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A Moving Boundary Problem Arising from the Diffusion of Oxygen in Absorbing Tissue

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Approximate analytical and numerical solutions of a partial differential equation are obtained which describe the diffusion of oxygen in an absorbing medium. Essential mathematical difficulties are associated with the presence of a moving boundary which marks the furthest penetration of oxygen into the medium and also with the need to allow for an initial distribution of oxygen through the medium.

1. Introduction

THE CLASSICAL moving-boundary problem in heat flow which has been most thoroughly studied is one in which a change of state occurs on the moving interface. The velocity of the boundary is determined by the physical requirement that the latent heat required for the change of phase must be supplied or removed by conduction. Such problems are often referred to as "Stefan problems" after J. Stefan who published a paper on the subject towards the end of the nineteenth century. There is an extensive literature dating from that time. An excellent survey is given by Muehlbauer & Sunderland (1965).

The present paper concerns a problem arising from the diffusion of oxygen in a medium which simultaneously consumes the oxygen. A moving boundary is an essential feature of this problem also, but the conditions which determine its movement are different. Not only is the concentration of oxygen always zero at the boundary but, in addition, no oxygen diffuses across the boundary at any time. There is thus no relationship which contains the velocity of the moving boundary explicitly. A combination of analytical and numerical methods are applied to this problem and the results are finally expressed in the form of an approximate polynomial expression.

The work is of immediate interest in medical research concerning the uptake of oxygen by tissue and the problem was suggested to us by Dr N. T. S. Evans at the Medical Research Council's Experimental Radiopathology Unit, Hammersmith Hospital.

2. Statement of the Problem

First, oxygen is allowed to diffuse into a medium, and some of the oxygen is absorbed by the medium, thereby being removed from the diffusion process. The concentration of oxygen at the surface of the medium is maintained constant. This first 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 further 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, recedes towards the sealed surface. The major problem is that of tracing the movement of the boundary during this phase and of determining the distribution of oxygen through the medium as a function of time. A secondary problem in the application of numerical techniques is associated with the discontinuity in the derivative boundary condition which results from the abrupt sealing of the surface.

The diffusion-with-absorption process is represented by the partial differential equation

$$\frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} - m, \tag{2.1}$$

where $C(X, T)$ denotes the concentration of the oxygen free to diffuse at a distance X from the outer surface of the medium at time T, D is a constant diffusion coefficient and m, the rate of consumption of oxygen per unit volume of the medium, is also assumed constant.

The problem has two parts:—

(a) Steady-state solution

During the initial phase, when the oxygen is entering through the surface, the following boundary condition is satisfied,

$$C = C_0, \quad X = 0, \quad T \geqslant 0, \tag{2.2}$$

where C_0 is a constant.

A steady-state is achieved in which the concentration at every point in the medium becomes independent of time, i.e. $\partial C/\partial T = 0$ everywhere, when the gradient of concentration becomes zero at the point, X_0, in the medium where the concentration itself is zero. No oxygen can then diffuse beyond this point and we have the conditions,

$$C = 0, \quad X \geqslant X_0, \tag{2.3}$$

$$\frac{\partial C}{\partial X} = 0, \quad X \geqslant X_0, \tag{2.4}$$

for $T \geqslant 0$.

The steady-state is defined by a solution of

$$D\frac{\partial^2 C}{\partial X^2} - m = 0 \tag{2.5}$$

which satisfies the boundary conditions (2.2), (2.3) and (2.4). This solution is readily seen to be

$$C = \frac{m}{2D}(X - X_0)^2, \tag{2.6}$$

where

$$X_0 = \sqrt{\left(\frac{2DC_0}{m}\right)}. \tag{2.7}$$

(*b*) *Moving Boundary Problem*

After the surface $X = 0$ has been sealed, oxygen which is already in the medium, in the range $0 \leqslant X \leqslant X_0$, continues to be consumed. Consequently, the point of zero-concentration which was initially given by (2.7) recedes towards $X = 0$. Let the position of this point at any time, T, be represented by $X_0(T)$. The second phase of the problem can be expressed by the equation,

$$\frac{\partial C}{\partial T} = D\frac{\partial^2 C}{\partial X^2} - m, \qquad 0 \leqslant X \leqslant X_0(T), \tag{2.8}$$

with the following conditions,

$$\frac{\partial C}{\partial X} = 0, \qquad X = 0, \qquad T \geqslant 0, \tag{2.9}$$

$$C = \frac{\partial C}{\partial X} = 0, \qquad X = X_0(T), \qquad T \geqslant 0, \tag{2.10}$$

$$C = \frac{m}{2D}(X - X_0)^2, \qquad 0 \leqslant X \leqslant X_0, \qquad T = 0, \tag{2.11}$$

where $T = 0$ is the moment when the surface is sealed. Making the changes of variables,

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

and denoting by $x_0(t)$ the value of x corresponding to $X_0(T)$, the above system is reduced to the following non-dimensional form,

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - 1, \qquad 0 \leqslant x \leqslant x_0(t), \tag{2.12}$$

with the corresponding boundary conditions,

$$\frac{\partial c}{\partial x} = 0, \qquad x = 0, \qquad t \geqslant 0, \tag{2.13}$$

$$c = \frac{\partial c}{\partial x} = 0, \qquad x = x_0(t), \qquad t \geqslant 0, \tag{2.14}$$

$$c = \tfrac{1}{2}(1 - x)^2, \qquad 0 \leqslant x \leqslant 1, \qquad t = 0, \tag{2.15}$$

where $x_0(0) = 1$. The subscript t in $x_0(t)$ is dropped in the following discussions.

3. Short-time Solution

The condition (2.15) shows that in the steady-state a negative unit gradient of concentration exists at the surface. When the surface is sealed a zero surface gradient is instantaneously imposed in accordance with (2.13). Because of this discontinuity in the surface-gradient numerical methods based on finite differences are liable to give inaccurate solutions in the neighbourhood of the surface for short times. There will be an interval of time, however, before the disturbance at the surface has an effect on the solution in the neighbourhood of $x = 1$ to any specified degree of accuracy. Thus an analytical solution can be obtained which will provide a suitable approximation for small times, by assuming that the boundary, $x_0 = 1$, does not move initially.

The solution of (2.12) subject to the initial condition (2.15) and the boundary conditions (2.13) and

$$c = 0, \quad x = 1, \quad t \geqslant 0 \tag{3.1}$$

is found by using Laplace Transforms to be

$$c(x, t) = \tfrac{1}{2}(1-x)^2 + 2\sqrt{\left(\frac{t}{\pi}\right)} \sum_{n=0}^{\infty} (-1)^n \left[\exp\left\{-\left(\frac{2n+2-x}{2\sqrt{t}}\right)^2\right\} - \exp\left\{-\left(\frac{2n+x}{2\sqrt{t}}\right)^2\right\}\right] - \sum_{n=0}^{\infty} (-1)^n \left\{(2n+2-x)\operatorname{erfc}\left(\frac{2n+2-x}{2\sqrt{t}}\right) - (2n+x)\operatorname{erfc}\left(\frac{2n+x}{2\sqrt{t}}\right)\right\}, \quad 0 \leqslant x \leqslant 1, \quad t \geqslant 0. \tag{3.2}$$

Values of $c(x, t)$ have been computed for $x = 0\ (0{\cdot}05)\ 1.0$. The typical curves of Fig. 1 demonstrate the general shape and confirm that the concentration has not changed within the accuracy of plotting near the boundary at $x = 1$.

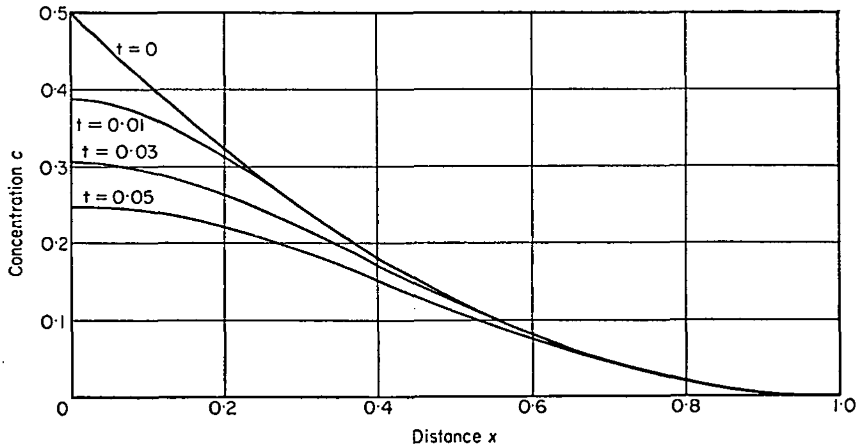

FIG. 1. Concentration distributions for $t < 0{\cdot}05$ before the boundary moves within the accuracy of plotting.

In computing $c(x, t)$ from (3.2), it is seen that the convergence of the infinite series is very rapid, so that the terms corresponding to $n = 0$ are sufficient over an appreciable interval of time, when the terms less than 10^{-6} are neglected. Furthermore, for $0 \leqslant t \leqslant 0{\cdot}020$, the second and the third series can be ignored to obtain an accuracy nowhere worse than 10^{-5}. The concentration for $0 \leqslant t \leqslant 0{\cdot}020$ can therefore be represented fairly accurately by the approximate expression,

$$c(x, t) = \tfrac{1}{2}(1-x)^2 - 2\sqrt{\left(\frac{t}{\pi}\right)} \exp\left\{-\left(\frac{x}{2\sqrt{t}}\right)^2\right\} + x \operatorname{erfc}\left(\frac{x}{2\sqrt{t}}\right), \quad 0 \leqslant x \leqslant 1. \tag{3.3}$$

4. Numerical Method

Once the boundary has started to move we resort to numerical methods of solution. Several methods have been proposed. Douglas & Gallie (1955) introduced a method of variable time step, keeping the size of the space mesh fixed. Murray & Landis (1959) used a variable space mesh and kept the time step fixed. Ehlrich (1958) employed implicit formula at the intermediate points and Taylor's expansions near the moving boundary in both time and space directions. Lotkin (1960) made use of subdivided differences while Crank (1957) suggested a three-point Lagrange interpolation formula near the moving boundary.

In the present analysis, the concentrations at the intermediate points between the two boundaries have been calculated by using simple explicit finite-difference formulae. Near the moving boundary a Lagrange-type formula has been used, as suggested by Crank (1957) because of convenience in calculation. The location of the moving point itself is determined by a Taylor's series. The method is described below in detail.

The whole region, $0 \leqslant x \leqslant 1$, is subdivided into M intervals each of width δx and we take $x_r = r\delta x$ where $0 \leqslant r \leqslant M(M\delta x = 1)$.

4.1. *Concentrations at the Intermediate Points*

We assume that the concentrations at each of the grid points, at the jth time level are known and the position of the moving boundary at that time is somewhere in the rth interval between x_{r-1} and x_r, given by $x_0 = (r-1)\delta x + p^j \delta x$ where p^j is positive and usually less than one, and is also known (Fig. 2). Then the concentrations at the

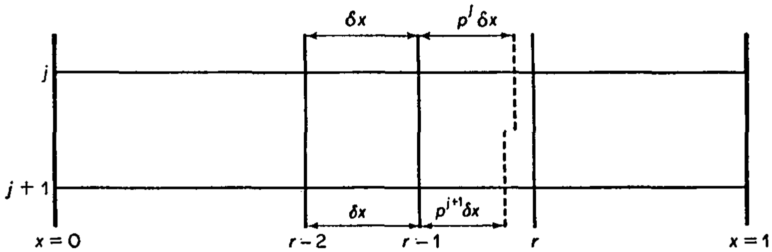

FIG. 2.

$(j+1)$th time level, up to and including the mesh point $r-2$ can be calculated using the well known explicit formulae,

$$\frac{c_0^{j+1} - c_0^j}{\delta t} = \frac{2}{(\delta x)^2}(c_1^j - c_0^j) - 1, \tag{4.1}$$

$$\frac{c_k^{j+1} - c_k^j}{\delta t} = \frac{1}{(\delta x)^2}(c_{k-1}^j - 2c_k^j + c_{k+1}^j) - 1, \tag{4.2}$$

for $k = 1, 2, \ldots, (r-2)$, where δt is the size of the time-step and c_k^j denotes the concentration at point $k\delta x$ at time $j\delta t$.

4.2. *Concentration in the Neighbourhood of the Moving Boundary*

Let $f(a_0)$, $f(a_1)$ and $f(a_2)$ be any function values corresponding to the arguments a_0, a_1 and a_2. A three-point Lagrangian interpolation formula can be written as

$$f(x) = \frac{(x-a_1)(x-a_2)}{(a_0-a_1)(a_0-a_2)}f(a_0)+\frac{(x-a_0)(x-a_2)}{(a_1-a_0)(a_1-a_2)}f(a_1)+\frac{(x-a_0)(x-a_1)}{(a_2-a_0)(a_2-a_1)}f(a_2).$$

Differentiating the above twice with respect to x, we get

$$\frac{\partial^2 f}{\partial x^2} = \frac{2f(a_0)}{(a_0-a_1)(a_0-a_2)}+\frac{2f(a_1)}{(a_1-a_0)(a_1-a_2)}+\frac{2f(a_2)}{(a_2-a_0)(a_2-a_1)}. \tag{4.3}$$

Application of (4.3) at the points $(r-2)\delta x$, $(r-1)\delta x$ and the moving point, and remembering the boundary condition (2.14), gives,

$$\frac{\partial^2 c}{\partial x^2} = \frac{2}{(\delta x)^2}\left(\frac{c_{r-2}}{1+p}-\frac{c_{r-1}}{p}\right)-1,$$

and the appropriate finite-difference replacement at the point $(r-1)\delta x$ leads to

$$\frac{c_{r-1}^{j+1}-c_{r-1}^{j}}{\delta t} = \frac{2}{(\delta x)^2}\left(\frac{c_{r-2}^{j}}{1+p^j}-\frac{c_{r-1}^{j}}{p^j}\right)-1, \tag{4.4}$$

an explicit expression for c_{r-1}^{j+1}.

4.3. *Position of the Moving Boundary*

In order to determine the location of the moving boundary, $x_0(t)$, we first derive some extra conditions there. Differentiation of (2.14) with respect to t, gives

$$\frac{dc}{dt} = \left(\frac{\partial c}{\partial x}\right)_{x=x_0}\left(\frac{dx_0}{dt}\right)+\left(\frac{\partial c}{\partial t}\right)_{x=x_0} = 0. \tag{4.5}$$

By using (2.12) and (2.14) in (4.5) we obtain

$$\frac{\partial^2 c}{\partial x^2} = 1, \qquad x = x_0. \tag{4.6}$$

Differentiating (2.12) with respect to x, we get

$$\frac{\partial^2 c}{\partial x \partial t} = \frac{\partial^3 c}{\partial x^3}. \tag{4.7}$$

Again, we have from (2.14)

$$\frac{d}{dt}\left(\frac{\partial c}{\partial x}\right)\left(\frac{\partial^2 c}{\partial x^2}\right)_{x=x_0}\frac{dx_0}{dt}+\left(\frac{\partial^2 c}{\partial t \partial x}\right)_{x=x_0} = 0,$$

and hence using (4.6) and (4.7) in the above and assuming that order of differentiation by x and t can be interchanged we obtain

$$\frac{\partial^3 c}{\partial x^3} = -\frac{dx_0}{dt}, \qquad x = x_0,$$

Similarly

$$\frac{\partial^4 c}{\partial x^4} = \left(\frac{dx_0}{dt}\right)^2, \qquad \frac{\partial^5 c}{\partial x^5} = -\frac{d^2 x_0}{dt^2}-\left(\frac{dx_0}{dt}\right)^3 \text{ etc.}$$

TABLE 4.1

Values of 10^6c *and the positions of the moving boundary. For each time the upper entry corresponds to* $\delta x = 0{\cdot}05$ *and the lower entry* $\delta x = 0{\cdot}10$

t \ x	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9	Moving boundary
0·010	387497 393371	365668 369057	310719 311105	243726 243388	179927 179787	125000 124980	80000 79999	45000 45000	20000 20000	5000 5000	1·00000 1·00000
0·020	340661 344573	326222 329324	287180 288631	233793 234012	176960 176757	124370 124193	79905 79831	44991 44970	19999 19996	5000 4999	1·00000 0·99999
0·050	247841 250246	240358 242563	219089 220778	187264 188310	149327 149802	109945 110039	73208 73118	42199 42067	18955 18852	4673 4620	0·99709 0·99612
0·100	143287 144974	139414 141031	128228 129651	110966 112108	89502 90330	66112 66643	43228 43515	23232 23345	8342 8344	619 546	0·93518 0·93304
0·120	109228 110768	106125 107613	97149 98489	83265 84387	65963 66832	47115 47733	28827 29224	13324 13544	2924 2987	0 0	0·87885 0·87729
0·140	77937 79368	75442 76833	68233 69507	57105 58206	43322 44216	28536 29210	14730 15187	4249 4489	0 0	0 0	0·79756 0·79476
0·160	48893 50243	46912 48230	41212 42437	32511 33595	21996 22900	11346 12036	2890 3271	0 0	0 0	0 0	0·68128 0·68089
0·180	21824 23119	20328 21597	16096 17289	9950 11010	3506 4285	0 0	0 0	0 0	0 0	0 0	0·49607 0·49257
0·190	9039 10319	7827 9082	4575 5703	750 1353	0 0	0 0	0 0	0 0	0 0	0 0	0·33873 0·35201
0·195	2880 4153	1909 3138	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0·16128 0·17922

Now, the Taylor's series for c_{r-1} obtained by expanding about the moving point can be written as

$$c_{r-1} = c(x_0) - p\delta x\left(\frac{\partial c}{\partial x}\right)_{x=x_0} + \tfrac{1}{2}(p\delta x)^2\left(\frac{\partial^2 c}{\partial x^2}\right)_{x=x_0} - \tfrac{1}{6}(p\delta x)^3\frac{\partial^3 c}{\partial x^3} + \dots$$

$$= \tfrac{1}{2}(p\delta x)^2 + \tfrac{1}{6}(p\delta x)^3\frac{dx_0}{dt} + \dots . \tag{4.8}$$

Provided the boundary is not moving too quickly the first term of the series provides a reasonable approximation and gives

$$p = \frac{\sqrt{(2c_{r-1})}}{\delta x}. \tag{4.9}$$

We shall see later that the boundary moves faster towards the end of the process and we then replace the finite-difference solution by an analytical expression.

When c_{r-1}^{j+1} has been calculated from (4.4), the relation (4.9) gives the position of the moving point at the $(j+1)$th time level.

4.4. *Moving Boundary Crossing a Mesh Line*

As c_{r-1} goes on decreasing we look for either of the two possibilities (i) $c_{r-1}^{j+1} \leqslant 0$ or (ii) $c_{r-1}^{j+1} > c_{r-1}^{j}$. With regard to the first condition it is physically impossible for c_{r-1} to go negative. When the second condition is detected, it shows that the numerical process has become unstable. A stability analysis is presented in the appendix to this paper. When either of the two conditions arises, the $(r-1)$th mesh point is given up at the $(j-1)$th time level and onwards. The Lagrange formula is then applied to

TABLE 4.2

Comparison between analytical and numerical ($\delta x = 0{\cdot}05$) solutions for small times. For each time the upper entry corresponds to the analytical solution and the lower entry to numerical solutions. Tabulated values are $10^6 c$

t \ x	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9
0·001	464318	404606	320000	245000	180000	125000	80000	45000	20000	5000
	460000	405000	320000	245000	180000	125000	80000	45000	20000	5000
0·002	449538	401927	319973	245000	180000	125000	80000	45000	20000	5000
	452000	405000	320000	245000	180000	125000	80000	45000	20000	5000
0·003	438197	397811	319760	244998	180000	125000	80000	45000	20000	5000
	437600	398000	320000	245000	180000	125000	80000	45000	20000	5000
0·004	428636	393157	319212	244981	180000	125000	80000	45000	20000	5000
	429600	394760	320000	245000	180000	125000	80000	45000	20000	5000
0·005	420213	388238	318302	244924	179999	125000	80000	45000	20000	5000
	420320	389128	318976	245000	180000	125000	80000	45000	20000	5000
0·010	387164	365073	309950	243276	179804	124986	79999	45000	20000	5000
	387497	365668	310719	243726	179927	125000	80000	45000	20000	5000
0·050	247691	240179	218845	186955	148992	109636	72962	42030	18856	4628
	247841	240358	219089	187264	149327	109945	73208	42199	18955	4673

recalculate c_{r-2}^{j} using a new value of p at the $(j-1)$th time which is taken to be the old value of p^{j-1} plus one. This process is continued until there are at least two mesh points including the sealed surface. At the end, however, an approximate solution may be useful which is discussed in the next section.

Concentrations have been computed for $\delta x = 0{\cdot}10$, $0{\cdot}05$ and $\delta t = 0{\cdot}001$. A comparison is given in Table 4.1 to indicate the order of accuracy of the results. Table 4.2 shows that the values obtained by using $\delta x = 0{\cdot}05$, are in a very good agreement with those calculated from the Laplace solution, for small times. It should be noted that the numerical solutions involve large errors in the beginning at the surface due to discontinuity in the gradient there at zero time, but they very soon become consistent with the Laplace solutions. At $t = 0{\cdot}050$, the difference between the numerical and the Laplace solutions is not more than $0{\cdot}0003$ anywhere when the boundary x_0 has moved a distance of $0{\cdot}003$ from its original position $x_0 = 1$.

5. Integral Method

In this section we look for simple analytical expressions for the concentration-distribution as well as for the location of the moving boundary at any given time. We shall make use of an approximate method that was introduced by Goodman (1958) and is usually referred to as the "Integral Method". A review of integral methods and their applications to a variety of transient-heat-transfer problems is to be found in Irvine & Hartnett (1964).

5.1. *Description of Integral Method*

In applying the Integral Method to the present problem we choose a profile which satisfies all the known conditions. This profile involves the position of the moving point as a parameter to be determined. In order to find a moving point versus time relationship we integrate both sides of the differential equation (2.12) with respect to x over the range for which it is valid, i.e. $0 \leqslant x \leqslant x_0$. This means that the differential equation is to be satisfied on average only and not at each point. Thus we obtain

$$\int_0^{x_0} \frac{\partial c}{\partial t}\, dx = \int_0^{x_0} \frac{\partial^2 c}{\partial x^2}\, dx - \int_0^{x_0} \quad dx. \tag{5.1}$$

Substituting the concentration profile in (5.1) and after a certain amount of manipulation we get an ordinary differential equation for the position of the moving boundary, x_0, with t as the independent variable. Once the position of the moving point, x_0, is determined at any time, substitution of this value for the parameter x_0 in the profile gives the concentration distribution at that time.

5.2. *Determination of Surface Concentration*

Integral methods are not very amenable in cases of non-uniform initial distributions. In the present problem the discontinuity in the surface gradient is an additional difficulty. In order to apply an integral method we first get an expression for the surface concentration and use it as an additional condition to obtain the profile. We refer to the analytical solution (3.2) which has been obtained assuming the boundary, x_0, fixed at $x = 1$. As described in Section 3, this solution is true everywhere for small times i.e. until the boundary has not moved within the range of working accuracy. However, it is observed that the concentrations near the sealed surface have a close agreement with those obtained from the numerical solutions for $\delta x = 0{\cdot}05$ for all times. Therefore, an expression for surface concentration can be obtained by putting $x = 0$ in (3.2). A closer examination of that expression reveals that the concentration varies linearly with the square-root of the time to an accuracy of 5×10^{-4}, as compared with the numerical solutions, and is given by

$$c(0, t) = \tfrac{1}{2} - 2\sqrt{\frac{t}{\pi}}. \tag{5.2}$$

Comparative figures are given in the following table for (i) analytical solution (3.2); (ii) numerical solution for $\delta x = 0{\cdot}05$ and (iii) approximate solution given by (5.2).

TABLE 5.1

Comparisons of 10^6c at the sealed surface

Solutions \ Time	0·04	0·08	0·12	0·16	0·18	0·19
Analytical	274328	180852	109134	48771	21546	8546
Numerical	274496	180969	109228	48893	21834	9039
Approximate	274324	180846	109118	48648	21269	8151

It may be mentioned here that the total time, t_1, for the concentration everywhere to become zero is given by $c(0, t_1) = 0$ and is equal to $\pi/16$ from (5.2).

5.3. *Choosing a Polynomial Profile*

A polynomial profile of fourth degree is now chosen containing five unknown parameters which might be functions of time and which are determined using (2.13), (2.14), (4.6) and (5.2). On writing c_0 for $c(0, t)$ the equation for the polynomial becomes

$$c(x, x_0) = (1-x/x_0)^2\{\tfrac{1}{2}x^2+4c_0(1-x/x_0)-3c_0(1-x/x_0)^2\}. \tag{5.3}$$

This contains the position of the moving point, x_0, which still has to be determined.

5.4. *Determination of the Moving Boundary*

To obtain x_0 as a function of time we refer back to the equation (5.1) which gives

$$\int_0^{x_0} \frac{\partial c}{\partial t}\,dx = \frac{\partial}{\partial t}\int_0^{x_0} c\,dx = -x_0, \tag{5.4}$$

since $\partial c/\partial x = 0$ at $x = 0, x_0$.

Writing $c(x, x_0)$ from (5.3) in (5.4) and using (5.2) we get, after some manipulation

$$\frac{dx_0}{dt} = -\frac{\{20-8/\sqrt{(\pi t)}\}x_0}{x_0^2+4-16\sqrt{(t/\pi)}}. \tag{5.5}$$

We know that $dx_0/dt \leqslant 0$. This condition will not be true until

$$20-\frac{8}{\sqrt{(\pi t)}} \geqslant 0, \tag{5.6}$$

since the term in the denominator of (5.5) is positive for $0 \leqslant x_0 \leqslant 1$ and $t \leqslant t_1$, where t_1 is obtained from (5.2).

The inequality (5.6) gives the minimum time t_0 for the condition $dx_0/dt \leqslant 0$ to hold as $4/25\pi$. It should be noted that as the moving point x_0 approaches the sealed surface, its speed dx_0/dt tends to infinity as t tends to t_1.

We have found that the numerical solution of (5.5) obtained by using a Runge-Kutta algorithm can be approximated by the expression,

$$x_0 = 1 - \exp\left\{-2\left(\frac{t_1 - t}{t - t_0}\right)^{\frac{1}{2}}\right\}. \tag{5.7}$$

Table 5.2 below provides a comparison for the position of the moving boundary as obtained from (i) numerical evaluation of (5.5) using Runge-Kutta method (ii) approximation (5.7) and (iii) numerical method of Section 4.

TABLE 5.2

Comparison for $10^4 x_0$ at different times

Time	0·051	0·060	0·080	0·100	0·120	0·140	0·160	0·180	0·190	0·195
Numerical Solution of (5·5)	10000	9974	9750	9321	8686	7817	6634	4892	3505	2331
Approximate solution (5·7)	10000	9996	9817	9393	8779	7962	6848	5092	3478	1760
Numerical Method of section 4.	9967	9922	9719	9352	8788	7975	6812	4959	3381	1618

It is seen from the above table that the numerical solution of (5.5) agrees with the exponential profile for the moving boundary (5.7) very well except for very large times. But the profile (5.7) has a very good agreement with the values obtained from the numerical method for all times. Therefore, (5.2) and (5.3) together with (5.7) constitute an approximate solution. It should be noted that this solution is applicable for the time interval $4/25\pi \leqslant t \leqslant \pi/16$ only. For $t \leqslant 4/25\pi$, Laplace solutions (3.2) and (3.3) give analytical solutions when it has been assumed that the boundary has not moved from its original position $x_0 = 1$. Thus we have got now an analytical solution of the problem for all times.

6. Results and Discussion

The concentrations in the medium at various times together with the position of the moving boundary have been compared in Table 6.1 for numerical and the approximate solutions. A very close agreement is seen between the two solutions. The approximate method would specially be useful (a) to calculate the concentration and the position of the moving boundary at an arbitrary time and (b) at the end when the numerical method would not work because too few mesh points remain. Graphs have been drawn to show the concentration-distributions at various times (Fig. 3) and the progress of the moving boundary with respect to time (Fig. 4).

TABLE 6.1

Comparison of concentrations 10^6c and the distances of the moving boundary from the sealed surface. For each time the upper entry shows values obtained from the approximate solution and the lower entry values from the numerical solution ($\delta x = 0{\cdot}05$)

t \ x	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9	Moving boundary
0·051	245176	236403	213648	181831	145308	107868	72736	42571	19469	4957	1·00000
	245329	237966	217026	185652	148186	109216	72788	41981	18854	4635	0·99673
0·060	223605	215950	195945	167714	137974	101028	68767	40671	18809	4837	0·99957
	223746	217330	198992	171251	137684	102227	68548	39645	17705	4186	0·99220
0·100	143175	138758	126795	109243	88096	65385	43176	23569	8703	751	0·93934
	143287	139414	128338	110996	89502	66112	43228	23232	8342	619	0·93518
0·150	62981	61083	55236	45725	33529	20315	8443	962	0	0	0·74538
	63157	60928	54494	44602	32453	19668	8298	1007	0	0	0·74487
0·180	21269	20771	17750	11681	4387	42	0	0	0	0	0·50925
	21824	20328	16096	9950	3506	0	0	0	0	0	0·49607
0·190	8151	8028	5315	925	0	0	0	0	0	0	0·34776
	9039	7827	4575	750	0	0	0	0	0	0	0·33873
0·195	1721	1307	0	0	0	0	0	0	0	0	0·17598
	2880	1909	0	0	0	0	0	0	0	0	0·16128

Note. For $t < 0{\cdot}050$ see Table 4.2.

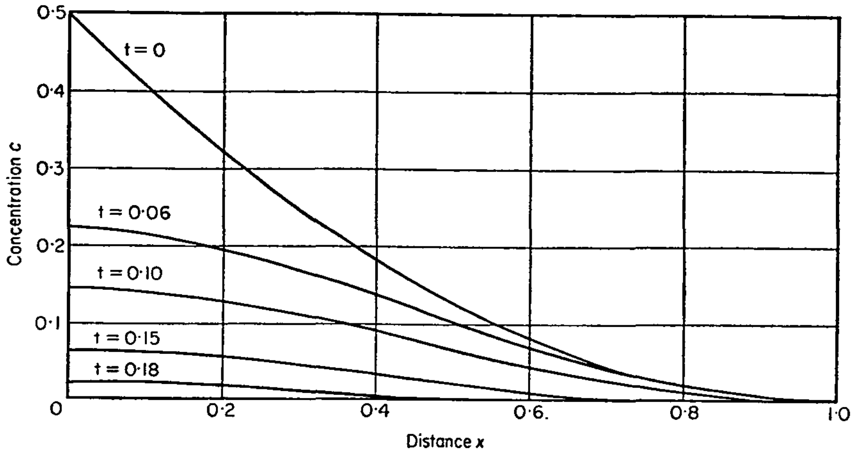

FIG. 3. Concentration distributions for the steady-state ($t = 0$) and for $t > 0{\cdot}05$.

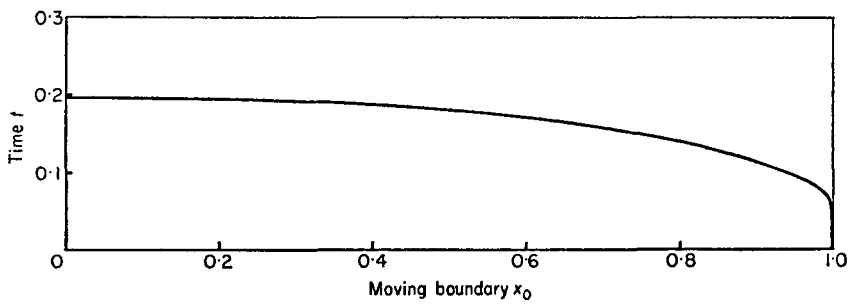

FIG. 4. Position of the moving boundary with respect to time.

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Appendix. Stability Analysis

The set of difference equations connecting values of c at two consecutive time levels can be written in the following matrix form ($r = \delta t/(\delta x)^2$),

$$\begin{bmatrix} c_0^{j+1} \\ c_1^{j+1} \\ \cdot \\ \cdot \\ \cdot \\ c_{N-2}^{j+1} \\ c_{N-1}^{j+1} \end{bmatrix} = \begin{bmatrix} 1-2r & 2r & & & \\ r & 1-2r & r & 0 & \\ & \cdot & \cdot & & \\ & & \cdot & \cdot & \\ & & & \cdot & \\ & 0 & r & 1-2r & r \\ & & & \dfrac{2r}{1+p^j} & 1-\dfrac{2r}{p^j} \end{bmatrix} \begin{bmatrix} c_0^j \\ c_1^j \\ \cdot \\ \cdot \\ \cdot \\ c_{N-2}^j \\ c_{N-1}^j \end{bmatrix} - \begin{bmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ 1 \\ 1 \end{bmatrix} .\delta t \tag{1}$$

or

$$\mathbf{c}^{j+1} = \mathbf{A}_j\mathbf{c}^j - \mathbf{U}\delta t \tag{2}$$

where $\mathbf{A}_j$ is a square matrix of order N which varies with N and $\mathbf{U}$ is a column vector each element of which is unity. We see that elements in the last row of $\mathbf{A}_j$ are dependent on j and therefore in order to make analysis possible we first replace p^j by a constant value p. Later on conditions are imposed on p in order to make the scheme stable. Equation (2) is then written as

$$\mathbf{c}^{j+1} = \mathbf{A}\mathbf{c}^j - \mathbf{U}\delta t. \tag{3}$$

We denote the computed values by $\boldsymbol{\psi}$ so that we have actually solved the equations

$$\boldsymbol{\psi}^{j+1} = \mathbf{A}\boldsymbol{\psi}^j - \mathbf{U}\delta \mathrm{t}. \tag{4}$$

The computational error is then given by subtracting (4) from (3). If the error introduced at the kth step is denoted by the vector $\mathbf{e}^k$, then

$$\mathbf{c}^{j+1} - \boldsymbol{\psi}^{j+1} = \mathbf{A}(\mathbf{c}^j - \boldsymbol{\psi}^j),$$

i.e.

$$\mathbf{e}^{j+1} = \mathbf{A}\mathbf{e}^j. \tag{5}$$

The recurrence relation (5) gives

$$\mathbf{e}^{j+1} = (\mathbf{A})^{j+1}\mathbf{e}^0, \tag{6}$$

where $\mathbf{e}^0$ is an error vector for the starting values.
Let us express $\mathbf{e}^0$ as the linear combination of the eigenvectors of $\mathbf{A}$, such that

$$\mathbf{e}^0 = \sum_{s=1}^{N} a_s \mathbf{v}_s,$$

where $\mathbf{v}_s$ is an eigenvector of A corresponding to the eigenvalue λ_s and a's are constants. It is easy to show that

$$\mathbf{e}^n = \sum_{s=1}^{N} a_s \lambda_s^n \mathbf{v}_s.$$

For $\mathbf{e}^n$ to tend to zero, as n increases, it follows that the largest of $|\lambda_1|, |\lambda_2|, \ldots, |\lambda_N|$ must be less than unity. If Q_s is the sum of the moduli of the terms along the sth row excluding the diagonal term a_{ss} in matrix A then by Brauer's theorem every eigenvalue of A lies inside or on the boundary of at least one of the circles $|\lambda - a_{ss}| = Q_s$.

As we are interested in the bounds of p, applying Brauer's theorem to the last row of **A** that contains p, we have

$$Q_s = \frac{2r}{1+p}, \qquad a_{ss} = 1-\frac{2r}{p},$$

so that

$$\left|\lambda-\left(1-\frac{2r}{p}\right)\right| \leqslant \frac{2r}{1+p}.$$

The bounds for λ are given by

$$\lambda_1 = 1-\frac{2r}{p(1+p)}; \qquad \lambda_2 = \frac{2r(1+2p)}{p(1+p)}-1.$$

For stability we require $|\lambda_1| \leqslant 1$, $|\lambda_2| \leqslant 1$, and hence

$$-1 \leqslant 1-\frac{2r}{p(1+p)} \leqslant 1 \quad \text{giving} \quad \frac{r}{p(1+p)} \leqslant 1,$$

and

$$-1 \leqslant \frac{2r(1+2p)}{p(1+p)} \leqslant 1 \quad \text{giving} \quad \frac{r(1+2p)}{p(1+p)} \leqslant 1.$$

Since p is always positive, the condition for stability is given by the second inequality because the first one is then satisfied automatically. Therefore, for overall stability

$$p^2+(1-2r)p-r \geqslant 0.$$

Since $r \leqslant \frac{1}{2}$ for the stability of the simple explicit scheme used at the intermediate points, it can be shown that

$$p \geqslant r-\tfrac{1}{2}+\sqrt{(\tfrac{1}{4}+r^2)}. \tag{7}$$

For $\delta x = 0{\cdot}1$, $\delta t = 0{\cdot}001$ we get the stability condition $p \geqslant 0{\cdot}11$ and for $\delta x = 0{\cdot}05$, $\delta t = 0{\cdot}001$ we have $p \geqslant 0{\cdot}54$. This suggests that an instability may arise when the moving point is nearer than 0·011 to the neighbouring mesh point in the first case and 0·027 in the second case ($\delta x = 0{\cdot}05$). This confirms the need for the stability check described in Section 4.4.

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