$$k_{n+1}=\frac{h^2}{4T_{n-1,n+1}}\left[T_{n-1,n+1}+4\beta+\sqrt{\left(T_{n-1,n+1}+4\beta\right)^2+16\beta T_{n-1,n+1}}\right] \qquad (21)$$

The procedure now is to assume any value for k_{n+1}, to obtain $T_{n,n+1}$ and solve the tridiagonal system as before. Knowing $T_{n-1,n+1}$, obtain the root of the quadratic and repeat the process. It took five or six iterations for the process to convergent. In [10], it was not established the convergence of iterative process. Convergence of both VTFS method and one of [10] can be established with the help of the theorem by Koneru and Lalli [18].

Suppose we have $(n - 1)$ relations involving n variables $x_1, x_2, x_3, .., x_n$, that is

$$x_j=\phi_j\left(x_1,x_2,x_3,\cdots,x_n\right),\ j=1,2,\cdots n-1 \qquad (22)$$

And another relation

$$x_n=p\left(x_1,x_2,x_3,\cdots,x_{n-1}\right) \qquad (23)$$

Let the eigen values of the Jacobi matrix of the $(n - 1)$ functions in (i) be less than unity in magnitude, then the value is a neighborhood of the true solution of (i) with x_n given by (ii). The iteration defined by (I) converges if we start in that neighborhood and after every iteration x_n is obtained from (ii). This is established in [18].

Applying this result to our method, we obtain the system (22) to be linear. The tri diagonal system occurring in the problem is a diagonally dominant and the Jacobi matrix is a convergent one. Any Jacobi based iteration, e.g. Gauss-Seidel or *SOR*, converges for any initial approximation for the variables. Rather than carrying one iteration we solve the tri diagonal system (thereby implying that iteration is carried until convergence) and then obtain x_n. For any given x_n if there exists a set of $x_1, x_2, x_3, .., x_{n-1}$ we can then take any arbitrary value for x_n for starting the process. That means that we can use any step size h in our main problem (1-4).

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References

1. Crank, J. (1984). Free and moving boundary problems, Clarendon Press, Oxford.
2. Pathella, D., Naidu, V.G. (2015). A New Finite Difference Front Tracking Method for Two Phase 1-D Moving Boundary Problems. Procedia Engineering, 127, 1034-1040.
3. Andreucci, D. Lecture notes on the Stefan problem. http://www.dmmm.uniroma1.it /pubblicazioni/doc/phd_quaderni/02-1-and.pdf. Accessed 21.03.2016. (2002).
4. Gupta, S. C. (2003). The Classical Stefan Problem - Basic Concepts, Modelling and Analysis. Elsevier Science B.V, Amsterdam.
5. Douglas, Jr. Jim, and Gallie, T.M. (1955). On the numerical integration of parabolic

differential equations subject to a moving boundary condition. Duke Math. J., 22, 557-571.
6. Gupta, P.S., and Kumar, D. (1980). A modified variable time step method for one dimensional Stefan problem. Comp. Math. Appl. Mech. Engineering, 23, 101-108.
7. Kutluay, S., Bahadir, A.R., and Ozdes, A. (1997). The numerical solution of one phase classical Stefan problem. J. Compute. Appl. Math., 81, 135-144.
8. Javierre, E., and Vuik, C., and Vermolen, F.J., and van der Zwaag, S. (2006). A comparison of models for one-dimensional Stefan problems. J. Comp. Appl. Math., 192, 445-459.
9. Mitchel, S. L., and Vynnycky. (2009). Finite difference method with increased accuracy and correct initialization for 1-dimensional Stefan problem. Applied Mathematics and Computation, 215, 1609 - 1621.
10. Alliabadi, M.H., and Ortiz, E.L. (1998). Numerical Treatment of moving and free boundary value problems with the Tau method. Computers Math. Applic., 35, 53-61.
11. Mayer, G.H. (1977). One dimensional parabolic free boundary problems. SIAM review, 119, 17-34.
12. Larsson, S., and Thomée, V. (2005). Partial Differential Equations with Numerical Methods. Springer, Berlin.
13. Pearson, C.E. (1965). Impulsive end conditions for diffusion equation. Math. Comp., 19, 572-576.
14. Koneru, S.R., and Lalli, B.S. (1971). On Convergence of iteration for fixed points of repulsive type. Canad. Math. Bulletin, 14, 353-357.
15. V. Voller, and M. Cross. (1980). Accurate solutions of moving boundary problems using Enthalpy Method. Int. J. Heat Mass Transfer, 24, 545-556.
16. Vuik, C., Segal, G., and Vermolen, F.J. (2000). A conserving discretization for a Stefan problem with an interface reaction at the free boundary. Comput. Visual Sci., 3, 109-114.