NUMERICAL SOLUTION OF EQUATIONS OF THE DIFFUSION TYPE WITH DIFFUSIVITY CONCENTRATION-DEPENDENT. II

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Summary

A new procedure is developed for the numerical solution of the equation

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

with D and K single-valued functions of θ and the conditions $\theta=\theta_n$, $t=0$, $x>0$; $\theta=\theta_0$, $x=0$, $t\geqslant 0$. Difficulties inherent in the one method previously suggested are avoided, the problem being reduced to one of solving a set of ordinary differential equations.

The solution is found in a form implicit in θ and t, with x expressed as a power series in $t^{\frac{1}{2}}$ with the " coefficients " functions of θ obtained as the solution of the ordinary equations. For problems of interest to the author this series converges rapidly, so that solution of only the first few ordinary equations is needed. A simple and rapid numerical process is given for solving these equations.

The truncation error of this process is studied empirically and the convergence of the power series in $t^{\frac{1}{2}}$ examined briefly.

I. INTRODUCTION

This paper describes a method for the numerical solution of the equation

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x}\left(D\frac{\partial\theta}{\partial x}\right)-\frac{\partial K}{\partial x}, \quad \text{(1.1)}$$

subject to the conditions

$$\left.\begin{array}{lll}\theta=\theta_n, & t=0, & x>0,\\ \theta=\theta_0, & x=0, & t\geqslant 0.\end{array}\right\} \quad \text{(1.2)}$$

D and K are both single-valued functions of θ.

Equation (**1.1**) is a generalized form of the Fokker-Planck equation and is relevant, for example, to diffusion phenomena modified by an external force field (Chandrasekhar 1943). In particular, the equation describes the vertical isothermal movement of a liquid and its vapour in a homogeneous stable porous medium under the potential gradient arising from capillarity and gravity (Klute 1952 ; Philip 1955*b*). Solutions of (**1.1**) by the present method are applied to the microhydrological problem of infiltration in a series of papers to be published elsewhere (Philip 1957). These solutions agree with experiment and provide important improvements in the understanding of this phenomenon.

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Klute (1952) suggested that a method developed by Crank and Nicholson (1947) might be adapted to give numerical solutions of (**1.1**). Essentially, these authors replaced derivatives both with respect to x and with respect to t by finite difference ratios, and on Q occasions solved P simultaneous equations to obtain values of θ at PQ points of the net formed by P intervals in x and Q in t. They also used an improved finite difference form of $\partial^2\theta/\partial x^2$.

The necessary procedure to solve (**1.1**) in this way was worked out by the author, but it was found that the method promised to give poor accuracy even at the expense of much labour.

II. Present Method

The present method follows that developed in an earlier paper (Philip 1955*a*, which will be referred to as Part I) in taking θ as the independent variable. The equation

$$\frac{\partial\theta}{\partial t}=\frac{\partial}{\partial x'}\left(D\frac{\partial\theta}{\partial x'}\right), \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (2.1)$$

subject to the conditions

$$\left.\begin{array}{lll}\theta=\theta_n, & t=0, & x'>0,\\ \theta=\theta_0, & x'=0, & t\geqslant 0,\end{array}\right\} \quad \ldots\ldots\ldots\ldots \quad (2.2)$$

is introduced. Its solution is of the form

$$x'=\varphi t^{\frac{1}{2}}, \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2.3)$$

where φ is a function of θ only. φ is readily evaluated by the method of Part I. Solution (**2.3**) is used to provide a first estimate of x. A partial D.E. is set up in θ, t, and the residual error $(x-x')$. An approximate solution of this equation is found by means of an approximation and a substitution suggested by dimensional analysis. At the same time a new partial D.E. is found which specifies the new residual error exactly. The new equation is amenable to the same treatment and the process may be repeated with new residual errors as often as required to give the necessary accuracy.

III. Introduction of Residual y and Approximate Residual y'

We use the well-known identity

$$\left(\frac{\partial\theta}{\partial t}\right)_x\cdot\left(\frac{\partial x}{\partial\theta}\right)_t=-\left(\frac{\partial x}{\partial t}\right)_\theta \quad \ldots\ldots\ldots\ldots\ldots \quad (3.1)$$

to introduce forms of (**1.1**) and (**2.1**) with θ as the independent variable. (Where necessary for clarity we employ the symbolism $(\partial a/\partial b)_c$ to denote the partial derivative of variable a with respect to variable b, with variable c held constant.) These are:

$$-\frac{\partial x}{\partial t}=\frac{\partial}{\partial\theta}\left(D\frac{\partial\theta}{\partial x}\right)-\frac{\partial K}{\partial\theta}, \quad \ldots\ldots\ldots\ldots\ldots \quad (3.2)$$

$$-\frac{\partial x'}{\partial t}=\frac{\partial}{\partial\theta}\left(D\frac{\partial\theta}{\partial x'}\right). \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.3)$$

In these equations the derivatives of the left-hand sides are for θ held constant and those of the right-hand sides are for t held constant. For simplicity we write $\partial\theta/\partial x$, $\partial\theta/\partial x'$ for $1/(\partial x/\partial\theta)$, $1/(\partial x'/\partial\theta)$. Subtraction gives

$$-\frac{\partial y}{\partial t}=\frac{\partial}{\partial\theta}\left[D\left(\frac{\partial\theta}{\partial x}-\frac{\partial\theta}{\partial x'}\right)\right]-\frac{\partial K}{\partial\theta}, \qquad (3.4)$$

where

$$y=x-x'. \qquad (3.5)$$

Now

$$\frac{\partial\theta}{\partial x}-\frac{\partial\theta}{\partial x'}=-\frac{\partial\theta}{\partial x'}\cdot\frac{\partial y}{\partial x}, \qquad (3.6)$$

where $\partial y/\partial x$ is written for $(\partial y/\partial x)_t$, so that (**3.4**) becomes

$$\frac{\partial y}{\partial t}=\frac{\partial}{\partial\theta}\left(D\frac{\partial\theta}{\partial x'}\cdot\frac{\partial y}{\partial x}\right)+\frac{\partial K}{\partial\theta}. \qquad (3.7)$$

(**3.7**) is subject to the conditions (**3.8**), in which K_0, K_n are written for the values of K at $\theta=\theta_0$, θ_n.

$$\left.\begin{aligned}\int_{\theta_n}^{\theta_0} y\,d\theta&=\int_0^t\left[D\frac{\partial\theta}{\partial x'}\cdot\frac{\partial y}{\partial x}\right]_{\theta=\theta_0}dt+(K_0-K_n)t,\\ y=0,\quad \theta&=\theta_0,\quad t\geqslant 0.\end{aligned}\right\} \qquad (3.8)$$

The first of these conditions (interpreted physically) states that the increase in the total amount of diffusing substance in the semi-infinite region due to the presence of the external force field is equal to the time integral of the increased flux entering the region across $x=0$ less the integrated flux leaving the region at infinity. The second condition follows directly from the second of each of conditions (**1.2**) and (**2.2**), provided x is a single-valued function of θ, a condition fulfilled in the present problem.

We now introduce the approximation

$$\partial y/\partial x=\partial y/\partial x' \qquad (3.9)$$

into (**3.7**), which then becomes

$$\frac{\partial y'}{\partial t}=\frac{\partial}{\partial\theta}\left[D\left(\frac{\partial\theta}{\partial x'}\right)^2\cdot\frac{\partial y'}{\partial\theta}\right]+\frac{\partial K}{\partial\theta}. \qquad (3.10)$$

y' is now written for y since the use of approximation (**3.9**) implies that (**3.10**) cannot give y exactly. (**3.10**) is subject to a modified form of (**3.8**):

$$\left.\begin{aligned}\int_{\theta_n}^{\theta_0} y'\,d\theta&=\int_0^t\left[D\left(\frac{\partial\theta}{\partial x'}\right)^2\cdot\frac{\partial y'}{\partial\theta}\right]_{\theta=\theta_0}dt+(K_0-K_n)t,\\ y'=0,\quad \theta&=\theta_0,\quad t\geqslant 0.\end{aligned}\right\} \qquad (3.11)$$

Using (**2.3**), we rewrite (**3.10**) as

$$\frac{\partial y'}{\partial t}=\frac{1}{t}\,\frac{\partial}{\partial\theta}\left(P\frac{\partial y'}{\partial\theta}\right)+\frac{\partial K}{\partial\theta}, \qquad (3.12)$$

where P is the function of θ given by

$$P = D(\mathrm{d}\theta/\mathrm{d}\varphi)^2. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.13)$$

It will be recalled that φ is a known function of θ, found by applying the method of Part I to (**2.1**) subject to (**2.2**). P is thus also a known function.

The substitution suggested by dimensional analysis

$$\chi = y' t^{-1}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.14)$$

where χ is a function of θ only, eliminates t from conditions (**3.11**), so that (**3.12**) has a solution of this type which may be presumed unique. (**3.14**) thus enables (**3.12**) subject to (**3.11**) to be reduced to

$$\chi = \frac{\mathrm{d}}{\mathrm{d}\theta}\left(P\frac{\mathrm{d}\chi}{\mathrm{d}\theta}\right) + \frac{\mathrm{d}K}{\mathrm{d}\theta}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.15)$$

subject to the conditions

$$\left.\begin{aligned} \int_{\theta_n}^{\theta_0} \chi \mathrm{d}\theta &= \left(P\frac{\mathrm{d}\chi}{\mathrm{d}\theta}\right)_{\theta=\theta_0} + (K_0 - K_n), \\ \theta &= \theta_0, \quad \chi = 0. \end{aligned}\right\}. \quad \ldots\ldots \quad (3.16)$$

Integration gives a form suitable for numerical solution

$$\int_{\theta_n}^{\theta} \chi \mathrm{d}\theta = P\mathrm{d}\chi/\mathrm{d}\theta + (K - K_n), \quad \ldots\ldots\ldots\ldots \quad (3.17)$$

subject to the condition

$$\theta = \theta_0, \quad \chi = 0. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (3.18)$$

Details of the numerical solution of (**3.17**) subject to (**3.18**) are given in Section VI. For the present we assume that χ and therefore y' have been evaluated and proceed to consider further improvement of the solution.

IV. The Second Approximation

Subtraction of (**3.10**) from (**3.7**) gives

$$\frac{\partial z}{\partial t} = \frac{\partial}{\partial \theta}\left[D\frac{\partial \theta}{\partial x'}\left(\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'}\right)\right], \quad \ldots\ldots\ldots\ldots \quad (4.1)$$

where the new residual z is given by

$$z = y - y'. \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4.2)$$

Since

$$\frac{\partial y}{\partial x} - \frac{\partial y'}{\partial x'} = \frac{\partial z}{\partial x} - \frac{\partial y}{\partial x} \cdot \frac{\partial y'}{\partial x'}, \quad \ldots\ldots\ldots\ldots\ldots\ldots \quad (4.3)$$

(**4.1**) becomes

$$\frac{\partial z}{\partial t} = \frac{\partial}{\partial \theta}\left[D\frac{\partial \theta}{\partial x'}\left(\frac{\partial z}{\partial x} - \frac{\partial y}{\partial x} \cdot \frac{\partial y'}{\partial x'}\right)\right]. \quad \ldots\ldots\ldots \quad (4.4)$$

In these equations $\partial y'/\partial x'$, $\partial z/\partial x$ are written for $(\partial y'/\partial x')_t$, $(\partial z/\partial x)_t$. (**4.4**) is subject to the conditions

$$\left.\begin{aligned}\int_{\theta_n}^{\theta_0} z\mathrm{d}\theta=\int_0^t\left[D\frac{\partial\theta}{\partial x'}\left(\frac{\partial z}{\partial x}-\frac{\partial y}{\partial x}\cdot\frac{\partial y'}{\partial x'}\right)\right]_{\theta=\theta_0}\mathrm{d}t,\\ \theta=\theta_0,\quad z=0,\quad t\geqslant 0.\end{aligned}\right\}\qquad(\mathbf{4.5})$$

If the approximations

$$\partial z/\partial x=\partial z/\partial x'\,;\quad \partial y/\partial x=\partial y'/\partial x' \qquad(\mathbf{4.6})$$

are put into (**4.4**), the result is

$$\frac{\partial z'}{\partial t}=\frac{\partial}{\partial\theta}\left[D\frac{\partial\theta}{\partial x'}\left\{\frac{\partial z'}{\partial x'}-\left(\frac{\partial y'}{\partial x'}\right)^2\right\}\right], \qquad(\mathbf{4.7})$$

in which z' is written for z, since the use of approximations (**4.6**) implies that (**4.7**) cannot give z exactly. The modified conditions are

$$\left.\begin{aligned}\int_{\theta_n}^{\theta_0} z'\mathrm{d}\theta=\int_0^t\left[D\frac{\partial\theta}{\partial x'}\left\{\frac{\partial z'}{\partial x'}-\left(\frac{\partial y'}{\partial x'}\right)^2\right\}\right]_{\theta=\theta_0}\mathrm{d}t,\\ \theta=\theta_0,\quad z'=0,\quad t\geqslant 0.\end{aligned}\right\}\qquad(\mathbf{4.8})$$

Now, introducing φ, χ, and P, we may rewrite (**4.7**)

$$\frac{\partial z'}{\partial t}=\frac{\partial}{\partial\theta}\left[\frac{P}{t}\,\frac{\partial z'}{\partial\theta}-Qt^{\frac{1}{2}}\right], \qquad(\mathbf{4.9})$$

where

$$Q(\theta)=D\frac{\mathrm{d}\theta}{\mathrm{d}\varphi}\left(\frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\right)^2. \qquad(\mathbf{4.10})$$

It will be noted that Q, a function of θ, is simply evaluated once φ and χ are known.

In the same way as (**3.14**) enabled the solution of (**3.10**) to be found, the substitution

$$\psi=z't^{-3/2} \qquad(\mathbf{4.11})$$

allows (**4.9**) to be reduced to the ordinary equation

$$\frac{3}{2}\psi=\frac{\mathrm{d}}{\mathrm{d}\theta}\left[P\frac{\mathrm{d}\psi}{\mathrm{d}\theta}-Q\right]. \qquad(\mathbf{4.12})$$

Integrating (**4.12**) and using (**4.11**) in (**4.8**) leads to a form suitable for numerical solution

$$\frac{3}{2}\int_{\theta_n}^{\theta}\psi\mathrm{d}\theta=P\mathrm{d}\psi/\mathrm{d}\theta-Q, \qquad(\mathbf{4.13})$$

subject to the condition

$$\theta=\theta_0,\quad \psi=0. \qquad(\mathbf{4.14})$$

Details of the numerical solution of (**4.13**) subject to (**4.14**) are given in Section VI. For the present we shall assume that ψ, and therefore z', have been evaluated.

V. Higher Approximations

Provided the procedure developed above is convergent, its continued application will enable x to be evaluated to any desired degree of accuracy. For example, the next step is to introduce the residual

$$w = z - z'. \qquad (5.1)$$

Then, if w' is the approximation to w and the substitution

$$\omega = w' t^{-2} \qquad (5.2)$$

is employed, we obtain the equation

$$2\int_{\theta_n}^{\theta} \omega \mathrm{d}\theta = P\mathrm{d}\omega/\mathrm{d}\theta - R, \qquad (5.3)$$

where

$$R(\theta) = D\frac{\mathrm{d}\theta}{\mathrm{d}\varphi} \cdot \frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\left[2\frac{\mathrm{d}\psi}{\mathrm{d}\varphi} - \left(\frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\right)^2\right] = Q\left[2\frac{\mathrm{d}\psi}{\mathrm{d}\chi} - \frac{\mathrm{d}\chi}{\mathrm{d}\varphi}\right]. \qquad (5.4)$$

(**5.3**) is subject to the condition

$$\theta = \theta_0, \quad \omega = 0, \qquad (5.5)$$

and like (**3.17**) and (**4.13**) will be found to lend itself readily to numerical solution. See Section VI for details of this.

Continuing to repeat this procedure gives the series

$$x = x' + y' + z' + w' + \ldots + \ldots + g_m(\theta, t) + \ldots, \qquad (5.6)$$

which may be written

$$x = \varphi t^{\frac{1}{2}} + \chi t + \psi t^{3/2} + \omega t^2 + \ldots + f_m(\theta) t^{m/2} + \ldots \qquad (5.7)$$

$f_m(\theta)$ is given by

$$\tfrac{1}{2}m\int_{\theta_n}^{\theta} f_m \mathrm{d}\theta = P\frac{\mathrm{d}}{\mathrm{d}\theta}(f_m) - R_m, \qquad (5.8)$$

subject to the condition

$$\theta = \theta_0, \quad f_m = 0. \qquad (5.9)$$

R_m is a function of θ which may be determined from $D, \varphi, \chi, \psi, \omega, \ldots, \ldots, f_{m-1}$.

It will be noted that an alternative procedure for obtaining the solution of (**1.1**) subject to (**1.2**) is to assume its existence in the form (**5.7**). Then, if (**5.7**) is substituted in (**3.2**) and successive powers of $t^{\frac{1}{2}}$ equated, equation (**2.6**) of Part I and equations (**3.15**), (**4.12**), (**5.3**), (**5.8**) of the present paper are found, all subject to the appropriate conditions. This is a much more direct method of securing the equations, but is open to the objection that there seems to be no *a priori* reason for assuming the form (**5.7**).

Before considering numerical examples and the convergence of (**5.7**), it is desirable to treat the numerical methods of obtaining χ, ψ, ω, etc.

VI. Numerical Solution of Equations (3.15), (4.12), (5.3), (5.8)

The procedure developed for computing these functions has some affinities with the method of Part I. Here again the finite difference equations and organization of the computations are simple, and an analytical solution is used to avoid difficulty close to $\theta=\theta_n$. In the present method, however, the linear form of the finite difference equations enables the result to be obtained directly, rather than by the process of trial and iterative improvement usual in the solution of equations subject to two-point boundary conditions.

It will be noticed that equations (**3.15**), (**4.12**), (**5.3**), (**5.8**) and their conditions may all be written in the form

$$\int_{\theta_n}^{\theta} f\mathrm{d}\theta=\alpha\mathrm{d}f/\mathrm{d}\theta-\beta, \qquad \text{(6.1)}$$

subject to

$$\theta=\theta_0, \quad f=0. \qquad \text{(6.2)}$$

α and β are known functions of θ.

We proceed to discuss the numerical solution of (**6.1**) subject to (**6.2**), realizing that the procedure for this general case may be applied to any one of the above equations by substituting the appropriate functions for α, β, f. Certain matters arising in the computation of the coefficients of these equations are discussed in Section VII.

Let the interval θ_0 to θ_n be divided into n equal steps $\delta\theta$.

Let

$$\theta_r=\theta_0-r\delta\theta, \qquad \text{(6.3)}$$

and let the suffix r appended to a quantity denote its value at $\theta=\theta_r$.

Replacing the $f(\theta)$ curve by the polygon with (θ_r, f_r) as vertices produces the finite difference approximation

$$\int_{\theta_r}^{\theta_{r+\frac{1}{2}}} f\mathrm{d}\theta=-\tfrac{1}{4}(f_{r+1}+3f_r)\cdot\tfrac{1}{2}\delta\theta. \qquad \text{(6.4)}$$

We also use the approximation

$$(\alpha\mathrm{d}f/\mathrm{d}\theta)_{r+\frac{1}{2}}=(\bar{\alpha}_{r+\frac{1}{2}}/\delta\theta)(f_r-f_{r+1}), \qquad \text{(6.5)}$$

where

$$\bar{\alpha}_{r+\frac{1}{2}}=\int_{\theta_{r+1}}^{\theta_r}\alpha\mathrm{d}\theta\Big/\!\!\Big/\int_{\theta_{r+1}}^{\theta_r}\mathrm{d}\theta. \qquad \text{(6.6)}$$

Putting (**6.4**) and (**6.5**) in (**6.1**) for $\theta=\theta_{r+\frac{1}{2}}$ gives

$$\int_{\theta_n}^{\theta_r} f\mathrm{d}\theta-\tfrac{1}{4}(f_{r+1}+3f_r)\cdot\tfrac{1}{2}\delta\theta=(\bar{\alpha}_{r+\frac{1}{2}}/\delta\theta)(f_r-f_{r+1})-\beta_{r+\frac{1}{2}}, \qquad \text{(6.7)}$$

which may be written

$$f_{r+1}-f_r=-(\beta_{r+\frac{1}{2}}/\delta\theta+I_{r+\frac{1}{2}})/\{\bar{\alpha}_{r+\frac{1}{2}}/(\delta\theta)^2-\tfrac{1}{8}\}, \qquad \text{(6.8)}$$

where

$$I_{r+\frac{1}{2}}=(1/\delta\theta)\int_{\theta_n}^{\theta_r} f d\theta-\tfrac{1}{2}f_r. \qquad (6.9)$$

Also, the polygonal approximation to the $f(\theta)$ curve gives

$$I_{r+\frac{1}{2}}=I_{r-\frac{1}{2}}-f_r. \qquad (6.10)$$

It is convenient to introduce the quantity I_n, defined by

$$I_n=I_{n-\frac{1}{2}}-\tfrac{1}{2}f_n. \qquad (6.11)$$

The polygonal approximation requires that $I_n=0$.

Now the linear form of (**6.8**) and (**6.10**) implies that the values of f_r ($r=1$ to n), f'_r, obtained by assuming a value of $I_{\frac{1}{2}}$, $I'_{\frac{1}{2}}$, and alternately using (**6.8**) and (**6.10**), are linear functions of $I'_{\frac{1}{2}}$. I'_n, the value arrived at for I_n, is also a linear function of $I'_{\frac{1}{2}}$. Thus the required solution may be obtained *exactly* (i.e. subject only to truncation errors) by evaluating the sets of f- and I-values corresponding to any two assumed values of $I_{\frac{1}{2}}$ and then interpolating (or extrapolating) linearly to $I_n=0$.

An equivalent procedure involving less computation has been used by the author and is described below.

(i) Tabulate $\{\bar{\alpha}_{r+\frac{1}{2}}/(\delta\theta)^2-\frac{1}{8}\}$ and $(\beta_{r+\frac{1}{2}}/\delta\theta)$ from the known α and β functions.

(ii) Taking the initial values $I_{\frac{1}{2}}=0$, $f_0=0$, alternately apply (**6.8**) and (**6.10**) to evaluate a set of f-values and finally I_n. Denote these values by f'_r, I'_n.

(iii) Repeat the procedure with $I_{\frac{1}{2}}=-1$ and $f_0=0$, but this time disregard the tabulated values of $\beta_{r+\frac{1}{2}}/\delta\theta$ and proceed as if this quantity were always zero. Denote the new f- and I- values by f''_r ,I''_n.

(iv) Then the true values of $I_{\frac{1}{2}}$ and f_r are given by (**6.12**) and (**6.13**) :

$$I_{\frac{1}{2}}=I'_n/I''_n, \qquad (6.12)$$

$$f_r=f'_r-I_{\frac{1}{2}}\cdot f''_r. \qquad (6.13)$$

(v) The computation may be checked for numerical errors by feeding the value of $I_{\frac{1}{2}}$ from (**6.12**) into the procedure of (ii). f's evaluated in this way should equal those given by (**6.13**), and I_n should be zero.

VII. Computation of $\bar{P}_{r+\frac{1}{2}}$, $Q_{r+\frac{1}{2}}$, etc. Especially near $\theta=\theta_n$

In applying the method of Section VI to equations (**3.15**), (**4.12**), (**5.3**), (**5.8**) it is necessary to compute the relevant quantities $\bar{\alpha}_{r+\frac{1}{2}}$, $\beta_{r+\frac{1}{2}}$. Certain points arising in this connexion seem worthy of mention.

Computation of $\bar{P}_{r+\frac{1}{2}}$. For (**3.15**), $\alpha=P$. Now from (**3.13**) and (**6.6**)

$$\bar{P}_{r+\frac{1}{2}}=(1/\delta\theta)\int_{\theta_{r+1}}^{\theta_r} D(d\theta/d\varphi)^2 d\theta. \qquad (7.1)$$

$\bar{P}_{r+\frac{1}{2}}/(\delta\theta)^2$ is then simply computed from the approximation

$$\frac{\bar{P}_{r+\frac{1}{2}}}{(\delta\theta)^2}=\frac{\bar{D}_{r+\frac{1}{2}}}{(\varphi_r-\varphi_{r+1})^2}, \qquad (7.2)$$

except for $r=n-1$. Since φ_n is infinite, (**7.2**) would give $\bar{P}_{n-\frac{1}{2}}=0$. It is preferable to use the analytical solution (equation (**4.3**) of Part I),

$$\varphi=2(\bar{D}_{n-\frac{1}{2}})^{\frac{1}{2}} \text{ inverfc}\left[\frac{\theta}{\delta\theta}\frac{\theta_n}{}\text{ erfc }\{\varphi_{n-1}/2(\bar{D}_{n-\frac{1}{2}})^{\frac{1}{2}}\}\right], \qquad (7.3)$$

which leads to

$$\frac{\bar{P}_{n-\frac{1}{2}}}{(\delta\theta)^2}=B\left[\frac{\varphi_{n-1}}{2(\bar{D}_{n-\frac{1}{2}})^{\frac{1}{2}}}\right], \qquad (7.4)$$

where

$$B(x)=\frac{1}{\sqrt{3\pi}}\,\frac{\text{erfc }\sqrt{3}x}{(\text{erfc } x)^3}. \qquad (7.5)$$

The asymptotic expansion (large x) of $B(x)$ is given in (**7.6**)

$$B(x)=\frac{x^2}{3}\left\{1+\frac{4}{3}\left(\frac{1}{x}\right)^2-\frac{11}{12}\left(\frac{1}{x}\right)^4+\frac{11}{36}\left(\frac{1}{x}\right)^6-\frac{249}{16}\left(\frac{1}{x}\right)^8+\ldots\right\}. \qquad (7.6)$$

It will be found frequently that B is more simply and accurately computed from (**7.6**) than by the use of the tables of erf x commonly available.

Computation of $Q_{r+\frac{1}{2}}$. For (**4.12**), $\beta=2Q/3$. A simple approximation follows from (**4.10**)

$$\frac{Q_{r+\frac{1}{2}}}{\delta\theta}=D_{r+\frac{1}{2}}\frac{(\chi_r-\chi_{r+1})^2}{(\varphi_r-\varphi_{r+1})^3}. \qquad (7.7)$$

(**7.7**) fails for $r=n-1$, since φ_n is infinite. However, since χ_n is finite, we may write

$$\frac{Q_{n-\frac{1}{2}}}{\delta\theta}=\frac{D_{n-\frac{1}{2}}(\chi_{n-1}-\chi_n)^2}{(\delta\theta)^3}\left(\frac{d\theta}{d\varphi}\right)^3_{n-\frac{1}{2}}. \qquad (7.8)$$

We may now use in (**7.8**) the value of $\left(\frac{d\theta}{d\varphi}\right)_{n-\frac{1}{2}}$ available from (**7.3**)

$$\left(\frac{d\theta}{d\varphi}\right)_{n-\frac{1}{2}}=-\frac{\delta\theta\exp\,[-\varphi^2_{n-\frac{1}{2}}/4\bar{D}_{n-\frac{1}{2}}]}{(\pi\bar{D}_{n-\frac{1}{2}})^{\frac{1}{2}}\text{ erfc }[\varphi_{n-1}/2\bar{D}^{\frac{1}{2}}_{n-\frac{1}{2}}]}. \qquad (7.9)$$

It will be noted that, since $(d\theta/d\varphi)_n=0$ and $(d\chi/d\theta)_n$ is finite, $Q_n=0$. R_n, and apparently all $(R_m)_n$, are also zero.

In computing $R_{n-\frac{1}{2}}$, and apparently all $(R_m)_{n-\frac{1}{2}}$, difficulty due to the proximity to θ_n may be avoided by employing (**7.9**).

VIII. A Numerical Example

The accuracy and rate of convergence of the processes developed here have been studied empirically by applying them to problems of liquid movement in porous media with known D and K functions. In addition, a control solution has been carried out for one (necessarily simple) problem for which an analytical solution was obtained also. Details of the latter problem (Example 1) follow.

Example 1

Solve (**1.1**) subject to (**1.2**) for D constant and $\partial K/\partial\theta=\rho=$constant. It is convenient to introduce the dimensionless quantities:

$$c=(\theta-\theta_n)/(\theta_0-\theta_n)\,;\quad T=\rho^2 t/D\,;\quad \zeta=\rho x/D. \qquad \textbf{(8.1)}$$

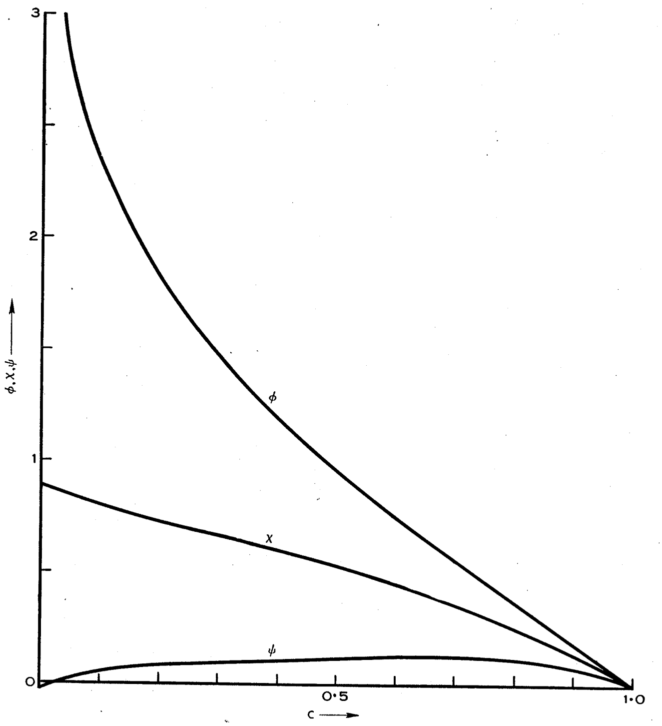

Fig. 1.—φ-, χ-, and ψ-curves for Example 1.

Then, for Example 1, (**1.1**) becomes

$$\partial c/\partial T=\partial^2 c/\partial\zeta^2-\partial c/\partial\zeta, \qquad \textbf{(8.2)}$$

and the new conditions are

$$\left.\begin{array}{lll} c=0, & T=0, & \zeta>0\,; \\ c=1, & \zeta=0, & T\geqslant 0. \end{array}\right\}. \qquad \textbf{(8.3)}$$

It will be of advantage to discuss the problem and its solution in this dimensionless form.

(i) *Analytical Solution.*—The transformation (**8.4**)

$$u=ce^{-(\zeta/2-T/4)} \qquad \textbf{(8.4)}$$

reduces (**8.2**) to

$$\partial u/\partial T = \partial^2 u/\partial \zeta^2, \qquad \text{(8.5)}$$

subject to the conditions

$$\left.\begin{array}{lll} u=0, & T=0, & \zeta>0\,; \\ u=e^{T/4}, & \zeta=0, & T\geqslant 0. \end{array}\right\} \qquad \text{(8.6)}$$

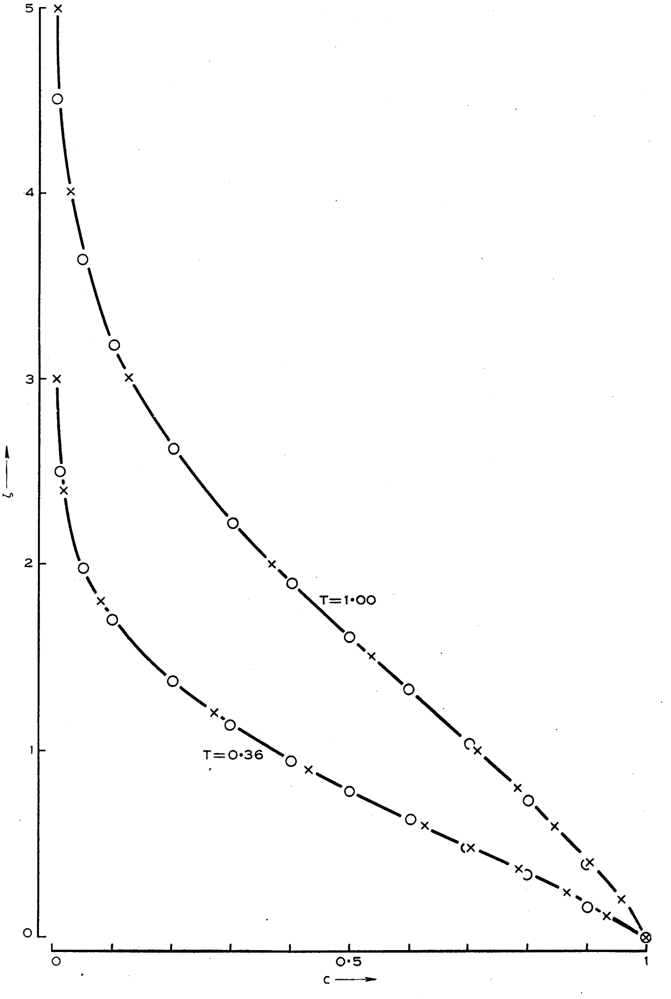

Fig. 2.—Comparison of analytically and numerically computed concentration-distance curves for $T=0\cdot36$, $T=1\cdot00$. Numerical computations based on first three terms only of (**5.7**). Analytical points $\times$, numerical points $\bigcirc$.

The solution of (**8.5**) subject to (**8.6**) is (Carslaw and Jaeger 1947)

$$u=\tfrac{1}{2}e^{T/4}[e^{-\zeta/2}\operatorname{erfc}\{(\zeta-T)/2T^{\frac{1}{2}}\}+e^{\zeta/2}\operatorname{erfc}\{(\zeta+T)/2T^{\frac{1}{2}}\}], \qquad \text{(8.7)}$$

that is

$$c=\tfrac{1}{2}[\operatorname{erfc}\{(\zeta-T)/2T^{\frac{1}{2}}\}+e^{\zeta}\operatorname{erfc}\{(\zeta+T)/2T^{\frac{1}{2}}\}]. \qquad \text{(8.8)}$$

(ii) *Numerical Solution.*—For this example

$$\varphi=2 \text{ inverfc } c. \qquad \ldots\ldots\ldots\ldots\ldots\ldots \quad (8.9)$$

This analytical value of φ was used since the present work is intended, not as a further check of the method of Part I, but as an examination of the process developed for evaluating χ, ψ, etc. and of the convergence of series (**5.7**).

Numerical solutions for χ were then carried out for $\delta c=0\cdot05$ and $\delta c=0\cdot1$, the h^2-extrapolation of Richardson (1927) being used to estimate truncation errors and obtain a final best numerical solution. The computations are simply organized in tabular form similar to Table 2 of Part I.

The solution for χ was then used in evaluating ψ, also for $\delta c=0\cdot05$ and $\delta c=0\cdot1$. The h^2-extrapolation was again used. The final solutions for χ and ψ, together with the analytical solution for φ, are shown in Figure 1.

Figure 2 compares the analytical solution and the numerical solution using the first three terms of (**5.7**) only, for times $T=0\cdot36$ and $T=1\cdot00$. In soil water problems D and $\partial K/\partial\theta$ are of such order of magnitude that (were they constant, which they are not) t would be of order 10^6 sec for $T=1$. Most problems of interest in this connexion deal with phenomena lasting a few hours or at most a few days, so that the errors resulting from using only the first three terms of (**5.7**) might be expected to be very much less than the small errors revealed in Figure 2.

IX. Accuracy of the Method

The present discussion of errors excludes those arising in the computation of φ, which have been treated in Part I. It suffices to remark that the employment of two or three iterations combined with the h^2-extrapolation provides φ to an accuracy adequate for most purposes, and that the order of accuracy increases very rapidly with n and the number of iterations.

The errors which concern us here are of two types:

(i) truncation errors of the numerical process used to evaluate χ, ψ, ω, etc.;

(ii) errors due to incomplete convergence (or even divergence) of series (**5.7**).

The truncation errors determined for Example 1 are given in (**9.1**). In each case $\lambda(I_{\frac{1}{2}})_{\text{trunc.}}$ is written for the fractional truncation error in $I_{\frac{1}{2}}$.

$$\left.\begin{aligned}&\text{In evaluating } \chi: \ \lambda(I_{\frac{1}{2}})_{\text{trunc.}}=0\cdot13n^{-2},\\&\text{In evaluating } \psi: \ \lambda(I_{\frac{1}{2}})_{\text{trunc.}}=0\cdot08n^{-2}.\end{aligned}\right\} \quad \ldots\ldots \quad (9.1)$$

These values are smaller than those found in Part I for the evaluation of φ. As before, these estimates take no account of additional truncation errors produced in more general problems by the replacement of continuous D- and K-functions by n-step functions. In any case, use of the h^2-extrapolation will enable truncation errors to be virtually eliminated.

In discussing the convergence of series (**5.7**) it is convenient to introduce the integral form

$$\int_x = t^{\frac{1}{2}}\int_\varphi + t\int_\chi + t^{3/2}\int_\psi + t^2\int_\omega + \ldots + \ldots + t^{m/2}\int_{f_m} \ldots, \quad \ldots (\mathbf{9.2})$$

where the notation $\int_f$ denotes $\int_{\theta_n}^{\theta_0} f \mathrm{d}\theta$.

In numerical examples computed to date (in all of which $\partial K/\partial\theta$ has been positive) it has been found that

$$\int_{f_m} \Big/ \int_\varphi < \left[\int_\chi \Big/ \int_\varphi\right]^{m-1}. \quad \ldots\ldots\ldots\ldots (\mathbf{9.3})$$

If (**9.3**) is valid, (**9.2**) may be shown by comparison with the geometric series to converge for

$$t < \left[\int_\chi \Big/ \int_\varphi\right]^2. \quad \ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{9.4})$$

On the (dubious) basis of (**9.3**) the fractional error in $\int_x$ produced by using only the first m terms of (**9.2**) is given by

$$\left|\lambda\left(\int_x\right)\right| \leqslant \left|\frac{\int_\chi}{\int_\varphi} t^{\frac{1}{2}}\right|^m. \quad \ldots\ldots\ldots\ldots (\mathbf{9.5})$$

The case of $\partial K/\partial\theta$ negative has not been studied in any detail. In this case the solution of (**1.1**) subject to (**1.2**) approaches (**9.6**) in the limit as $t \to \infty$.

$$x = -\int_\theta^{\theta_0} \frac{D}{K+a} \mathrm{d}\theta, \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{9.6})$$

where a is a constant of integration. When the denominator of the integrand of (**9.6**) is non-zero throughout some range of θ, θ_0 to θ_r (as it is in the immediate extension of the present work to the problem of " capillary rise "), $\lim_{t\to\infty} x$ is finite for this range of θ. This result suggests the failure of convergence of (**5.7**) at rather smaller values of t than in the case of $\partial K/\partial\theta$ positive.

Supplementary to the present approach, a study has been made of the solution in the limit as $t \to \infty$ (Philip 1957). It has been found possible to use this limit to give good approximate solutions for large t. In consequence, failures of series solution (**5.7**) at large t are unimportant. Comparison of solutions by the two methods suggests that errors in the series solution due to incomplete convergence are rather less than (**9.5**) would indicate.

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XI. References

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Philip, J. R. (1955*a*).—*Trans. Faraday Soc.* **51**: 885. Two misprints in this paper may be misleading. The corrigenda are:

p. 888. Fifth line from bottom of page, read: " (iii) Use $I_{\frac{1}{2}}$ and φ_1 in (**3.9**) . . . ".

p. 889. Equation (**6.1**), read for denominator of right-hand side: " $(\theta_0—\theta_n)^2$ ".

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