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On a Moving Boundary Problem from Biomechanics

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A moving boundary problem arising in biomechanical diffusion theory which has previously been investigated by Crank & Gupta (1972*a*, *b*) is studied using a different method of solution. The method is based on an integral equation for the function defining the position of the moving boundary and an integral formula for the concentration. The integral equation is solved asymptotically for small times and numerically during the entire motion of the boundary. The concentration is estimated asymptotically for small times and computed by numerical quadrature at later instants. The results are compared with those of Crank & Gupta. In most cases the agreement is fair.

1. Introduction

IN TWO recent papers Crank & Gupta (1972*a*, *b*) studied a moving boundary problem arising from absorption and diffusion of oxygen in tissue. In the following their papers are referred to as I and II respectively. They used a one-dimensional model where the tissue occupies the interval $0 \leqslant x < \infty$, and the absorption rate F (amount of absorbed oxygen per unit length and time) was assumed to depend on the concentration c of oxygen in the following manner:

$$F(c) = \begin{cases} 1 & \text{if } c > 0 \\ 0 & \text{if } c = 0. \end{cases} \tag{1.1}$$

(Throughout the present paper the non-dimensional quantities defined in I are used.) During a diffusion and absorption process the on–off character of this absorption rate will cause the medium to be divided into two regions, one in which $c > 0$ everywhere, and one in which $c \equiv 0$. In general the boundary between the two regions will be moving in the course of the process and it becomes part of the problem to determine its position as a function of time.

With the absorption rate given by (1.1) the non-dimensional equation for the concentration $c = c(x, t)$ becomes

$$\frac{\partial^2 c}{\partial x^2} - \frac{\partial c}{\partial t} = 1 \tag{1.2}$$

in the region where $c > 0$. Since no diffusion takes place into the region where $c \equiv 0$, c and $\partial c/\partial x$ must vanish on the boundary. Thus, if $x = x_0(t)$ is the equation of the boundary in the (x, t) plane, the following relations hold:

$$c(x_0(t), t) = \partial c/\partial x(x_0(t), t) = 0 \qquad \text{for } t \geqslant 0. \tag{1.3}$$

In the problem studied in I and II it is supposed that during a long interval of time ending at $t = 0$ the concentration at $x = 0$ has been maintained at the value $\frac{1}{2}$.

Therefore, the concentration at $t = 0$ is put equal to the time-independent solution of (1.2) which satisfies the conditions (1.3) and for which $c = \frac{1}{2}$ at $x = 0$. So, the initial condition is

$$c(x, 0) = \tfrac{1}{2}(1-x)^2 \qquad \text{for } 0 \leqslant x \leqslant 1, \tag{1.4}$$

and $c(x, 0) = 0$ for $x > 1$. It is further supposed that the surface is sealed off at time $t = 0$ so that

$$\frac{\partial c}{\partial x}(0, t) = 0 \qquad \text{for } t > 0. \tag{1.5}$$

The relations (1.2)–(1.5) define the problem we shall consider. As seen from (1.4), $x_0(0) = 1$.

In I three methods are applied to this problem. The first is an approximate analytic method based upon the assumption that in the beginning of the process the boundary will move extremely slowly so that the concentration may be computed approximately for small t by replacing the present problem by one where the boundary stays at $x = 1$. The second method is a finite difference method with the step length of x being the same everywhere except at the interval next to the boundary. The third one is a so-called integral method. In this method the concentration is approximated by a fourth degree polynomial. Applying the results of the approximate analytic method mentioned above and satisfying (1.2) in an average sense an approximate differential equation for x_0 is derived which is solved numerically. In II a finite difference method is used again, the main difference being that the interval of variable length is now placed next to the fixed boundary at $x = 0$.

In the present paper we shall also solve the problem given by (1.2)–(1.5) but using a different method. We derive an integral equation for x_0 and an integral formula for c in terms of x_0. The integral equation is solved asymptotically for $t \to 0$ and numerically for all t. Thus, in our method the determination of the motion of the boundary which is the characteristic feature of this problem is disconnected from the computation of the concentration. Once x_0 is found, $c(x, t)$ is computed from the integral formula. We also derive a simple formula for the integral of x_0 taken over the time interval of the entire absorption process. This formula is used as a partial check of the results from the numerical solution of the integral equation.

Essentially the results we obtain using this method agree well with those found by Crank & Gupta. However, our method allows us to find some additional results. Thus for example from the very form of our expression for the concentration it can be concluded that certain of Crank & Gupta's numerical results are less accurate than those obtained from their approximate analytical solution. Also, by solving our integral equation numerically we have been able to trace the moving boundary closer to the termination value $x_0 = 0$ than has been reported in I and II.

Integral equation methods have been applied previously by several authors in connection with the classical Stefan problem and similar freezing or melting problems. Some of them are concerned with problems of existence and similar matters while others solve concrete problems. Among the latter ones we mention Lightfoot (1930) who used physical reasoning to set up an integral equation for the position of the freezing front in the one-dimensional freezing problem. He solved the equation approximately by making a special assumption about the functional dependence of the position on time. Portnov (1962) treated the same problem. He used Laplace-transform technique to set up an integral equation and found the position for small times by series expansion. His method was subsequently used by Jackson (1964) and Westphal (1966). Evans, Isaacson & MacDonald (1950) used a method similar to Portnov's on a generalized version of the one-dimensional freezing problem. Rathjen & Jiji (1971) extended Lightfoot's method and obtained an integral equation for the two-dimensional problem of freezing of a rectangular corner. They solved the equation approximately by assuming a special functional form of the equation of the freezing front and obtained rather extensive numerical results. For other applications of integral equation methods we refer the reader to a recent review by Noble (1971).

2. An Integral Equation Formulation of the Problem

As mentioned in the introduction, we shall apply an integral equation method to solve the problem defined by (1.2)–(1.5). The use of such a method is especially advantageous in the case of a linear problem since then it reduces the problem to one involving only the values of the unknowns on the boundary of the domain considered in the problem. In case of non-linear boundary value problems the same is in general not true.

The absorption rate F defined in (1.1) makes the problem under consideration a non-linear one. However, the dependence of F on c is such, that the problem is linear in c as long as only one of the regions where $c > 0$ or $c \equiv 0$ is considered. Therefore we may set up an integral formula expressing c everywhere in the interior and on the boundary of the region where $c > 0$ in terms of the known boundary values of c and $\partial c/\partial x$ and the unknown function x_0. From this formula we may then derive an integral equation for x_0.

In order to obtain the integral formula for c we use a Green's function technique. Let G be Green's function defined by

$$G(x, x', t'-t) = \frac{1}{2\sqrt{\pi(t'-t)}}\left\{\exp\left[-\frac{(x-x')^2}{4(t'-t)}\right]+\exp\left[-\frac{(x+x')^2}{4(t'-t)}\right]\right\} \tag{2.1}$$

for $t' > t$ and

$$G(x, x', t'-t) = 0 \tag{2.2}$$

for $t > t'$. For x and $x' \geqslant 0$ and for all t, G satisfies the equation

$$\frac{\partial^2 G}{\partial x^2}+\frac{\partial G}{\partial t} = -\delta(x-x')\delta(t'-t), \tag{2.3}$$

where δ denotes the Dirac delta function. For $x' > 0$ and for all t it satisfies the boundary condition

$$G_x(0, x', t'-t) = 0. \tag{2.4}$$

Now consider the integral

$$\int_0^{t'}\int_0^{x_0(t)}\left[G\left(\frac{\partial^2 c}{\partial x^2}-\frac{\partial c}{\partial t}\right)-c\left(\frac{\partial^2 G}{\partial x^2}+\frac{\partial G}{\partial t}\right)\right]dx\,dt, \tag{2.5}$$

where $G = G(x, x', t'-t)$. In virtue of equations (1.2) and (2.3) this integral is equal to

$$\int_0^{t'}\int_0^{x_0(t)} G(x, x', t'-t)\, dx\, dt + c(x', t'). \tag{2.6}$$

Integrating by parts and using (2.2) we may also rewrite the integral in (2.5) as

$$\int_0^{t'} \left[G\frac{\partial c}{\partial x} - c\frac{\partial G}{\partial x}\right]_{x=0}^{x=x_0(t)} dt - \int_0^1 [G\,c]_{t=0}^{t=t_0(x)}\, dx. \tag{2.7}$$

Here $t = t_0(x)$ denotes the inverse of the function $x = x_0(t)$. Because of the boundary conditions (1.3), (1.5), and (2.4) the first integral in (2.7) and the contribution from $t = t_0(x)$ in the second one vanish. Inserting $c(x, 0)$ from (1.4) and equating (2.6) and (2.7) we thus obtain the formula

$$c(x', t') = -\int_0^{t'}\int_0^{x_0(t)} G(x, x', t'-t)\, dx\, dt + \tfrac{1}{2}\int_0^1 G(x, x', t')(1-x)^2\, dx. \tag{2.8}$$

As described in the Appendix, this formula may be put in the following form:

$$c(x', t') = \tfrac{1}{2}(1-x')^2 - 2\sqrt{\frac{t'}{\pi}}\exp\left(-\frac{x'^2}{4t'}\right) + x'\operatorname{erfc}\left(\frac{x'}{2\sqrt{t'}}\right) + R(x', t'), \tag{2.9}$$

where

$$R(x', t') = \tfrac{1}{2}\int_0^{t'}\left\{\operatorname{erfc}\left[\frac{x_0(t)-x'}{2(t'-t)^{\frac{1}{2}}}\right] - \operatorname{erfc}\left[\frac{1-x'}{2(t'-t)^{\frac{1}{2}}}\right] + \operatorname{erfc}\left[\frac{x_0(t)+x'}{2(t'-t)^{\frac{1}{2}}}\right] - \operatorname{erfc}\left[\frac{1+x'}{2(t'-t)^{\frac{1}{2}}}\right]\right\} dt. \tag{2.10}$$

Once the function $x = x_0(t)$ has been determined, c can be computed from (2.9) everywhere in the region where $c > 0$. In order to find $x_0(t)$ we may let x' in (2.9) approach $x_0(t')$. Noting that $c(x_0(t'), t') = 0$ we thereby obtain an integral equation for the function $x = x_0(t)$. Another integral equation is obtained by differentiating (2.9) with respect to x' and employing the boundary condition $\partial c/\partial x(x_0(t'), t') = 0$. Since the conditions $c(x_0(t), t) = \partial c/\partial x(x_0(t), t) = 0$ imply that $\partial c/\partial t(x_0(t), t) = 0$ a third integral equation may be obtained by differentiating (2.9) with respect to t and putting $x' = x_0(t')$. The second of these equations turns out to be somewhat simpler than the two others. Therefore, we shall use it for the determination of $x_0(t)$. The equation, of which the derivation is indicated in the Appendix, may be written in the following form:

$$\begin{aligned} x' = {} & 1 - 2\operatorname{erfc}\left(\frac{x'}{2\sqrt{t'}}\right) + (1-x')\operatorname{erf}\left(\frac{1-x'}{2\sqrt{t'}}\right) + (1+x')\operatorname{erfc}\left(\frac{1+x'}{2\sqrt{t'}}\right) \\ & - 2\sqrt{\frac{t'}{\pi}}\left\{1 - \exp\left[-\frac{(1-x')^2}{4t'}\right] + \exp\left[-\frac{(1+x')^2}{4t'}\right]\right\} \\ & - \frac{1}{\sqrt{\pi}}\int_0^{t'} \frac{1}{(t'-t)^{\frac{1}{2}}}\left\{\exp\left[-\frac{(x-x')^2}{4(t'-t)}\right] - 1 - \exp\left[-\frac{(x+x')^2}{4(t'-t)}\right]\right\} dt. \end{aligned} \tag{2.11}$$

Here for brevity, x, and x' stand for $x_0(t)$ and $x_0(t')$, respectively.

We conclude this section by deriving a formula which may serve as a partial check of the numerical evaluation of the function x_0.

In I (equation 5.4) the following formula is derived:

$$\frac{d}{dt}\int_0^{x_0(t)} c(x,t)\,dx = -x_0(t). \tag{2.12}$$

The reader may convince himself about the validity of (2.12) by the following argument: since $c(x, t) = 0$ for $x > x_0(t)$, the left-hand side is equal to the increase per unit of time of the total content of oxygen in the interval $0 < x < \infty$. The oxygen escapes by absorption only. Therefore, this increase is equal to minus the integral of the absorption rate F over the same interval. Since, from (1.1), $F = 1$ for $x < x_0(t)$ and $F = 0$ for $x > x_0(t)$, this integral is equal to $x_0(t)$.

By integrating (2.12) we get that

$$\int_0^{x_0(t)} c(x,t)\,dx = -\int_0^t x_0(\tau)\,d\tau + K. \tag{2.13}$$

When in this formula we put $t = 0$ and use the fact that $x_0(0) = 1$ together with the initial condition (1.4), the constant K is found to be

$$K = \int_0^1 c(x,0)\,dx = \int_0^1 \tfrac{1}{2}(1-x)^2\,dx = \tfrac{1}{6}. \tag{2.14}$$

Inserting this value in (2.13) and putting t equal to the termination time t_1 i.e. the value of t for which $x_0(t) = 0$ we obtain the formula

$$\int_0^{t_1} x_0(\tau)\,d\tau = \tfrac{1}{6}. \tag{2.15}$$

Physically, (2.15) expresses the obvious fact that the amount of oxygen absorbed during the entire process equals the total content of oxygen at $t = 0$.

3. An Asymptotic Solution for Small t

In the problem we are considering the boundary condition at $x = 0$ is changed at time $t = 0$ from being $c(0, t) = \frac{1}{2}$ for $t < 0$ to $\partial c/\partial x(0, t) = 0$ for $t > 0$. Experience from other problems involving the heat equation indicates that for t positive but small this change will cause the concentration to be less than its value at $t = 0$ by an amount of order $\exp(-\frac{1}{4}x^2/t)$. This dependence on x and t is reflected in the form of the Green's function given by (2.1). We may therefore expect that for t small the moving boundary will move away from $x_0(0) = 1$ through a distance which is of order $\exp(-(4t)^{-1})$. Indeed, as we prove in the Appendix, for $t \to 0$ (2.11) has the asymptotic solution

$$x_0(t) = 1 - 2\,\mathrm{erfc}\left(\frac{1}{2\sqrt{t}}\right) + O\left(\exp\left(-\frac{1}{2t}\right)\right). \tag{3.1}$$

As $t \to 0$,

$$x_0(t) = 1 - 4\sqrt{\frac{t}{\pi}}\exp\left(-\frac{1}{4t}\right)\left(1 + O\left(\frac{1}{t}\right)\right), \tag{3.2}$$

which shows that the shift of the moving boundary is of the anticipated exponential order of size.

In Fig. 1 the function x_0 as determined from (3.1) is compared with results found by the numerical solution of equation (2.11) which is described in Section 4. The figure also shows an iterated asymptotic solution of (2.11), this solution being defined as the right-hand side of (2.11) with the expression (3.1) inserted for x and x'. In evaluating the iterated asymptotic solution the integral on the right-hand side of (2.11) was computed numerically using Romberg's method with double precision.

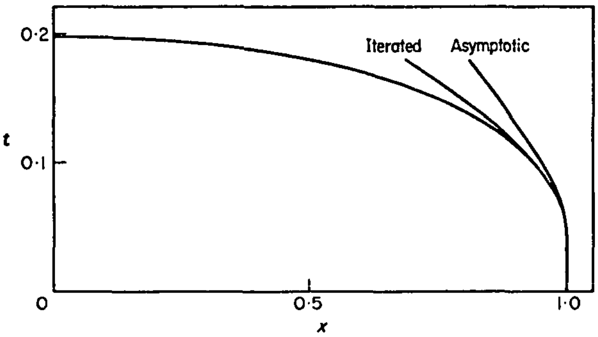

FIG. 1. The moving boundary as determined by numerical solution of (2.11). The curve denoted *asymptotic* corresponds to the asymptotic solution (3.4). The curve denoted *iterated* is determined from (2.11) with x and x' on the right-hand side inserted from (3.4).

As shown in the Appendix, one may use (3.2) to derive the following asymptotic representation of $c(x', t')$, valid for $1-x' \gg 1-x_0(t')$ with a relative error of $O(t')$:

$$c(x', t') \sim \tfrac{1}{2}(1-x')^2-2\sqrt{\frac{t'}{\pi}}\exp\left(-\frac{x'^2}{4t'}\right)+x' \operatorname{erfc}\left(\frac{x'}{2\sqrt{t'}}\right)$$
$$+4\sqrt{\frac{t'^3}{\pi}}\left[\frac{1}{(2-x')^2}\exp\left(-\frac{(2-x')^2}{4t'}\right)+\frac{1}{(2+x')^2}\exp\left(-\frac{(2+x')^2}{4t'}\right)\right]. \quad (3.3)$$

We shall now discuss some of the results obtained so far.

Formula (2.9) for the concentration may be compared with the corresponding result derived in I by an approximate analytic method applicable for small t. In this method the two boundary conditions (1.3) are replaced by the single one $c(1, t) = 0$ for $t \geqslant 0$, and (1.2) is assumed to hold also for $c \leqslant 0$. By these changes of the original problem one obtains a classical solvable one. Solving this problem by a Laplace transform technique Crank & Gupta find that for small t the concentration is approximately given by

$$c(x', t') = \tfrac{1}{2}(1-x')^2-2\sqrt{\frac{t'}{\pi}}\exp\left[-\frac{x'^2}{4t'}\right]+x' \operatorname{erfc}\left(\frac{x'}{2\sqrt{t'}}\right) \quad (3.4)$$

(equation (3.3) in I). Comparing this formula with (2.9) we see that they are identical except for the term $R = R(x', t')$ in (2.9). Therefore the various terms in (2.9) may be interpreted as follows. The first term is the concentration at $t = 0$. The two next terms account for the change of c due to the fact that at $t = 0$ the boundary condition at $x = 0$ is changed from $c = 0$ to $\partial c/\partial x = 0$. Finally, R accounts for the change of c caused by the motion of the boundary.

With regard to the term R two remarks are appropriate. The first one is that as seen from (2.10), R is positive for all $t' > 0$ and all x' between 0 and $x_0(t')$. This means that the concentration is everywhere larger than that given by (3.4) which, as was mentioned, is a result derived from the approximate analytical method in I. The fact that this method leads to a lower bound for the concentration agrees with the following physical consideration. In the original problem the absorption ceases to take place when c becomes zero. On the other hand, when c becomes zero in the problem considered in the approximate analytical method, the absorption is assumed to continue so that c is allowed to become negative, and because of the diffusion this extra reduction of c is transmitted to all points in the region where $c > 0$. We shall return to this point in connection with Table 4.

The second remark we wish to make about R is that as seen from (3.3), R increases extremely slowly from its value zero at $t = 0$. The formula shows that at a distance $y = 1-x$ from the boundary the change of the concentration caused by the motion of the boundary is of order $\exp(-\frac{1}{4}(1+y)^2/t)$ for small t. This may be compared with the fact that the change of the boundary condition at $x = 0$ from $c = 0$ to $\partial c/\partial x = 0$ at $t = 0$ gives rise to a change of c which is of order $\exp(-\frac{1}{4}x^2/t)$ for small t. The fact that there is a difference in order is understandable on physical grounds since while the change of boundary condition at $x = 0$ happens abruptly the motion of the boundary away from $x = 1$ is very slow in the beginning of the process. Of course, strictly speaking (3.3) can only be relied upon for small times. Still, in the authors' opinion this asymptotic result, together with the physical mechanism to which we have ascribed it above, throws some light on the remarkable fact, which is pointed out in I, that during the entire process, (3.4) agrees very well with results obtained from numerical methods. That this is so will be seen later from Table 4.

4. Numerical Solution

We now describe the numerical procedure which has been used for determining the moving boundary, that is the function $x = x_0(t)$, and the concentration. As mentioned in Section 2, x_0 is found from the integral equation (2.11) and thereafter c is evaluated from (2.9).

We wish to find $x_0(t_i)$ for $t_i = ih$, where $i = 1, 2, \ldots$ and h is a suitable time step. For $t_i < 0{\cdot}02$, $x_0(t_i)$ is computed from the asymptotic formula (3.4). For larger values of t_i, $x_0(t_i)$ is found from (2.11) by an iterative procedure. Approximating the integral in (2.11) by a sum, we write (2.11) as

$$f_i = \frac{N(f_i, t_i)}{D(f_i, t_i)}. \tag{4.1}$$

Here

$$f_i = 1 - x_0(ih),$$

$$N(f_i, t_i) = \frac{1}{\sqrt{\pi}} \sum_{j=1}^{i} \frac{\alpha_j}{(t_i - t_j)^{\frac{1}{2}}} \left\{ \exp\left[-\frac{(f_i - f_j)^2}{4(t_i - t_j)}\right] - 1 - \exp\left[-\frac{(2 - f_i - f_j)^2}{4(t_i - t_j)}\right] \right\}$$
$$+ 2\,\mathrm{erfc}\left[\frac{1 - f_i}{2\sqrt{t_i}}\right] - 2\,\mathrm{erfc}\left[\frac{2 - f_i}{2\sqrt{t_i}}\right] + 2\sqrt{\frac{t_i}{\pi}} \left\{ 1 + \exp\left[-\frac{(2 - f_i)^2}{4t_i}\right] - \exp\left[-\frac{f_i^2}{4t_i}\right] \right\}, \tag{4.2}$$

and

$$D(f_i, t_i) = 1+\text{erf}\left[\frac{f_i}{2\sqrt{t_i}}\right]-\text{erfc}\left[\frac{2-f_i}{2\sqrt{t_i}}\right]. \quad (4.3)$$

The coefficients α_j depend on the quadrature formula applied. In the present case the standard Simpson integration formula was used together with Newton's $\frac{3}{8}$ rule since this method was available as a standard routine on the IBM 370/165 computer which was used for the numerical work.

TABLE 1

Position of the moving boundary as function of time

Time	INT-EQ	FGL	IM	FDS	FDP
0·0100	1·00000	1·00000			
0·0200	1·00000	1·00000			
0·0400	0·99918	0·99920		0·9993	0·9992
0·0500	0·99679	0·99709			
0·0510	0·99642	0·99673	1·0000		
0·0600	0·99180	0·99220			
0·0800	0·97155		0·9750		
0·1000	0·93501	0·93518	0·9321	0·9327	0·9344
0·1200	0·87916	0·87885	0·8686	0·8739	0·8780
0·1400	0·79891	0·79756	0·7817	0·7892	0·7968
0·1500	0·74668	0·74487			
0·1600	0·68337	0·68128	0·6634	0·6664	0·6798
0·1800	0·50109	0·49607	0·4892	0·4680	0·4948
0·1850	0·43341	0·41780		0·3917	0·4258
0·1900	0·34537	0·33873	0·3505		
0·1950	0·20652	0·16128	0·2331		
0·1955	0·18708				
0·1960	0·16266				
0·1965	0·13284				
0·1970	0·09175				
0·1972	0·06708				

A straightforward iterative procedure comes out of (4.1) as

$$f_i^{(n+1)} = \frac{N(f_i^{(n)}, t_i)}{D(f_i^{(n)}, t_i)}, \quad (4.4)$$

the starting value $f_i^{(0)}$ being obtained by quadratic extrapolation from the three preceding values f_{i-1}, f_{i-2} and f_{i-3}. The iterative cycle is stopped and f_i is put equal to $f_i^{(n+1)}$ when $|f_i^{(n+1)}-f_i^{(n)}| \leqslant \varepsilon f^{(n)}$, where ε is an error parameter, or when n becomes equal to a prescribed maximum number K.

Following the scheme just described, computations were carried out for different values of the parameters h, ε and K. It was found that the iterative process is monotonic and, when t is not close to t_1, quite fast.

For $t' \leqslant 0{\cdot}1950$ the parameter values were $h = 5.10^{-4}$, $\varepsilon = 10^{-9}$, and $K = 40$. The number of iterations required to reach this accuracy was less than 8 for $t' \leqslant 0{\cdot}160$

and increased to 26 for $t' = 0{\cdot}1950$. With these values of h and ε the highest value of t' for which the required accuracy could be reached with $K = 40$ was $t' = 0{\cdot}1960$. Therefore, for $t' > 0{\cdot}1950$, h was reduced to 10^{-4} while ε and K were unaltered. For $t' = 0{\cdot}1972$ the required accuracy was then reached after 39 iterations.

TABLE 2

Tabulated values are $10^6 c$ for small times. The first row on each time level gives values obtained from (2.9), *the second row shows values computed by the approximate formula* (3.19) *and the third row values which are taken from I, where the FGL-method has been used*

$t \backslash x$	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9
	464318	404606	320000	245000	180000	125000	80000	45000	20000	5000
0·001	464318	404606	320000	245000	180000	125000	80000	45000	20000	5000
	460000	405000	320000	245000	180000	125000	80000	45000	20000	5000
	449537	401927	319973	245000	180000	125000	80000	45000	20000	5000
0·002	449537	401927	319973	245000	180000	125000	80000	45000	20000	5000
	452000	405000	320000	245000	180000	125000	80000	45000	20000	5000
	438196	397811	319760	244998	180000	125000	80000	45000	20000	5000
0·003	438196	397811	319760	244998	180000	125000	80000	45000	20000	5000
	437600	398000	320000	245000	180000	125000	80000	45000	20000	5000
	428635	393156	319211	244981	180000	125000	80000	45000	20000	5000
0·004	428635	393156	319211	244981	180000	125000	80000	45000	20000	5000
	429600	394760	320000	245000	180000	125000	80000	45000	20000	5000
	420212	388337	318302	244924	179999	125000	80000	45000	20000	5000
0·005	420212	388337	318302	244924	179999	125000	80000	45000	20000	5000
	420320	389128	318976	245000	180000	125000	80000	45000	20000	5000
	387162	365072	309949	243275	179804	124986	79999	45000	20000	5000
0·010	387162	365072	309949	243275	179804	124986	79999	45000	20000	5000
	387497	365668	310719	243726	179927	125000	80000	45000	20000	5000
	340423	325881	286674	233277	176604	124198	79847	44977	19997	5000
0·020	340423	325881	286674	233277	176604	124198	79847	44977	19997	5000
	340661	326222	287180	233793	176960	124370	79905	44991	19999	5000
	247687	240175	218841	186952	148990	109634	72961	42029	18856	4629
0·050	247687	240175	218841	186952	148990	109634	72961	42027	18845	4588
	247841	240358	219089	187264	149327	109945	73208	42199	18955	4673

Table 1 shows values of the function x_0 as computed by the present authors compared with those obtained in I and II. The columns denoted FGL and IM are taken from I; these results were obtained by a finite difference method with a Lagrangian interpolation and by an integral method, respectively. The last two columns are taken from II where finite difference methods using cubic splines (FDS) and cubic polynomials (FDP) were applied.

It is seen that over most of the time interval the agreement is fair. However, when t becomes large the differences between the values compared increase, our computations being larger than those of I and II. When our calculations were repeated with the smaller time step $h = 10^{-4}$ (expecting this to improve the accuracy) it was found that the values of x_0 changed less than 0·01% for $0 \leqslant t \leqslant 0{\cdot}160$ and less than 0·8% for $t \leqslant 0{\cdot}195$. In all cases the changes were towards larger values. In the authors' opinion this indicates that the values calculated by Crank & Gupta are too small. Our observation is supported by the fact that as seen from I their values found by the FGL-method were increased when the mesh-width was diminished.

Since we were able to trace the moving boundary closer to the termination point than has been reported in I and II, no comparison was possible for the last five of our results shown in the table.

In order to carry out the check made possible by (2.17) an estimate of t_1 is necessary. Since none of the methods compared offers an acurate way of finding t_1, approximate bounds for this quantity were obtained by linear extrapolation from the two last of our results in Table 1. We hereby found that $0{\cdot}1972 < t_1 < 0{\cdot}1977$. Using $t_1 = 0{\cdot}1974$ the integral in (2.18) was found to be equal to 0·166645 for $h = 5.10^{-4}$ and 0·166661 for $h = 10^{-4}$, which should be compared with the exact value $\frac{1}{6}$.

After x_0 had been found the concentration c was computed from (2.9) using the standard Simpson's integration formula together with Newton's $\frac{3}{8}$ rule. The results are shown in Tables 2 and 3.

In Table 2 on each time level the values in the top line are computed from (2.9), those in the middle line correspond to (3.19) i.e. the approximate analytical solution of I, and those in the bottom line are the results from the finite difference method as given in Table 4.2 of I. As will be noted, our results and those from the approximate analytical method are very close. This means that the quantity R in (2.10) which is equal to the difference between these two set of results is very small for $t \leqslant 0{\cdot}050$. Since x_0, which is the only quantity in (2.9) which was not known from the beginning, only enters in c through R, it may be concluded that these two sets of results are very close to the true values for t less than or equal to 0·050.

For larger values of x the agreement with the results from the finite difference method in I is excellent while, when x becomes smaller, the latter results deviate somewhat from ours. Especially this is so when t too is small. The explanation probably is that, as pointed out in I, the change of the boundary condition at $x = 0$ from $c = 0$ to $\partial c/\partial x = 0$ at $t = 0$ gives rise to computational difficulties for $x \simeq t \simeq 0$ as far as the finite difference method is concerned. Since we compute c from an explicit integral formula such difficulties are avoided in our method of attack.

In Table 3 on each time level the top and the bottom lines again give our results and those from the finite difference method of I, respectively, while the middle line is found from the integral method as given in Table 6.1 of I. As is seen, the agreement between our results and those from the finite difference method is quite good everywhere except again when both x and t are small. Here our results agree better with those of the integral method. In this connection it should be borne in mind that the values from the integral method of I are so adjusted that they agree with $c(0, t)$ as determined from the approximate analytical method.

In Table 4 results for the concentration at the sealed surface ($x = 0$) obtained by means of different methods are compiled. The results in the first row have been obtained from (2.9) while those in the next three rows are taken from II, the abbreviations of the various methods being explained in connection with Table 1. The results denoted Approx. are computed from (3.4) which, as mentioned earlier, is identical with a

TABLE 3

Tabulated values are 10^6c. *The first row on each time level gives values obtained from* (2.9), *the second row shows values from the so-called integral-method of I and the third row values from the FGL-method of I*

$t \backslash x$	0·0	0·1	0·2	0·3	0·4	0·5	0·6	0·7	0·8	0·9
	245176	237786	216782	185345	147853	108906	72539	41808	18752	4590
0·051	245176	236403	213648	181831	145308	107868	72736	42571	19469	4957
	245329	237966	217026	185652	148186	109216	72788	41981	18854	4635
	223605	217168	198777	170979	137379	101928	68291	39451	17581	4129
0·060	223605	215950	195945	167714	137974	101028	68767	40671	18809	4837
	223746	217330	198992	171251	137684	102227	68548	39645	17705	4186
	143177	139294	128082	110787	89295	65892	43018	23059	8232	603
0·100	143175	138758	126795	109243	88096	65385	43176	23569	8703	751
	143287	139414	128338	110996	89502	66112	43228	23232	8342	619
	109129	106019	97025	83117	65795	46941	28667	13204	2873	0
0·120	—	—	—	—	—	—	—	—	—	—
	109228	106125	97149	83265	65963	47115	28827	13324	2924	0
	77850	75351	68130	56988	43197	28416	14638	4204	0	0
0·140	—	—	—	—	—	—	—	—	—	—
	77937	75442	68233	57105	43322	28536	14730	4249	0	0
	63078	60845	54403	44503	32353	19583	8251	1005	0	0
0·150	62981	61083	55236	45725	33529	20315	8443	962	0	0
	63157	60928	54496	44602	32453	19668	8298	1007	0	0
	48823	46840	41136	32434	21927	11304	2890	0	0	0
0·160	—	—	—	—	—	—	—	—	—	—
	48893	46912	41212	32511	21996	11346	2890	0	0	0
	21781	20287	16066	9942	3523	0	0	0	0	0
0·180	21269	20771	17750	11681	4387	42	0	0	0	0
	21824	20328	16096	9950	3506	0	0	0	0	0
	9021	7817	4578	799	0	0	0	0	0	0
0·190	8151	8028	5315	925	0	0	0	0	0	0
	9039	7827	4575	750	0	0	0	0	0	0
	2884	1914	32	0	0	0	0	0	0	0
0·195	1721	1304	0	0	0	0	0	0	0	0
	2880	1909	0	0	0	0	0	0	0	0

formula obtained from Crank & Gupta's approximate analytical method. Finally, the last row denoted Asymp. contains results computed from (3.3) in which a correction found from our asymptotic solution of the integral equation has been added to the results denoted Approx.

The table shows that some of the results obtained by the various finite difference methods of Crank & Gupta are smaller than those denoted Approx. although, as pointed out earlier, the latter ones constitute lower bounds for the exact values. In the authors' opinion, the fact that Crank & Gupta's approximate analytical method in certain cases leads to more correct results than some of the finite difference methods illustrates the very high degree to which the physical idea underlying the approximate method is able to account for a large part of the diffusion process. A further illustration of this is given by the fact that when the asymptotic correction is added, the discrepancy from the results obtained from our integral equation method becomes still smaller.

TABLE 4

Tabulated values are 10^6c at the sealed surface. The values computed by the integral-equation method are compared to those obtained by the various finite-difference methods of Crank & Gupta and to values computed from the approximate formula (3.19) *and from the asymptotic formula* (3.16)

Method \ Time	0·040	0·060	0·100	0·120	0·140	0·160	0·180	0·185
INT.–EQ.	2743	2236	1432	1091	779	488	218	153
FGL ($\Delta x = 0{\cdot}05$)	2742	2234	1430	1089	777	486	216	151
FDP ($\Delta x = 0{\cdot}10$)	2745	2238	1434	1093	780	490	219	155
FDP ($\Delta x = 0{\cdot}05$)	2742	2234	1429	1089	776	486	216	151
FDS ($\Delta x = 0{\cdot}10$)	2736	2277	1424	1083	771	481	210	145
Approx.	2743	2236	1432	1091	778	486	213	147
Asymp.	2743	2236	1432	1091	778	488	216	151

The numerical computations described in this paper were carried out on the IBM 370/165 computer of the Northern Europe University Computing Center.

Appendix

In this Appendix we describe the derivation of some of the formulas in Sections 2 and 3.

In order to write (2.8) in the form given by (2.9) and (2.10) we use the formula

$$G(x, x', t') = \int_0^\infty \left[\delta(x-x')\delta(t-t') + \frac{\partial^2 G}{\partial x^2}(x, x', t'-t)\right] dt \qquad \text{(A1)}$$

which follows immediately from (2.3) and (2.2). Substituting $G(x, x', t')$ in the second integral of (2.8) by the right-hand side of (A1) and using the fundamental property of the delta function we rewrite (2.8) as

$$c(x', t') = \tfrac{1}{2}(1-x')^2 - \int_0^{t'} \int_0^{x_0(t)} G(x, x', t'-t)\, dx\, dt$$
$$+\tfrac{1}{2} \int_0^{\infty} \int_0^1 \frac{\partial^2 G}{\partial x^2}(x, x', t'-t)(1-x)^2\, dx\, dt. \quad \text{(A2)}$$

When the last integral in (A2) is twice integrated by parts with respect to x and (2.4) and (2.2) are used, (A2) becomes

$$c(x', t') = \tfrac{1}{2}(1-x')^2 - \int_0^{t'} G(0, x', t'-t)\, dt + \int_0^{t'} \int_{x_0(t)}^1 G(x, x\,, t'-t)\, dx\, dt. \quad \text{(A3)}$$

Here, when integrated by parts, the first integral becomes identical with the second and the third term in (2.9). In each term of $G(x, x', t'-t)$ in the second integral the square root of the exponent is introduced as a new variable of integration instead of x. This integral is thereby found to be equal to the quantity $R(x', t')$ given by (2.10).

The integral equation (2.11) is derived by differentiating (2.9) with respect to x' and putting $x' = x_0(t)$ so that $\partial c/\partial x\,(x', t') = 0$. In order to write the equation in the form given by (2.11) we integrate by parts two terms in $\partial R/\partial x\,(x', t')$ which contain $1 \mp x'$ in the exponent. We also introduce the term $-(t'-t)^{-\frac{1}{2}}$ in the integral, and the compensating term $-2(t'/\pi)^{\frac{1}{2}}$ outside, so that the integrand remains bounded in the limit $t \to t'$.

We prove that x_0 given by (3.1) is an asymptotic solution of (2.11) by estimating the various terms in (2.11) under the assumption that (3.1), and consequently (3.2), are true. By straightforward estimates using (3.2) it is found that the sum of all the terms on the right-hand side of (2.11) except the first two is $O(\sqrt{t'}\exp(-(2t')^{-1})$ for $t' \to 0$, so that (2.11) becomes

$$x_0(t') = 1 - 2\,\mathrm{erfc}\left(\frac{x_0(t')}{2\sqrt{t'}}\right) + O\left(\sqrt{t'}\exp\left(-\frac{1}{2t'}\right)\right). \quad \text{(A4)}$$

Using (3.2) again we find that

$$2\,\mathrm{erfc}\left(\frac{x_0(t')}{2\sqrt{t'}}\right) = 2\,\mathrm{erfc}\left(\frac{1}{2\sqrt{t'}}\right) + O\left(\exp\left(-\frac{1}{2t'}\right)\right). \quad \text{(A5)}$$

Inserting (A5) in (A4) we see that the assumption is confirmed.

In (3.3) the first three terms on the right-hand side are identical with the first three terms on the right-hand side of (2.9). Thus, in order to derive (3.3) we must show that the quantity $R(x', t')$ given by (2.10) is represented asymptotically by the rest of the right-hand side of (3.3) To do so we write

$$R(x', t') = Q(1-x', t') + Q(1+x', t') \quad \text{(A6)}$$

where

$$Q(a, t') = \tfrac{1}{2} \int_0^{t'} \mathrm{erfc}\left[\frac{a-f}{2(t'-t)^{\frac{1}{2}}}\right] dt - \tfrac{1}{2} \int_0^{t'} \mathrm{erfc}\left[\frac{a}{2(t'-t)^{\frac{1}{2}}}\right] dt. \quad \text{(A7)}$$

Here $f = f(t) = 1 - x_0(t)$. For $t' \to 0$ the difference between the two integrals in (A7) is exponentially smaller than each of them. Therefore, they must be combined into one integral containing a single exponential in order that standard methods of asymptotic evaluation can be applied. This may be done as follows. We introduce the monotone substitutions

$$y = \frac{a-f}{2(t'-t)^{\frac{1}{2}}} \quad \text{and} \quad z = \frac{a}{2(t'-t)^{\frac{1}{2}}} \tag{A8}$$

in the first and the second integral respectively and integrate by parts. Since $f(0) = 0$, the end point contributions cancel so that we get

$$Q(a, t') = -\frac{1}{4\sqrt{\pi}} \int_{a/2\sqrt{t'}}^{\infty} \frac{(a-f)^2}{y^2} \exp(-y^2)\, dy + \frac{1}{4\sqrt{\pi}} \int_{a/2\sqrt{t'}}^{\infty} \frac{a^2}{z^2} \exp(-z^2)\, dz. \tag{A9}$$

These two integrals may be combined into one to give

$$Q(a, t') = \frac{1}{4\sqrt{\pi}} \int_{a/2\sqrt{t'}}^{\infty} \frac{(2a-f(t))}{y^2} f(t) \exp(-y^2)\, dy, \tag{A10}$$

where t is related to y through the first formula in (A8). In (A10) we substitute $2a-f(t)$ by $2a$ and y by the variable z given by the second formula in (A8):

$$Q(a, t') \sim \frac{a}{2\sqrt{\pi}} \int_{a/2\sqrt{t'}}^{\infty} \frac{f(t)}{z^2} \exp(-z^2)\, dz. \tag{A11}$$

The relative errors introduced by these substitutions are exponentially small if $f(t') \ll a$. In (A11) we insert the asymptotic representation of $f(t) = 1-x_0(t)$ as given by (3.2) and introduce the variable $\tau = t/t'$. The integral in (A11) then becomes

$$Q(a, t') \sim \frac{2t'}{\pi} \int_0^1 \sqrt{\frac{\tau}{1-\tau}} \exp\left[-\frac{1}{4t'}\left(\frac{1}{\tau} + \frac{a^2}{1-\tau}\right)\right] d\tau, \tag{A12}$$

the relative error now being $O(t')$. The asymptotic representation of this integral may be evaluated by Laplace's method (Erdélyi 1956: 36). The result is

$$Q(a, t') \sim 4\sqrt{\frac{t'^3}{\pi}} \frac{1}{(1+a)^2} \exp\left(-\frac{(1+a)^2}{4t'}\right). \tag{A13}$$

The relative error is still $O(t')$. (3.3) is now obtained when (A13) is used in (A6) and the resulting expression for $R(x', t')$ in turn is inserted in (2.9) for $c(x', t')$.

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