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NEW INSIGHTS IN SOLVING DISTRIBUTED SYSTEM EQUATIONS BY THE QUADRATURE METHOD—II. NUMERICAL EXPERIMENTS

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Abstract—The results of a series of numerical experiments are presented to verify some of the important points made in Part I of this paper. First, the numerical solutions of various linear and nonlinear differential equations, which were obtained by following the proposed general procedure, are compared with the analytical solutions. It can be observed that a high degree of accuracy is achieved in every case. Second, quadrature coefficients determined by using the explicit formulae derived in this work are shown to be more superior than those by the conventional approach of inverting the Vandermonde matrix. Third, the suggested grid point placement scheme is demonstrated to be better than any other available choice, including the one adopted in the orthogonal collocation method. Finally, the developed techniques are applied to obtain the solution of a chemical engineering problem.

INTRODUCTION

The objective of this part of the paper is to illustrate the implementation of the general procedure and to support the analysis presented in Part I (Quan and Chang, 1989) by using numerical examples. The proposed general procedure has been carried out in all examples and is explained with details in Example 1. The convenience of having the proposed explicit formulae and the ease of implementing the suggested procedure are clearly demonstrated here. For this particular problem, the task of obtaining the numerical values of the analytical solutions is considered to be harder than solving the equations by the proposed method.

Then, the reliability of the proposed techniques is established by comparing the analytical and numerical solutions of a large number of linear and nonlinear differential equations. A list of the problems considered in this work is presented in the Appendix. The results of this exercise are summarized in Table 1.

The advantages of using the explicit formulae derived in the first part of this paper in calculating the quadrature coefficients are shown in Example 3 and in Tables 2–4. It can be observed that the solutions obtained by adopting the suggested techniques are clearly more accurate than those obtained through inverting the Vandermonde matrix.

In Part I of this paper, the zeros of the Chebyshev polynomial (first kind) were considered as the most logical candidates to be chosen for grid points. This proposition was confirmed by numerical experiments carried out for Examples 2–5, 7 and 8 (Quan, 1988). The results of Example 5 are presented in Tables 5–7. It can be seen that this approach yields consistently better results than the orthogonal collocation method does.

To demonstrate that the proposed procedure can be applied to typical chemical engineering problems, a set of nonlinear partial differential equations describing the behavior of a steady-state catalytic reactor are solved. This example shows that reasonable results are obtained with efficiency.

IMPLEMENTATION OF THE GENERAL PROCEDURE

For illustration purposes, the solution steps of two partial differential equations coupled through a common boundary condition is presented here to demonstrate the ease of implementing the proposed procedure. The solutions of other examples in this paper were obtained by using the same approach and will not be detailed.

Example 1

$$\frac{\partial u_1(t,r)}{\partial t} = D_1\left(\frac{\partial^2 u_1(t,r)}{\partial r^2} + \frac{2}{r}\frac{\partial u_1(t,r)}{\partial r}\right) \qquad 0 < r < R_1 \quad 0 < t < t_f, \tag{1a}$$

$$\frac{\partial u_2(t,r)}{\partial t} = D_2\left(\frac{\partial^2 u_2(t,r)}{\partial r^2} + \frac{2}{r}\frac{\partial u_2(t,r)}{\partial r}\right) \qquad R_1 < r < R_2 \quad 0 < t < t_f, \tag{1b}$$

with initial conditions

$$u_1(0,r) = u_0 \quad 0 \leqslant r \leqslant R_1, \tag{1c}$$

$$u_2(0,r) = u_0 \quad R_1 \leqslant r \leqslant R_2, \tag{1d}$$

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and boundary conditions

$$u_1(t, R_1) = u_2(t, R_1) \quad 0 \leqslant t \leqslant t_f, \tag{1e}$$

$$K\frac{\partial u_1(t, R_1)}{\partial r} = \frac{\partial u_2(t, R_1)}{\partial r} \quad 0 \leqslant t \leqslant t_f, \tag{1f}$$

$$u_2(t, R_2) = 0 \quad 0 \leqslant t \leqslant t_f, \tag{1g}$$

$$\frac{\partial u_1(t, 0)}{\partial r} = 0 \quad 0 \leqslant t \leqslant t_f, \tag{1h}$$

where:

$$t_f = 2, \quad R_1 = 0.7, \quad R_2 = 1, \quad u_0 = 20, \quad D_1 = 0.1,$$

$$D_2 = 0.3, \quad K = 0.75.$$

The analytical solutions to this problem are in the form of infinite series (Carslaw and Jaeger, 1959). Notice that obtaining a numerical answer from the analytical expressions in itself is a hard task. A root-finding technique must be implemented to locate a sequence of eigenvalues. Extreme care must be exercised to avoid bypassing any one in this sequence. In addition, the infinite series in the analytical solutions converge very slowly for small values of t.

On the other hand, the effort required in obtaining the numerical solutions by the proposed method is considerably less. Let us distinguish between the two different regions by using superscripts, e.g. $\alpha_{ij}^{(1)}$ is used for $0 < r < R_1$ and $\alpha_{ij}^{(2)}$ is used for $R_1 < r < R_2$. The initial and final grid points in the first region are set to be 0 and R_1, respectively. Similarly, for the second region, $r_1^{(2)} = R_1$ and $r_n^{(2)} = R_2$.

Using equation (2) in Part I, one can transform equations (1a) and (1b) into two sets of ordinary differential equations:

$$\frac{\mathrm{d}u_k(t, r_i^{(k)})}{\mathrm{d}t} \cong D_k\Bigg[\beta_{i1}^{(k)}u_k(t, r_1^{(k)}) + \sum_{j=2}^{n-1}\beta_{ij}^{(k)}u_k(t, r_j^{(k)}) + \beta_{in}^{(k)}u_k(t, r_n^{(k)}) + \frac{2}{r_i^{(k)}}\Bigg(\alpha_{i1}^{(k)}u_k(t, r_1^{(k)}) + \sum_{j=2}^{n-1}\alpha_{ij}^{(k)}u_k(t, r_j^{(k)}) + \alpha_{in}^{(k)}u_k(t, r_n^{(k)})\Bigg)\Bigg]$$

$$k = 1, 2 \quad i = 2, 3, \ldots, n-1. \tag{2}$$

The initial conditions of these equations can be obtained from equations (1c) and (1d), i.e.

$$u_k(0, r_i^{(k)}) = u_0 \quad k = 1, 2 \quad i = 2, 3, \ldots, n-1. \tag{3}$$

The values of the dependent variables at the boundary points, i.e. $u_1(t, r_1^{(1)})$, $u_1(t, r_n^{(1)})$, $u_2(t, r_1^{(2)})$ and $u_2(t, r_n^{(2)})$, can be determined by the boundary conditions. More specifically, equations (1e–h) can be approximated by:

$$u_1(t, r_n^{(1)}) = u_2(t, r_1^{(2)}) \tag{4a}$$

$$K\Bigg[\alpha_{n1}^{(1)}u_1(t, r_1^{(1)}) + \sum_{j=2}^{n-1}\alpha_{nj}^{(1)}u_1(t, r_j^{(1)}) + \alpha_{nn}^{(1)}u_1(t, r_n^{(1)})\Bigg] \cong \alpha_{11}^{(2)}u_2(t, r_1^{(2)}) + \sum_{j=2}^{n-1}\alpha_{1j}^{(2)}u_2(t, r_j^{(2)}) + \alpha_{1n}^{(2)}u_2(t, r_n^{(2)}), \tag{4b}$$

$$u_2(t, r_n^{(2)}) = 0, \tag{4c}$$

$$\alpha_{11}^{(1)}u_1(t, r_1^{(1)}) + \sum_{j=2}^{n-1}\alpha_{1j}^{(1)}u_1(t, r_j^{(1)}) + \alpha_{1n}^{(1)}u_1(t, r_n^{(1)}) \cong 0. \tag{4d}$$

From these four equations, we can solve for the values of u at the first and last grid points in each region. As a result, equation (2) can be solved easily by a numerical integrator. This calculation was carried out by Quan (1988) and reported in detail. The "average" errors of the numerical solutions are presented in Table 1 in the next section.

ACCURACY OF NUMERICAL SOLUTIONS

In order to demonstrate the reliability of the proposed procedure, a wide variety of problems were solved. A list of these problems is provided in the Appendix. Among them, Examples 1–7 are formulated by linear partial differential equations. Example 8 involves the solution of a nonlinear ordinary differential equation. Nonlinear partial differential equations can be found in Examples 9 and 10.

The first step in solving all these problems is to approximate the first and second spatial derivatives by linear combinations of the values of the dependent variable at the grid points (Quan and Chang, 1989). Thus, the original formulations can always be transformed into an initial-value problem (e.g. Examples 1–5 and 9), a two-point boundary-value problem (e.g. Examples 6 and 10) or a system of algebraic equations (e.g. Examples 7 and 8).

Next, standard algorithms were used to solve the resulting equations. In this work, a fifth-order Runge–Kutta procedure with adaptive step size control was used to integrate ordinary differential equations that form initial-value problems. The shooting method implemented by Press *et al.* (1988) was adopted to handle two-point boundary-value problems. The solutions of linear algebraic equations can be obtained easily by the Gaussian elimination procedure. Nonlinear algebraic equations were solved by the Levenberg–Marquardt algorithm implemented in the IMSL subroutines.

The numerical solutions were then compared with the analytical solutions. For the purpose of discussion, let us define several error terms. The error of

Table 1. Accuracy of the numerical solutions

Example No.	Equation type	Number and location of grid points	Transformed problem	$\bar{\epsilon}_{mn}$
1	Linear PDE	t: 11, evenly-spaced $r^{(1)}$: 13, Chebyshev (1st kind) $r^{(2)}$: 13, Chebyshev (1st kind)	IVP	5.44×10^{-4} 8.86×10^{-4}
2	Linear PDE	t: 11, evenly-spaced x: 13, Chebyshev (1st kind)	IVP	1.45×10^{-7}
3	Linear PDE	t: 11, evenly-spaced x: 13, Chebyshev (1st kind)	IVP	2.64×10^{-6}
4	Linear PDE	t: 11, evenly-spaced r: 7, Chebyshev (1st kind)	IVP	2.56×10^{-5}
5	Linear PDE	t: 11, evenly-spaced r: 13, Chebyshev (1st kind)	IVP	2.17×10^{-6}
6	Linear PDE	r: 11, evenly-spaced θ: 7, Chebyshev (1st kind)	TPBVP	1.08×10^{-5}
7	Linear PDE	x: 7, Chebyshev (1st kind) y: 7, Chebyshev (1st kind)	Linear algebraic equations	7.83×10^{-4}
8	Nonlinear ODE	x: 5, Chebyshev (1st kind)	Nonlinear algebraic equations	5.80×10^{-4}
9	Nonlinear PDE	x: 21, evenly-spaced y: 13, Chebychev (1st kind)	IVP	1.65×10^{-4}
10	Nonlinear PDE	x: 11, evenly-spaced y: 5, Chebychev (1st kind)	TPBVP	4.61×10^{-4}

a numerical solution at a given point (t, y) in a 2-D domain can be defined as:

$$\epsilon(t, y) = \frac{|u^c(t, y) - u^a(t, y)|}{|u^a(t, y)|}, \tag{5a}$$

where u^c and u^a represent the numerical and analytical solutions, respectively. In addition to this local error, two other "average" errors are used in this work. For a given t, the "spatial average error" is defined as:

$$\bar{\epsilon}_n(t) = \frac{1}{n} \sum_{j=1}^{n} \epsilon(t, y_j), \tag{5b}$$

where the y_js represent the locations of grid points. Finally, for a given solution domain, an "overall average error" can be determined by:

$$\bar{\epsilon}_{mn} = \frac{1}{m \times n} \sum_{i=1}^{m} \sum_{j=1}^{n} \epsilon(t_i, y_j), \tag{5c}$$

where the t_is indicate the values of the solutions at evenly-spaced times. The analytical solution of each problem can be found in the references cited in the Appendix. Due to the limitation of space, only the overall average errors $\bar{\epsilon}_{mn}$ are reported in Table 1. The local error ϵ and the spatial average error $\bar{\epsilon}_n$ are published elsewhere (Quan, 1988). From the magnitudes of the errors presented in Table 1, it can be concluded that the numerical solutions obtained by using the proposed techniques are extremely accurate and the suggested procedure is suitable for solving a wide range of problems.

ACCURACY OF THE QUADRATURE COEFFICIENTS

As mentioned in Part I of this paper, the Vandermonde matrix becomes ill-conditioned if a large number of grid points are used (Mingle, 1977; Civan and Sliepcevich, 1983). This problem can be overcome by using the explicit formulae developed in this work. To demonstrate the advantage of the proposed approach, Example 3 was solved using the quadrature coefficients determined by two different approaches. First, the grid points were selected at the zeros of a Chebyshev polynomial of the first kind. Equations (B5–B8) in Appendix B of Part I (Quan and Chang, 1989) were used to calculate the values of quadrature coefficients, i.e. α_{ij}s and β_{ij}s. The same grid points were used in the second approach. The inverse of the Vandermonde matrix was obtained by following Hamming's procedure (Hamming, 1973). The quadrature coefficients were then determined by pre-multiplying the vectors on the right-hand-side of equations (11) and (12) in Part I by $\mathbb{V}^{-1}$. In this example, the solutions of the two approaches are compared with the analytical solutions for several values of n, the number of grid points. For comparison purposes, let us define:

$$\Delta_1 = \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} |\alpha_{ij}^C - \alpha_{ij}^V|}{n^2} \tag{6a}$$

and

$$\Delta_2 = \frac{\sum_{i=1}^{n} \sum_{j=1}^{n} |\beta_{ij}^C - \beta_{ij}^V|}{n^2} \tag{6b}$$

where the superscripts C and V correspond to the Chebyshev and Vandermonde cases, respectively. As we can observe from Table 2, the average absolute deviations of first- and second-order coefficients increases with an increasing number of grid points. As

Table 2. Average absolute deviations in the entries of matrices $\mathbb{A}$ and $\mathbb{B}$

n	Δ_1	Δ_2
7	3.5402×10^{-8}	1.2376×10^{-6}
9	2.0997×10^{-7}	6.5553×10^{-6}
11	5.7619×10^{-6}	2.3555×10^{-4}
13	1.7839×10^{-4}	7.9647×10^{-3}
15	7.8575×10^{-3}	6.4497×10^{-1}
17	3.3060×10^{-1}	3.2097×10^{1}
19	6.9511×10^{0}	5.6557×10^{2}

Table 3. Spatial average errors $\bar{\epsilon}_n \times 10^6$ (Chebyshev, first kind)

t	$n = 11$	$n = 13$	$n = 15$	$n = 17$
0.05	9.2734	4.7569	3.7069	1.1778
0.10	1.4319	1.8872	18.2312	0.6430
0.15	50.8209	2.0164	1.8173	3.6039
0.20	1.7268	6.9188	23.1078	1.7263
0.25	1.0903	2.1511	1.7686	0.9326
0.30	18.0938	2.9141	1.4017	6.3601
0.35	0.4956	2.1771	1.5157	2.4534
0.40	3.0118	1.6458	16.6729	1.6605
0.45	0.4286	0.9555	1.0280	5.1099
0.50	5.8723	1.0015	15.8796	1.7971

Table 4. Spatial average errors $\bar{\epsilon}_n \times 10^6$ (Vandermonde)

t	$n = 11$	$n = 13$	$n = 15$	$n = 17$
0.05	1.5915	43.335	2818.1	50,989.1
0.10	2.1601	60.122	5522.8	63,464.8
0.15	55.8733	74.352	8356.5	74,763.2
0.20	3.1392	91.657	11,366.5	85,391.0
0.25	45.5064	114.135	14,560.8	95,664.7
0.30	4.4562	140.867	17,928.6	105,815.4
0.35	5.0203	173.146	21,477.8	116,005.4
0.40	17.6134	204.321	25,207.6	126,350.1
0.45	5.8806	243.060	29,126.3	136,934.8
0.50	8.1035	276.583	33,238.3	149,375.0

expected, the deviations of the β_{ij}s are greater than those of the α_{ij}s.

In Tables 3 and 4, the spatial average absolute errors defined by equation (5b) for several values of n are presented for the Chebyshev and Vandermonde cases, respectively. It can be observed from Table 3 that the solutions remain stable as n increases, if the suggested formulae are used. On the other hand, if the conventional approach is followed, the solutions at $n = 15$ and $n = 17$ are clearly unacceptable (Table 4).

COMPARISON WITH THE ORTHOGONAL COLLOCATION METHOD

The accuracy of the numerical solutions is dependent upon the locations of the grid points. It has been well recognized that the orthogonal collocation method yields more accurate solutions than the general collocation method with equally-spaced nodes (Villadsen and Michelsen, 1978). Since the quadrature method and the collocation method are basically equivalent except for the different choices of grid points, it is to our interest to compare their performances. For this purpose, several examples were reworked using three different node placement schemes for several values of n. In the first scheme, the orthogonal collocation method was used. The interior grid points were chosen as the zeros of a shifted $(n-2)$th degree Legendre polynomial. The general formulae, equations (18–21), derived in the first part of this paper were used to calculate the quadrature coefficients. In the second and third scheme, the zeros of the shifted nth degree Legendre and Chebyshev (first kind) polynomials were selected as the locations of grid points. The domains of these orthogonal polynomials were determined by equations (44) and (45) in Part I of this paper. The corresponding explicit formulae, i.e. equations (B1–B8) in Part I, were then used to calculate the quadrature coefficients.

The average errors resulting from the above three schemes for Example 5 are presented in Tables 5–7. It can be observed that, in general, the differential quadrature method performs better, especially for small values of n. The best results are obtained by the differential quadrature method using Chebyshev polynomials. Similar results were reported by Quan (1988) for Examples 2–4 and 7. Also, in the case of Example 8, the spatial average errors corresponding to different placement schemes were calculated by using five grid points. If the interior nodes are placed at the zeros of a third-degree Legendre polynomial according to the orthogonal collocation method, the value of the average error is 2.75×10^{-3}. However, if the proposed procedure is followed, the error can be reduced to 5.80×10^{-4}. Thus, from the evidence we have gathered so far, the techniques developed in Part I of this paper should be considered better than the orthogonal collocation method in terms of efficiency and accuracy.

APPLICATION EXAMPLE

The solution of initial-value problems arising in chemical engineering applications can be obtained with relative ease using the method of differential quadrature. For illustration purposes, we adopt the partial differential equations used to model the steady-state temperature and concentration profiles in a packed bed reactor by Buchanan and Sundaresan (1987). The specific reaction considered is butane oxidation over the catalyst vanadium phosphate:

$$\text{butane} \xrightarrow{r_1} \text{maleic anhydride} \xrightarrow{r_3} \text{CO, CO}_2,$$

$$\text{butane} \xrightarrow{r_2} \text{CO, CO}_2.$$

Table 5. Spatial average errors for Example 5 (orthogonal collocation, Legendre)

t	$n = 5$	$n = 7$	$n = 9$	$n = 11$
0.1	0.0070157724	0.0010687526	0.0007317606	0.0001708534
0.2	0.0091076356	0.0020559955	0.0003089055	0.0000519404
0.3	0.0066407025	0.0013312957	0.0001219449	0.0000092381
0.4	0.0033139335	0.0004024027	0.0000613005	0.0000061655
0.5	0.0008454230	0.0003683775	0.0000472253	0.0000030899
0.6	0.0016465982	0.0003549155	0.0000251803	0.0000009896
0.7	0.0029377743	0.0002782768	0.0000104697	0.0000012284
0.8	0.0036037179	0.0002136375	0.0000039429	0.0000004395
0.9	0.0038174329	0.0001550866	0.0000045995	0.0000001714
1.0	0.0037326825	0.0001061122	0.0000039305	0.0000000863

Table 6. Spatial average errors for Example 5 (differential quadrature, Legendre)

t	$n=5$	$n=7$	$n=9$	$n=11$
0.1	0.0053113381	0.0006091974	0.0005213998	0.0001102474
0.2	0.0022336979	0.0010114794	0.0001116469	0.0000305658
0.3	0.0009888917	0.0005446990	0.0000901398	0.0000075769
0.4	0.0014213024	0.0002068286	0.0000433664	0.0000043355
0.5	0.0017499901	0.0000896354	0.0000209243	0.0000023767
0.6	0.0017973357	0.0001070997	0.0000085003	0.0000010117
0.7	0.0016501215	0.0001057352	0.0000068820	0.0000011328
0.8	0.0014344237	0.0000920667	0.0000047198	0.0000004050
0.9	0.0012052304	0.0000738707	0.0000034842	0.0000002020
1.0	0.0009893673	0.0000566823	0.0000026275	0.0000001196

Since the reactions are highly exothermic, the possibility of a runaway hotspot near the reactor entrance is high under certain operating conditions. This situation can be prevented by diluting the catalyst. The behavior of the reactor for a specific catalyst dilution profile is examined.

The packed bed reactor is modelled by the following set of partial differential equations:

$$\frac{\partial y_1(z,r)}{\partial z} = \frac{d_p L}{R^2 \mathrm{Pe}_m}\left(\frac{\partial^2 y_1(z,r)}{\partial r^2} + \frac{1}{r}\frac{\partial y_1(z,r)}{\partial r}\right) + \psi(z)\frac{L\rho_b}{vC_{ref}}(r_1 + r_2), \tag{7}$$

$$\frac{\partial y_2(z,r)}{\partial z} = \frac{d_p L}{R^2 \mathrm{Pe}_m}\left(\frac{\partial^2 y_2(z,r)}{\partial r^2} + \frac{1}{r}\frac{\partial y_2(z,r)}{\partial r}\right) + \psi(z)\frac{L\rho_b}{vC_{ref}}(r_1 - r_3), \tag{8}$$

$$\frac{\partial y_3(z,r)}{\partial z} = \frac{Lk_{er}}{R^2 v C_p \rho_g}\left(\frac{\partial^2 y_3(z,r)}{\partial r^2} + \frac{1}{r}\frac{\partial y_3(z,r)}{\partial r}\right) + \psi(z)\frac{L\rho_b}{v\rho_g C_p T_{ref}}\left((-\Delta H_1)r_1 + (-\Delta H_2)r_2 + (-\Delta H_3)r_3\right), \tag{9}$$

where the rate expressions are given by:

$$r_1 = k_{01}\exp\left(-\frac{E_1}{R_g y_3(z,r) T_{ref}}\right)\frac{y_1(z,r)C_{ref}}{p}, \tag{10}$$

$$r_2 = k_{02}\exp\left(-\frac{E_2}{R_g y_3(z,r) T_{ref}}\right)\frac{y_1(z,r)C_{ref}}{p}, \tag{11}$$

$$r_3 = k_{03}\exp\left(-\frac{E_3}{R_g y_3(z,r) T_{ref}}\right)\frac{y_2(z,r)C_{ref}}{p}, \tag{12}$$

with

$$p = 1 + \frac{K_1 y_1(z,r) + K_2 y_2(z,r)}{O_2}, \tag{13}$$

$$O_2 = \frac{4.1}{C_{ref}} - 4.2\left(\frac{F_B}{C_{ref}} - y_1(z,r)\right). \tag{14}$$

The initial conditions are:

$$y_1(0,r) = y_{10} \quad y_2(0,r) = y_{20} \quad y_3(0,r) = y_{30}, \tag{15}$$

and the boundary conditions are:

$$\frac{\partial y_1(z,0)}{\partial r} = \frac{\partial y_2(z,0)}{\partial r} = \frac{\partial y_3(z,0)}{\partial r} = 0, \tag{16}$$

$$\frac{\partial y_1(z,1)}{\partial r} = \frac{\partial y_2(z,1)}{\partial r} = 0, \tag{17}$$

$$\frac{\partial y_3(z,1)}{\partial r} = \frac{hR}{k_{er}}\left(\frac{T_c}{T_{ref}} - y_3(z,1)\right). \tag{18}$$

In the above equations, $y_1(z,r)$ and $y_2(z,r)$ are the dimensionless butane and maleic anhydride concentrations, respectively, and $y_3(z,r)$ is the dimensionless temperature. These state variables are defined as follows:

$$y_1(z,r) = \frac{C_1(z,r)}{C_{ref}}, \quad y_2(z,r) = \frac{C_2(z,r)}{C_{ref}}, \quad y_3(z,r) = \frac{T(z,r)}{T_{ref}}. \tag{19}$$

The function $\psi(z)$ represents the catalyst dilution profile and is only a function of z, for practical purposes. For simplicity, a piecewise linear function, shown in Fig. 1, was used to represent one possible profile.

Table 7. Spatial average errors for Example 5 (differential quadrature, Chebyshev-first kind)

t	$n=5$	$n=7$	$n=9$	$n=11$
0.1	0.0051076758	0.0009371251	0.0003687343	0.0000963376
0.2	0.0022537371	0.0008758178	0.0001272661	0.0000184993
0.3	0.0012765720	0.0004071388	0.0000623725	0.0000045276
0.4	0.0016770279	0.0001554707	0.0000274437	0.0000026320
0.5	0.0017621578	0.0001338407	0.0000126810	0.0000014808
0.6	0.0017360715	0.0000939165	0.0000063052	0.0000006029
0.7	0.0015425658	0.0000805949	0.0000038482	0.0000009608
0.8	0.0013010266	0.0000659588	0.0000024703	0.0000003096
0.9	0.0010609210	0.0000502050	0.0000019602	0.0000001253
1.0	0.0008447294	0.0000371285	0.0000014696	0.0000000618

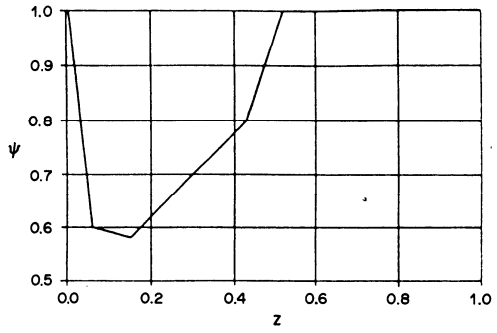

Fig. 1. Catalyst dilution profile.

After approximating the partial derivatives with respect to r in the above equations using differential quadrature, the resulting system of ODEs was integrated from $z = 0$ to $z = 1$ with grid points located at the zeros of an eleventh-degree Chebyshev polynomial (first kind). An example of the output is shown in Fig. 2, where cubic spline interpolation was used for plotting purposes. The obtained temperature profile shows the expected behavior, i.e. there is a sharp increase in temperature near the entrance of the reactor with higher values at $r = 0$. The proposed method is more appealing than previous approaches since less implementation effort is required to obtain accurate solutions for this problem. This is due to the availability of explicit formulae for the quadrature coefficients and better approximation of boundary conditions through the use of a new grid point placement scheme.

CONCLUSIONS

A number of important conclusions concerning the method of differential quadrature can be drawn from the results of the numerical experiments presented in this paper. The use of explicit formulae for determining the quadrature coefficients has been shown to be more accurate and efficient than the conventional technique of inverting the Vandermonde matrix. The approach of positioning the grid points at the zeros of a Chebyshev polynomial of the first kind has been shown to be consistently better than any other choice under consideration, including the method of orthogonal collocation. Although the convergence of iteration cannot be guaranteed, the feasibility of treating the extension problems as two-point boundary-value problems has also been demonstrated. Based on the above observations, the degree of accuracy achieved in all the examples, and the ease in the implementation, it is safe to say that the proposed procedure is suitable for solving a wide range of the distributed system equations arising in chemical engineering applications.

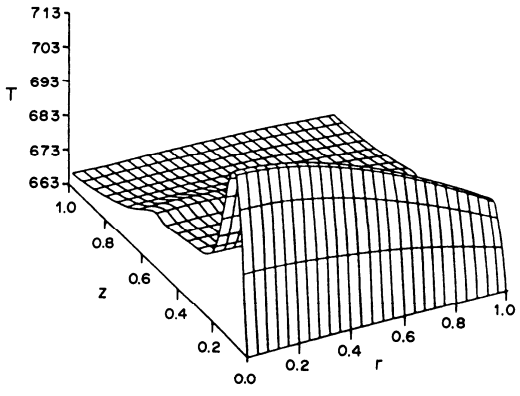

Fig. 2. Reactor temperature (K).

NOMENCLATURE

a, b = Lower and upper bounds of a finite interval, $a < b$
C_i = Concentration of species i
C_p = Mean specific heat (0.26 kcal kg^{-1} K^{-1})
C_{ref} = Reference concentration (0.1 mol m^{-3})
D_{er} = Effective radial diffusivity (7.14×10^{-4} m^2 s^{-1})
d_p = Catalyst particle diameter (0.00476 m)
E_1 = Activation energy for reaction 1 (29.875 kcal mol^{-1})
E_2 = Activation energy for reaction 2 (34.655 kcal mol^{-1})
E_3 = Activation energy for reaction 3 (43.020 kcal mol^{-1})
F_B = Feed butane (0.318 mol m^{-3})
h = Heat transfer coefficient (15.0 kcal h^{-1} m^{-2} K^{-1})
k_{01} = Rate constant for reaction 1 (7.06×10^{10} m^3 kg cat^{-1} h^{-1})
k_{02} = Rate constant for reaction 2 (1.22×10^{12} m^3 kg cat^{-1} h^{-1})
k_{03} = Rate constant for reaction 3 (6.12×10^{13} m^3 kg cat^{-1} h^{-1})
K_1 = Model constant (59)
K_2 = Model constant (26)
k_{er} = Effective radial thermal conductivity (1.0 kcal h^{-1} m^{-1} K^{-1})
L = Total reactor length (3 m)
n = Total number of grid points
Pe_m = Peclet number for radial mass transfer ($vd_p/D_{er} = 10$)
r = Independent variable, radial distance in cylindrical or spherical coordinates
R = Reactor tube radius (0.0127 m)
R_g = Gas constant (1.9872 cal mol^{-1} K^{-1})
r_i = Rate for reaction i
t = Independent variable, $0 \leqslant t < \infty$
T = Reactor temperature
T_c = Coolant temperature (663 K)
T_{ref} = Reference temperature (1000 K)
u = Dependent variable
v = Superficial fluid velocity (1.5 m s^{-1})
x = Independent variable, distance in rectangular coordinates
y = Independent variable, shifted distance in rectangular coordinates $a \leqslant y \leqslant b$
y_i = Dimensionless state variable i
y_{10} = Initial value for dimensionless butane concentration (3.18)
y_{20} = Initial value for dimensionless maleic anhydride concentration (0.0)
y_{30} = Initial value for dimensionless temperature (0.663)
z = Independent variable, reactor axial distance

Greek letters

α_{ij} = The first-order quadrature coefficients
β_{ij} = The second-order quadrature coefficients
ϵ = The absolute value of the relative error defined by equation (5a)
$\bar{\epsilon}_n$ = The spatial average error defined by equation (5b)
$\bar{\epsilon}_{mn}$ = Overall average error defined by equation (5c)
Δ_1 = Average absolute value of the deviations between the α_{ij}s obtained by using the explicit formulae and those by inverting the Vandermonde matrix
Δ_2 = Average absolute value of the deviations between the β_{ij}s obtained by using the explicit formulae and those by inverting the Vandermonde matrix
$(-\Delta H_1)$ = Heat released by reaction 1 (297 kcal mol^{-1})
$(-\Delta H_2)$ = Heat released by reaction 2 (461 kcal mol^{-1})
$(-\Delta H_3)$ = Heat released by reaction 3 (164 kcal mol^{-1})
ρ_b = Bulk density of catalyst and inert material (1000 kg cat^{-1} m^{-3})
ρ_g = Mean fluid density (0.573 kg m^{-3})
θ = Independent variable, angular position in cylindrical coordinates, $0 \leqslant \theta \leqslant \pi$
ψ = Catalyst dilution profile

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APPENDIX

Example Problems

Example 2 (Farlow, 1982)

$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial^2 u(t,x)}{\partial x^2} + \sin(3\pi x) \quad 0 < x < 1 \quad 0 < t < t_f. \tag{A1}$$

Initial condition:

$$u(0,x) = \sin(\pi x) \quad 0 \leqslant x \leqslant 1. \tag{A2}$$

Boundary conditions:

$$u(t,0) = 0 \quad u(t,1) = 0 \quad 0 < t \leqslant t_f, \tag{A3}$$

where $t_f = 0.05$.

Example 3 (Evans, 1987)

$$\frac{\partial u(t,x)}{\partial t} = \frac{\partial^2 u(t,x)}{\partial x^2} \quad 0 < x < 1 \quad 0 < t < t_f. \tag{A4}$$

Initial condition:

$$u(0,x) = \sin(x) + \cos(x) \quad 0 \leqslant x \leqslant 1. \tag{A5}$$

Boundary conditions:

$$\frac{\partial u(t,0)}{\partial x} = e^{-t} \quad \frac{\partial u(t,1)}{\partial x} = e^{-t}[\cos(1) - \sin(1)] \quad 0 < t \leqslant t_f, \tag{A6}$$

where $t_f = 0.5$.

Example 4 (Luikov, 1968)

$$\frac{\partial u(t,r)}{\partial t} = D\left(\frac{\partial^2 u(t,r)}{\partial r^2} + \frac{2}{r}\frac{\partial u(t,r)}{\partial r}\right) \quad 0 < r < R \quad 0 < t < t_f. \tag{A7}$$

Initial condition:

$$u(0,r) = u_0 \quad 0 \leqslant r \leqslant R. \tag{A8}$$

Boundary conditions:

$$-\frac{\partial u(t,R)}{\partial r} + H[u_a - u(t,R)] = 0 \quad \frac{\partial u(t,0)}{\partial r} = 0 \quad 0 < t \leqslant t_f, \tag{A9}$$

where

$$t_f = 2, \quad u_0 = 80, \quad u_a = 50, \quad D = 0.2, \quad R = 0.8, \quad H = 1.25.$$

Example 5 (Luikov, 1968)

$$\frac{\partial u(t,r)}{\partial t} = D\left(\frac{\partial^2 u(t,r)}{\partial r^2} + \frac{2}{r}\frac{\partial u(t,r)}{\partial r}\right) \quad 0 < r < R \quad 0 < t < t_f. \tag{A10}$$

Initial condition:

$$u(0,r) = u_0 \quad 0 \leqslant r \leqslant R. \tag{A11}$$

Boundary conditions:

$$u(t,R) = u_a \quad \frac{\partial u(t,0)}{\partial r} = 0 \quad 0 < t \leqslant t_f, \tag{A12}$$

where

$$t_f = 1, \quad u_0 = 60, \quad u_a = 50, \quad D = 0.05, \quad R = 1.$$

Example 6 (Myint-U, 1988)

$$\frac{\partial^2 u(r,\theta)}{\partial r^2} + \frac{1}{r}\frac{\partial u(r,\theta)}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u(r,\theta)}{\partial \theta^2} = 0 \quad 1 < r < 2 \quad 0 < \theta < \pi. \tag{A13}$$

Boundary conditions:

$$u(1,\theta) = \sin(\theta) \quad u(2,\theta) = 0 \quad 0 \leqslant \theta \leqslant \pi, \tag{A14}$$

$$u(r,0) = u(r,\pi) = 0 \quad 1 < r < 2. \tag{A15}$$

Example 7

$$\frac{\partial^2 u(x,y)}{\partial x^2}+\frac{\partial^2 u(x,y)}{\partial y^2}=-1 \quad -1<x<1 \quad -1<y<1. \tag{A16}$$

Boundary conditions:

$$u(-1,y)=u(1,y)=0 \quad -1\leqslant y\leqslant 1, \tag{A17}$$

$$u(x,-1)=u(x,1)=0 \quad -1\leqslant x\leqslant 1. \tag{A18}$$

Example 8 (Finlayson, 1980)

$$\frac{\mathrm{d}}{\mathrm{d}x}\left[(1+u)\frac{\mathrm{d}u}{\mathrm{d}x}\right]=0 \quad 0<x<1. \tag{A19}$$

Boundary conditions:

$$u(0)=0, \quad u(1)=1. \tag{A20}$$

Example 9

$$\frac{\partial u(x,y)}{\partial x}+\left(\frac{\partial u(x,y)}{\partial y}\right)^2=\sqrt{y}\cos(x)+\frac{\sin^2(x)}{4y}, \quad 0<x<\pi/2 \quad 1<y<3. \tag{A21}$$

Initial condition:

$$u(0,y)=0 \quad 1\leqslant y\leqslant 3. \tag{A22}$$

Example 10

$$\frac{\partial^2 u(x,y)}{\partial x^2}+\frac{\partial u(x,y)}{\partial x}\frac{\partial^2 u(x,y)}{\partial y^2}= \mathrm{e}^{-xy}[xy^2-2y+x^3\mathrm{e}^{-xy}-x^4y\mathrm{e}^{-xy}], \quad 0<x<1 \quad 0<y<1. \tag{A23}$$

Boundary conditions:

$$u(0,y)=y \quad u(1,y)=\mathrm{e}^{-y}+y \quad 0\leqslant y\leqslant 1. \tag{A24}$$