CONCENTRATION-DEPENDENT DIFFUSION III. AN APPROXIMATE SOLUTION*

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In the papers [1, 2], hereafter referred to as I and II respectively, we discussed the similarity solution of the one-dimensional diffusion equation $c_t = (Dc_x)_x$ when the diffusion coefficient D is a function of the concentration c. The physical problem that concerns us is the diffusion of a substance into a semi-infinite medium after the substance is introduced at the face at a given concentration level which is maintained thereafter. Normalizing and introducing the similarity variable $\eta = x/\sqrt{t}$ leads to the problem

$$\frac{d}{d\eta}\left(D(c)\,\frac{dc}{d\eta}\right) + \frac{\eta}{2}\frac{dc}{d\eta} = 0, \tag{1}$$

$$c(0) = 1, \qquad c(\infty) = 0. \tag{2}$$

In addition to (1, 2) a solution must have a continuous flux $f(\eta) = D(c(\eta))c'(\eta)$. We suppose $D(c) \in C^1[0, 1]$ and that $D(c) > 0$ for $c > 0$. If $D(0) = 0$, the problem is said to be singular and there may then be an η_0 such that the solution $c(\eta) \equiv 0$ for $\eta \geq \eta_0$. This η_0 represents the location of a "front" of a nonlinear wave of the diffusant.

Bounds on the initial flux of the solution are useful in two ways. They were necessary in I and II for computing the solution. They are quite useful physically because of their relation to the uptake, which is a quantity readily measured: the total amount of diffusant which has crossed $x = 0$ by time t, M_t, is

$$M_t = \int_0^\infty c(x, t)\,dx = \sqrt{t}\int_0^\infty c(\eta)\,d\eta.$$

Using the conservation law

$$-f(0) = \frac{1}{2}\int_0^\infty c(\eta)\,d\eta \tag{3}$$

which we proved for both singular and non-singular cases, we see that

$$M_t = -f(0)2\sqrt{t}.$$

By physical reasoning Macey [3] derived an approximate solution of (1, 2) which in our notation is

$$f^* = -\left(\frac{1}{2}\int_0^1 \tau D(\tau)\,d\tau\right)^{1/2}, \tag{4}$$

$$\eta^*(c) = \left(\int_c^1 D(\tau)\,d\tau\right)\Big/(-f^*) \quad \text{for} \quad c \geq 0. \tag{5}$$

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Here $f^* \doteq f(0)$. He observes that in his computations $f^* > f(0)$, and we reported the same observation in II. This is plausible from the physical arguments. The approximation $c^*(\eta)$ is defined implicitly by (5) and is supplemented by $c^*(\eta) \equiv 0$ for $\eta \geq \eta_0^*$ where

$$\eta_0^* = \left(\int_0^1 D(\tau)\, d\tau\right)/(-f^*). \tag{6}$$

In this note we shall prove by simple means that the quantity f^* of (4) is an upper bound on the initial flux. Furthermore, if any f^* which is a *lower* bound for the initial flux is used in (5), the approximation $c^*(\eta)$ so defined satisfies $c(\eta) > c^*(\eta)$ for all $\eta > 0$. Lower bounds are easy to obtain, e.g. in II we derived $f(0) \geq -(\Delta/\pi)^{1/2}$ where $\Delta = \max_{0 \leq c \leq 1} D(c)$. Study of Macey's plots of the approximation $c^*(\eta)$ of (4, 5) shows that in every case there is a number δ such that for $0 < \eta < \delta$, $c^*(\eta) > c(\eta)$ and for $\delta < \eta$, $c^*(\eta) < c(\eta)$. We shall prove this qualitative behavior is always true. In particular, we shall prove that if the problem exhibits a front at η_0, then η_0 is at least as large as the η_0^* of (6).

In I and II we proved there is a unique solution to (1, 2) which strictly decreases from 1 to 0. Introducing the flux as a dependent variable and the concentration as the independent variable, we see that the solution satisfies, for $1 \geq c > 0$,

$$d\eta/dc = D(c)/f, \qquad \eta(1) = 0,$$

$$df/dc = -\eta/2, \qquad 0 > f(1) \text{ given.}$$

Now the approximation (5) is the solution of

$$d\eta^*/dc = D(c)/f^*, \qquad \eta^*(1) = 0,$$

$$df^*/dc = 0, \qquad 0 > f^*(1) = f^* \text{ given}$$

(Since $f^*(c) \equiv f^*$, we shall just write f^* in what follows.) The flux $f(c)$ obviously is strictly increasing as c decreases to 0 and in I and II it is shown to tend to zero. Evidently if $0 > f(1) \geq f^*$, we shall have $f(c) > f^*$ for all $c < 1$. But then

$$d(\eta - \eta^*)/dc = D(c)(1/f - 1/f^*) \tag{7}$$

is negative for $c < 1$ which implies $\eta(c) > \eta^*(c)$. Returning to c as the dependent variable, we have shown that if f^* is a lower bound for the initial flux, then the approximation $c^*(\eta)$ of (5) is a strict lower bound for $c(\eta)$ as long as $c(\eta)$ is positive.

The way Macey chooses the initial flux f^* is to insist $c^*(\eta)$ satisfy

$$-f^* = \frac{1}{2}\int_0^\infty c^*(\eta)\, d\eta,$$

so as to imitate the behavior (3) of the true solution. This requirement results in the expression (4). It is now easy to see that f^* so chosen is an upper bound for the initial flux. If it were not, the preceding analysis would imply $c(\eta) > c^*(\eta)$ as long as $c(\eta) > 0$, hence

$$-f^* = \frac{1}{2}\int_0^\infty c^*(\eta)\, d\eta < \frac{1}{2}\int_0^\infty c(\eta)\, d\eta = -f(0),$$

and $0 > f^* > f(0)$, contrary to our assumption.

If we suppose that $f^* > f(1)$, then since $f(c)$ strictly increases to zero as c decreases, there is a unique point ζ for which $f(\zeta) = f^*$. Thus, according to (7), $\eta^*(c) - \eta(c)$ strictly increases as c decreases from 1 to ζ and then strictly decreases as c decreases from ζ to 0. Returning to the concentration as the dependent variable, we have that $c^*(\eta)$ cannot intersect $c(\eta)$ more than once. However, using Macey's approximation $c^*(\eta)$ must cross $c(\eta)$ at least once. Otherwise we would have $c^*(\eta) > c(\eta)$ for all $\eta > 0$ which implies

$$-f^* = \frac{1}{2} \int_0^\infty c^*(\eta)\, d\eta > \frac{1}{2} \int_0^\infty c(\eta)\, d\eta = -f(0),$$

and the consequence that $f(0) > f^*$ is a contradiction. Thus there is a $\delta > 0$ such that $c^*(\eta) > c(\eta)$ for $0 < \eta < \delta$ and $c^*(\eta) < c(\eta)$ for $\delta < \eta$.

We have seen that any f^* less than the initial flux leads to a $c^*(\eta)$ from (5) which is less than $c(\eta)$. Naturally, then, the η_0^* of (6) is a lower bound for the location η_0 of a front of $c(\eta)$, should one exist. The qualitative picture of Macey's approximation shows that using the f^* of (4) leads to an η_0^* of (6) which must also be a lower bound for η_0. The η_0^* of (6) is an increasing function of f^* so Macey's approximation gives the best bound.

References

[1] L. F. Shampine, *Concentration-dependent diffusion*, Quart. Appl. Math. **30**, 441–452 (1973)

[2] ————, *Concentration-dependent diffusion II. Singular problems*, Quart. Appl. Math. **31**, 287–293 (1973)

[3] R. I. Macey, *A quasi-steady state approximation method for diffusion problems: I. Concentration-dependent diffusion coefficients*, Bull. Math. Biophys. **21**, 19–32 (1959)