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Approximate method for the oxygen diffusion problem

RADHEY S. GUPTA and N. C. BANIK
Department of Mathematics, University of Roorkee, Roorkee 247 667, India

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1. INTRODUCTION

DUE TO the inherent nonlinearity involved in moving boundary problems (MBPs), it is extremely difficult to obtain their analytical solutions. Therefore, approximate analytical methods, which are quite versatile, are generally used to solve them. Approximate methods have been in use in the field of boundary layer theory in fluid flow since they were first introduced by Karman and Pohlhausen. A general account of the Karman–Pohlhausen method and the original reference may be found in Schlichting [1]. Goodman [2] introduced the 'heat balance integral method' which is very popular due to its simple forms. A detailed review of the integral methods and their application to a variety of heat transfer problems including MBPs may be found in Goodman [3]. Reynolds and Dolton [4] also developed the heat balance integral method independently. For improvement of the integral methods Noble [5] suggests repeated spatial subdivision, whereas Bell [6] makes equal subdivisions of the dependent variable, temperature range, instead of subdividing the space domain.

In MBPs, generally, three boundary conditions are prescribed. One condition is prescribed at the fixed end and the other two at the moving boundary interface. While dealing with MBPs by the integral method we can select a linear profile using two of these conditions and the remaining third condition at the moving boundary interface may be used to determine the position of the moving boundary. But a linear profile, obviously, will not give a desirable solution. Therefore, to increase the degree of the polynomial profile some extra conditions are derived at the moving boundary. But derivation of all extra conditions at the moving boundary only cannot take into account the behaviour at the fixed end. In the present note we suggest taking higher moments in place of or in addition to derived conditions based on the method of moments originally proposed by Fujita (see Crank [7]) for solving heat conduction problems in a fixed domain. Two simultaneous differential equations in two unknowns are arrived at—one being the position of the moving boundary interface and the other being a parameter defined at the fixed end. This parameter is either the temperature–concentration if the flux is prescribed or the flux if the temperature–concentration is prescribed. Due to involvement of this extra constraint at the fixed end let us refer to this technique as the constrained integral method (CIM) in further discussions.

For testing this method we consider the oxygen diffusion problem of ref. [8] which is not amenable to approximate methods, firstly because of the fact that it possesses a discontinuity in the surface gradient and secondly a non-uniform distribution is provided at zero time. As will be seen the numerical results obtained from the present method compare satisfactorily with those due to earlier authors who solved the problem by other techniques. We would also like to add that as the basic equation is satisfied on average (or weighted average) only the accuracy of the solution cannot be guaranteed. The efficacy of the method can only be tested by its application to typical worked out examples. There are other methods for solving heat conduction problems which use different weight factors but we shall not elaborate on them here as they deal only with the fixed domains, i.e. not MBPs.

2. THE PROBLEM

The problem, known as the Crank and Gupta problem [8], arises from the diffusion of oxygen in the body tissue which absorbs it at a constant rate. The problem itself is different from the usual moving boundary problem in the sense that there is no latent heat type condition available at the moving boundary. It has also been dealt with by many other authors namely, Hansen and Hougaard [9], Ferris and Hill [10], Berger *et al.* [11], Miller *et al.* [12], Gupta and Kumar [13, 14] and Dahmardah and Mayers [15]. In non-dimensional form the problem is defined by the following differential equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - 1, \quad 0 \leqslant x \leqslant s(t),\ t \geqslant 0 \tag{1}$$

with associated boundary conditions

$$\frac{\partial u}{\partial x} = 0 \text{ at the surface } x = 0 \tag{2}$$

$$u = \frac{\partial u}{\partial x} = 0 \text{ at the moving boundary } x = s(t),\ t \geqslant 0 \tag{3}$$

and the initial condition

$$u = \tfrac{1}{2}(1-x)^2, \quad 0 \leqslant x \leqslant 1,\ t = 0 \tag{4}$$

with $s(0) = 1$.

Here $u(x, t)$ denotes the oxygen concentration at a point x, at time t and $s(t)$, the position of the moving boundary at this time.

3. METHOD OF SOLUTION

An extra condition, as derived in ref. [8], at the moving boundary is given by

$$\frac{\partial^2 u}{\partial x^2} = 1, \quad x = s(t). \tag{5}$$

A polynomial of the fourth degree is chosen containing five unknown parameters which are in general functions of time. On writing u_0 for the surface concentration $u(0, t)$ the equation of the polynomial becomes

$$u(x, u_0, s) = \tfrac{1}{2}(s^2 - 6u_0)\left(\frac{x}{s}\right)^4 + (8u_0 - s^2)\left(\frac{x}{s}\right)^3 + \tfrac{1}{2}(s^2 - 12u_0)\left(\frac{x}{s}\right)^2 + u_0 \tag{6}$$

which satisfies conditions (2), (3) and (5).

NOMENCLATURE

s position of the moving boundary interface
t time
Δt time step
u temperature
x Cartesian coordinate.

The position of the moving point, s, and the surface concentration, u_0, in equation (6) are still to be determined. To obtain u_0 and s as functions of time we take the zeroth and first moments, i.e.

$$\int_0^s \frac{\partial u}{\partial t}\,dx = \int_0^s \left(\frac{\partial^2 u}{\partial x^2} - 1\right) dx \tag{7}$$

and

$$\int_0^s x\frac{\partial u}{\partial t} = \int_0^s x\left(\frac{\partial^2 u}{\partial x^2} - 1\right) dx. \tag{8}$$

Writing $u(x, u_0, s)$ from equation (6) in equations (7) and (8) and using conditions (2) and (3) we obtain

$$(s^2+8u_0)\frac{ds}{dt} + 8s\frac{du_0}{dt} = -20s \tag{9}$$

and

$$s(s^2+6u_0)\frac{ds}{dt} + 3s^2\frac{du_0}{dt} = 30u_0 - 15s^2 \tag{10}$$

respectively.

Equations (9) and (10) readily provide

$$\frac{du_0}{dt} = -\frac{(5s^4+30s^2u_0+240u_0^2}{s^2(5s^2+24u_0)} \tag{11}$$

and

$$\frac{ds}{dt} = -\frac{60(s^2-4u_0)}{s(5s^2+24u_0)}. \tag{12}$$

We can obtain the numerical solution of simultaneous equations (11) and (12) by standard methods for solving differential equations if $u_0(0)$ and $s(0)$ are known.

Table 1. Comparison of position of the moving boundary

Time, t	Crank and Gupta [8]	Hansen and Hougaard [9]	Miller *et al.* [12]	Dahmardah and Mayers [15]	Present
0.051	0.9967	0.9964	—	—	1.0000
0.060	0.9922	0.9918	0.9920	—	0.9969
0.080	0.9719	0.9716	0.9717	—	0.9756
0.100	0.9352	0.9350	0.9356	0.9350	0.9350
0.120	0.8789	0.8792	0.8796	0.8792	0.8743
0.140	0.7976	0.7989	0.7992	0.7989	0.7896
0.150	0.7449	0.7467	0.7467	—	0.7356
0.160	0.6813	0.6834	0.6832	0.6835	0.6710
0.180	0.4961	0.5011	0.4985	0.5013	0.4879
0.190	0.3388	0.3454	0.3397	0.3460	0.3300
0.195	0.1613	0.2065	—	0.2085	0.1708
0.1955	—	0.1871	—	—	0.1380

Note: the dashes (--) indicate that the corresponding figures are not available.

Table 2. Comparative figures for the concentration at the sealed surface

Method	Time						
	0.051	0.06	0.10	0.15	0.18	0.19	0.195
Crank and Gupta [8]:							
Numerical	0.245329	0.223746	0.143287	0.063157	0.021824	0.009039	0.002880
Approximate	0.245176	0.223605	0.143175	0.062981	0.021269	0.008151	0.001721
Hansen and Hougaard [9]	0.245176	0.223605	0.143177	0.063078	0.021781	0.009021	0.002884
Miller *et al.* [12]	—	—	0.143150	0.063020	—	0.008930	—
Dahmardah and Mayers [15]	—	—	0.143177	—	0.021781	0.009021	0.002883
Present	0.245176	0.223778	0.142312	0.060392	0.018827	0.006417	0.000744

Note: the dashes (—) indicate that the corresponding figures are not available.

4. NUMERICAL RESULTS AND DISCUSSION

We know from the physics of the problem that $ds/dt \leqslant 0$, since s should decrease as time increases. As the term in the denominator of equation (12) is positive for $0 \leqslant s \leqslant 1$, this condition will not be fulfilled until

$$s^2 - 4u_0 \geqslant 0. \tag{13}$$

Reference [8] has shown that the boundary marking zero concentration does not move until some time within the accuracy of working. We have taken the initial position of the moving boundary, $s = 1.0$, and surface concentration, $u_0 = 0.245176$, at time, $t = 0.051$, from ref. [8]. This is also in accordance with condition (13). Numerical values for s and u_0 have been computed for $\Delta t = 0.001$ using the fourth-order Runge–Kutta method. Comparative figures for the position of the moving boundary and concentration at the sealed surface $x = 0$ at different times are given in Tables 1 and 2, respectively. As may be seen, the agreement between our results and those due to earlier authors is reasonably good. Reference [8] solved the problem by the integral method also. An empirical expression for the surface concentration was used, which may not be obtained in other problems or even in the same problem with different boundary conditions. In contrast the present method is a general one which may be applied to any one-dimensional problem. In the present method s and u_0 are computed as part of the solution. That is, the concentration at any time t may be obtained from equation (6) after u_0 and s are computed from equations (11) and (12). Further it may be noted that although a closed form solution for equation (12) is possible, it may not be economical computationally.

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