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Quasilinearization Technique for Solution of Unsteady State Diffusion Problems

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A new iterative method is given for the numerical solution of the diffusion equation

$$\partial C/\partial t = \partial/\partial x(D\partial C/\partial x)$$

in a semi-infinite medium.

The nonlinear partial differential equations for unsteady state diffusion problems with variable diffusion coefficients are transformed into nonlinear ordinary differential boundary value problems. It is shown that the quasilinearization technique (also known as the generalized Newton–Raphson method) is an effective tool for solving these nonlinear ordinary differential boundary value problems. The versatility and convergence properties of this method are demonstrated by the solution of several representative cases. The following cases discussed herein for which the diffusion coefficients are functions of concentration possess solutions with differing stabilities and rates of convergence:

$$D = D_0(1 + \alpha C/C_0),\ D_0(1 + \alpha C/C_0 + \beta C^2/C_0^2),\ D_0/(1 + \alpha C/C_0 + \beta C^2/C_0^2),$$

$$D_0/(1 - \alpha C/C_0),\ D_0/(1 - \alpha C/C_0)^2,\ D_0 e^{\alpha C/C_0} \text{ and } D_0(\alpha + \beta \log(\gamma + \delta C/C_0)).$$

I. INTRODUCTION

One-dimensional unsteady-state diffusion problems in a semi-infinite medium for which the diffusion coefficient is a function of concentration may be solved by a variety of methods [1]. Generally, the methods reduce the nonlinear partial

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differential equations to ordinary differential equations by means of Boltzmann's transformation followed by a numerical solution of the resulting nonlinear equations. For example, Heaslet and Alksne [2] have solved the case of diffusion from a fixed surface with $D = D(C^n)$ by means of an elegant series expansion of the so transformed nonlinear ordinary differential equation. However, the use of alternative similarity variables based on transformation group concepts and depending on the form of the diffusion coefficient and on the boundary conditions has been suggested by Ames [3].

In this paper we present the results of a new iterative method for numerically solving the one-dimensional unsteady-state diffusion equation with concentration-dependent diffusion coefficient. Our work also employs Boltzmann's transformation to obtain the nonlinear ordinary differential boundary value form of the one-dimensional diffusion equation. We also introduce an additional transformation, an error function transformation, which is able to reduce the computation time and overcome the difficulty of determining the finite value of distance at which the concentration vanishes. The resulting boundary value problems are then solved by a finite difference method or superposition method combined with a quasilinearization technique developed by Bellman and Kalaba [4] for obtaining numerical solutions of certain classes of nonlinear differential equations.

The nonlinear ordinary differential equation for diffusion is a two-point boundary-value problem. Such equations have been solved by others, barring analytical solution, by shooting methods (trial and error) or by the finite-difference method. Each method has its advantages and disadvantages and there is still no established numerical technique for this problem in general [5, 6]. Essentially, the quasilinearization algorithm is a generalization of the Newton–Raphson scheme applicable to functional equations [7, 8]. By quasilinearization we imply that through a functional Taylor's series expansion a nonlinear ordinary differential equation may be converted to a linear differential equation with variable coefficients for which a recursion relation may be constructed which is able to be solved numerically as a linear boundary-value problem by the finite-difference or superposition method. By quasilinearizing the nonlinearity difficulties associated with the finite-difference or superposition methods are circumvented. The advantage of this technique is that a recursive solution of the linearized equations has the property of quadratic convergence. Using this technique we can solve cases with a variety of diffusion coefficients. With an approximate initial guess of the concentration distribution and by a rough estimation of the finite distance at which the concentration vanishes, only four to nine iterations are needed to obtain a five digit accuracy.

II. Mathematical Development

The equation for one-dimensional diffusion when the diffusion coefficient D is a function of concentration C is

$$\partial C/\partial t = \partial/\partial x[D(\partial C/\partial x)], \tag{1}$$

where t is time, and x is distance. We select the boundary conditions (semi-infinite medium)

$$\begin{aligned} C &= C_0, \quad & x &= 0, \quad & t &> 0 \\ C &= 0, \quad & t &= 0, \quad & &\text{all } x. \end{aligned} \tag{2}$$

By Boltzmann's transformation, C may be expressed in terms of a single variable and Eq. (1) may be reduced to an ordinary differential equation. Define

$$c = C/C_0 \quad \text{and} \quad \bar{y} = x/(4D_0t)^{1/2},$$

then Eq. (1) becomes

$$d/d\bar{y}(D\, dc/d\bar{y}) + 2\bar{y}(dc/d\bar{y}) = 0 \tag{3}$$

with boundary conditions

$$\begin{aligned} c &= 1, \quad & \bar{y} &= 0, \\ c &= 0, \quad & \bar{y} &= \infty. \end{aligned} \tag{4}$$

Equation (3) may be expressed as

$$d^2c/d\bar{y}^2 + f(c)(dc/d\bar{y})^2 + 2\bar{y}g(c)\, dc/d\bar{y} = 0, \tag{5}$$

where

$$\begin{aligned} f(c) &= 1/D(c)(dD(c)/dc) = g(c)(dD(c)/dc), \\ g(c) &= 1/D(c). \end{aligned}$$

An additional transformation, an error function transformation, arises from the solution of the unsteady state diffusion problem in a semi-infinite medium with constant diffusion coefficient.

Define

$$z = \operatorname{erf} k\bar{y} = \operatorname{erf} y, \tag{6}$$

where k is an arbitrary constant and erf is the error function. If we substitute Eq. (6) into Eq. (5), we obtain

$$d^2c/dz^2 + f(c)(dc/dz)^2 + \sqrt{\pi}\, ye^{y^2}[g(c)/k^2 - 1]\, dc/dz = 0, \tag{7}$$

i.e.,

$$d^2c/dz^2 = F(dc/dz, c, y) \tag{7'}$$

with boundary conditions

$$c = 1, \qquad z = 0,$$
$$c = 0, \qquad z = 1.$$

1. *Quasilinearization Combined With Finite Difference Method* [7]

Now let us consider the functional equation given by Eq. (7)′ with accompanying boundary conditions, Eq. (4). By applying the quasilinearization technique we may linearize Eq. (7)′ to the form

$$d^2c_{n+1}/dz^2 = F(dc_n/dz, c_n, y) + F_{c'}(dc_n/dz, c_n, y)(dc_{n+1}/dz - dc_n/dz) + F_c(dc_n/dz, c_n, y)(c_{n+1} - c_n). \tag{8}$$

$F_{c'}$ and F_c represent differentiation of F with respect to dc/dy and c, respectively. The subscript n denotes the n-th iteration. Upon substituting Eq. (8) into Eq. (7) we obtain

$$d^2c_{n+1}/dz^2 + P_n(dc_{n+1}/dz) + Q_n c_{n+1} = R_n, \tag{9}$$

where

$$P_n = 2f(c_n)\, dc_n/dz + \sqrt{\pi}\, ye^{y^2}\, [g(c_n)/k^2 - 1],$$
$$Q_n = df(c_n)/dc_n\, (dc_n/dz)^2 + \sqrt{\pi}\, ye^{y^2}/k^2(dg(c_n)/dc_n)(dc_n/dz),$$
$$R_n = f(c_n)(dc_n/dz)^2 + c_n(df(c_n)/dc_n)(dc_n/dz)^2 + \sqrt{\pi}\, ye^{y^2}/k^2\, (dg(c_n)/dc_n)(dc_n/dz)\, c_n .$$

In order to solve the system of equations given by Eq. (9) the finite-difference method is utilized to avoid stability difficulties. Let $c_n(m)$ denote the value of c at position $m\Delta y$ in the n-th iteration; then, the first- and second-order derivatives, dc_{n+1}/dz and d^2c_{n+1}/dz^2, can be replaced by the following difference equations:

$$dc_{n+1}/dz = 1/2(\Delta z)[c_{n+1}(m+1) - c_{n+1}(m-1)], \tag{10}$$
$$d^2c_{n+1}/dz^2 = 1/(\Delta z)^2[c_{n+1}(m+1) - 2c_{n+1}(m) + c_{n+1}(m-1)]. \tag{11}$$

z is divided into N equal intervals. Upon substituting Eqs. (10) and (11) into Eq. (9) the following $N - 1$ simultaneous algebraic equations are obtained:

$$(1 + P_n(m)\, \Delta z/2)\, c_{n+1}(m+1) + (-2 + Q_n(m)(\Delta z)^2)\, c_{n+1}(m) + (1 - P_n(m)\, \Delta z/2)\, c_{n+1}(m-1) = (\Delta z)^2\, R_n(m). \tag{12}$$

Defining

$$E_m = 1 + P_n(m)\,\Delta z/2,$$
$$B_m = -2 + Q_n(m)(\Delta z)^2,$$
$$A_m = 1 - P_n(m)\,\Delta z/2,$$

the $N - 1$ simultaneous algebraic equations can be represented by

$$\mathbf{AC} = \mathbf{B}, \tag{13}$$

where matrix **A** is tridiagonal. The matrices **A**, **C** and **B** can be represented as

$$\mathbf{A} = \begin{pmatrix} B_1 & E_1 & & & & \\ A_2 & B_2 & E_2 & & & \\ & \cdot & \cdot & \cdot & & \\ & & \cdot & \cdot & \cdot & \\ & & & & A_{N-1} & B_{N-1} \end{pmatrix}$$

$$\mathbf{C} = \begin{pmatrix} c_{n+1}(1) \\ c_{n+1}(2) \\ \vdots \\ c_{n+1}(N-1) \end{pmatrix},$$

$$\mathbf{B} = \begin{pmatrix} -A_1 c_{n+1}(0) + (\Delta z)^2 R_n(1) \\ (\Delta z)^2 R_n(2) \\ \cdot\ \cdot\ \cdot \\ \cdot\ \cdot\ \cdot \\ (\Delta z)^2 R_n(N-1) - E_{N-1} c_{n+1}(N) \end{pmatrix}.$$

From the boundary conditions, Eq. (4), matrix **B** is reduced to

$$\mathbf{B} = \begin{pmatrix} -A_1 + (\Delta y)^2 R_n(1) \\ (\Delta y)^2 R_n(2) \\ \cdot\ \cdot\ \cdot \\ \cdot\ \cdot\ \cdot \\ (\Delta y)^2 R_n(N-1) \end{pmatrix}.$$

In Eq. (12), c_{n+1} is the unknown variable. The value of c_n is considered known and is obtained from the previous iteration. Since c_n is known, c_{n+1} can be obtained by solving Eq. (13). With c_{n+1} known, the results of the next iteration c_{n+2} can be obtained by the same prodecure. Iteration is continued until satisfactory convergence is obtained.

2. *Quasilinearization Technique Combined With The Superposition Method*

It is difficult to obtain a convergent solution for some cases when we employ the above technique. For such cases in order to solve the system of equations given by Eq. (7) the superposition method is utilized. We employ a further transformation, the s-transformation [1]. The new variable s, defined by the relation

$$s = \int_0^c D dc' \Big/ \int_0^1 D dc',$$

enables some improvement in the rate of convergence. On using the s-transformation, Eq. (7) becomes

$$(d^2s/dz^2) + \sqrt{\pi}\, y e^{y^2}/k^2\, g(s)(ds/dz) = 0 \tag{14}$$

with boundary condition

$$\begin{aligned} s &= 1, \qquad z = 0, \\ s &= 0, \qquad z = 1. \end{aligned} \tag{15}$$

Equation (14) can be reduced to a system of first-order differential equations by the substitutions

$$\begin{aligned} ds/dz &= w, \\ d^2s/dz^2 &= dw/dz. \end{aligned} \tag{16}$$

Equation (14) is now reduced to the following equivalent system of two first-order equations:

$$\begin{aligned} ds/dz &= w, \\ dw/dz &= -\sqrt{\pi}\, y e^{y^2} [g(s)/k^2 - 1]\, w. \end{aligned} \tag{17}$$

By using the quasilinearization technique, Eq. (17) can be linearized to

$$\begin{aligned} ds_{n+1}/dz &= w_{n+1}, \\ dw_{n+1}/dz &= -\bar{P} w_{n+1} - \bar{Q} s_{n+1} + \bar{R}, \end{aligned} \tag{18}$$

where

$$\begin{aligned} \bar{P} &= \sqrt{\pi}\, y e^{y^2} [g(s_n)/k^2 - 1], \\ \bar{Q} &= \sqrt{\pi}\, y e^{y^2}/k^2\, (dg(s_n)/ds_n)\, w_n, \\ \bar{R} &= \sqrt{\pi}\, y e^{y^2}/k^2\, (dg(s_n)/ds_n)\, w_n s_n \end{aligned}$$

with boundary conditions

$$\begin{aligned} s_{n+1} &= 1, \qquad z = 0, \\ s_{n+1} &= 0, \qquad z = 1. \end{aligned} \tag{19}$$

The system represented by Eqs. (18) and (19) constitutes a linear boundary value problem which can be solved by the superposition method. Let $s_{p,n+1}$ and $w_{p,n+1}$ be any set of particular solutions of Eq. (18). Let $s_{hj,n+1}$ and $w_{hj,n+1}$, $j = 1, 2$ be any two sets of nontrivial and distinct homogeneous solutions of the homogeneous equations

$$\begin{aligned} ds_{n+1}/dz &= w_{n+1}, \\ dw_{n+1}/dz &= -\bar{P}w_{n+1} - \bar{Q}s_{n+1}. \end{aligned} \tag{20}$$

Then the solution of Eq. (18) can be represented by

$$\begin{aligned} s_{n+1} &= s_{p,n+1} + a_1 s_{h1,n+1} + a_2 w_{h1,n+1}, \\ w_{n+1} &= w_{p,n+1} + a_1 w_{h1,n+1} + a_2 w_{h2,n+1}, \end{aligned} \tag{21}$$

where the unknown constants, a_1 and a_2 will be determined by using boundary condition, Eq. (19). The set of particular solutions and the two sets of homogeneous solutions can be obtained by numerically integrating Eqs. (18) and (20), respectively.

If the initial conditions used in obtaining the particular and homogeneous solutions satisfy the given initial condition of Eq. (19), the number of homogeneous solutions is reduced to one only. Hence Eq. (21) can be reduced to

$$\begin{aligned} s_{n+1} &= s_{p,n+1} + a s_{h,n+1}, \\ w_{n+1} &= w_{p,n+1} + a w_{h,n+1}, \end{aligned} \tag{22}$$

where the unknown constants a can be determined by $-s_{p,n+1}/s_{h,n+1}$. Once a is obtained, the general solution of Eq. (18) can be obtained by using Eq. (22) and the newly obtained particular and homogeneous solutions. With s_{n+1} and w_{n+1} known, the results of next iteration s_{n+2} and w_{n+2} can be obtained by the same procedure. The initial conditions used are

$$\begin{pmatrix} s_{p,n+1} \\ w_{p,n+1} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \tag{23}$$

and

$$\begin{pmatrix} s_{h,n+1} \\ w_{h,n+1} \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{24}$$

III. Numerical Results and Discussion

The verification of the validity of the method developed above was obtained by solving the diffusion equation for constant diffusivity.

If the diffusion coefficient is constant, Eq. (1) reduces to

$$\partial C/\partial t = D(\partial^2 C/\partial x^2), \tag{25}$$

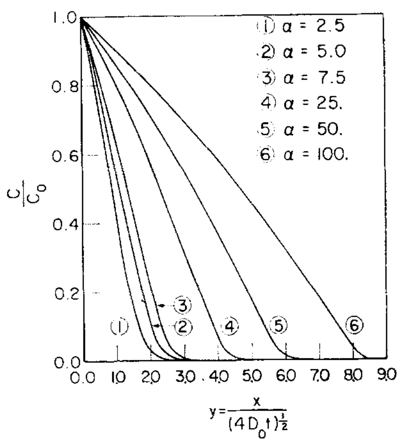

Fig. 1. Concentration-distance curve for $D = D_0(1 + \alpha C/C_0)$.

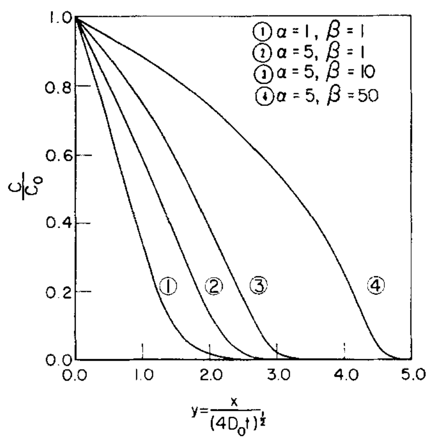

Fig. 2. Concentration-distance curve for $D = D_0(1 + \alpha C/C_0 + \beta C^2/C_0^2)$.

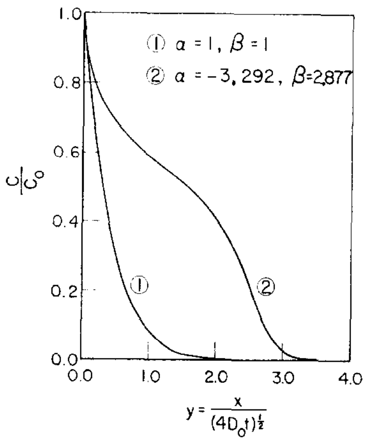

FIG. 3. Concentration-distance curve for $D = D_0/(1 + \alpha C/C_0 + \beta C^2/C_0^2)$.

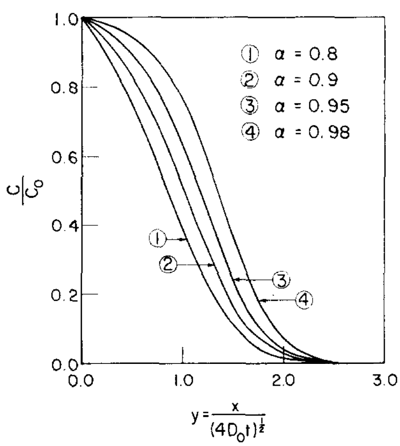

FIG. 4. Concentration-distance curve for $D = D_0/(1 - \alpha C/C_0)$.

with, for example, boundary conditions given by Eq. (2). The exact solution of Eq. (25) with these boundary conditions is

$$C/C_0 = \operatorname{erfc} x/(4D_0t)^{1/2}, \tag{26}$$

i.e.,

$$C = \operatorname{erfc} \bar{y},$$

where erfc is the complementary error function. We may compare, in this case, the quasilinearization solution of Eq. (25) with the exact solution. The difference between the numerical and exact solutions was found to be less than 4×10^{-5} over the entire range of reduced concentration variable.

To illustrate the use of the quasilinearization scheme as applied to the general nonlinear diffusion equation with variable (concentration dependent) diffusion coefficients we consider the following representative cases: $D = D_0(1 + \alpha C/C_0)$, $D_0(1 + \alpha C/C_0 + \beta C^2/C_0^2)$, $D_0/(1 - \alpha C/C_0)$, $D_0/(1 - \alpha C/C_0)^2$, $D_0 e^{\alpha C/C_0}$, and $D_0(\alpha + \beta \log(\gamma + \delta C/C_0))$, where α, β, γ, and δ are constants. In this notation D_0 is the diffusion coefficient for the concentration $C = C_0$ at $x = 0$.

The numerical results for these cases are shown in Figs. 1–7. The data are

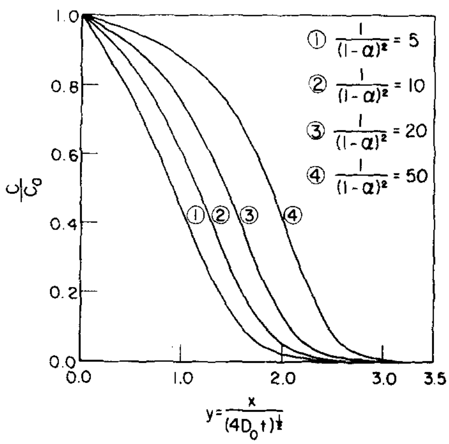

FIG. 5. Concentration-distance curve for $D = D_0/(1 - \alpha C/C_0)^2$.

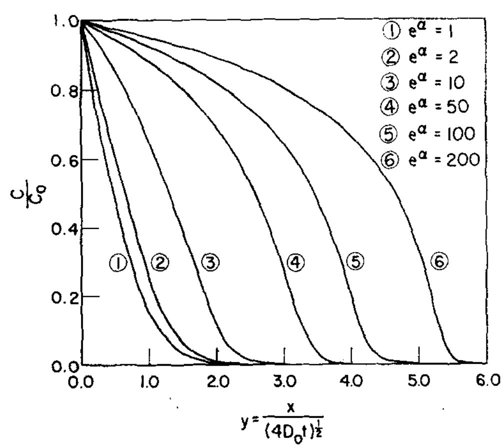

FIG. 6. Concentration-distance curve for $D = D_0 e^{\alpha C/C_0}$.

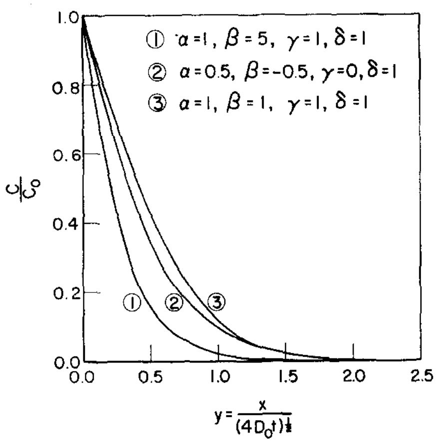

FIG. 7. Concentration-distance curve for $D = D_0[\alpha + \beta \log(\gamma + \delta C/C_0)]$.

presented in a form similar to that used by Crank to which we refer the reader for comparison [1, Chap. 12]. The results are plotted as c versus $\bar{y}$. The method of quasilinearization combined with the finite difference method can be applied to solve all cases shown in Figs. 1–7 except $D = D_0 e^{\alpha C/C_0}$ if $e^\alpha = 200$ and $D = D_0(1 + \alpha C/C_0)$ if $\alpha = 50$ and 100. It is difficult to get convergent solutions for these three cases when the quasilinearization technique is combined with the finite difference method. The quasilinearization technique combined with the superposition method is used to solve the above three cases.

The initial guess of the concentration profile is $1 - z$; i.e., erfc $k\bar{y}$. This is based on the analytic solution of the diffusion equation with constant diffusivity, Eq. (26). The transformation from $\bar{y}$ to z is given by $z = \operatorname{erf} k\bar{y}$, where k is a constant. By this error function transformation the semi-infinite range is transformed into the range between 0 and 1. Hence the size of the mesh is reduced and the required computer storage space and computation time are considerably reduced. The choice of k depends upon $\bar{y}_0$, the finite value of $\bar{y}$ at which the concentration vanishes. However, as we need not know the exact value of $\bar{y}$ it is estimated; the value of k is chosen to make $\operatorname{erf} k\bar{y}_0 \approx 1$. For example, for the $e^\alpha = 10$ case the range of k is from 0.4 to 1; i.e., the rough value of $\bar{y}_0$ is from 2.8 to 7.0. The results for this case are independent of the value of k in this range.

When the quasilinearization technique combined with the finite difference method is employed, the size of Δz is 0.005. With $1 - z$ as initial guess the correct solutions are obtained in four to nine iterations, with accuracy to the fifth decimal place. The rate of convergence of the concentration distribution function for

$D = D_0 e^{\alpha C/C_0}$ and $D = D_0/(1 + C/C_0 + C^2/C_0^2)$ is shown in Figs. 8 and 9, respectively.

When the employ the quasilinearization technique combined with the superposition method, the Runge–Kutta fourth-order integration method is used to obtain the particular and homogeneous solutions with the initial conditions given by Eqs. (23) and (24). The integration interval is taken to be 0.0001. Only four to nine iterations are needed to obtain a five-digit accuracy.

The method of quasilinearization combined with the superposition method is unstable under certain conditions [8]. For example, during the process of iteration

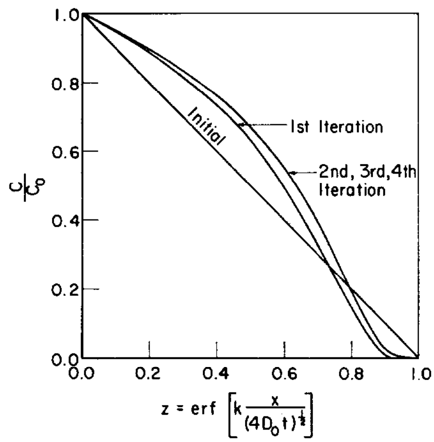

FIG. 8. Convergence rate of C/C_0 for $D = D_0 e^{\alpha C/C_0}$ with $e^\alpha = 10$ and $k = 0.5$.

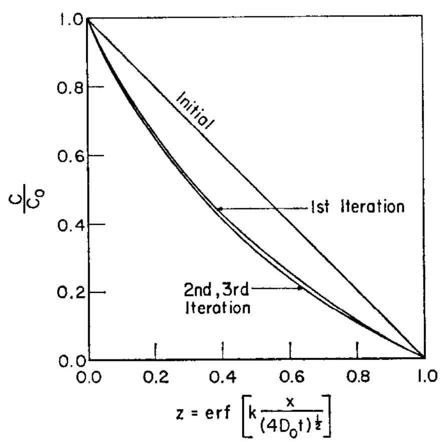

FIG. 9. Convergence rate of C/C_0 for $D = D_0/(1 + C/C_0 + C^2/C_0^2)$ with $k = 1.0$.

one or more values of the particular and homogeneous solution can become unreasonable. Extremely large or small values at the end point of the problem are encountered so that the final boundary condition cannot be fulfilled. Since the linear differential equation is obtained by approximation from complex nonlinear differential equations, these unreasonable values should be expected under certain conditions. These difficulties can be overcome by the use of the finite difference scheme.

In general, the quasilinearization technique combined with the finite difference method is an effective tool for solving unsteady state diffusion problems with variable diffusion coefficients. However, in the finite difference scheme we must calculate first-order derivatives [cf. Eq. (9)]. The numerical evaluation of derivatives by a digital computer is inaccurate. When a function has an abrupt discontinuity in its derivative as in Fig. 10, the finite difference method is not suitable. If quasi-

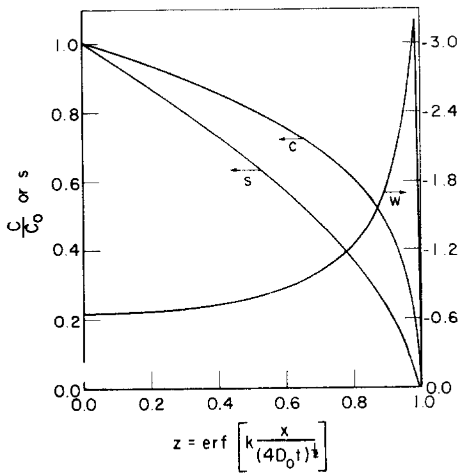

FIG. 10. Concentration and its slope distribution for $D = D_0(1 + \alpha C/C_0)$ with $\alpha = 100$ and $k = 0.238$.

linearization is combined with the superposition method, it is necessary to solve simultaneous first-order differential equations. The calculation of first-order derivatives is then obviated. Although an s-variable transformation can improve the rate of convergence, the relationship between s and c is nonlinear in some cases. The solution of nonlinear algebraic equations influences the accuracy of c and requires additional computation time. Figure 10 also shows the relationship between c, s, w and z for $D = D_0(1 + \alpha C/C_0)$ with $\alpha = 100$ and $k = 0.238$.

Even if the boundary conditions are nonlinear we can apply the quasilinearization technique to linearize the boundary conditions. We may thus avoid the cumbersome traditional analyses [1] for solving concentration-dependent unsteady-state diffusion problems. The method used here is also applicable to heat conduction when thermal conductivity is a function of temperature. More detailed discussion of the advantage and disadvantages of the quasilinearization technique can be found in the literature [4, 6–9].

Acknowledgments

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