An approximate method for oxygen diffusion in a sphere with simultaneous absorption

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Received May 1998
Revised January 1999
Accepted February 1999

Keywords *Oxygen, Boundary conditions, Diffusion theory, Absorption*

Abstract *The oxygen diffusion problem is usually formulated in two stages: first, the steady state and second, the moving boundary stage. In this paper, we will consider the solution of the second stage in which a new semi-analytical method for solving such a problem was developed. The present method starts by assuming a polynomial representing the profile of oxygen concentration, and then by some mathematical manipulation a system of linear equations is obtained. Numerical solution for the system with a simple scheme relating the moving boundary and its velocity leads to the unknown functions in the assumed polynomial.*

Introduction

Under certain conditions, the phenomenon of oxygen diffusion from blood into oxygen-consuming tissue gives rise to a moving boundary. A typical example arises when studying tumour tissue-oxygen interaction. Generally, in moving boundary problems, the velocity of the moving boundary is determined by the physical requirement that the latent heat required for the change of phase must be supplied or removed by conductions.

In the oxygen diffusion problem, a moving boundary is an essential feature of the problem, but conditions that determine its movement are different. Not only is the concentration of oxygen alyways zero at the moving boundary, but also no oxygen diffuses across it at any time.

Crank and Gupta (1972a), who studied the moving boundary problem arising from the diffusion of oxygen into absorbing tissue, first reported the problem of oxygen diffusion. First the oxygen is allowed to diffuse into a medium, some of the oxygen is absorbed by the medium, thereby being removed from the diffusion process, and the concentration of oxygen at the surface of the medium is maintained constant.

This phase of the problem continues until a steady state is reached in which the oxygen does not penetrate any further into the medium. The supply of oxygen is then cut off and the surface is sealed so that no oxygen passes in or out, the medium continues to absorb the available oxygen already in it and, as a consequence, the boundary marking the furthest depth of penetration in the steady state starts to recede towards the sealed surface.

The major problem is that of tracking the movement of the moving boundary during this stage of the process as well as determining the distribution of oxygen throughout the medium at any instant in time. This type of problem, also known as an implicit moving boundary problem, has been addressed by Crank and Gupta (1972a); initially when the moving boundary is moving slowly they used an approximate analytical solution and a numerical scheme once the velocity of the moving boundary has increased.

Their numerical scheme consists of using a fixed grid network and calculating the concentration at each node using Euler equation. For the grid near the moving boundary, a Langrange type formula is used and the location of the moving boundary is determined using a Taylor series expansion.

In another paper (Crank and Gupta, 1972b) the same authors used a uniform grid system which moves with the velocity of the moving boundary; this has the effect of transferring the unequal interval from the neighborhood of the moving boundary to the surface of the medium and therefore gives an improvement in the smoothness of the calculated motion of the moving boundary. They evaluated the concentration distribution at the new grid points by interpolation using either cubic splines or ordinary polynomials.

Hansen and Hougaard (1974) used an integral equation for the function defining the position of the moving boundary and an integral formula for the concentration distribution. The integral equation is solved asymptotically during the entire motion of the moving boundary whereas the concentration integral is solved asymptotically for small times, and computed by numerical quadrature at later times.

Many other authors have dealt with the problem by various methods; for instance, Berger *et al.* (1975) used a truncation method, whilst Miller *et al.* (1978) used finite elements. More references relating to the oxygen diffusion problem involving a moving boundary can be found in Furzeland (1980) and Crank (1984).

The common feature of the numerical methods (Crank and Gupta, 1972a; 1972b; Hansen and Hougaard, 1974; Berger *et al.*, 1975; Miller *et al.*, 1978; Furzeland, 1980; Crank, 1984) is that they adopt a fixed space-time grid network, and utilize both numerical computation and analytical approximation. In order to prevent the oxygen concentration from taking negative values, which causes instability, these methods often resort to small time steps. This not only increases the CPU-time, but also the array size.

Furthermore, the numerical procedures can not be used up to the end of the absorption process, due to the lack of necessary mesh points when the moving boundary is close to the sealed surface. Therefore, in all methods extrapolation is used to evaluate the time at which the moving boundary reaches the sealed surface.

Gupta and Kumar (1981), by using a variable time step grid network, avoid the large number of time steps generally required for the methods in Crank and Gupta (1972a; 1972b); Hansen and Hougaard (1974), Berger *et al.* (1975), Miller *et al.* (1978), Furzeland (1980) and Crank (1984). Their method computes the concentration distribution using the Crank-Nicolson implicit finite difference scheme. Due to the implicit boundary condition, an integral equation is used to determine the time steps; this gives rise to convergence difficulties because it is very sensitive to a change in concentration. Zerroukat and Chatwin (1992) modified the explicit variable time step method to solve the oxygen diffusion as an example of implicit moving boundary problems.

One of the most important semi-analytical methods is that proposed first in 1988 by Gupta and Banik (1989) to solve the implicit moving boundary problems, which is called constrained integral method (CIM). They solved the diffusion of oxygen in a sphere as an example of implicit moving boundary problem. In their method they assumed the distribution of the oxygen concentration as a polynomial of even degree in which four unknown functions should be determined as a part of the required solution. They expressed these unknowns in terms of the concentration at the outer surface of the sphere, which was still unknown and to be determined. Finally, they reduced the unknowns to two unknowns, the concentration at the outer surface and the position of the moving boundary.

In the present paper, a major modification is developed to the constrained integral method, and the present method takes the name of "modified constrained integral method" or simply (MCIM). The present method starts by assuming a polynomial representing the profile of oxygen concentration. Herein this polynomial is taken as that assumed by Gupta and Banik (1989) just for the purpose of comparison. Moments are then taken, starting from the first one to avoid time differentiation for the unknowns in the assumed polynomial. The number of moments will be equal to the number of unknowns in the polynomial. After some mathematical manipulation, a system of linear equations is obtained, their solution leads to the unknowns directly and subsequently the position of the moving boundary.

Problem description and formulation

Consider a radially symmetric spherical tissue (an absorbing medium in general) of radius k that consumes oxygen at a constant rate A everywhere. The sphere, which is assumed to be free of oxygen at time zero, is subjected to unit concentration at its outer surface $r = k$, as shown in Figure 1.

As soon as oxygen penetrates the tissue, absorption starts taking place in the region that has a non-zero concentration. The diffusion process coupled

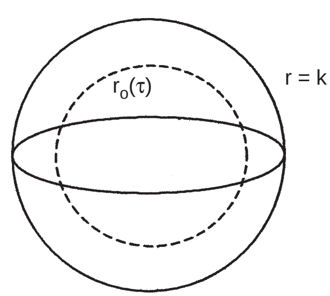

Figure 1.
Problem configuration

with absorption may be defined by Gupta and Baik (1990):

$$\frac{\partial U}{\partial \tau} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(Dr^2\frac{\partial U}{\partial rr}\right) - A \quad \mathrm{r_0}\ (\tau)\ < \mathrm{r} < \mathrm{k} \tag{1}$$

Where

$r_0(\tau)$ Radius of the spherical boundary at time τ

D Constant of diffusion coefficient

A Constant rate of consumption of oxygen

Because there is no flow beyond $r_0(\tau)$ into the sphere, we have:

$$\mathrm{U} = \frac{\partial U}{\partial r} \qquad \mathrm{r} = \mathrm{r_0}(\tau) \tag{2}$$

The condition at the surface r = k and the initial condition may be written as:

$$\mathrm{U}(\mathrm{r},\tau) = 1 \qquad \mathrm{r} = \mathrm{k}, \qquad \tau > 0 \tag{3}$$

and

$$\mathrm{U}(\mathrm{r},\tau) = 0 \qquad 0 \le \mathrm{r} \le \mathrm{k}, \qquad \tau = 0 \tag{4}$$

with

$$\mathrm{r_0}(0) = \mathrm{k} \tag{5}$$

Gupta and Banik (1990) introduced the following change of variable:

$$\mathrm{v} = \mathrm{Ur} \tag{6-a}$$

to reduce equation (1) to linear space, however, the constant absorption terms in the sphere must be transformed in the linear space to terms equivalent to the distance from the origin. Because of that Gupta and Banik (1990) introduced:

$$\mathrm{x} = \mathrm{r}/\mathrm{k} \tag{6–b}$$

$$\mathrm{t} = \mathrm{D}\tau/\mathrm{k}^2 \tag{6-c}$$

$$\mathrm{u} = \mathrm{Dv}/\mathrm{Ak}^3 \tag{6-d}$$

Then, the system (1)-(5) becomes:

$$\frac{\partial \mathrm{u}}{\partial \mathrm{t}} = \frac{\partial^2 \mathrm{u}}{\partial \mathrm{x}^2} - \mathrm{x} \qquad \mathrm{s}(\mathrm{t})\ \le \mathrm{x} \le 1 \tag{7}$$

$$\mathrm{u}(\mathrm{x},\mathrm{t}) = 0 \qquad \mathrm{x} = \mathrm{s}(\mathrm{t}) \tag{8-a}$$

$$\frac{\partial u}{\partial x} = 0 \qquad x = s(t) \tag{8-b}$$

$$u(x,t) = \text{constant} = u_c(\text{say}) \quad \text{at } x = 1, t > 0 \tag{9}$$

$$u(x,t) = 0 \qquad 0 \le x \le 1, t = 0 \tag{10}$$

$$s(0) = 1 \tag{11}$$

Where s(t) is the position of the moving boundary in linear space corresponding to $r_0(t)$ in spherical boundary. We first let the system reach steady state and then seal off the surface x = 1, so that no oxygen can get into the medium or can come out of it.

However, the process of absorption still continues, and the point of zero concentration, which was originally at x = 0, starts moving away from it. The problem is to determine the location of the point of zero concentration, which is the position of the moving boundary and the concentration in the medium at different times.

The second stage may be described by the following equations:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - x \qquad s(t) < x < 1 , \ t > 0 \tag{12}$$

$$u(x,t) = 0 \qquad \text{at } x = s(t), \quad t > 0 \tag{13}$$

$$\frac{\partial u}{\partial x}(x, t) = 0 \qquad \text{at } x = s(t), \ t > 0 \tag{14}$$

$$\frac{\partial u}{\partial x}(x, t) = 0 \qquad \text{at } x = 1, \ t > 0 \tag{15}$$

$$u(x,t) = x^3/6 \qquad 0 \le x \le 1, t = 0 \tag{16}$$

$$s(0) = 0 \tag{17}$$

Equation (16) represents the steady state solution. The initial condition (17) corresponds to the second case in the analysis given by Gupta and Banik (1990), where u_c in equation (9) equals 1/2 which states that the steady-state is obtained when oxygen just reaches the center of the sphere.

The proposed modified constrained integral method (MCIM)

Since the gradient is zero at the outer surface of sphere, i.e. at x = 1, then assume a concentration profile in (1 – x) of the form (Gupta and Banik, 1989):

$$u(x,\ t)\ = a(t)\ +\ b(t)\left(\frac{1-x}{1-s(t)}\right)^2 + c(t)\left(\frac{1-x}{1-s(t)}\right)^4 + d(t)\left(\frac{1-x}{1-s(t)}\right)^6, \quad s(t)\ < x\ < 1 \tag{18}$$

where a(t), b(t), c(t), d(t) and s(t) are five unknowns to be determined. The next step is to take moments as proposed first by Gupta and Banik (1990), but the treatment in the present method will be different as will be seen next.

The general formula for the moments of order n is:

$$\int_{s(t)}^{1} (1-x)^n \frac{\partial u}{\partial t}\ dx\ =\ \int_{s(t)}^{1} \left\{(1-x)^n\left[\frac{\partial^2 u}{\partial x^2} - x\right]\right\}dx \tag{19}$$

in which n = 0 corresponding to zero moment, n = 1 corresponds to first moment, ... etc. In the present paper we will start with the first moment to avoid getting the differentiation with respect to time for the unknowns' a(t), b(t), c(t) and d(t), which is the first major difference between the present method and the constrained integral method, as follows:

$$\int_{s}^{1} (1-x)\frac{\partial u}{\partial t}dx\ =\ \int_{s}^{1} (1-x)\left[\frac{\partial^2 u}{\partial x^2} - x\right]\ dx \tag{20}$$

Integrating both sides, and applying the Leibniz's rule to the left-hand side, gives:

$$\frac{d}{dt}\left[\int_{s}^{1} (1-x)\ u\ dx\right] - \left[(1-s)\ u(s,t)\ \frac{ds}{dt}\right] = (1-x)\left[\frac{\partial u}{\partial x} - \frac{x^2}{2}\right]_s^1 + \int_s^1 \left(\frac{\partial u}{\partial x} - \frac{x^2}{2}\right)\ dx \tag{21}$$

Substituting in the assumed polynomial for x = s, gives:

$$u(s,\ t)\ =\ a(t)\ +\ b(t)\ +\ c(t)\ +\ d(t) \tag{22}$$

Substituting equation (22) into (21), simplifying the integration and then differentiating leads to:

$$-s^{\bullet}\ (1-s)\ a(t)\ + [1-\ s^{\bullet}\ (1-s)\ ]\ (b\ +\ c\ +\ d) = \frac{1}{2}s^2(1-s) - \frac{1}{6}(1-s^3) \tag{23}$$

Following the same procedure for the second leads to the following equation:

$$
\begin{aligned}
&-s^{\bullet}(1-s)^2 a(t) + b(t)\left[\frac{4}{3}(1-s) - s^{\bullet}(1-s)^2\right] \\
&+ c(t)\left[\frac{8}{5}(1-s) - s^{\bullet}(1-s)^2\right] + d(t)\left[\frac{12}{7}(1-s) - s^{\bullet}(1-s)^2\right] \\
&= \frac{1}{2}s^2(1-s)^2 + \frac{1}{3}s^3(1-s) - \frac{1}{12}(1-s^4)
\end{aligned}
\tag{24}
$$

For the third moment:

$$[3 - s^{\bullet}(1-s)](a(t) + b(t) + c(t) + d(t)) = \frac{1}{2}s^2 \tag{25}$$

And finally for the fourth moment:

$$
\begin{aligned}
&a(t)[16(1-s)^3 - s^{\bullet}(1-s)^4] + b(t)[8(1-s)^3 - s^{\bullet}(1-s)^4] \\
&\quad + c(t)\left[\frac{32}{5}(1-s)^3 - s^{\bullet}(1-s^4)\right] \\
&\quad + d(t)\left[\frac{40}{7}(1-s)^3 - s^{\bullet}(1-s)^4\right] \\
&\quad = \frac{1}{2}s^2(1-s)^4 + \frac{2}{3}s^3(1-s)^3 + \frac{1}{2}(1-s)^2(1-s)^4
\end{aligned}
\tag{26}
$$

Equations (23), (24), (25) and (26) can be written in the following matrix form:

$$
\begin{bmatrix} A_{11} & A_{12} & A_{13} & A_{14} \\ A_{21} & A_{22} & A_{23} & A_{24} \\ A_{31} & A_{32} & A_{33} & A_{34} \\ A_{41} & A_{42} & A_{43} & A_{44} \end{bmatrix}
\begin{bmatrix} a(t) \\ b(t) \\ c(t) \\ d(t) \end{bmatrix}
=
\begin{bmatrix} C_1 \\ C_2 \\ C_3 \\ C_4 \end{bmatrix}
\tag{27}
$$

Where:

$$A_{11} = -s^{\bullet}(1-s) \tag{28}$$

$$A_{12} = A_{13} = A_{14} = 1 - s^{\bullet}(1-s) \tag{29}$$

$$A_{21} = -s^{\bullet}(1-s)^2 \tag{30}$$

$$A_{22} = (4/3)(1-s) - s^{\bullet}(1-s)^2 \tag{31}$$

$$A_{23} = (8/5)(1-s) - s^{\bullet}(1-s)^2 \tag{32}$$

$$A_{24} = (12/7)(1 - s) - s^{\bullet}(1 - s)^2 \tag{33}$$

$$A_{31} = A_{32} = A_{33} = A_{34} = 3 - s^{\bullet}(1 - s) \tag{34}$$

$$A_{41} = 16(1 - s)^3 - s^{\bullet}(1 - s)^4 \tag{35}$$

$$A_{42} = 8(1 - s)^3 - s^{\bullet}(1 - s)^4 \tag{36}$$

$$A_{43} = \frac{32}{5}(1 - s)^3 - s^{\bullet}(1 - s)^4 \tag{37}$$

$$A_{44} = \frac{40}{7}(1 - s)^3 - s^{\bullet}(1 - s)^4 \tag{38}$$

$$C_1 = \frac{1}{2}s^2(1 - s) - \frac{1}{6}(1 - s^3) \tag{39}$$

$$C_2 = \frac{1}{2}s^2(1 - s)^2 + \frac{1}{3}s^3(1 - s) - \frac{1}{12}(1 - s^4) \tag{40}$$

$$C_3 = \frac{1}{2}s^2 \tag{41}$$

$$C_4 = \frac{1}{2}s^2(1 - s)^4 + \frac{2}{3}s^3(1 - s)^3 + \frac{1}{2}(1 - s)^2(1 - s)^4 \tag{42}$$

It is clear that all the coefficients in the system (27) are functions of the moving boundary and its velocity. This system must be solved at each time step iteratively.

At the beginning an initial guess for the velocity of the moving boundary is assumed, after that a linear variation between time and the position of the moving boundary is assumed according to the following relation (Ahmed and Wrobel, 1995; Ahmed, 1997):

$$\frac{ds(t)}{dt} = \frac{s_{j+1}(t) - s_j(t)}{t_{j+1} - t_j} \tag{43}$$

The flow chart describing the numerical procedure for solving the system given in equation (27) is shown in Figure 2.

In which

- j Time step
- i Iteration number.

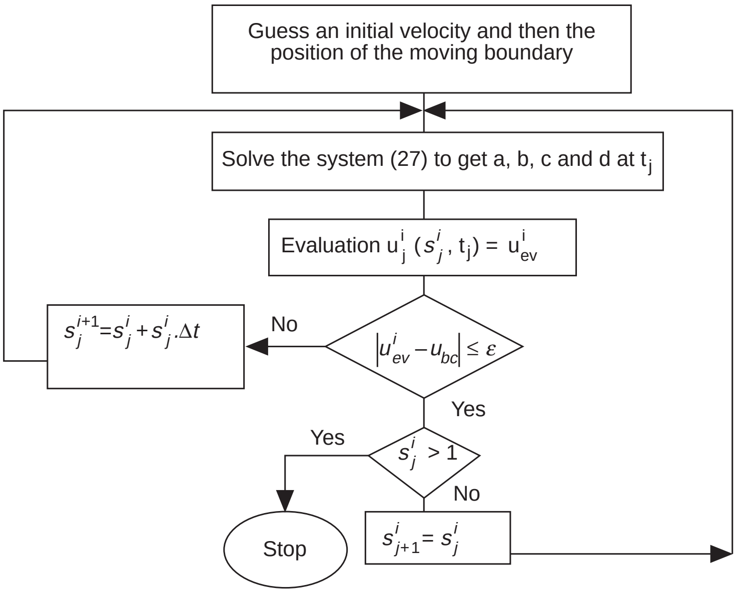

Figure 2.
Flow chart

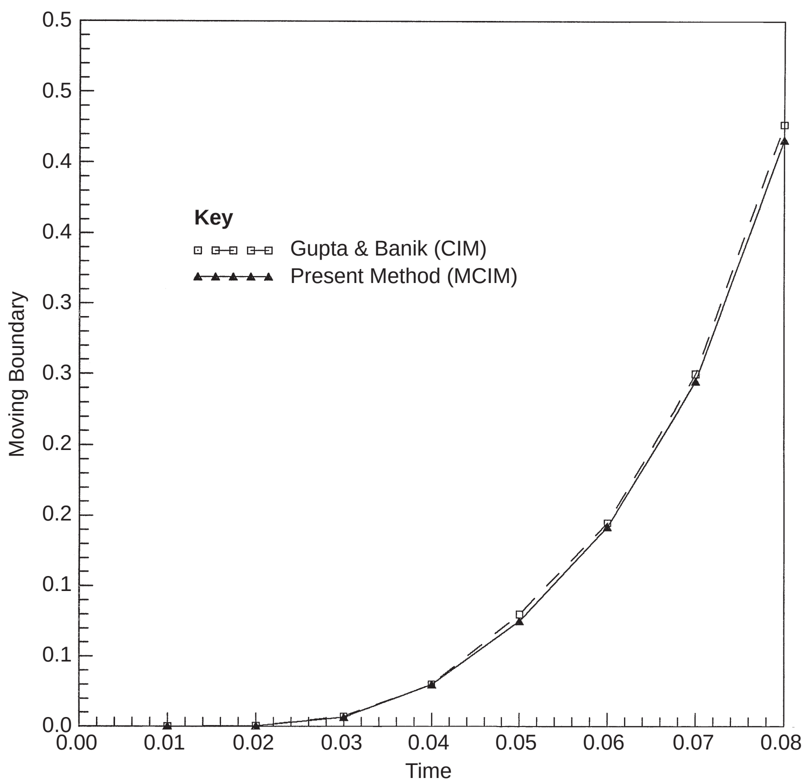

Figure 3.
Position of the moving boundary

u_{ev} Concentration evaluated at the moving boundary

u_{bc} Concentration given as a boundary condition

Numerical results and discussions

Various authors, beginning with Murray and Landis (1959), Crank and Gupta (1972a; 1972b), and Gupta and Banik (1989; 1990) solved the problem under consideration. The last one developed what is called the constrained integral method (CIM) on which the comparison will be restricted.

The moving boundary versus time graph in Figure 3 shows that the boundary moves very slowly in the beginning, while its movement becomes very fast in the last stages. It is clear the agreement between the present method MCIM and the constrained integral method CIM in the behaviour of the movement with slightly small error can be neglected.

The variation of oxygen concentration with depth was made at different times, t = 0.01, 0.03 and 0.05 as shown in Figure 4. The error in variation between the two methods is slightly large only at the beginning time step, this being due to numerical solution of the system of equations obtained.

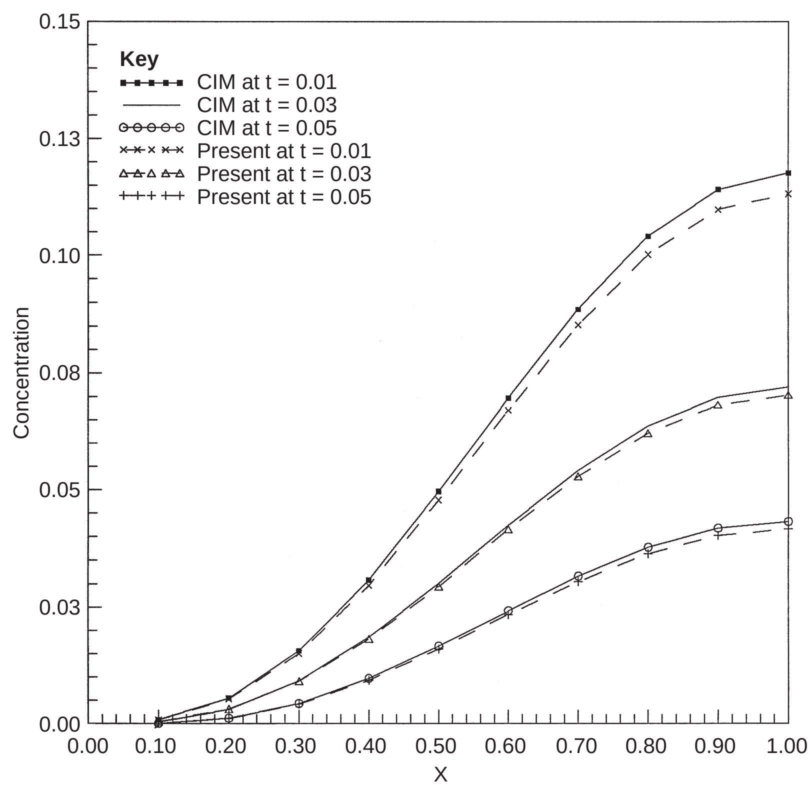

Figure 4.
Oxygen concentration versus depth

Another comparison between the two methods is made as shown in Figure 5, in which the variation of oxygen concentration with time is calculated at different depths and shows a slightly large error occurs only at the beginning time step and then decreases.

Conclusion

The present method is semi-analytical and can be applied to any moving boundary problem in which the moving boundary is either implicit or explicit. It transforms the state equation with the associate boundary and initial conditions to a system of linear equations.

It can be seen from the results obtained by the present method that the error is small compared with the constrained integral method (CIM) and can be neglected. Also, to apply the present method there is no need to solve inequalities as is done in the constrained integral method (CIM) to avoid negative values for the velocity of the moving boundary, which is inconsistent physically.

The error obtained in the present method comes from the numerical solution of the system of linear equations and from the assumption of linear variation of

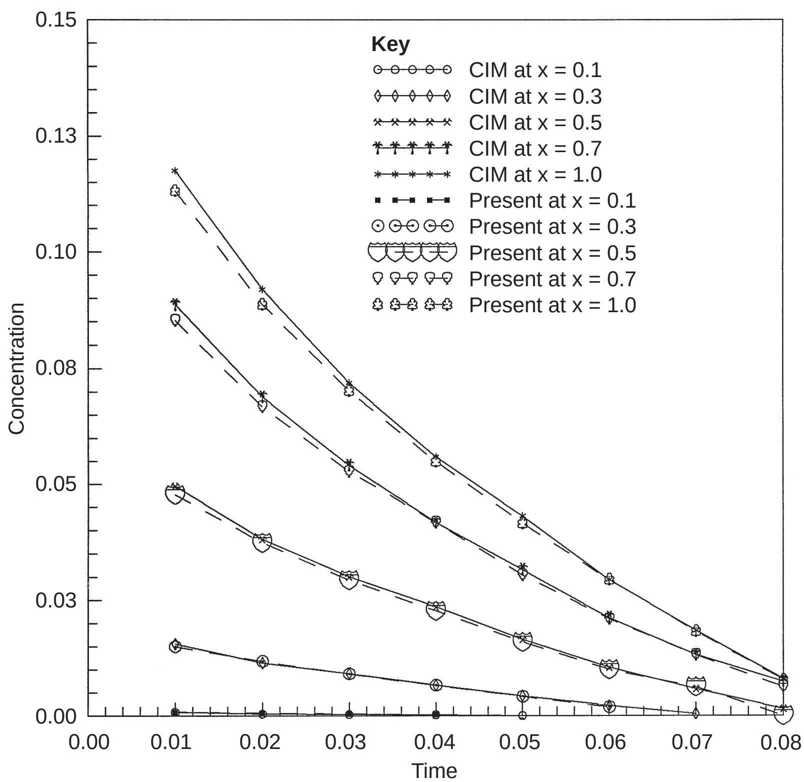

Figure 5. Oxygen concentration versus times

the moving boundary velocity with time. The last one can be reduced by taking small time steps and by decreasing the prescribed tolerance when solving the system of the obtained linear equations.

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