An Extrapolation Method for Oxygen Diffusion Problem

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Abstract— We consider the oxygen diffusion equation. Oxygen diffusion in a sike cell with simultaneous absorption is an important problem. Oxygen diffusion has a wide range of medical applications. Numerical solutions of its partial differential equation are obtained by extrapolation method with the vector of values V approximating to C (diffusion) at the mesh points. And the results gave a good agreement with the previous methods [1,2,3]. And L_0 stability method of analysis of the stability is also investigated.
Keywords— Oxygen Diffusion Problem, Pade approximates, finite difference, L_0 stability.
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1. Introduction

The diffusion with absorption model accounts for the presence of moving boundary which marks the furthest penetration of oxygen into the absorbing medium and also allows for an initial distribution of oxygen through the absorbing tissue. The model predictions may be used in the development of time variant radiation treatments of cancerous tumors, so that the dosage of radiation could be varied with the changing oxygen concentration. Simple expressions are also presented for evaluating the surface oxygen concentration the rate of consumption of oxygen per unit volume of absorbing tissue, and the point of innermost oxygen penetration.

Crank and Gupta [1] studied the moving boundary problem arising from the diffusion of oxygen into absorbing tissue. Crank and Gupta [4] also employed an uniform space grid moving with the boundary and the necessary interpolations are performed with either cube splines or polynomials, Liapis et al. [5] proposed an orthogonal collocation for solving the partial differential equation of the diffusion of oxygen in absorbing tissue. Gülkaç studied two numerical methods for oxygen diffusion problem [3]. More references to this problem can be found in references [6-16].

This paper is organized as follows in section 2 describes the oxygen diffusion problem. Section 3 describes the method and contains the extrapolation method for the oxygen diffusion problem. Section 4 describes stability of extrapolation method for the oxygen diffusion problem. Section 5 presents the numerical results and conclusions.

2. Desciription of Problem

Mathematical model of biological diffusion problem was made first by Crank and Gupta [1].

The procedure consists of two levels mathematically. At the first level, the stable condition occurs when the cell surface is isolated after the oxygen is injected into either from the inside or outside of the cell.

At the second level, the absorption of injected oxygen by tissues starts. This condition causes the moving boundary problem. The goal of this procedure is to find a balance position and to define the time dependent moving boundary position.

In one dimension, the diffusion with absorption process is presented by parabolic partial differential equation [1]

$$\frac{\partial c}{\partial T} = D\frac{\partial^2 c}{X^2} - m \qquad (1)$$

Where c(x,T) denotes the concentration of oxygen that is free to diffuse at distance x from the outer surface of medium at time T, D is a constant diffusion coefficient, and m a constant rate of consumption of oxygen per unit volume of absorbing medium. This problem has two parts.

1. Steady-state solution

When the oxygen enters through the surface during the initial phase, the boundary conditions is given by the expression [3, 12]

$$c = c_{0,}\ \ X = 0, T \geq 0 \qquad (2)$$

where c_0 is a constant.

The steady state is defined by a solution of

$$D\frac{d^2 c}{X^2} - m = 0 \qquad (3)$$

which satisfies the conditions

$$c = \frac{\partial c}{\partial X} = 0, X \geq X_0 \qquad (4)$$

where X_0 the innermost extend of oxygen penetration. The required solution is obtained to be

$$c = \frac{m(X - X_0)^2}{2D} \qquad (5)$$

where

$$X_0 = \sqrt{\frac{2Dc_0}{m}} \qquad (6)$$

2. After the surface X=0 has been sealed, the position of the receding boundary is denoted by
$X_0(T)$ and problem can be expressed by the equation

$$\frac{\partial c}{\partial T} = D\frac{\partial^2 c}{\partial X^2} - m, 0 \leq X \leq X_0(T) \qquad (7)$$

$$\frac{\partial c}{\partial X} = 0, X = 0, T \geq 0 \qquad (8)$$

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$$c = \frac{\partial c}{\partial X} = 0, X = X_0(T), T \geq 0 \quad (9)$$

$$c = \frac{m}{2D}(X - X_0(T))^2, 0 \leq X \leq X_0, T = 0 \quad (10)$$

where T=0 is the time when the surface is sealed. By changing the variables

$$x = \frac{X}{X_0},\ t = \frac{D}{X_0^2}T, c = \frac{CD}{mX_0^2} = \frac{C}{2C_0}$$

and denoting by s(t) the value of x corresponding to $X_0(T)$, the above system is (7)-(10) reduced to the following non-dimensional form [3]:

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - 1, 0 \leq x \leq s(t) \quad (11)$$

$$\frac{\partial C}{\partial x} = 0,\ x = 0,\ t \geq 0 \quad (12)$$

$$C = \frac{\partial C}{\partial x} = 0,\ x = s(t),\ t \geq 0 \quad (13)$$

and

$$C = 0.5(1 - x)^2,\ 0 \leq x \leq 1,\ t = 0 \quad (14)$$

where C is concentration of the oxygen free to diffuse [1].

3. Extrapolation Method For The Oxygen Diffusion Problem

3.1 Be converted into ordinary differential equations systems of partial differential equation

If the x derivative at (x, t) for $\frac{\partial^2 c}{\partial x^2}$ is replaced by

$$\frac{1}{h^2}\{C(x - h,t) - 2C(x,t) - C(x + t)\} + O(h^2)$$

in equation (11) and x is considered a constant equation (11) can be written as the ordinary differential equation,

$$\frac{dC(t)}{dt} = \frac{1}{h^2}\{C(x - h,t) - 2C(x,t) + C(x + h,t)\} - 1 + O(h^2) \quad (15)$$

Subdivide the interval $0 \leq x \leq 1$ into N equal subintervals by the grid lines x_i=ih, i=0(1)N, where Nh=x and write down equation (12) at every mesh points x_i=ih, i=1(1)N-1 along time-level t. It then follows that the values $V_i(t)$ approximating to $C_i(t)$ will be exact solution values of the system of (N-1) ordinary differential equations .
Therefore

$$\frac{dV_1(t)}{dt} = \frac{1}{h^2}\{V_0 - 2V_1 + V_2\} - 1$$
$$\frac{dV_2(t)}{dt} = \frac{1}{h^2}\{V_1 - 2V_2 + V_3\} - 1 \quad (16)$$
.
.
.
$$\frac{dV_{N-1}(t)}{dt} = \frac{1}{h^2}\{V_{N-2} - 2V_{N-1} + V_N\} - 1$$

V_0 and V_N are known boundary values.

We can write this equation system (16) in matrix form as,

$$\frac{d}{dt}\begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-1} \end{bmatrix} = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & & \ddots & & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}\begin{bmatrix} V_1 \\ V_2 \\ \vdots \\ V_{N-1} \end{bmatrix} + \frac{1}{h^2}\begin{bmatrix} V_0 \\ 0 \\ \vdots \\ 0 \\ V_N \end{bmatrix} - 1 \quad (17)$$

and, we can write as

$$\frac{dV(t)}{dt} = AV(t) + b \quad (18)$$

or equation (18) can be write as

$$\frac{dV}{dt} = AV + b \quad (19)$$

where $V(t)=[V_1, V_2,\ldots V_{N-1}]^T$, b is a column vector of zeros and known boundary values and matrix A of order (N-1).
Equation (19) is scalar differential equation. A and b are independent of t and V(t) satisfies the initial condition V(0)=g, equation (19) is easily solved by method of separation of variables, to be

$$V(t) = -\frac{b}{A} + (g + \frac{b}{A})e^{At}$$

or

$$V(t) = -A^{-1}b + e^{tA}(g + A^{-1}b) \quad (20)$$

therefore, iteration equation for the equation (20) can be written follows

$$V(t + k) = -A^{-1}b + e^{(t+k)A}(g + A^{-1}b) \quad (21)$$

or

$$V(t + k) = -A^{-1}b + e^{kA}(V(t) + A^{-1}b) \quad (22)$$

Because all boundary values is zero (see eqn.(12) and eqn.(13)) then b=-1 and

$$V(t + k) = A^{-1} + e^{kA}V(t) - A^{-1} \quad (23)$$

or

$$V(t + k) = e^{kA}V(t) + A^{-1}(I - e^{kA}) \quad (24)$$

The boundary values can be always be eliminated if we are concerned more, say, with stability than with a particular numerical solution.
Perturb the vector of initial values from g to g^*. By equation (20) the solution $V^*(t)$ is

$$V^*(t) = -A^{-1}b + e^{tA}(g^* + A^{-1}b) \quad (25)$$

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Let perturbation vector E(t) can be written as equation (26) with equation (20) and (25)

$$V^*(t) - V(t) = e^{tA}(g^* - g) \qquad (26)$$

Hence the perturbation vector $E(t) = V^*(t) - V(t)$ at time t is related to the initial perturbation vector $E(0)=g^*-g$ by $E(t)=e^{tA}E(0)$.

As before

$E(t+k)=e^{kA}E(t)$.

3.2 Extrapolation method for oxygen diffusion problem

If the exponential is approximated by its (1,0) Pade approximant, the vector of values $C=[C_1, C_2, \ldots, C_{N-1}]^T$ approximating V will be solution of the implicit backward difference equations [14]

$$C(t+k)=(I-kA)^{-1}C(t)-B \qquad (27)$$

Where A matrix defined is

$$A=\frac{1}{h^2}\begin{bmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & & \ddots & \\ & & 1 & -2 \end{bmatrix}$$

and B is defined $B=A^{-1}(I-Ak)^{-1}$. Over a time-interval of 2k this gives

$$C^{(1)}(t+2k)=(I-2kA)^{-1}C(t)-A^{-1}(I-2kA)^{-1} \qquad (28)$$

Alternatively, the application of equation (27) twice, each over a time-interval of k, leads to the implicit equations,

$$C^{(2)}(t+2k)=(I-kA)^{-1}C(t+k)=(I-kA)^{-1}[(I-kA)^{-1}C(t)-B] \qquad (29)$$

$$C^{(2)}(t+2k)=(I-kA)^{-2}C(t)-(I-kA)^{-1}B \qquad (30)$$

$$C^{(2)}(t+2k)=(I-kA)^{-2}C(t)-A^{-1}(I-kA)^{-2} \qquad (31)$$

Equations (28) and (31) are two different backwards difference schemes for calculating approximations to $C_i(t+2k)$, i=1(1)N-1.

The binomial expansion of the matrix inverse of (28) and (31) can be written as

$$C^{(1)}(t+2k)=(I+2kA+4k^2A^2)C(t)-(I+2kA+4k^2A^2)A^{-1}+O(k^3) \qquad (32)$$

and

$$C^2(t+2k)=(I+2kA+3k^2A^2)C(t)-(I+2kA+3k^2A^2)A^{-1}+O(k^3) \qquad (33)$$

But the Maclaurin expansion of exp(2kA) in $V(t+2k)=e^{2kA}V(t)-A^{-1}e^{2kA}$ an equation giving a more accurate approximation to $C_i(t+2k)$ than either (32) or (33), i=1(1)N-1,

$$V(t+2k)=(I+2kA+2k^2A^2)V(t)-A^{-1}(I+2kA+2k^2A^2)+O(k^3) \qquad (34)$$

Comparison of equations (32), (33) and (34) shows that neither (32) nor (33) is accurate to terms of order k^2. A simple linear combination of (32) and (33) will however, produce an extrapolated vector $C^{(E)}$ that is second order accurate in t, i.e. with a leading error term $O(k^3)$, namely,

$C^{(E)}(t+2k)=2C^{(2)}(t+2k)-C^{(1)}(t+2k)+F$

Where F is $F=-A^{-1}(I+2kA+2k^2A^2)$.

$C^{(E)}=(I+2kA+2k^2A^2)C(t)+F$

The algorithm for the extrapolation is therefore

$$(I-2kA)C^{(1)}(t+2k)=C(t)-A^{-1} \qquad (35)$$

$$(I-2kA)^2C^{(2)}(t+2k)=C(t)-A^{-1} \qquad (36)$$

and

$$C^{(E)}(t+2k)=2C^{(2)}-C^{(1)}+F \qquad (37)$$

Naturally, the extrapolated solution values are used as the starting values for the extrapolation procedure over the next two time-levels.

4. Stability of Extrapolation Method

If equation (37) is written in the form

$C^{(E)}(t+2k)=S_{1,0}(kA)C(t)+F$

$=[2(I-kA)^{-2}-(I-2kA)^{-1}]C(t)$

then

$S_{1,0}(kA)=2(I-kA)^{-2}-(I-2kA)^{-1}$

Therefore the symbol $S_{1,0}(-z)$ of the extrapolation method is,

$$S_{1,0}(-z)=\frac{2}{(1+z)^2}-\frac{1}{1+2z}=\frac{1+2z-z^2}{1+4z+5z^2+2z^3}$$

Division of the numerator and denominator by z^2 shows that $S_{1,0}(-z)\to 0$ as $z\to\infty$.

$|S_{1,0}(-z)|<1$ for all z>0.

Hence the extrapolation method is L_0-stable. The symbol is small and negative for $z>1+\sqrt{2}$, which implies that small oscillations of fluctuations could occur in the numerical solution for $z=-k/_{s\P}>1+\sqrt{2}$. In this case, visibility reduces calculations, because $S_{1,0}(-z)$ is very small for these values of z. Therefore, only L_0-stable methods are worth extrapolating.

5. Numerical Results and Conclusion

In this work we proposed an efficient method of determining extrapolation by using pade approximates. We also showed the stability analysis to prove the merit of our proposed numerical scheme. As one would expect, L_0-stable difference methods of third and fourth accuracy in the t can be achieved by extrapolating over considered in Crank [1].

The computation procedure showed that the present method is easy to handle with minimum error. A good agreement between the present method and previous methods was also shown.

The calculations performed with $d_x = 0.05$, $d_x = 0.1$ and $d_t = 0.001$ are given in Figures 1 and 2 which shows that the values obtained are in very good agreement with those calculated from earlier works [1, 2, 3].

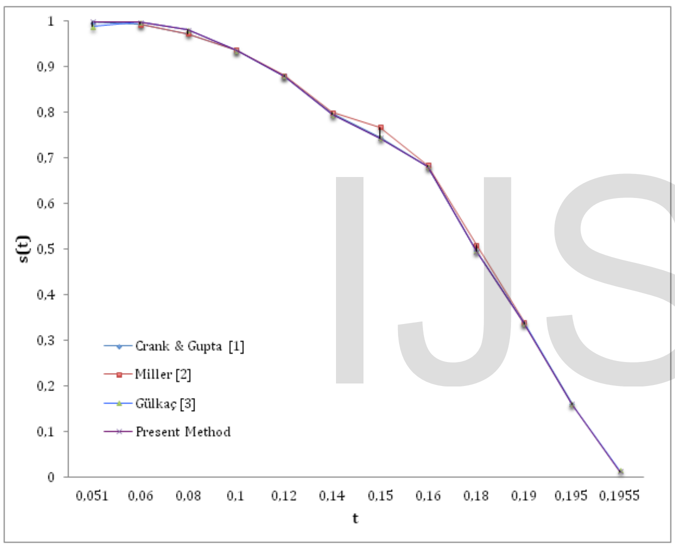

Figure 1. Position of moving boundary s(t)

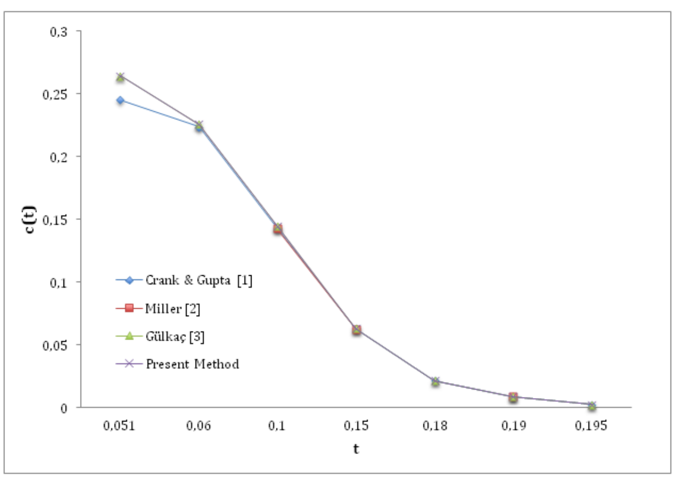

Figure 2. Surface concentration c

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