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One Phase Moving Boundary Problem

P. Kanakadurga Devi, V. G. Naidu

Abstract: ***In this paper we introduced a variable time step method to obtain interface to moving boundary problem for Slab and Sphere. We present the basic difficulty, apart from the need to find the moving boundary, that there is no domain for the space variable. This difficulty is handled by the age old principles of basic mathematics. Naturally, giving symbolic names to the unknowns develop equations involving them and solve it using the conditions of the problem. High order accurate initial time step sizes for given space step size are obtained with the help of Green's theorem. The Subsequent time steps are obtained by an iterative scheme. This variable time step method handles Dirichlet's problem of freezing or melting of a Slab and spherical droplet.***

Keywords: ***interface, Finite difference method, Crank-Nicolson scheme, stefan problem, variable time step.***

I. INTRODUCTION

If thin rod of a solid material is melted by suppling heat, at one end, melting takes and the interface keeps moving.
When a spherical ball is frozen (or melted), the equation for the heat diffusion along a radial line is governed by [1].The spherical polar coordinates governing equations are reduced to

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

$$T(0,t) = -1 \tag{2}$$

$$T(s(t),t) = 0 \tag{3}$$

$$s(0) = 0 \tag{4}$$

$$\frac{\partial T}{\partial x} = \beta(1-x)\frac{ds}{dt} \tag{5}$$

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. The basic methodology will be developed in section 2.In section 3, we derive two equations involving the two unknowns using **Green's theorem** for the given problem and obtained $T_{1,2}$ to start the solution procedure. Once we do this, we can find $T_{1,3}$, $T_{2,3}$ provided k_3. This can be continued to solve the diffusion equation for n = 3, 4, 5…. . The number of points along the line parallel to x-axis increases one by one for increasing *n*. In section 4, iterative procedure to find k_n, for $n \geq 3$ and the computational procedure as an algorithm is given in this section. Consideration of the convergence to find k_n is done in section 5 and an example is given in section 6. The well known one phase problem of freezing (or melting) of a spherical droplet is given as an example.
Stewartson and Waechter [10] obtained solution by asymptotic expansion of the variables and discussed the results qualitatively. Similar exercise was done by Soward [9]. Davis and Hill [1] is one of the few researchers, who gave quantitative details about the time taken for the interface to reach the centre. Numerical Methods to obtain approximate solution relevant to our work, was first introduced by Douglas and Gallie [2]. Although no specific results were presentedfor a fixed space step, they used variable time step sizes to track the front. Gupta and Kumar [3] and Marshall [6] have subsequently improved the iterative procedure of [2] for finding the time step. Kutluay [5] obtained numerical solution of a specific problem with variable space grid; even these front tracking methods have made certain transformations of the original problem [11-12].

II. BASIC FRAME WORK OF COMPUTATIONAL METHODOLOGY

For a fixed space step size, the time intervals needed for the interface can be fine. 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 temperature on the interface.

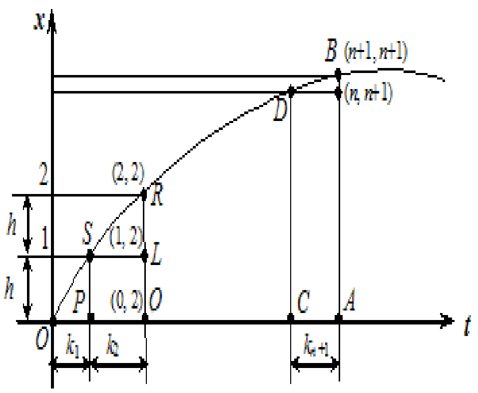

Fig. 1. Moving boundary with variable time step.

Using theCrank-Nicolson scheme the diffusion equation becomes

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

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

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$$\frac{T_{i,n+1} - T_{i,n}}{k_{n+1}} = \frac{1}{h^2}\left(T_{i-1,n+1} - 2T_{i,n+1} + T_{i+1,n+1}\right) \quad (7)$$

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; $T_{0,2}$ is given in the problem, $T_{2,2} = 0$ and $T_{1,2}$ is not known. To know these starting ingredients, we need to find k_1 andk_2.

This is a first order approximation in x and t. Apply the Green's theorem in the region OPS in the first cell. In the process, we need the second degree polynomial to the interface passing through the points $(0,0), (k_1, h)$ and $(k_1 + k_2, 2h)$ as

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

$$\frac{ds}{dt}_{t=0} = \dot{s}(0) = h\frac{[k_2^2 - k_1^2 + 2k_1k_2]}{k_1k_2(k_1+k_2)} = \frac{1}{\beta(1-x)}T_{x(0,0)} \quad (8)$$

$$\frac{ds}{dt}_{t=t_1} = \dot{s}(t_1) = h\frac{[k_2^2 + k_1^2]}{k_1k_2(k_1+k_2)} = \frac{1}{\beta(1-x)}T_{x(1,1)} \quad (9)$$

$$\frac{ds}{dt}_{t=t_2} = \dot{s}(t_2) = h\frac{[k_1^2 - k_2^2 + 2k_1k_2]}{k_1k_2(k_1+k_2)} = \frac{1}{\beta(1-x)}T_{x(2,2)} \quad (10)$$

We know that by Green's Theorem

$$\oiint_R [T_{xx} - T_t]dxdt = 0 => \int_C [T_x dt + T dx] = 0 ,$$

Where c is the boundary of R and $c = OP \cup PS \cup SO$

$$I_1 = \int_{OP} [T_x dt + T dx] = \int_0^{k_1} [T_x dt] = \frac{k_1}{2}[T_x|_O + T_x|_P]$$

Therefore$I_1 = \frac{k_1}{2}\left[-\frac{g(k_1)}{h} + \beta(1-h)h\frac{[k_2^2 - k_1^2 + 2k_1k_2]}{k_1k_2(k_1+k_2)}\right]$

Here, we approximated $T_x|_P$ by $\frac{T_S - T_P}{h} = \frac{0 - g(k_1)}{h}$, $T_x|_O = \beta(1-x)\dot{s}(0)$ and

$$I_2 = \int_{PS} [T_x dt + T dx] = \int_0^{h} [T dx] = \frac{h}{2}[T|_P + T|_S]$$

Thus $I_2 = \frac{h}{2}g(k_1)(T_s = 0$ being on the interface)

Now$I_3 = \int_{SO} [T_x dt + T dx] = \int_{k_1}^{0} [T_x dt]$ $(T = 0$ at$S)$

$$I_3 = \int_{k_1}^{0}\left[\beta(1-x)\frac{ds}{dt}dt\right] = -\frac{\beta h}{2}(2-h)$$

Thus $I_3 = -\frac{\beta h}{2}(2-h)$

By the green's theorem $I_1 + I_2 + I_3 = 0$

$$\frac{k_1}{2}\left[-\frac{g(k_1)}{h} + \beta(1-h)h\frac{[k_2^2 - k_1^2 + 2k_1k_2]}{k_1k_2(k_1+k_2)}\right] + \frac{h}{2}g(k_1) - \frac{\beta h}{2}(2-h) = 0$$

We thus have one relation involving two unknowns k_1 and k_2 as

$$\boldsymbol{g(k_1)k_2(k_1+k_2)(h^2 - k_1) - \beta h^2(2-h)(k_1{}^2 + k_2{}^2) = 0} \quad (11)$$

To derive another equation involving $k_1$andk_2, we have from Stefan's condition at (2, 2) gives

$$\frac{2\beta h^2(1-2h)}{k_2} = 4T_{1,2} - g(t_2) \quad (12)$$

At (1, 2), from (7)$T_{1,2} = \frac{k_2 g(t_2)}{h^2 + 2k_2}$ (13)

Using the equation (13) in (12) we get

Thus

$$\boldsymbol{k_2 g(t_2)(2k_2 - h^2) + 2\beta h^2(1-2h)(2k_2 + h^2) = 0} \quad (14)$$

We can solve (11) and (14) to find k_1 and k_2 using the relation (13).

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 at (n+1, n+1) as

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

This can be written as:

$$4T_{n,n+1} - T_{n-1,n+1} = 2\beta(1-nh)\frac{h^2}{k_{n+1}} \quad (15)$$

With $i = n$ in the system (7), we have

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

On simplifying to (In fact, we cannot use Crank- Nicolson scheme at (n, n+1) since the point outside the domain occurs in the difference equation)

Thus $T_{n,n+1} = \frac{k_{n+1}}{(h^2 + 2k_{n+1})}T_{n-1,n+1}$ (16)

This, when substituted in (16), we get

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

Using (17) in (16) we get $T_{n,n+1} = \frac{2\beta h^2(1-nh)}{(h^2 - 2k_{n+1})}$ (18)

Considering (17) as a quadratic in k_{n+1}, the positive root can be obtained as:

$$k_{n+1} = \frac{h^2}{4T_{n-1,n+1}}\left[T_{n-1,n+1} - 4\beta(1-nh) - \sqrt{\left(T_{n-1,n+1} + 4\beta(1-nh)\right)^2 + 16\beta(1-nh)T_{n-1,n+1}}\right] \quad (19)$$

Choosing an initial approximation fork_{n+1}; calculate$T_{n,n+1}$ using (18). Solve the finite difference equations for $i = 1, 2\ldots n-1$ 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 (19). Calculate $T_{n,n+1}$ using (18) and solve the difference equations as earlier. Repeat the process until the desired degree of accuracy occurs.

III. CONVERGENCE

If $k_{n+1}$is chosen on the manifold given by equation (15) for every iteration, convergence of the solution of the method is assured by Koneru and Lalli [4]. But to reduce the computational effort, we have solved the system by Thomas algorithm. We have to make sure that k_{n+1}, after each such solution, has to be chosen satisfying (15), equivalently (17) and (18). Thus we calculate k_{n+1}using (19) satisfying (17) and obtain T_n from (18) with this k_{n+1} and use it as a boundary condition. After choosing k_{n+1} to start the iteration process, some value of $T_n$exists and lies on the manifold. Any starting value for k_{n+1} works, as this implies any starting values for T_{n-1} and $T_n$satisfying (17) and (18);

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and that means (15). We have to first calculate T_n and solve for $T_{n-1}, T_{n-2}, T_{n-3}, \ldots, T_2$, T_1.

IV. EXAMPLES

We obtained the numerical solution using the algorithm of section 2.Time for the interface to reach the centre with varying step sizes and for several values of the Stefan constant (β) are presented in the table 1. Results from Davis and Hill [1] with first three terms of the expansions are given in the last column. These obtained present results are compared well with ref. [1].

Table 1.Time taken for the interface to reach the centre for $g(t) = -1$

Present Results for different values of β					
β\h	0.04	0.02	0.01	0.005	Results of ref. [1]
0.25	0.1219	0.1270	0.1266	0.1265	0.131
0.5	0.1826	0.1805	0.1800	0.1799	0.190
1.0	0.2781	0.2760	0.2753	0.2752	0.290
5.0	0.9690	0.9678	0.9671	0.9667	0.987
10.0	1.8088	1.8092	1.8087	1.8084	1.83
50.0	8.4695	8.4851	8.4880	8.4886	8.50

The interface for the one phase sphere problem has been presented graphically with β =1, 10,50 in figure 2.The impact of Stefan number β is clearly seen from the graphs drawn.

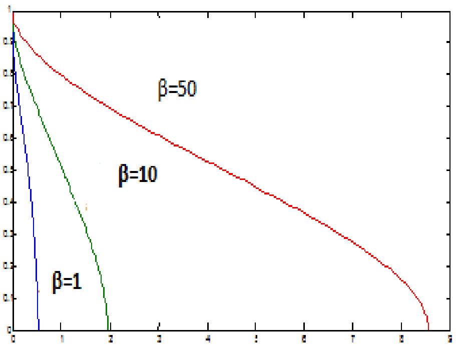

Fig 2. *Interface for the sphere proble*

It may be noted that even if the freezing process on the surface is time dependent, our algorithm works well without any difficulty. Indeed, this statement applies to all the problems considered by us. The computational method to obtain an approximate solution to the classical two-phase Stefan problem with quadratic polynomial approximation to the front has been discussed in [8].

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3	M.Sc(Applied Mathematics)	Andhra University, Vizag	2004-2006	70
4	B.Sc(Computer science)	Bapatla College of Arts and Science, Bapatla	2001-2004	72
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1	Assoc. Prof.	MLR Institute of Technology	2017	
2	Asst. Prof.	Vignan University,Guntur	2015	2017
3	Asst. Prof.	Vignan University,Guntur.	2009	2010
4	Asst. Prof.	Gudlavalleru Engineering College,Gudlavalleru.	2007	2009

Software Proficiency: Languages : FORTRAN, C, .NET

Professional Recognition/ Award/ Prize/ Certificate, Fellowship received by the applicant.

i. Selected as **Associative fellow** in AP science congress

ii. Got **1st** rank in **N U CET-2004** in Mathematics.

iii. **FET** (Faculty Eligibility Test) qualified in 2012.

iv. Completed Rastrabhasha Praveena in Hindi.

Publications:

Number of Publications: 7

1. Kanakadurga Devi P., Naidu.V.G. (2018). One Dimensional Two Phase Problem. IEEE Xplore.
2. Kanakadurga Devi P., Naidu.V.G. (2018). Free and Moving Boundary Problems of Heat and Mass Transfer . International Journal of Engineering & Technology, 7 (3.27) (2018) 18-19.
3. Kanakadurga Devi P., Naidu.V.G. (2018). Finite difference method for One dimensional Stefan Problem journal of Adv Research in Dynamical & Control systems, Vol. 10, 02-Special Issue, 2018.
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Participation/Presentation of papers in Conferences: 10

1. International Conference on Smart System and Inventive Technology (ICSSIT 2018), organized by Francis Xavier Engineering College, during December 13-14, 2018 at Tirunelveli, Tamilnadu, India.
2. Presented and selected for Best poster award in the Andhra Pradesh Science Congress held at Yogi Vemana University during 9-11 November, 2018.
3. Quality Improvement Program conducted by Nation Institute of Technical Teachers Training & Research in MLR institute of technology from 2nd to 7th Jult 2018.
4. World summit on advances in science, engineering and technology, university of Cambridge, united kingdom, one phase 1-d moving boundary problem for sphere 2018.
5. Two days Research Workshop at IIIT, Hyderabad on 26-27th August 2017.
6. International Workshop and Conference on Mathematical Computer Engineering (ICMCE-2016), December 16-17, 2016, organized by the school of Advanced Sciences, VIT University, Chennai.
7. International Workshop and Conference on Analysis and Applied Mathematics (IWCAAM)-2016, June 06-10, 2016, at department of Mathematics, National Institution of Technology, Tiruchirappalli.
8. International Conference on Computational Heat and Mass Transfer (ICCHMT)-2015, 30 Nov-2 Dec 2015, at department of Mathematics, National Institution of Technology, Warangal.
9. 102nd Indian Science Congress to be held at Mumbai University from 3rd to 7th January 2015.
10. II International Conference on Applications of Fluid Dynamics, 21st -23rd, July 2014 at department of Mathematics, Sri Venkateswara University, Tirupati.
11. National Conference on Applications of Mathematics in Engineering, Physical and Life Sciences, 7-9, December 2012 in Sri Venkateswara University, Tirupati.
12. Two-week ISTE WORKSHOP on Introduction to Research Methodologies conducted by Indian institute of Technology Bombay from 25th June to 04th July, 2012 in Gokaraju Rangaraju Institute of Engineering and Technology, Hyderabad.
13. Faculty development program (FDP) from 10th July to 15th July 2009 in VIGNAN UNIVERSITY, Guntur.

RESEARCH ACTIVITY

I have completed my M. Phil in the year 2012; topic entitled “Fourth Order Difference Methods for the System of 2-D Nonlinear Elliptic Partial Differential Equations” under the guidance of Prof. S.R.K Iyengar (Formerly Professor and Head, Dept of Mathematics, IIT, and New Delhi) and Prof. G. Viswanatha Reddy, Dept of Mathematics, Sri Venkateswara University, Tirupati.

After completion of M.Phil, registered for Ph. D project and awarded the thesis entitled “Front Tracking Methods for One and Two Phase Stefan Problems” under the guidance of Prof. S.R Koneru (Retired from IIT, Mumbai), Prof. V.G.S. Naidu and Prof. G. Viswanatha Reddy, Dept of Mathematics , Sri Venkateswara University, Tirupati.

This thesis is concerned with the development of computational methods for obtaining solutions of moving boundary problems. The moving boundary problems occur mostly during the heat flow with phase changes. The phenomena of solidification and melting are associated with many practical applications such as metal processing, solidification of castings, environmental engineering, thermal energy storage system in a space station and medical sciences (cryosurgery).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 solution process. These problems are also referred to as Stefan problems. If the diffusion of heat takes place in both phases (possibly with different diffusion rates), the problem is known as a two phase problem, which is realistic.

While attempting to solve this problem the moving boundary or interface that separates the two regions presents a major difficulty. A systematic and well defined methodology is developed in this work for solving both formulated partial differential equations, which cannot be solved by analytical methods.

Numerical methods usually applied for problems involving discretization of the independent variables with a fixed size in each of them. Techniques are available to make the discretization finer depending on the gradient of the dependent variable in certain parts of the domain. But in moving boundary value problems, domain itself is not known a priory. A variety of methods has been developed and is available in literature, namely Boundary immobilization method, Momentum integral method, Variable step method, enthalpy method etc.

I have developed an efficient simple Computational Technique to solve such moving boundary value problems and easy to implement using computer programming. The technique developed can handle problems with Dirichlet’s data; even problems with source (or sink) terms on the interface can be handled, provided, one is willing to develop equations. This method can be generalized and effectively used to obtain accurate solutions to two phase problems. Efforts in this direction have fructified and being reported for publication. The method developed can possibly be extended to multi-dimensional problems.

PROFILE

I am very glad to introduce myself as Dr. V.G. Naidu, working as an Associate Professor in Applied Mathematics, AdamaScience Technology University, Ethiopia.

I have completed my Ph. D degree in Applied Mathematics, thesis entitled “Study of some problems in Magneto-hydrodynamic (MHD) flows”, from Indian Institute of Technology Bombay, India, in 1989. Since then, I have been teaching for the last 30 years and working on numerical solutions of Boundary Value Problems, which arise in the calculation of Fluid Dynamics.

In the recent research work, aim is to introduce a new Computational method to obtain approximate solution to one phase Stefan problems. Several methods exist, but each of them is mostly specific problem oriented and is not general enough to be applicable to a wide range of problems. The work developed 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 an iterative process with assured convergence. For a non-thermal diffusion, Stefan condition is of implicit nature. For such class of two point boundary value problems, method of bisection is efficient to obtain their solutions. The methods are illustrated by presenting three examples one of which is much discussed oxygen diffusion problem, which is published. The procedure is general enough to be applicable to a broad class of moving boundary problems.

Publications: Published about **18** papers in National and International journals.

Attended/conducted **20** Workshops/conferences/seminars.

Professional Membership: Life member of "ISTE & APSMS

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Declaration: I, the undernoted signatory, hereby certify that the information provided above and in the attached documents is correct. I understand that any deliberate falsehood could lead to termination of my employment contract with the University and that any offer of employment is subject to the receipt of satisfactory references and security check.