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INVARIANT IMBEDDING APPROACH FOR THE DISSOLUTION OF A GAS BUBBLE IN A LIQUID

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Abstract

In the present work, the author has obtained the numerical solution of the moving boundary problem for the dissolution of a gas bubble in a liquid. The above boundary value problem is imbedded into a sequence of initial value problems involving ordinary differential equations by applying the invariant imbedding approach suggested by Meyer [1-4], but the location of the free boundary is determined at each time step by solving an intial value problem rather than a nonlinear scalar equation as mentioned in [1-4]. The numerical results obtained for the case of collapse of the bubble and for the case of its expansion are shown to be in good agreement with those obtained by other authors.

1. Introduction

The mathematical models of many problems in engineering and sciences involve governing equations of parabolic type subject to corresponding initial and boundary conditions. Certain boundary value problems of the above type must be solved subject to given boundary conditions specified on a priori unknown interface called the free or moving surface. The evolution of this interface is not known in advance but it is linked with the solution of the problem itself at each time instant. Such problems are called moving boundary problems of the Stefan type. Typical examples of these problems arise from studying phenomena such as melting or solidification processes, frost penetration into earth, ablation of solids, and diffusion of gas in liquids. The derivation of exact analytical solutions of these problems represents a very difficult task since the time dependent conditions prescribed on the moving boundary are usually nonlinear and depend on the solution of the corresponding problem.

Rubinstein [5] gives a comprehensive survey of the Stefan problem and related moving boundary problems together with their solutions. The state of art of the subject of moving boundary problems is given in the works by Ockendon and Hofgkins [6] and by Wilson et al [7]:

The present paper is concerned with the numerical solution of a special moving boundary problem of the Stefan type namely the one dimensional dissolution of a gas bubble in a liquid. This problem has been previously discussed by Rubinstein [5], and its numerical solution is also obtained by Varoglu and Finn [8] using element method. Recently the same problem is numerically solved by Gupta and Kumar [9] using two methods, the first is an improved version of the method suggested by Douglas and Gallie [10], while the second is a modified method derived from the variable time step approach previously introduced by Gupta and Kumar [11]. The central idea of the above variable time step techniques is to subdivide the region of interest into a finite number of fixed size space intervals. Then an approach is adopted to compute a sequence of time steps for each time level such that the movement of the free boundary is restricted to only one complete space mesh step as time varies from one level to the next by the previously computed time step. Since the evolution of the free boundary depends on the solution, it is expected that these time steps will vary from one time level to the next. The determination of each corresponding suitable time step is done by an iterative process [9].

The implementation of any numerical technique for the solution of moving boundary problems on digital computers imposes certain requirements on the method itself such as being computationaly fast, flexible, mechanically applicable and at the same time mathematically sound. It turns out that an approach which is very suitable for moving boundary problems and possesses the above features is the invariant imbedding technique discussed by Meyer [1] which he used to obtain very encouraging results for various free and moving boundary problems for example [2-4]. In the present paper the invariant imbedding method as discussed in [2] is adopted but the tracking of the free boundary is achieved differently as will be demonstrated in the next sections.

2. Statement of The Problem And Governing Equations

In this paper we consider the isothermal process of dissolution of a spherical gas bubble in a liquid. Following Rubinstein [5] it is assumed that the redistribution of concentration of the dissolving gas is due to diffusion only without convection. The governing mathematical model of this process is based on the fact that the change of pressure in the bubble is due to the change of its curvature and that the surface tension of the gas-liquid interface is taken as constant. The dimensionless equations governing the above phenomenon [5] are as follows:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad S(t) < x < \infty, \quad t > 0, \tag{2.1}$$

with the initial conditions

$$u(x,0) = \varphi(x), \tag{2.2}$$

$$S(0) = 1, \tag{2.3}$$

while the boundary conditions are

$$u(S(t),t) = \beta(1 - S(t)), \tag{2.4}$$

$$\frac{dS}{dt} = \frac{a}{S+b} \cdot \left.\frac{\partial u}{\partial x}\right|_{S(t)} - \frac{c(1-S)}{S(S+b)}, \tag{2.5}$$

and at infinity we have

$$\lim_{x\to\infty} \frac{\partial u}{\partial x} = 0, \tag{2.6}$$

where $u(x,t)$ represents the dimensionless concentration of the dissolved gas in the liquid at distance x and time t. The radius of the bubble at any time t is represented by the dimensionless linear distance of the interface S(t). The constants β ,a,b and c in equations (2.4) and above depend on the properties of the liquid and the diffusing gas [5]. As in the works by Rubinstein [5] and Gupta and Kumar [9] we take

$$\varphi(x) = \begin{cases} 0 & 0 \le x < 1 \\ \gamma x & 1 < x < \infty \end{cases} , \tag{2.6a}$$

where γ is a parameter the sign of which determines the character of the dissolution process. If γ is negative then the process corresponds to a monotonically decreasing bubble, but if γ is positive this represents the case of growth of the bubble. The conditions (2.4) and (2.5) are consequences of the material balance at the bubble surface and accordingly the mass velocity of the dissolving bubble is equal to the diffusion rate of the gas within the liquid at the bubble surface. It is evident that for practical computational reasons the condition at infinity given by (2.6) must be considered at some sufficiently large distance x = p at which the quantity $\partial u/\partial x$ does not change appreciably from its initial value as time passes. As in the work by Gupta and Kumar [7] the point x = 5 is chosen and accordingly condition (2.6), in view of the initial condition (2.2) and (2.6a), is replaced by

$$\frac{\partial u}{\partial x}(5,t) = \gamma \quad . \tag{2.6b}$$

3. Algorithm Based On Invariant Imbedding Approach

As a first step, toward the numerical solution of the free boundary problem described in the above section, the method of straight lines formulation [12-14] is introduced. This amounts to the definition of a fixed partition $\{0 = t_o < \ldots < t_N = T\}$ of $[0,T]$ where T is some final time. For simplicity these subintervals are taken of equal size, the time step $\Delta t = t_j - t_{j-1}$, $j = 1,2,\ldots N$. A straight forward discretization due to the method of lines yields the following approximations

$$\frac{\partial u}{\partial t}(x,t_j) \approx \frac{u_j(x) - u_{j-1}(x)}{\Delta t}, \tag{3.1a}$$

and

$$\frac{dS}{dt}(t_j) \approx \frac{S_j - S_{j-1}}{\Delta t}, \tag{3.1b}$$

where $u_j(x) \approx u(x,t_j)$ and $S_j = S(t_j)$. As a result of this step the free boundary problem (2.1) - (2.6) is imbedded into the sequence of free boundary problems involving ordinary differential equations given by

$$u_j''(x) = \frac{u_j(x) - u_{j-1}(x)}{\Delta t}, \quad S_j < x < \infty, \tag{3.2}$$

for $j = 1,2,\ldots, N$

subject to the initial conditions

$$u_o(x) = \varphi(x), \tag{3.3}$$

$$S_o = 1, \tag{3.4}$$

while the boundary conditions are

$$u_j(S_j) = \beta(1 - S_j) \tag{3.5}$$

$$\frac{S_j - S_{j-1}}{\Delta t} = \frac{a}{S_j+b} \cdot u'_j(S_j) - \frac{c(1-S_j)}{S_j(S_j+b)} , \tag{3.6}$$

and the condition at infinity which is replaced by

$$u'_j(5) = \gamma . \tag{3.7}$$

It should be mentioned that equations (3.2)-(3.7) represent a fully implicit approximation of order Δt. Higher order approximations, for example a Crank-Nicolson type, would be equally possible. A discussion of stability and convergence of the above by lines approximations is given by Meyer [2].

The next step is the central idea of the invariant imbedding approach which depends on the linearity of the differential equation (3.2). It is shown by Meyer [1-2] that the theory of characteristics leads to the relation between $u'_j(x)$ and $u_j(x)$

$$u'_j(x) = R_j(x) . u_j(x) + W_j(x) , \tag{3.8}$$

where R_j and W_j are functions of x that can be determined by substituting (3.8) into (3.2). Since the resulting equation is valid for all values of x then it can be separated into the following equations

$$R' = \frac{1}{\Delta t} - R^2 , \qquad R(5) = 0 , \tag{3.9}$$

and

$$W'_j = - R.W_j - \frac{u_{j-1}}{\Delta t} , \quad W_j(5) = \gamma \quad , \tag{3.10}$$

The index j for the function R in equation (3.9) has been omitted since it is independent of time. The two conditions for R and W_j at x = 5 given in (3.9) and (3.10) respectively are direct consequences of equations (3.7) and (3.8). Equations(3.9) and (3.10) are called the invariant imbedding equations, and they can be integrated in the backward direction of x subject to the corresponding initial conditions at x = 5 up to x = 0. While equation (3.9) has the closed form solution

$$R(x) = \frac{1}{\sqrt{\Delta t}} \tanh \frac{(x-5)}{\sqrt{\Delta t}} , \tag{3.11}$$

the second equation is numerically integrated by any suitable ordinary differential equation solver. In the present paper both the trapezoidal rule and the fourth order Runge Kutta method have been used, results from both methods do not differ appreciably.

Once the values of R and W_j are available, at predetermined equidistant points along the x direction such that $0 = x_o < x_1 < x_2 \ldots < x_M = 5$, the third step is to determine the location of the free boundary at each time level $t = t_j$. Following Meyer [2] the relation (3.8) is valid for all values of x, hence in particular at $x = S_j$ we obtain from (3.5) and (3.8).

$$u_j'(S_j) = R(S_j).\, \beta (1 - S_j) + W_j\,(S_j). \tag{3.12}$$

Substituting from (3.12) into (3.6) we obtain

$$H(S_j) \equiv \frac{S_j - S_{j-1}}{\Delta t} - \frac{a}{S_j+b} \cdot [R(S_j)\,\beta\,(1-S_j)+W_j(S_j)] + \frac{c\,(1-S_j)}{S_j(S_j+b)} = 0 \qquad (3.13)$$

The technique used by Meyer [1-4] to find the solution S_j of $H(S_j)=0$ for each time level $t = t_j$ is to use linear interpolation between successive x mesh points between which H given by (3.13) changes sign for the first time. This approach has been tested but results were not very satisfactory.

In this paper the differential equation (2.5) that corresponds to (3.13) above is written as

$$\left.\frac{dS}{dt}\right|_j = \frac{a}{S+b}\,[R(S).\ \beta(1-S) + W_j\ (S)] - \frac{c(1-S)}{S(S+b)}, \qquad (3.14)$$

which is solved as an initial value problem for $t_{j-1} < t < t_j$ subject to the initial condition $S(t_{j-1}) = S_{j-1}$. The numerical solution of (3.14) is obtained by an iterative process of an Euler type method. We initiate the procedure by supplying a guess for S_j namely $S_j^{(0)} = S_{j-1}$ where the upper index denotes the iteration step. Thus the resulting algorithm for (3.14) is

$$S_j^{(k)} = S_{j-1} + \Delta t \left\{ \frac{a}{\tilde{S}+b}\,[R(\tilde{S})\,\beta(1-\tilde{S}) + \tilde{W}\,(\tilde{S})] - \frac{c(1-\tilde{S})}{\tilde{S}(\tilde{S}+b)} \right\} \qquad (3.15)$$

where $\tilde{S}$ is a linear combination of S_{j-1} and $S_j^{(k-1)}$. In the present paper we take

$$\tilde{S} = \tfrac{1}{2}\,(S_{j-1} + S_j^{(k-1)}).$$

Hence (3.11) gives

$$R(\tilde{S}) = \frac{1}{\sqrt{\Delta t}} \tanh \frac{(\tilde{S} - 5)}{\sqrt{\Delta t}} .$$

The term $\tilde{W}(\tilde{S})$ in equation (3.15) above is the interpolated value of $W_j(x)$ obtained from the integration of (3.10) using the corresponding values of W_j at the x mesh points surrounding the interval $[S_j^{(k-1)}, \quad S_{j-1}]$. In the present paper a simple linear interpolation is used. The convergence is obtained when a predetermined degree of accuracy is achieved between two successive answers for the location of the free surface S_j.

Upon finding the interface position the value of the concentration of the dissolved gas at time $t = t_j$ is obtained by integrating equation (3.8) from $S_j < x < 5$ subject to the initial condition (3.5) where S_j is now known and a fourth order Runge-Kutta method is used for that purpose.

4. Numerical Results And Conclusion

The Stefan problem for the dissolution of a gas bubble in a liquid described in section two is numerically solved using the invariant imbedding approach presented in section three above. Two cases are considered, the first is the case of collapse of the bubble while the second is for a growing bubble, this corresponds to taking γ equals to -0.39 and 0.11 respectively. The values of the constants a,b,c and β are taken as 0.0247, 0.0933, 0.00346 and 0.14 respectively. These values were also taken by Gupta and Kumar [9] and previously by Rubinstien [5] and also Varoglu and Finn [8]. In this paper a fixed time step of $\Delta t = 0.1$ and fixed space mesh size of $\Delta x = 0.1$ are used. The convergence of the iterative procedure for the determination of S_j is considered achieved when two successive answers differ by less than 10^{-5}.

Nummerical results for the interface positions at various times calculated by the present method as well as by other authors for the case of collapse and growth of the bubble are given in Tables 1 and 2 respectively. In order to obtain the corresponding values at the same time level a simple interpolation is used. Results are shown to be in good agreement with those obtained by other methods. The concentration profiles for the dissolving gas in liquid at some chosen time levels as functions of the distance x are given in Figures 1 and 2 for the case of collapse and growth of the bubble respectively. Corresponding curves obtained by other methods are also displayed for each case.

It should be mentioned that numerical experiments for the same problem with smaller values of Δx and Δt were performed for the case of collapse and growth of the gas bubble, and the resulting numerical solution did not vary appreciably than those obtained above.

Table 1. Location of interface S(t) for collapse of the bubble (X = 0.1, t = 0.1)

t	S(t) in [5]	S(t) in [9] IDG Method	S(t) in [9] MVTS Method	S(t)
0	1	1	1	1
1.00	0.982	0.989	0.989	0.982
2.00	0.969	0.977	0.979	0.968
5.24	0.931	0.941	0.941	0.929
9.24	0.885	0.895	0.896	0.884
12.24	0.850	0.858	0.858	0.852
16.24	0.802	0.808	0.809	0.803
18.24	0.777	0.782	0.783	0.779
23.24	0.711	0.718	0.720	0.715
27.24	0.653	0.661	0.663	0.659
31.24	0.589	0.601	0.603	0.595
39.24	0.428	0.437	0.442	0.431
43.24	0.304	0.313	0.322	0.305

IDG denotes improved Douglas-Gallie method.

MVTS denotes modified variable time step method, both methods use Crank Nicolson discretization.

Table 2. Location of interface S(t) for growth of the bubble (X = 0.1, t = 0.1)

t	S(t) in [5]	S(t) in [9] IDG Method	S(t) in [9] MVTS Method	S(t)
0	1	1	1	1
5	1.02	1.01	1.01	1.02
10	1.03	1.03	1.03	1.03
20	1.06	1.05	1.05	1.06
30	1.09	1.08	1.08	1.09
50	1.15	1.13	1.13	1.14
100	1.30	1.26	1.26	1.27
200	1.58	1.51	1.51	1.52
300	1.85	1.75	1.74	1.76
400	2.10	1.97	1.97	1.985
500	2.34	2.18	2.17	2.31

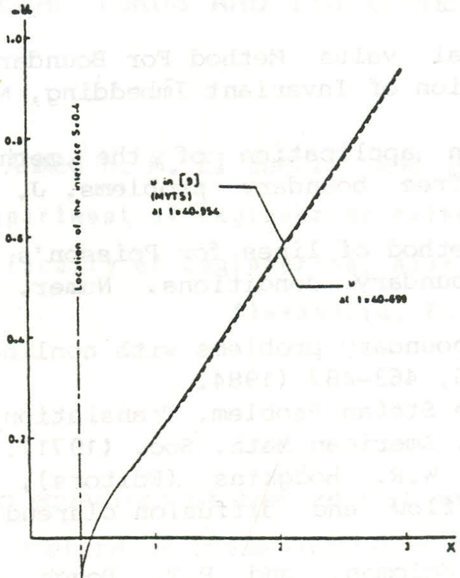

Fig. 1. Concentration Profile for Collapse of Bubble.

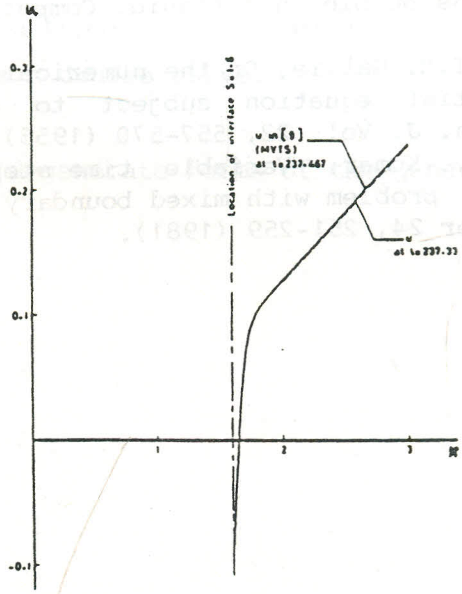

Fig. 2. Concentration Profile for Growth of Bubble.

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