GENERAL METHOD OF EXACT SOLUTION OF THE CONCENTRATION-DEPENDENT DIFFUSION EQUATION

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Summary

Only three forms of $D(\theta)$ have previously been known to yield exact solutions of the equation

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left(D(\theta)\frac{\partial\theta}{\partial x}\right),$$

subject to the conditions $\theta=0,\ x>0,\ t=0$; $\theta=1,\ x=0,\ t>0$. The present paper reports a general method of establishing a very large class of $D(\theta)$ functions which yield exact solutions. A similar method enables exact solutions of the same equation subject to the conditions $\theta=0$, $x>0$, and $\theta=1$, $x<0$, $t=0$; $\int_0^1 x\mathrm{d}\theta=0$, $t\geqslant 0$. In this case also a very large class of $D(\theta)$ functions yield exact solutions. Examples are given for both cases.

Many of the exact solutions which are most readily found tend to lead to zero or infinite values of D at one or two points of the θ-range. Means of avoiding this difficulty are devised. Practical use of the method is discussed.

I. INTRODUCTION

Hitherto, the mathematics of concentration-dependent diffusion has depended almost exclusively on numerical analysis. According to Crank (1956, p. 166), the only known " formal solutions " in concentration-dependent diffusion are due to Fujita (1952*a*, 1952*b*, 1954). They provide solutions of the equation

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left(D(\theta)\frac{\partial\theta}{\partial x}\right), \qquad \textbf{(1.1)}$$

subject to the conditions

$$\left.\begin{array}{l}\theta=0,\ x>0,\ t=0\ ;\\ \theta=1,\ x=0,\ t>0\ ;\end{array}\right\} \qquad \textbf{(1.2)}$$

and are for the following $D(\theta)$ functions :

$$D=D_0/(1-\lambda\theta)\ ;\quad D=D_0/(1-\lambda\theta)^2\ ;\quad D=D_0/(1+2a\theta+b\theta^2).$$

Philip (1955) showed how (**1.1**) subject to (**1.2**) could be solved analytically for D, an n-step function of θ. However, the method is cumbersome when n is large.

This paper presents a very general method of obtaining exact solutions of (**1.1**) subject to (**1.2**). It embraces all possible exact solutions, including as particular cases those of Fujita and those implicit in Philip (1955). The method

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is also applicable to all possible exact solutions of (**1.1**) subject to the following conditions, which are also of practical importance:

$$\theta=0,\ x>0 \text{ and } \theta=1,\ x<0,\ t=0;\ \int_0^1 x\mathrm{d}\theta=0,\ t\geqslant 0. \quad \ldots . \quad (\mathbf{1.3})$$

Extension of the results of this paper to the slightly more general cases of (**1.2**) and (**1.3**) with $\theta=\theta_n$, $\theta=\theta_0$, in place of $\theta=0$, $\theta=1$, is trivial, involving only the introduction of the linear transformation $\theta_*=(\theta-\theta_n)/(\theta_0-\theta_n)$ and solution in terms of θ_*.

II. Exact Solutions and Exact Functions

The use of the adjective "exact" to distinguish solutions obtainable in terms of the functions of analysis from those obtainable only numerically is well established (e.g. Carslaw and Jaeger 1959, p. 91). This usage is convenient and unambiguous, though no definition of the term seems to have been given in the literature.

For the purposes of the present work, it is desirable to define an *exact function* of a real variable. We say that y is an exact function of the real variable x in some interval of x, provided y can be specified without approximation for all values of x in the given interval by means of a finite number of explicit formulae.

Further, we may then define an *exact solution* as a solution expressible in the form of an exact function.

III. General Principles of the Method

It is well known (cf. Philip 1955) that the substitution

$$\varphi=xt^{-\frac{1}{2}} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{3.1})$$

enables (**1.1**) subject to either (**1.2**) or (**1.3**) to be reduced to

$$\int_0^\theta \varphi\mathrm{d}\theta=-2D\mathrm{d}\theta/\mathrm{d}\varphi, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{3.2})$$

that is,

$$D=-\tfrac{1}{2}\mathrm{d}\varphi/\mathrm{d}\theta.\int_0^\theta \varphi\mathrm{d}\theta. \quad \ldots\ldots\ldots\ldots \quad (\mathbf{3.3})$$

It follows that the solution of (**1.1**), subject to either (**1.2**) or (**1.3**), $\varphi(\theta)$, exists in exact form, so long as $D(\theta)$ is of the form

$$D=-\tfrac{1}{2}\mathrm{d}F/\mathrm{d}\theta.\int_0^\theta F\mathrm{d}\theta, \quad \ldots\ldots\ldots\ldots\ldots \quad (\mathbf{3.4})$$

where F is any single-valued exact function of θ in the interval $0\leqslant\theta\leqslant 1$, which satisfies certain, not very restrictive, conditions, which we indicate in the following paragraphs.†

† Note that D is expressible in terms of known functions if F (as well as satisfying these conditions) is integrable in terms of known functions.

(i) *Conditions imposed by Conditions governing* (**1.1**).—Evidently, the exact solution for $D(\theta)$ of form (**3.4**) is simply $\varphi=F$. F must therefore satisfy the conditions to be imposed on (φ in) equation (**3.2**). It follows that, for (**1.1**) subject to (**1.2**),

$$F(1)=0, \qquad \ldots\ldots\ldots\ldots \quad (3.5)$$

and that, for (**1.1**) subject to (**1.3**),

$$\int_0^1 F\mathrm{d}\theta=0. \qquad \ldots\ldots\ldots\ldots \quad (3.6)$$

(ii) *Conditions imposed by Requirement that* D *Exists.*—For D to exist for all values of θ in the range $0\leqslant\theta\leqslant1$, it is necessary that $\int_0^\theta F\mathrm{d}\theta$ and $\mathrm{d}F/\mathrm{d}\theta$ exist throughout this θ-range. (However, if a finite number of discontinuities in D are allowable, or if D is permitted to be infinite at a finite number of points in the range $0<\theta\leqslant1$, $\mathrm{d}F/\mathrm{d}\theta$ may either not exist or be infinite at the appropriate finite number of points in the θ-range.)

(iii) *Condition imposed by Requirement that* D$\geqslant$0.—The flux of the diffusing entity in the sense x positive, Q, is equal to $-D\partial\theta/\partial x=-t^{-\frac{1}{2}}D\mathrm{d}\theta/\mathrm{d}\varphi$. Now both (**1.2**) and (**1.3**) describe phenomena in which for $D\geqslant0$, $Q\geqslant0$. It follows that $\mathrm{d}\theta/\mathrm{d}\varphi\leqslant0$ in both cases. Accordingly we have, for the two cases we consider, the further condition

$$\mathrm{d}F/\mathrm{d}\theta\leqslant0 \quad (0\leqslant\theta\leqslant1). \qquad \ldots\ldots\ldots\ldots \quad (3.7)$$

IV. Solutions of (1.1), (1.2)

It is seen that exact solutions of (**1.1**) subject to (**1.2**) may be established at will, simply by selecting F functions satisfying the conditions set out in Section III. Some typical results of this elementary process are given in Table 1.

It will be observed that the D functions in this table tend to have $\lim_{\theta\to0} D(\theta)$ either zero or infinite.* It would be a serious limitation on the generality of the present methods if none of our exact solutions were for $D(0)$ non-zero, but finite.† Accordingly, we now give some attention to this question.

A well-known result in linear diffusion (Carslaw and Jaeger 1959, p. 59) for phenomena governed by (**1.2**) is equivalent, from the present viewpoint, to the statement that

$$\text{for } F=2D_0^{\frac{1}{2}}\,\text{inverfc}\,\theta,\ D=\text{constant}=D_0. \qquad \ldots\ldots \quad (4.1)$$

The notation inverfc denotes the inverse of erfc (Philip 1955).

* From this point on we shall write $D(0)$ for $\lim_{\theta\to0} D(\theta)$. Note that we use the form $\lim_{\theta\to0} D(\theta)$ since, strictly, the value of D at $\theta=0$ is irrelevant to the phenomena. We are concerned only with values of $D(\theta)$ in the interval $0<\theta\leqslant1$.

† This is not to imply that no practical interest attaches to cases with $D(0)=0$. For a discussion of such cases and certain applications see Philip (1956, 1957).

We therefore put

$$F = 2D_0^{\frac{1}{2}} \text{ inverfc } \theta + f(\theta)\,; \quad D_0 \text{ finite, non-zero} \quad \ldots . \quad (4.2)$$

in (3.4), and obtain

$$D = D_0 + \tfrac{1}{2} D_0^{\frac{1}{2}} \left(\frac{2}{B} \int_0^\theta f \mathrm{d}\theta - B \frac{\mathrm{d}f}{\mathrm{d}\theta} \right) - \tfrac{1}{2} \frac{\mathrm{d}f}{\mathrm{d}\theta} \cdot \int_0^\theta f \mathrm{d}\theta, \quad \ldots\ldots \quad (4.3)$$

where

$$B(\theta) = 2\pi^{-\frac{1}{2}} \exp\left[-(\text{inverfc } \theta)^2\right]. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4.4)$$

Table 1

SOME SIMPLE CASES OF EXACT SOLUTIONS OF (1.1), (1.2)

No.	D	φ	Remarks
1	$\frac{1}{2} n\theta^n [1 - \theta^n/(1+n)]$	$1 - \theta^n$	$n > 0$
2	$\dfrac{n}{2(n+1)} [(1-\theta)^{n-1} - (1-\theta)^{2n}]$	$(1-\theta)^n$	$n > 0$
3	$\frac{1}{2} n\theta^{-n} \left[\dfrac{\theta^{-n}}{1-n} - 1 \right]$	$\theta^{-n} - 1$	$0 < n < 1$
4	$\frac{1}{2} \sin^2 \frac{1}{2}\pi\theta$	$\cos \frac{1}{2}\pi\theta$	
5	$\frac{1}{2} \cos \frac{1}{2}\pi\theta [\cos \frac{1}{2}\pi\theta + \frac{1}{2}\pi\theta - 1]$	$1 - \sin \frac{1}{2}\pi\theta$	
6	$\frac{1}{2} \left(\dfrac{\theta \cos^{-1}\theta + 1}{\sqrt{(1-\theta^2)}} - 1 \right)$	$\cos^{-1}\theta$	
7	$\frac{1}{2} \left(\dfrac{\frac{1}{2}\pi - (1-\theta)\sin^{-1}(1-\theta)}{\sqrt{(2\theta-\theta^2)}} - 1 \right)$	$\sin^{-1}(1-\theta)$	
8	$\frac{1}{4}\theta \left(\theta + \dfrac{\sin^{-1}\theta}{\sqrt{(1-\theta^2)}} \right)$	$\sqrt{(1-\theta^2)}$	
9	$\frac{1}{8} \sin \pi\theta (\pi\theta + \sin \pi\theta)$	$\cos^2 \frac{1}{2}\pi\theta$	
10	$\frac{1}{16} \sin^2 \pi\theta (5 + \cos \pi\theta)$	$\cos^3 \frac{1}{2}\pi\theta$	
11	$\frac{1}{2} e^{n\theta} [1 - e^{n\theta} + n\theta e^n]$	$e^n - e^{n\theta}$	$n > 0$
12	$\frac{1}{2} e^{-n\theta} [1 - e^{-n\theta} - n\theta e^{-n}]$	$e^{-n\theta} - e^{-n}$	$n > 0$
13	$\frac{1}{2}(1 - \log \theta)$	$-\log \theta$	
14	$\dfrac{n}{2\theta} (-\log \theta)^{n-1} \times \{\Gamma(n+1) - \Gamma(-\log\theta,\ n+1)\}$	$(-\log \theta)^n$	$n > 0$. $\Gamma(x,p)$ denotes the incomplete Γ-function $\int_0^x e^{-x} x^{p-1} \mathrm{d}x$.

This result depends on the following relationships, which are readily established :

$$\frac{\mathrm{d}}{\mathrm{d}\theta} (\text{inverfc } \theta) = -\frac{1}{B}\,; \quad \int_0^\theta \text{inverfc } \theta \ \mathrm{d}\theta = \tfrac{1}{2} B. \quad .. \quad (4.5)$$

The properties of inverfc θ and $B(\theta)$ are treated in more detail in Philip (1960). Tables of these two functions are also given there.

Reverting to (**4.3**), we are concerned with the conditions under which $D(0)$ is finite, non-zero. Evidently, it is a sufficient condition that both

$$\lim_{\theta\to 0}\left(\frac{1}{B}\int_0^\theta f\,\mathrm{d}\theta\right) \text{ and } \lim_{\theta\to 0}\left(B\frac{\mathrm{d}f}{\mathrm{d}\theta}\right)$$

be finite (including zero). The slightly stronger condition that these limits be *zero* ensures that $D(0)$ is equal to D_0. Evidently, the imposition on f of the conditions

$$\lim_{\theta\to 0}\left(\frac{1}{B}\int_0^\theta f\,\mathrm{d}\theta\right)=0, \qquad \ldots\ldots\ldots\ldots\ldots (4.6)$$

$$\lim_{\theta\to 0}\left(B\frac{\mathrm{d}f}{\mathrm{d}\theta}\right)=0, \qquad \ldots\ldots\ldots\ldots\ldots (4.7)$$

ensures that the inverfc term in (**4.2**) accounts completely for the finite but non-zero value of $D(0)$ in (**4.3**).

It is simply shown that (**4.6**) and (**4.7**) are equivalent to the single condition that

$$\lim_{\theta\to 0}\frac{f}{\operatorname{inverfc}\theta}=0. \qquad \ldots\ldots\ldots\ldots\ldots (4.8)$$

Note that since (Philip 1960)

$$\lim_{\theta\to 0}\frac{\operatorname{inverfc}\theta}{(-\log\theta)^{\frac{1}{2}}}=1, \qquad \ldots\ldots\ldots\ldots\ldots (4.9)$$

(**4.8**) is equivalent to

$$\lim_{\theta\to 0}\frac{f}{(-\log\theta)^{\frac{1}{2}}}=0. \qquad \ldots\ldots\ldots\ldots\ldots (4.10)$$

f is thus free to become infinite at $\theta=0$, but it must approach infinity more slowly than $(-\log\theta)^{\frac{1}{2}}$. Note that it is necessary, *but not sufficient*, that $f\to\infty$ more slowly than $\theta^{-\varepsilon}$, where ε is any non-zero positive quantity.

Accordingly, there exists an exact solution of (**1.1**) subject to (**1.2**) with $D(0)=D_0$ (finite, non-zero) corresponding to every $D(\theta)$ of the form (**4.3**) for which

(i) $(2D_0^{\frac{1}{2}}\operatorname{inverfc}\theta+f)$ satisfies the appropriate conditions on F set out in Section III;

(ii) f satisfies condition (**4.8**).

A further result is that, for

$$F=2D_0^{\frac{1}{2}}\operatorname{inverfc}\theta\pm f \quad (D_0 \text{ finite, non-zero}), \qquad \ldots\ldots (4.11)$$

$$D=D_0\pm\tfrac{1}{2}D_0^{\frac{1}{2}}\left(\frac{2}{B}\int_0^\theta f\,\mathrm{d}\theta-B\frac{\mathrm{d}f}{\mathrm{d}\theta}\right)-\tfrac{1}{2}\int_0^\theta f\,\mathrm{d}\theta\cdot\frac{\mathrm{d}f}{\mathrm{d}\theta}. \qquad \ldots\ldots (4.12)$$

For the results (**4.2**), (**4.3**), the restriction on $\mathrm{d}f/\mathrm{d}\theta$ was simply

$$\mathrm{d}f/\mathrm{d}\theta\leqslant 2D_0^{\frac{1}{2}}/B. \qquad \ldots\ldots\ldots\ldots\ldots\ldots (4.13)$$

We here require the somewhat stronger restriction

$$|\,\mathrm{d}f/\mathrm{d}\theta\,|\leqslant 2D_0^{\frac{1}{2}}/B. \quad\quad (4.14)$$

We note in passing that condition (**3.5**) reduces to the condition on f that

$$f(1)=0. \quad\quad (4.15)$$

It will be observed that a very large class of functions f satisfy these various requirements, and that many of them may be found by elementary means. Some typical results are presented in Table 2. It is, of course, a simple matter to extend this table to a much greater length; but there seems little purpose in enumerating further examples.

TABLE 2

SOME EXACT SOLUTIONS OF (**1.1**), (**1.2**) WITH $D(0)$ FINITE NON-ZERO

No.	D	φ	Remarks
1	$D_0+\frac{1}{2}n\theta^n\left(1-\dfrac{\theta^n}{1+n}\right)\pm\frac{1}{2}D_0^{\frac{1}{2}}\left[\dfrac{2\theta}{B}\left(1-\dfrac{\theta^n}{1+n}\right)+Bn\theta^{n-1}\right]$	$2D_0^{\frac{1}{2}}$ inverfc $\theta\pm(1-\theta^n)$	$n>0$. For minus sign $D_0\geqslant\pi n^2/16$
2	$D_0+\dfrac{n}{2(n+1)}[(1-\theta)^{n-1}-(1-\theta)^{2n}]\pm\frac{1}{2}D_0^{\frac{1}{2}}\left[\dfrac{2}{(n+1)B}[1-(1-\theta)^{n+1}]+Bn(1-\theta)^{n-1}\right]$	$2D_0^{\frac{1}{2}}$ inverfc $\theta\pm(1-\theta)^n$	$n>0$. For minus sign D_0 has lower limit
3	$D_0+\frac{1}{2}\sin^2\frac{1}{2}\pi\theta\pm\frac{1}{4}D_0^{\frac{1}{2}}\sin\frac{1}{2}\pi\theta\cdot\left[\dfrac{8}{\pi B}+\pi B\right]$	$2D_0^{\frac{1}{2}}$ inverfc $\theta\pm\cos\frac{1}{2}\pi\theta$	For minus sign $D_0\geqslant\pi/16$
4	$D_0+\frac{1}{2}e^{n\theta}[1-e^{n\theta}+n\theta e^n]\pm\frac{1}{2}D_0^{\frac{1}{2}}\left[\dfrac{2}{nB}(1-e^{n\theta}+n\theta e^n)+Bne^{n\theta}\right].$	$2D_0^{\frac{1}{2}}$ inverfc $\theta\pm(e^n-e^{n\theta})$	$n>0$. For minus sign $D_0\geqslant\pi n^2e^{2n}/16$

V. SOLUTIONS OF (1.1), (1.3)

Similarly, we may establish exact solutions of (**1.1**) subject to (**1.3**) at will, simply by selecting F functions satisfying the appropriate conditions stated in Section III. Typical results are given in Table 3. It will be noted that the entries 1 and 11 of the table are for $D(\theta)$ functions symmetrical about $\theta=\frac{1}{2}$. It is evident that these results follow immediately from Nos. 2 and 4 of Table 1, and that many more "symmetrical" exact solutions may be readily constructed from the results of the preceding section.

We here again encounter the difficulty which arose previously, namely, that F functions chosen without certain precautions tend to lead to zero or infinite values of D. In Section IV, this occurred only for $D(0)$; but here the trouble arises also for $D(1)$, which we write for $\lim\limits_{\theta\to 1} D(\theta)$.

In this case we may avoid the difficulty by using a known result for diffusion in composite media governed by conditions (**1.3**) (Carslaw and Jaeger 1959, p. 87). We find that, from the present viewpoint, this result is equivalent to the following statement.

Let F be specified by (**5.1**) below:

$$\left.\begin{array}{ll} 1\geqslant\theta>\theta', & F=-2D_1^{\frac{1}{2}}\,\mathrm{inverfc}\,\{(1-\theta)/(1-\theta')\}\,; \\ 0\leqslant\theta<\theta', & F=2D_0^{\frac{1}{2}}\,\mathrm{inverfc}\,(\theta/\theta')\,; \\ \text{where} & \\ & \theta'=D_1^{\frac{1}{2}}/(D_0^{\frac{1}{2}}+D_1^{\frac{1}{2}}). \end{array}\right\} \quad \ldots (\mathbf{5.1})$$

TABLE 3

SOME SIMPLE CASES OF EXACT SOLUTIONS OF (**1.1**), (**1.3**)

No.	D	φ	Remarks
1	$\dfrac{n}{2(n+1)}[(1-2\theta)^{n-1}-(1-2\theta)^{2n}]$	$(1-2\theta)^n$	$n=1, 3, 5, 7, \ldots$
2	$\dfrac{n\theta^n}{2(n+1)}(1-\theta^n)$	$\dfrac{1}{n+1}-\theta^n$	$n>0$
3	$\dfrac{n\theta^{-n}}{2(1-n)}(\theta^{-n}-1)$	$\theta^{-n}-\dfrac{1}{1-n}$	$0<n<1$
4	$\dfrac{n(1-\theta)^n}{2(n+1)}[1-(1-\theta)^n]$	$(1-\theta)^n-\dfrac{1}{n+1}$	$n>0$
5	$\dfrac{n(1-\theta)^{-n}}{2(1-n)}[(1-\theta)^{-n}-1]$	$\dfrac{1}{1-n}-(1-\theta)^{-n}$	$0<n<1$
6	$\frac{1}{2}\sin\frac{1}{2}\pi\theta(\sin\frac{1}{2}\pi\theta-\theta)$	$\cos\frac{1}{2}\pi\theta-2/\pi$	
7	$\frac{1}{2}\cos\frac{1}{2}\pi\theta[\cos\frac{1}{2}\pi\theta+\theta-1]$	$2/\pi-\sin\frac{1}{2}\pi\theta$	
8	$\frac{1}{2}\left[\dfrac{1+\theta\cos^{-1}\theta-\theta}{\sqrt{(1-\theta^2)}}+1\right]$	$\cos^{-1}\theta-1$	
9	$\frac{1}{2}\left[\dfrac{(1-\theta)\cos^{-1}(1-\theta)+\theta}{\sqrt{(2\theta-\theta^2)}}\right]$	$\sin^{-1}(1-\theta)-\frac{1}{2}\pi+1$	
10	$\frac{1}{4}\theta\left[\dfrac{\theta+\sin^{-1}\theta-\frac{1}{2}\pi\theta}{\sqrt{(1-\theta^2)}}\right]$	$\sqrt{(1-\theta^2)}-\frac{1}{4}\pi$	
11	$\frac{1}{2}\sin^2\pi\theta$	$\cos\pi\theta$	
12	$\dfrac{\sin^2\pi\theta}{16}[5+2\cos\pi\theta-4\theta\,\mathrm{cosec}\,\frac{1}{2}\pi\theta]$	$\cos^3\frac{1}{2}\pi\theta-4/3\pi$	
13	$\frac{1}{2}n^2e^{n\theta}[(e^n-1)\theta-(e^{n\theta}-1)]$	$e^n-1-ne^{n\theta}$	n may be either positive or negative
14	$-\frac{1}{2}\log\theta$	$-(\log\theta+1)$	
15	$\dfrac{n}{2\theta}(-\log\theta)^{n-1}$ $\times\{\Gamma(n+1)\cdot(1-\theta)-\Gamma(-\log\theta, n+1)\}$	$(-\log\theta)^n-\Gamma(n+1)$	$n>0$

Then the corresponding D function is:

$$\left.\begin{array}{ll} 1\geqslant\theta>\theta', & D=\text{constant}=D_1\,; \\ 0\leqslant\theta<\theta', & D=\text{constant}=D_0. \end{array}\right\} \qquad \text{(5.2)}$$

We therefore put F into the form (D_1, D_0 finite, non-zero)

$$\left.\begin{array}{ll} 1\geqslant\theta>\theta', & F=-2D_1^{\frac{1}{2}}\,\text{inverfc}\,\{(1-\theta)/(1-\theta')\}+f(\theta)\,; \\ 0\leqslant\theta<\theta', & F=2D_0^{\frac{1}{2}}\,\text{inverfc}\,(\theta/\theta')+f(\theta). \end{array}\right\} \qquad \text{(5.3)}$$

Using (**3.4**), we obtain the corresponding $D(\theta)$ for diffusion subject to conditions (**1.3**):

$$\left.\begin{array}{ll} 1\geqslant\theta>\theta', & D=D_1+\frac{1}{2}D_1^{\frac{1}{2}}\left[\dfrac{2}{(1-\theta')B\{(1-\theta)/(1-\theta')\}}\displaystyle\int_0^\theta f\,\mathrm{d}\theta-(1-\theta')B\left(\dfrac{1-\theta}{1-\theta'}\right)\dfrac{\mathrm{d}f}{\mathrm{d}\theta}\right] \\ & \qquad -\frac{1}{2}\dfrac{\mathrm{d}f}{\mathrm{d}\theta}\cdot\displaystyle\int_0^\theta f\,\mathrm{d}\theta\,; \\ 0\leqslant\theta<\theta', & D=D_0+\frac{1}{2}D_0^{\frac{1}{2}}\left[2/\theta'B(\theta/\theta')\displaystyle\int_0^\theta f\,\mathrm{d}\theta-\theta'B(\theta/\theta')\dfrac{\mathrm{d}f}{\mathrm{d}\theta}\right] \\ & \qquad -\frac{1}{2}\dfrac{\mathrm{d}f}{\mathrm{d}\theta}\cdot\displaystyle\int_0^\theta f\,\mathrm{d}\theta. \end{array}\right\} \qquad \text{(5.4)}$$

The condition that $D(0)=D_0$ reduces to

$$\lim_{\theta\to 0}\frac{f}{\text{inverfc}\,(\theta/\theta')}=0, \qquad \text{(5.5)}$$

entirely analogous to (**4.8**) in the previous Section. We have similarly that the condition that $D(1)=D_1$ is that

$$\lim_{\theta\to 1}\frac{f}{\text{inverfc}\,\{(1-\theta)/(1-\theta')\}}=0. \qquad \text{(5.6)}$$

It follows that there exists an exact solution of (**1.1**) subject to (**1.3**) with $D(0)=D_0$, $D(1)=D_1$ (both finite, non-zero) corresponding to every $D(\theta)$ of the form (**5.4**) for which

(i) F of the form (**5.3**) satisfies the appropriate conditions set out in Section III;

(ii) f satisfies conditions (**5.5**) and (**5.6**).

It will be noted that, in this case, when $\mathrm{d}f/\mathrm{d}\theta$ is continuous at $\theta=\theta'$, a discontinuity of magnitude D_1-D_0 occurs in $D(\theta)$ at this point. The condition that $\mathrm{d}F/\mathrm{d}\theta$, and therefore $D(\theta)$, is continuous at $\theta=\theta'$ is that

$$\frac{\mathrm{d}f}{\mathrm{d}\theta}(\theta'+)-\frac{\mathrm{d}f}{\mathrm{d}\theta}(\theta'-)=\left(\frac{\pi}{D_0D_1}\right)^{\frac{1}{2}}(D_1^{\frac{1}{2}}+D_0^{\frac{1}{2}})(D_1-D_0). \qquad \text{(5.7)}$$

That is, a discontinuity in $\mathrm{d}f/\mathrm{d}\theta$, defined in (**5.7**), is necessary if a discontinuity in $D(\theta)$ is to be avoided at $\theta=\theta'$. It is seen that usually f will be required to satisfy this further condition.

It is therefore helpful to replace f by $g+f'$, where the discontinuity in $\mathrm{d}f/\mathrm{d}\theta$ at $\theta=\theta'$ is contained in $\mathrm{d}g/\mathrm{d}\theta$, with $\mathrm{d}f'/\mathrm{d}\theta$ continuous at this point. Condition (**3.6**) on F reduces here to the requirement that

$$\int_0^1 f\mathrm{d}\theta=0,$$

so that it is convenient to take g such that

$$\int_0^1 g\mathrm{d}\theta=0. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{5.8})$$

We then have as a condition on f' that

$$\int_0^1 f'\mathrm{d}\theta=0. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (\mathbf{5.9})$$

The family of linear g functions satisfying (**5.8**) is

$$\left.\begin{array}{ll} 1\geqslant\theta>\theta', & g=a+b(\theta-\theta')\,; \\ 0\leqslant\theta<\theta', & g=a+(b-c)(\theta-\theta'). \end{array}\right\} \quad \ldots\ldots\ldots \quad (\mathbf{5.10})$$

Here a is an arbitrary constant,

$$b=(D_1^{\frac{1}{2}}+D_0^{\frac{1}{2}})[2a/(D_1^{\frac{1}{2}}-D_0^{\frac{1}{2}})+(\pi D_1/D_0)^{\frac{1}{2}}],$$

and

$$c=(\pi/D_0D_1)^{\frac{1}{2}}(D_1^{\frac{1}{2}}+D_0^{\frac{1}{2}})(D_1-D_0).$$

We recall that g and f' must be such that $\mathrm{d}F/\mathrm{d}\theta\leqslant 0$.

It is evident that, despite these various restrictions, there still remains a wide range of permissible f functions. Figures 1 and 2 represent some simple exact solutions for the case $D_0=1$, $D_1=9$, $f'=0$, and several values of the parameter a.

We have here treated the case with both D_0 and D_1 finite non-zero. Evidently, when only *one* of these quantities is required to be finite non-zero, the conditions on F are weaker and the problem is correspondingly simpler.

VI. Practical Use of the Method

The typical mathematical problem arising in concentration-dependent diffusion is to compute $\varphi(\theta)$ when $D(\theta)$ is known (frequently determined experimentally). Effective use of the method developed here depends then on the ability to match any given $D(\theta)$ function with a member of the family of $D(\theta)$ functions yielding exact solutions.

This may be done, though rather brutally, by introducing (for the case of diffusion subject to (**1.2**)) an F function of the form

$$F=2D_0\,\mathrm{inverfc}\,\theta+\sum_1^n a_r(1-\theta)^r. \quad \ldots\ldots\ldots \quad (\mathbf{6.1})$$

The corresponding $D(\theta)$ function follows from (**3.4**). We may now match this computed $D(\theta)$ with its $(n+1)$ adjustable parameters, D_0 and a_r, at $(n+1)$

points of the given $D(\theta)$ curve. The problem reduces to solving $(n+1)$ simultaneous equations for $(n+1)$ unknowns. This is a possible, but not particularly attractive, manner of securing the solution. A similar method may be used for solving (**1.1**) subject to (**1.3**).

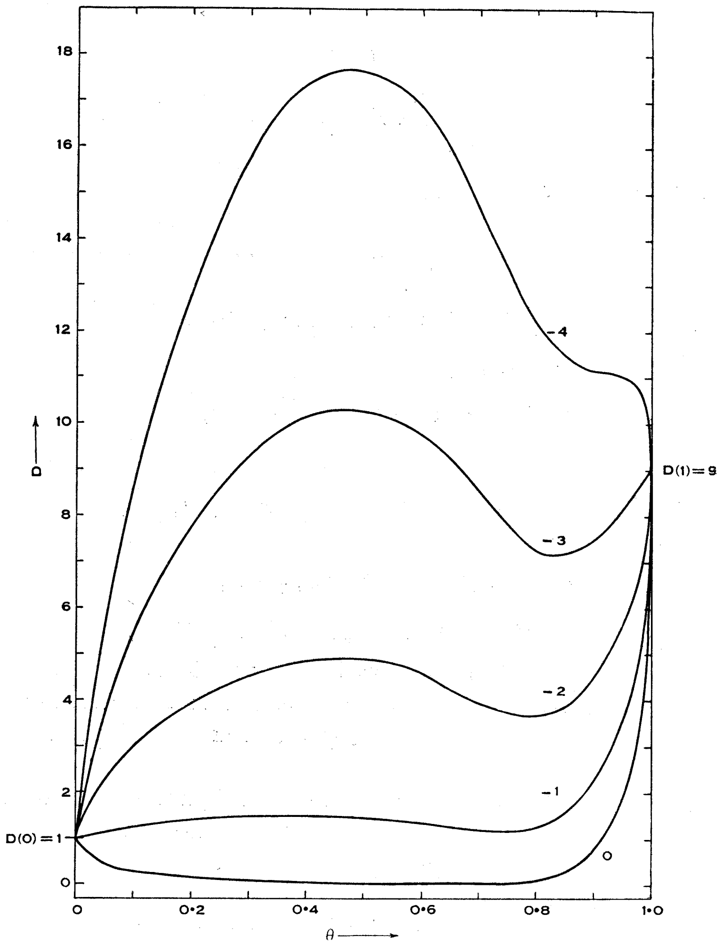

Fig. 1.—Parametric family of $D(\theta)$ functions defined as follows:
$1 \geqslant \theta > \frac{3}{4}$, $D = 9 + (1-\theta)[(2a+6\sqrt{\pi})\theta - 3\sqrt{\pi}]\{2a+6\sqrt{\pi} - 12/B(4-4\theta)\} - \frac{3}{4}(2a+6\sqrt{\pi})B(4-4\theta)$;
$0 \leqslant \theta < \frac{3}{4}$, $D = 1 - \theta[(2a+\frac{2}{3}\sqrt{\pi})\theta - (2a+\sqrt{\pi})]\{2a+\frac{2}{3}\sqrt{\pi} - 4/3B(4\theta/3)\} - \frac{3}{4}(2a+\frac{2}{3}\sqrt{\pi})B(4\theta/3)$.
Numbers on the curves denote values of a.

It appears to the author that (both in the case of (**1.1**), (**1.2**) and of (**1.1**), (**1.3**)) it is preferable to keep the number of disposable constants in the F function down to perhaps two or three, and to provide the desired range of shapes of $D(\theta)$ function by making use of the variety of the possible functional forms which F is free to assume. This requires the construction of a "library" in which are arrayed various F functions together with the corresponding D

functions. It should then be possible, by inspection, to select an appropriate functional form of F, and the problem then reduces to matching the given D function by solving for the small number of disposable parameters occurring in the F function. It is beyond the scope of the present paper to provide such a library. Its construction and presentation remain a task for the future.

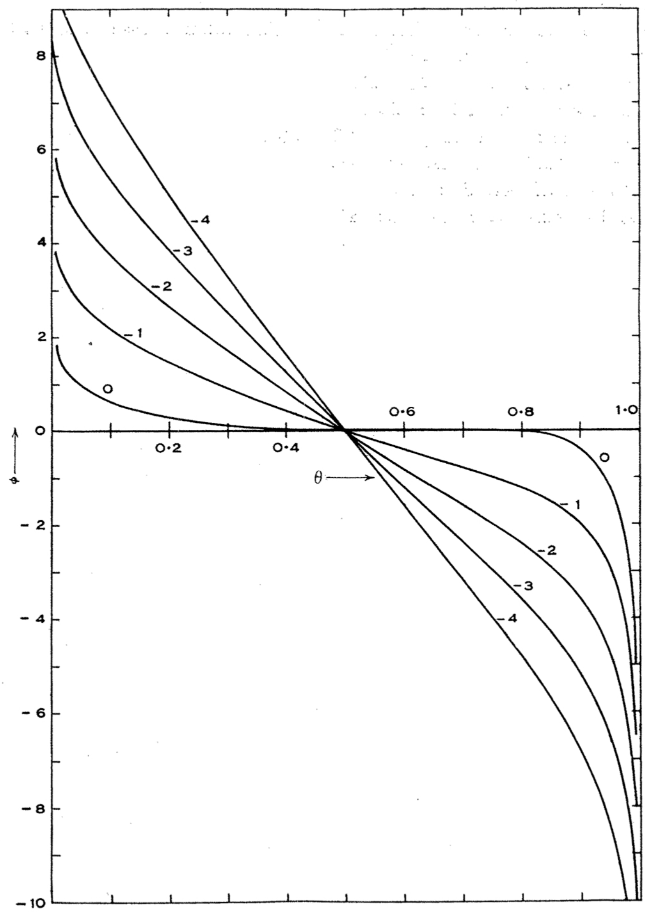

Fig. 2.—Parametric family of $\varphi(\theta)$ functions defined as follows :
$1 \geqslant \theta > \frac{3}{4}$, $\varphi = -6 \text{ inverfc } (4-4\theta) + a + 4(a+3\sqrt{\pi})(\theta - \frac{3}{4})$;
$0 \leqslant \theta < \frac{3}{4}$, $\varphi = 2 \text{ inverfc } 4\theta/3 + a + 4(a+\frac{1}{3}\sqrt{\pi})(\theta - \frac{3}{4})$.
Numbers on the curves denote values of a. These curves represent exact solutions of (**1.1**), (**1.3**) corresponding to the $D(\theta)$ functions of Figure 1.

VII. Discussion

In the present study we have made use of (**4.1**) and (**5.1**), (**5.2**) to avoid difficulties due to $D(\theta)$ becoming zero or infinite at one or both ends of the θ-interval ; but we have not provided a thorough investigation of such questions as the relationship (for diffusion subject to (**1.2**)) between the manner in which

$\varphi(\theta)$ behaves as $\theta \to 0$ and the behaviour of $D(\theta)$ close to $\theta = 0$. It is hoped to return to questions of this nature in a later communication (cf. Philip 1957 for an early approach).

VIII. References

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