JOURNAL OF MATHEMATICAL ANALYSIS AND APPLICATIONS 93, 206–221 (1983)

Application of Differential Quadrature to Transport Processes

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Submitted by W. Welsh

The methodology and numerical solution of problems concerning transport processes via the method of differential quadrature are presented. Application of the method is demonstrated by solving a simple one-dimensional, time-dependent (transient) diffusion process involving an irreversible reaction without any flux across the end boundary. In addition, the same technique is used (for the first time to the authors' knowledge) to solve a steady-state problem. For this purpose, a convection–diffusion problem involving an irreversible reaction is considered. The demonstration is carried out in two ways, (1) using the Bellman *et al.* technique which employs approximation formulas for higher order partial derivatives derived by iterating the linear quadrature approximation for the first order partial derivative, and (2) using individual quadratures to approximate the partial derivatives of first, as well as higher orders, as suggested by Mingle. Both approaches give the same results; however, the latter saves an appreciable amount of iterative computing effort despite the fact that it requires separate weighting coefficients for each individual quadrature. Since the technique of differential quadrature can produce solutions with sufficient accuracy even when using as few as three discrete points, both the programming task and computational effort are alleviated considerably. For these reasons the differential quadrature approach appears to be very practical in solving a variety of problems related to transport phenomena.

INTRODUCTION

Transport phenomena equations are the foundation for continuum mechanics. They have their origin in the partial differential equations expressing the conservation of mass, momentum and energy subject to specified initial and/or boundary conditions. To complete the mathematical model the thermal and the caloric equations of state and the constitutive relationships which define the physical properties of the system (such as viscosity and elasticity modulus) are required. In many cases the resulting mathematical models involve nonlinear partial differential equations for which exact solutions are frequently not available. Even when available it is often more expeditious to obtain solutions via numerical methods.

0022-247X/83 $3.00

Rapid advances in high speed computer hardware over the past three decades have stimulated the development of numerical methods for solving a complex set of partial differential equations. Much of this effort has focused on variants of the finite element and the finite difference techniques. More recently, Bellman *et al.* [1–6] have introduced the method of differential quadrature for the rapid solution of nonlinear partial differential equations, specifically for one- and two-dimensional, time-dependent (inital value) problems. Mingle [12, 13] applied differential quadrature to the solutions of the one-dimensional, time-dependent, (initial and boundary value) problem of nonlinear diffusion. Civan [8] extended and generalized the method of differential quadrature to one-, two-, and three-dimensional models for both time-dependent (initial or initial and boundary value) and for time-independent (boundary value) problems.

The objective of this paper is twofold: (1) To demonstrate the methodology for solving transport phenomenological models by the technique of differential quadrature; and (2) to demonstrate the computational effort and the accuracy of the solution for a time-independent (steady-state) and a time-dependent (transient-state) transport system.

Briefly the method of differential quadrature entails replacing each partial (space) derivative with a weighted linear sum of the values of the function at discrete points. The result is a set of algebraic equations for time-independent systems and a set of ordinary differential equations for time-dependent systems. In both instances numerical methods are available for solving the resulting set of equations.

Regardless of which method—differential quadrature or otherwise—is used to solve the transport model equations, it is recommended that they be normalized before initiating the solution for the following reasons:

(1) The final results will be applicable to all transport processes which reduce to the same normalized form.

(2) The size of the computational region is scaled downward, thereby reducing roundoff errors.

(3) The effect of roundoff errors which promote instability in the solution, such as the case where convection (bulk flow) terms dominate diffusion terms, or vice versa, can be circumvented by proper definition of the dimensionless time variable.

In the following, the methodology for generating numerical solutions based on differential quadrature is described and demonstrated by two simple examples (steady-state and transient-state) for which exact solutions are available for comparisons. The general procedure is outlined in Fig. 1.

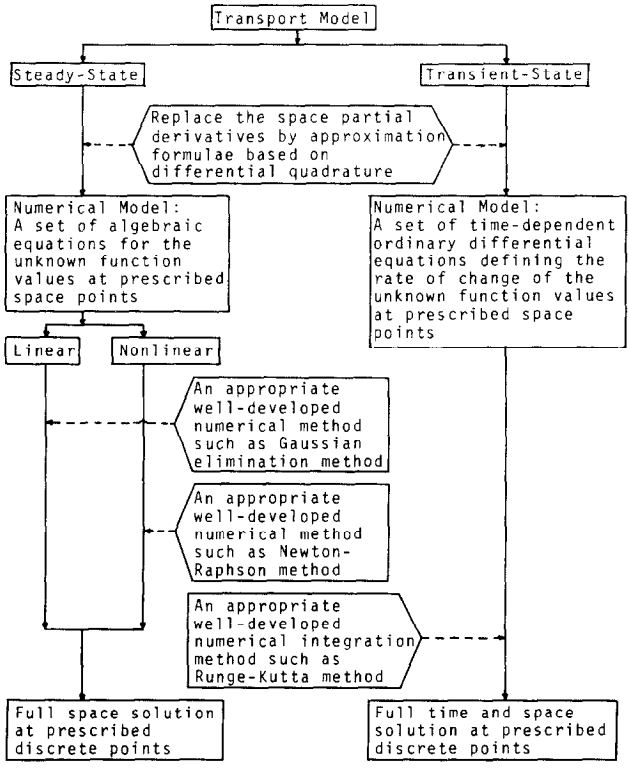

FIG. 1. A systematic approach for solving transport phenomenological models.

NUMERICAL SOLUTION OF STEADY-STATE MODELS

Although not mandatory, the recommended first step in the numerical solution is to normalize the transport model equations by converting all of the variables into appropriate dimensionless forms. Next, subdivide the computational domain into a grid by selecting discrete values for each of the space variables. Then, replace the derivatives in the differential equation and the derivative boundary conditions by approximation formulas based on differential quadrature as described by Bellman *et al.* [1–6], Mingle [12, 13], Civan [8], or Civan and Sliepcevich [9]. The weighting coefficients for the approximation formulas can be either calculated or obtained directly from the foregoing references.

The intermediate result is a set of algebraic equations. If they are linear, they can be solved by available methods, such as Gaussian elimination. If

they are nonlinear, an iterative technique, such as Newton–Raphson, will be required.

In order to demonstrate the procedure for calculation and the accuracy of the numerical results, via the technique of differential quadrature, a simplified one-dimensional model of a steady-state, convection–diffusion process involving an irreversible reaction is chosen since an exact solution giving concentration as a function of distance is available for comparison purposes. Specifically, the governing transport equations in *normalized* form is taken to be

$$\frac{dc}{dx} = \frac{d^2c}{dx^2} - \alpha c^m, \qquad 0 \leqslant x \leqslant 1 \tag{1}$$

subject to the boundary conditions

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

$$dc(1)/dx = 0, \tag{3}$$

where

c = dimensionless concentration, C/C_0,

x = dimensionless distance, $X/(D/U)$,

α = system parameter, DKC_0^{m-1}/U^2,

in which the actual variables are

C = concentration,

C_0 = inlet concentration at $X = 0$,

X = distance, $0 \leqslant X \leqslant (D/U)$,

D = diffusivity coefficient,

K = reaction rate constant,

U = uniform bulk velocity in the X direction,

m = order of the reaction involved.

Exact Solution of Steady-State Example

For a first order reaction, $m = 1$, the analytical result is given by

$$c(x) = (\beta_2 e^{\beta_2 + \beta_1 x} - \beta_1 e^{\beta_1 + \beta_2 x})/(\beta_2 e^{\beta_2} - \beta_1 e^{\beta_1}), \tag{4}$$

where

$$\beta_{1,2} = (1 \pm \sqrt{1 + 4\alpha})/2. \tag{5}$$

Numerical Solution of Steady-State Example by the Bellman et al. Technique

This solution follows the technique of differential quadrature as introduced by Bellman *et al.* [1–6]. The solution domain $0 \leqslant x \leqslant 1$ is decomposed into N assumed discrete points. Then the first and second order partial derivatives are replaced, respectively, by

$$\left.\frac{dc}{dx}\right|_{x=x_i} \cong \sum_{j=1}^{N} a_{ij} c_j \tag{6}$$

and

$$\left.\frac{d^2c}{dx^2}\right|_{x=x_i} \cong \sum_{k=1}^{N} a_{ik} \sum_{j=1}^{N} a_{kj} c_j \tag{7}$$

so that the transport equation (1) and the boundary condition involving the derivative Eq. (3) reduce to algebraic equations as follows:

$$\sum_{j=1}^{N} a_{ij} c_j = \sum_{k=1}^{N} a_{ik} \sum_{j=1}^{N} a_{kj} c_j - \alpha c_i^m, \qquad i = 2, 3, \ldots, (N-1) \tag{8}$$

$$c_1 = 1 \qquad \text{at point} \quad i = 1 \tag{9}$$

$$\sum_{j=1}^{N} a_{Nj} c_j = 0 \qquad \text{at point} \quad i = N. \tag{10}$$

Equation (8) can be expanded as

$$\sum_{j=1}^{N} a_{ij} c_j = \sum_{k=1}^{(N-1)} a_{ik} \sum_{j=1}^{N} a_{kj} c_j + a_{iN} \sum_{j=1}^{N} a_{Nj} c_j - \alpha c_i^m. \tag{11}$$

The middle term in Eq. (11) drops out by virtue of Eq. (10). Collecting the terms involving c_1 on the right of Eq. (11) and substituting $c_1 = 1$ from Eq. (9) into Eqs. (11) and (10) results in

$$\sum_{j=2}^{N} a_{ij} c_j - \sum_{k=1}^{(N-1)} a_{ik} \sum_{j=2}^{N} a_{kj} c_j + \alpha c_i^m = \sum_{k=1}^{(N-1)} a_{ik} a_{k1} - a_{i1}, \qquad i = 2, 3, \ldots, (N-1) \tag{12}$$

and

$$\sum_{j=2}^{N} a_{Nj} c_j = -a_{N1} \qquad \text{at point} \quad i = N. \tag{13}$$

Equations (12) and (13) constitute $(N-1)$ algebraic equations with $(N-1)$ unknowns c_i (since $i=2, 3,..., N$) for which the elements of the Jacobian matrix are from Eq. (12)

$$\frac{\partial g_i}{\partial c_j} = a_{ij} - \sum_{k=1}^{(N-1)} a_{ik}a_{kj} + \alpha m c_i^{m-1}\delta_{ij}, \tag{14}$$

where g_i are the left sides of Eq. (12) and $i=2, 3,...,$ $(N-1)$ and $j=2, 3,..., N$. Here δ_{ij} is the Kronecker delta whose value is 1 when $i=j$ and zero when $i \neq j$. Similarly, the elements of the Jacobian matrix corresponding to $i=N$ are, from Eq. (13),

$$\partial g_N/\partial c_j = a_{Nj}, \qquad j=2, 3,..., N, \tag{15}$$

where a_{Nj} represent numerical constants and g_N is the left side of Eq. (13).

If a first order reaction is considered $(m=1)$, since Eq. (14) gives numerical constants, Eqs. (12) and (13) form linear algebraic equations which can be expressed as

$$\sum_{j=2}^{N} c_j \frac{\partial g_i}{\partial c_j} = h_i, \qquad i=2, 3,..., N, \tag{16}$$

where h_i represent the right sides of Eqs. (12) and (13). Equation (16) can be solved simultaneously for $(N-1)$ unknown values of concentration c_i (since $i=2, 3,..., N$) by the method of Gaussian elimination [11], for example. (Had a second or higher order reaction been involved, the resulting set of nonlinear algebraic equations would have had to have been solved by an iterative method such as Newton–Raphson.)

Numerical solutions were obtained for a fixed number of equally spaced discrete points N while varying the system parameter α, and for a fixed value of the system parameter α while varying the number of discrete points N. These results were compared with the corresponding results obtained from the exact solution, represented by Eq. (4) by defining the relative error ε as the absolute value of the ratio

$$\varepsilon = \left| \frac{c_{\text{num}} - c_{\text{ex}}}{c_{\text{ex}}} \right|, \tag{17}$$

where c_{num} is the result of the numerical solution and c_{ex} is the result from the exact solution.

Some authors prefer to express the errors as the difference between the numerical and exact solutions, i.e., as a deviation rather than as a relative error. For solution values that are relatively small, the deviation will likewise be small, consequently its magnitude is not a true representation of the error.

TABLE I

Relative Errors for System Parameter, $\alpha = 1$

Number of sample points, N	Relative error: $\lvert(c_{num} - c_{ex})/c_{ex}\rvert$	
	At midpoint, ε_m	At end point, ε_e
3	8.25×10^{-3}	2.47×10^{-2}
5	2.68×10^{-4}	9.20×10^{-4}
7	3.67×10^{-6}	1.25×10^{-5}
11	1.51×10^{-8}	5.06×10^{-8}
15	7.74×10^{-6}	3.37×10^{-5}

For this reason, the relative error, which is a more severe indicator of the error, will be used in this paper.

Numerical calculations have been carried out on an IBM 370/158 computer at the University of Oklahoma using double-precision with a Gaussian elimination method as described by Forsythe [11]. (If these computations were made on a large computer, the accuracy would increase significantly.)

The relative errors at the midpoint ε_m, and at the end point ε_e, are presented in Tables I and II. As would be expected the maximum error always occurs at the end point, where the no-flux boundary condition Eq. (3) is exposed. As can be seen in Table I, for a fixed value of the system parameter α the relative error first decreases with increasing values of N, passes through a minimum and thereafter increases. This result is not unexpected. For small values of N, the quadrature approximation is weak. As N increases, the relative error becomes very small, less than 10^{-7}. At this level of relative error, the function is most closely represented by the quadrature, and at the same time, the conditioning in weighting coefficients is properly

TABLE II

Relative Errors for $N = 7$ Sample Points

System parameter, α	Relative error: $\lvert(c_{num} - c_{ex})/c_{ex}\rvert$	
	At midpoint, ε_m	At end point, ε_e
0	3.19×10^{-16}	3.33×10^{-15}
1	3.67×10^{-6}	1.25×10^{-5}
5	2.81×10^{-5}	1.81×10^{-4}
10	4.80×10^{-5}	1.52×10^{-3}

compromised. However, as N increases further, errors become larger due to the loss of significant digits in arithmetic calculations caused by ill-conditioning in the weighting coefficients, as pointed out by Bellman [3, pp. 231–232].

On the other hand, the relative error increases with increasing values of the system parameter α, for a fixed value of N (as shown in Table II) because of the increase in dominancy of the reaction term over the other terms.

Numerical Solution of Steady-State Example Using Individual Quadratures

The double summation on the right of Eq. (7) is a direct result of deriving the approximation formulas for second (and higher) order partial derivatives by iterating differential quadrature to the first order partial derivative Eq. (6) as introduced by Bellman *et al.* [1–6]. To alleviate the additional computational effort inherent in the double summation, Mingle [12] has proposed that the higher order derivatives be approximated directly by individual differential quadratures as

$$\left.\frac{dc}{dx}\right|_{x=x_i} \cong \sum_{j=1}^{N} a_{ij} c_j \tag{18}$$

and

$$\left.\frac{d^2c}{dx^2}\right|_{x=x_i} \cong \sum_{j=1}^{N} b_{ij} c_j, \tag{19}$$

where a_{ij} and b_{ij} are the weighting coefficients associated with the differential quadrature formulas for the first and second order partial derivatives, respectively. Note that in this approach two sets of weighting coefficients are required, whereas in the previously described Bellman *et al.* technique only one set is required. However, the combination of two sets of weighting coefficients with single summations usually represents an advantageous tradeoff in computational effort over the combination of one set of weighting coefficients with double summations.

Substituting Eqs. (18) and (19) into the transport model Eqs. (1) and (3) and rewriting Eq. (9) for $i = 1$ gives

$$\sum_{j=1}^{N} a_{ij} c_j = \sum_{j=1}^{N} b_{ij} c_j - \alpha c_i^m, \qquad i = 2, 3, \ldots, (N-1), \tag{20}$$

$$c_1 = 1, \tag{21}$$

$$\sum_{j=1}^{N} a_{Nj} c_j = 0 \qquad \text{at point} \quad i = N. \tag{22}$$

Collecting the terms involving c_1 on the right and substituting $c_1 = 1$ in Eqs. (20) and (22), we have

$$\sum_{j=2}^{N} a_{ij}c_j - \sum_{j=2}^{N} b_{ij}c_j + \alpha c_i^m = -a_{i1} + b_{i1} \qquad \text{for} \quad i = 2, 3,..., (N-1) \tag{23}$$

and

$$\sum_{j=2}^{N} a_{Nj}c_j = -a_{N1} \qquad \text{at point} \quad i = N. \tag{24}$$

As before, the elements of the Jacobian matrix for Eqs. (23) and (24) can be expressed as

$$\begin{aligned} \partial g_i/\partial c_j &= (a_{ij} - b_{ij} + \alpha m c_i^{m-1}\delta_{ij}), && \text{for} \quad i = 2, 3,..., (N-1), \\ &= a_{Nj}, && \text{for} \quad i = N \end{aligned} \tag{25}$$

and the right sides

$$\begin{aligned} h_i &= (-a_{i1} + b_{i1}), && \text{for} \quad i = 2, 3,..., (N-1), \\ &= -a_{N1}, && \text{for} \quad i = N. \end{aligned} \tag{26}$$

For a first order reaction, $m = 1$, Eqs. (23) and (24) can be written as

$$\sum_{j=2}^{N} c_j \frac{\partial g_i}{\partial c_j} = h_i, \qquad i = 2, 3,..., N. \tag{27}$$

It is apparent that Eq. (27) involves less computational effort than the corresponding equation (16), which was obtained by the earlier method, because of the simplicity of Eqs. (25) and (26).

Numerical solutions based on Eq. (27) were obtained for the same assigned values of the parameters α and N as before. Insofar as the numerical accuracy is concerned, the two methods agree exactly, as would be expected. However, the second method requires significantly less computing time.

Numerical Solutions of Transient-State Models

Figure 1 also applies to transient-state models. As before, the defined solution domain is discretized into N values for each space variable. Next, all of the partial derivatives with respect to the space coordinates in the

governing transport equation and the boundary conditions are replaced with the algebraic approximation formulas derived by differential quadrature. The resulting set of equations contains only the ordinary derivative with respect to time. The unknown boundary values, which are now expressed algebraically based on the differential quadrature in terms of the interior field values, can be eliminated throughout the ordinary differential equations. The resulting set of ordinary differential equations is then integrated with respect to time by an appropriate technique, such as Runge–Kutta, to obtain the solution of the interior field variables as a function of time and space from which the unknown boundary values can be calculated.

To illustrate the numerical solution of transient-state models and the accuracy obtainable by the method of differential quadrature the following simplified, one-dimensional model of time-dependent diffusion involving an irreversible reaction is chosen since an exact solution, giving concentration as a function of time and distance, is available for comparison purposes. The governing transport equation in *normalized* form is

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial x^2} - \alpha c^m, \qquad 0 \leqslant x \leqslant 1 \tag{28}$$

subject to the *normalized* initial and boundary conditions,

$$c(x, 0) = 0, \tag{29}$$

$$c(0, t) = 1, \tag{30}$$

$$\partial c(1, t)/\partial x = 0, \tag{31}$$

where

c = dimensionless concentration, C/C_0,

x = dimensionless distance, X/L,

t = dimensionless time, $T/(L^2/D)$,

α = system parameter, $KL^2C_0^{m-1}/D$,

in which the actual variables are

C = concentration,

C_0 = concentration at $X = 0$,

X = distance, $0 \leqslant X \leqslant L$,

T = time,

D = diffusivity coefficient,

K = reaction rate constant,

m = order of the reaction involved.

Exact Solution of Transient-State Example

The analytical solution adapted from Carslaw and Jaeger [7, Sect. 3.5, p. 105, Eq. (6)] for a first order reaction, $m = 1$, is

$$c(x, t) = \frac{\cosh[\alpha^{1/2}(x-1)]}{\cosh(\alpha^{1/2})} - 2\sum_{n=1}^{\infty} \frac{\lambda_n}{\alpha + \lambda_n^2} e^{-(\alpha+\lambda_n^2)t} \sin(\lambda_n x), \quad (32)$$

where

$$\lambda_n = (\tfrac{1}{2} + n)\pi. \quad (33)$$

Numerical Solution of Transient-State Example by the Bellman et al. Technique

Applying the method of differential quadrature as introduced by Bellman *et al.* [1–6] Eq. (28)–(31) become

$$\frac{dc_i}{dt} = \sum_{k=1}^{N} a_{ik} \sum_{j=1}^{N} a_{kj} c_j - \alpha c_i^m, \quad i = 2, 3, \ldots, (N-1), \quad (34)$$

$$c_i = 0 \qquad \text{at} \quad t = 0, \quad i = 1, 2, \ldots, N, \quad (35)$$

$$c_1 = 1, \quad (36)$$

$$\sum_{j=1}^{N} a_{Nj} c_j = 0. \quad (37)$$

Equation (34) can also be expressed as

$$\frac{dc_i}{dt} = \sum_{k=1}^{(N-1)} a_{ik} \sum_{j=1}^{N} a_{kj} c_j + a_{iN} \sum_{j=1}^{N} a_{Nj} c_j - \alpha c_i^m. \quad (38)$$

The middle term in Eq. (38) drops out by virtue of Eq. (37), so that

$$\frac{dc_i}{dt} = \sum_{k=1}^{(N-1)} a_{ik} \sum_{j=1}^{N} a_{kj} c_j - \alpha c_i^m, \qquad i = 2, 3, \ldots, (N-1) \quad (39)$$

in which the unknown c_N can be expressed in terms of the concentration values c_i, where $i = 1, 2, \ldots, (N-1)$, by solving Eq. (37) for c_N which gives

$$c_N = -\left(\sum_{j=1}^{(N-1)} a_{Nj} c_j\right) \Big/ a_{NN}. \quad (40)$$

TABLE III

Relative Errors for $\alpha = 1$ and Varying N Values[a]

$N = 3$			$N = 5$			$N = 11$			$N = 15$		
t	$10^3\varepsilon_m$	$10^2\varepsilon_e$	t	$10^4\varepsilon_m$	$10^4\varepsilon_e$	t	$10^7\varepsilon_m$	$10^6\varepsilon_e$	t	$10^5\varepsilon_m$	$10^5\varepsilon_e$
0.20	73.0	14.3	0.12	198.	1220.	0.11	3800.	2620.	0.11	37.9	279.
0.31	35.1	4.14	0.22	12.9	228.	0.19	2330.	1270.	0.21	22.8	117.
0.43	16.4	1.87	0.36	23.6	40.1	0.30	2050.	740.	0.31	20.3	71.2
0.56	7.82	1.22	0.60	4.82	1.29	0.55	1420.	333.	0.56	13.0	28.7
0.70	4.20	1.11	1.52	1.71	4.38	1.63	95.1	17.1	1.39	0.677	2.62
1.03	3.04	1.36	2.29	1.34	3.71	2.41	9.58	1.81	1.51	1.28	3.70
2.04	4.60	1.77	3.12	1.33	3.57	3.02	2.56	1.46	2.40	2.66	6.16
2.43	4.72	1.79	4.09	1.32	3.56	4.04	0.235	0.0453	3.00	2.76	6.23
2.94	4.76	1.80	$(\rightarrow\infty)$			$(\rightarrow\infty)$			3.38	2.77	6.30
3.66	4.77	1.80							$(\rightarrow\infty)$		
$(\rightarrow\infty)$											

[a] $|(c_{num} - c_{ex})/c_{ex}|$.

TABLE IV

Relative Errors for $N = 7$ and Varying α Values[a]

$\alpha = 0$			$\alpha = 1$			$\alpha = 5$			$\alpha = 10$		
t	$10^6\varepsilon_m$	$10^6\varepsilon_e$	t	$10^6\varepsilon_m$	$10^6\varepsilon_e$	t	$10^4\varepsilon_m$	$10^4\varepsilon_e$	t	$10^4\varepsilon_m$	$10^2\varepsilon_e$
0.11	1880.	9860.	0.11	2220.	3670.	0.12	13.6	28.4	0.12	0.965	2.71
0.20	12.5	4920.	0.19	354.	3340.	0.20	1.34	25.9	0.20	6.91	1.48
0.32	556.	1780.	0.32	226.	961.	0.34	1.65	11.5	0.35	7.83	1.14
0.54	404.	800.	0.56	164.	360.	0.58	1.48	8.78	0.59	7.74	1.09
1.68	47.2	75.2	1.65	7.75	20.	1.58	1.37	8.24	1.12	7.71	1.09
2.38	11.6	17.9	2.40	1.96	3.32	1.79	1.37	8.23	$(\rightarrow\infty)$		
3.13	2.16	3.73	3.11	0.88	2.23	$(\rightarrow\infty)$					
4.07	0.296	0.435	4.05	0.752	2.10						
4.57	0.0928	0.144	4.54	0.787	2.06						
5.08	0.0368	0.0405	5.00	0.786	2.05						
$(\rightarrow\infty)$			$(\rightarrow\infty)$								

[a] $|(c_{num} - c_{ex})/c_{ex}|$.

After eliminating c_N from Eq. (39) by means of Eq. (40) and substituting $c_1 = 1$, the resulting equation is expressed only in terms of the interior domain concentration values and represents $(N-2)$ ordinary differential equations subject to the initial conditions $c_i = 0$ at time $t = 0$ for the interior domain points $i = 2, 3, ..., (N-1)$. Therefore, these equations can be integrated simultaneously by an appropriate technique such as Runge–Kutta. Once the solution is obtained, the boundary values at the Nth point can be calculated from Eq. (40).

Integration of the resulting ordinary differential equations have been accomplished using a variable step Runge–Kutta–Fehlberg, four-five method [10]. In all of the calculations double-precision and an initial step size of 0.001 for dimensionless time have been used. A tolerance limit of 10^{-5} was assumed for the relative error as the criterion of convergence of solutions and for the stepsize adjustment.

As before, numerical calculations were performed for equally spaced grid points for various values of N at a fixed $\alpha = 1$ value and for different values of α at a fixed $N = 7$ value. For each calculation, relative errors, as defined before, were calculated as a measure of the accuracy of the numerical results compared to the exact solution given by Eq. (32). The values of relative errors at the midpoint ε_m and at the end point ε_e are shown in Tables III and IV as a function of dimensionless time. As can be seen the agreement among the results is very good; in fact the results using only three discrete points are more than adequate for most practical applications.

Table III shows that, for the same α value, the accuracy of the numerical solution first increases with increasing N, passes through a maximum, but then decreases if N is increased further. For a fixed N value, however, the accuracy decreases by increasing the value of the system parameter α. Both of these observations are similar to those obtained in the steady-state model solution and can therefore be explained as before.

Numerical Solution of the Transient-State Model Using Individual Quadratures

This calculation is analogous to the steady-state example described previously. Substituting Eq. (19), which approximates the second order partial derivative $\partial^2 c/\partial x^2$ into Eq. (28) permits writing

$$\frac{dc_i}{dt} \cong \sum_{j=1}^{N} b_{ij} c_j - \alpha c_i^m, \qquad i = 2, 3, ..., (N-1). \tag{41}$$

As in the first example b_{ij} represent the weighting coefficients. Note that the first order partial derivative with respect to space $\partial c/\partial x$ would still be given by Eq. (18) in terms of a_{ij} weighting coefficients. Eliminating c_N in Eq. (41) by Eq. (40) and substituting $c_1 = 1$ results in the equation for obtaining (via

an appropriate technique such as Runga–Kutta) the values for concentration c_i, where $i = 2, 3, \ldots, (N-1)$ for the interior domain, from which the concentration c_N at the end point is calculated by Eq. (40). Although the results are identical—as would be expected—to those obtained by using Eq. (39) of the Bellman *et al.* technique, significantly less computing time was required for the present approach despite the fact that two sets of weighting coefficients a_{ij} and b_{ij} had to be used.

Conclusions

Because of the reduction in programming effort and computational time, the technique of differential quadrature appears to enjoy substantial advantages over the conventional finite element and finite difference methods for solving problems related to transport phenomena.

Acknowledgments

The authors acknowledge the financial support of University Technologists, Inc. and the Merrick Computing Center of the University of Oklahoma.

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