



# Free and Moving Boundary Problems of Heat and Mass Transfer

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## Abstract

Bisection method is used to solve a moving boundary problem. This moving boundary problem was solved by the maze of mathematical manipulations by several authors. The method of using bisection is simple as compared to the lengthy mathematical manipulation of other methods. The procedure of the paper is useful in other moving boundary problems of heat and mass transfer, including boundary value problems involving ordinary differential equations with unknown interval length.

**Keywords:** Bisection method, interface, mass diffusion, one phase, two phase.

## 1. Introduction

The first method taught in a curriculum on the topic of finding isolated zeros of function of a real variable is perhaps the method of bisection. The main purpose of this presentation is to demonstrate the utility of this simple method in the development of computational methods to obtain approximate solutions of problems arising in several areas of engineering. We chose two problems to illustrate the use of bisection method.

In section II, we consider a two point boundary value problem which arises in mechanics. In section III, we consider the use of the bisection method in the development of a powerful computational method for solving an oxygen absorption problem occurring in medical engineering.

## 2. A Problem from Mechanics

A particle which is at rest is moved by applying a force  $f$  so that the particle moves and comes to rest after a specified distance 'X'. Mathematical model of this problem is

$$x'' = f(t, x, x'); \quad x'(0) = 0, \quad x(s) = X \text{ and } x'(s) = 0$$

where 's' is the time needed to come to rest and is to be found along with the solution. This problem was treated by Tau method [1], in which a perturbation function is introduced and a polynomial basis is used to approximate the solution of the perturbed problem. A sequence of functions is generated which converges to the solution of the original problem. But our approach is natural and simple using the bisection method.

With change of variable  $\theta = 1 - t/s$ , the problem takes the form  $x'' = s^2 f[s(1 - \theta), x, -x'/s]$ ;  $x(0) = X, x'(0) = 0$  and  $x'(1) = 0$ .  $\theta$  is the new independent variable. (Derivatives are with respect to this variable).

We can now comfortably solve this initial value problem for a given value of 's'. Starting with two values of s, we apply bisection to obtain the correct value using the sign of the discrete equivalent of the end condition  $x'(1) = 0$

$$x_{M-1} - 4x_{M-2} = 0 \quad (x_M = 0).$$

## 3. Mass Diffusion Problem

Oxygen is allowed to diffuse into a medium which absorbs and immobilizes oxygen at a constant rate. The concentration of oxygen at the surface of the medium is maintained constant. A moving boundary marks the innermost limit of oxygen penetration. This first phase of the problem continues until a steady state is reached in that the oxygen does not penetrate any further into the medium. The surface of the medium is then sealed so that no further oxygen passes in or out. The medium continues to absorb the available oxygen already diffused into it and as a consequence, the boundary marking the depth of penetration in the steady state recedes towards the sealed surface. Mathematical model for this problem is given by [2].

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \quad 0 \leq x \leq s(t), t \geq 0$$

$$\frac{\partial u}{\partial x}(0, t) = 0, t > 0 \text{ and } u(s, t) = 1$$

$$u = \frac{\partial u}{\partial x} = 0 \text{ along } x = s(t), t > 0$$

$$u(x, 0) = (1 - x)^2/2; \quad 0 \leq x \leq 1$$

This problem is slightly different from the classical Stefan problem in that the time derivative does not occur in the condition on the boundary. This difference poses a difficulty in the numerical method. Several authors tried to obtain approximate solutions. These efforts have been listed in the book [2]. The elaborate Tau method is used in [1] to tackle this problem.

The major problem is that of tracing the movement of the boundary and of determining the distribution of oxygen as a function of time.

Let space step  $h = \frac{1}{N}$ . We need to find the time step  $k_L (= \Delta t)$  to move from the line L-1 to L and u -values along the line L, knowing them along the line L-1... We thus have to find  $UF_j (j = 1, 2, \dots, M - 1: UF = 0)$  and the time step knowing  $UI_j$  along L-1 ( $j=1, 2 \dots M; UI_{M+1} = 0$ ), where  $M=N+2-L$ . This situation is similar to our dynamics problem. We need two conditions to solve the parabolic equation.

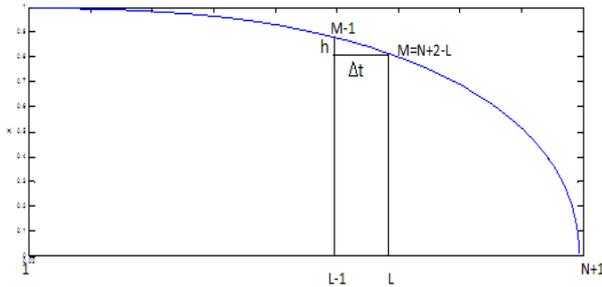


Fig. 1: Moving boundary

We use our simple method of bisection in the following manner. The fully implicit scheme incorporates the two of the three conditions  $u_x(0, t) = 0$  and  $u(s(t), t) = 0$ . The third condition,  $\frac{\partial u}{\partial x}(s(t), t) = 0$  is replaced by the three point approximation along the line L as  $UF_{M-1} - 4UF_{M-2} = 0 (UF_M = 0)$ . This approximation takes opposite sign when we obtain  $UF_j$  values with two values of  $k_L$ , between which correct values lies. In the very first step, we have taken, to be sure, the starting values of  $k_1$  as two extremes, such as 0.000001 and 0.1 and used the bisection method. For subsequent time step  $k_L$  we have taken  $0.5k_{L-1}$  and  $1.5k_{L-1}$ . Results obtained are presented in table 1. Numerical values are comparable very well with the results of all other methods. In fact, our results confirm that they are correct up to three significant digits.

Many researchers tried to obtain solution of this problem. About eight of them are available in [2]. Most of them have taken a fixed time step, often being as small as .00001. We have taken fixed space step size and found the required time. We had to do interpolation of our results for the purpose of comparison with the results of others. [8]

The results of the bisection method are used to obtain boundary points at specified times using Lagrange's interpolation with four points, two on either side of the point of interest. We have presented the results of few authors on this problem among several of them for comparison from ref.[1] and [2]. We followed similar procedure to present results of concentration along the line  $x = 0$ .

Table 1: Free Boundary Position

Method	Time								Step size	
	0.04	0.06	0.1	0.12	0.14	0.16	0.18	0.18		
HH	0.99 92	0.99 18	0.93 5	0.87 92	0.79 89	0.68 34	0.50 11	0.43 34	5	$\delta t=0.01$
MVT S	0.99 5	0.98 99	0.92 49	0.87 03	0.79 16	0.68 25	0.47 68	***	5	Var. step
FGL	0.99 88	0.99 05	0.93 12	0.87 47	0.79 12	0.67 56	0.48 49	0.40 14	5	$\delta t=0.01$
ML	0.99 58	0.99 04	0.93 09	0.87 4	0.79 3	0.67 76	0.49 74	0.43 08	5	$\delta t=0.01$
Tau	0.99 89	0.99 1	0.93 44	0.87 9	0.79 94	0.65 51	0.50 55	0.43 94	5	$\delta t=0.005$
Bisection	0.99 37	0.98 35	0.92 44	0.87 68	0.80 02	0.68 94	0.51 52	0.45 16	5	$h=0.02$
	0.99 3	0.98 26	0.92 84	0.87 6	0.79 98	0.68 93	0.51 55	0.45 2	5	$h=0.025$
	0.99 16	0.98 06	0.92 68	0.87 55	0.80 07	0.69 2	0.52 16	0.45 97	5	$h=0.04$

Total absorption time, accurate up to three significant digits, is 0.198 (based on the results with different step sizes).  $N=400$  was enough to achieve this accuracy.[7]

HH: Hansen and Hougaard; MVTS: Modified Variable Time Step; FGL: Fixed-Grid Lagrange; ML: Murray and Landis; Results of authors have been taken from the book of Crank (172; [2])  
Tau: Allabadi and Ortiz [1].

Tau: Table 2: Concentration  $u(0, t)$

Method	Time								
	0.04	0.06	0.1	0.12	0.14	0.16	0.18	0.18	
HH	0.27 43	0.22 36	0.14 32	0.10 91	0.07 79	0.04 88	0.02 18	0.01 53	5
FGL	0.27 45	0.22 38	0.14 34	0.10 94	0.07 81	0.04 9	0.02 2	0.01 56	5
ML	0.27 45	0.22 38	0.14 34	0.10 93	0.07 8	0.04 89	0.02 18	0.01 54	5
Tau	***	***	0.14 35	***	***	0.04 96	0.02 17	***	5
Bisection	0.28 44	0.22 98	0.14 64	0.11 17	0.08	0.05 07	0.02 34	0.01 69	5
	0.28 53	0.23 04	0.14 66	0.11 18	0.08	0.05 07	0.02 34	0.01 7	5
	0.28 83	0.23 26	0.14 79	0.11 29	0.08	0.05 15	0.02 42	0.01 77	5

### 4. Discussion

- (i) Simple bisection method is used to obtain solution of mass diffusion moving boundary problem and certain class of two point boundary value problems.
- (ii) Methodology presented in this article stems from the method developed by the authors [3,5] to solve the well-known classical two phase moving boundary problem
- (iii) It is noted that this simple bisection method is a powerful tool for solving many one and two phase moving boundary problems. This is so even if the conditions involved in the problem are nonlinear, as bisection works for nonlinear functions as well.
- (iv) Regulifalsi method, an improvement of bisection can be used. Our main purpose is to indicate the power of a simple method
- (v) Material in this article is a part of the Ph.D. dissertation [4] of the second author.

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