

See discussions, stats, and author profiles for this publication at:
<https://www.researchgate.net/publication/220561926>

Numerical solution of two-dimensional reaction-diffusion Brusselator system

Article in *Applied Mathematics and Computation* · February 2011

DOI: 10.1016/j.amc.2010.12.010 · Source: DBLP

CITATIONS

26

READS

255

2 authors:



R. C. Mittal

Indian Institute of Technology Roorkee

109 PUBLICATIONS 887 CITATIONS

SEE PROFILE



Dr Ram Jiwari

Indian Institute of Technology Roorkee

38 PUBLICATIONS 271 CITATIONS

SEE PROFILE



Numerical solution of two-dimensional reaction–diffusion Brusselator system

R.C. Mittal*, Ram Jiware

Department of Mathematics, Indian Institute of Technology Roorkee, Roorkee-247667, Uttarakhand, India

ARTICLE INFO

Keywords:

Reaction–diffusion Brusselator system
Differential quadrature method
System of ordinary differential equations
Runge–Kutta Method

ABSTRACT

In this paper, polynomial based differential quadrature method (DQM) is applied for the numerical solution of a class of two-dimensional initial-boundary value problems governed by a non-linear system of partial differential equations. The system is known as the reaction–diffusion Brusselator system. The system arises in the modeling of certain chemical reaction–diffusion processes. In Brusselator system the reaction terms arise from the mathematical modeling of chemical systems such as in enzymatic reactions, and in plasma and laser physics in multiple coupling between modes. The numerical results reported for three specific problems. Convergence and stability of the method is also examined numerically.

© 2010 Published by Elsevier Inc.

1. Introduction

The problem of dealing with chemical reactions of systems involving two variable intermediates, together with a number of initial and final products whose concentrations are assumed to be controlled throughout the reaction process is an important one under quite realistic conditions and is discussed by Nicolis and Prigogine in [1]. It is necessary to consider at least a cubic nonlinearity in the rate equations [2]. This model has been referred to as the trimolecular model or Brusselator [3]. The two-dimensional reaction–diffusion Brusselator system is the non-linear system of partial differential equations

$$\frac{\partial u}{\partial t} = B + u^2 v - (A + 1)u + \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right), \quad 0 < x, y < L, \quad (1)$$

$$\frac{\partial v}{\partial t} = Au - u^2 v + \alpha \left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right), \quad 0 < x, y < L, \quad (2)$$

for $u(x, y, t)$ and $v(x, y, t)$ in a two-dimensional region R bounded by a simple closed curve C subject to the initial-boundary conditions

$$(u(x, y, 0), v(x, y, 0)) = (f(x, y), g(x, y)) \quad (3)$$

and Neumann boundary conditions on the boundary ∂C of the square C defined by the lines $x = 0, y = 0, x = L, y = L$,

* Corresponding author.

E-mail address: rcmmmf@iitr.ernet.in (R.C. Mittal).

$$\begin{aligned}
\frac{\partial u(0,y,t)}{\partial x} &= \frac{\partial u(L,y,t)}{\partial x} = 0, & t \geq 0, \\
\frac{\partial u(x,0,t)}{\partial y} &= \frac{\partial u(x,L,t)}{\partial y} = 0, & t \geq 0, \\
\frac{\partial v(0,y,t)}{\partial x} &= \frac{\partial v(L,y,t)}{\partial x} = 0, & t \geq 0, \\
\frac{\partial v(x,0,t)}{\partial y} &= \frac{\partial v(x,L,t)}{\partial y} = 0, & t \geq 0,
\end{aligned} \tag{4}$$

where A , B and α are suitably given constants, $f(x,y)$ and $g(x,y)$ are suitably prescribed functions.

The non-linear system (1) and (2) represents a useful model for study of co-operative processes in chemical kinetics. Such Brusselator system arises in the formation of ozone by atomic oxygen via a triple collision. It also arises in the modeling of certain chemicals reaction–diffusion processes such as in enzymatic reactions, and in plasma and laser physics in multiple coupling between modes. Therefore these equations are of interest from the numerical point of view.

These types of problems have been solved by Dehghan and his coworkers in [4–9]. They proposed different numerical schemes for one dimensional heat and advection–diffusion equations, two dimensional transport equations, three dimensional advection–diffusion equations and coupled Burgers' equation. Many researchers have proposed methods for the numerical solutions and stability analyses of the Brusselator system (1) and (2). Twizell et al. [10] have given a second order finite-difference scheme for the Brusselator reaction–diffusion system. Adomain [11] and Wazwaz [12] have solved the system (1) by the decomposition method by taking initial conditions. Ang [13] has given the dual-reciprocity boundary element method for the numerical solution of the Brusselator system.

In this paper, we have applied a differential quadrature method (DQM) based polynomial to solve two-dimensional reaction–diffusion Brusselator system numerically. The equations are reduced into a system of non-linear ordinary differential equations by DQM. The obtained system of ordinary differential equations is then solved by a four-stage RK4 scheme given by Pike and Roe [14]. In order to demonstrate the accuracy of the present method, we have chosen three test problems given in the literature. The investigated results are reported in Figs. 1–3 and convergence of the method has been shown through the Tables 1–3 numerically. Obtained solutions are found to be very good and useful. To the best of authors' knowledge, this is the first attempt when the system is solved up to big time level $t = 50$.

2. Differential quadrature method

The differential quadrature method is a numerical technique for solving differential equations. It was firstly, introduced by Bellman et al. [15]. By this method, we approximate the derivatives of a function at any location by a linear summation of all the functional values at a finite number of grid points, then the equation can be transformed into a set of ordinary differential equations, if the equation is unsteady, otherwise a set of algebraic equations. The solutions can be obtained by applying standard numerical methods.

First the domain D is discretized by taking N points along x direction and M points along y direction.

According to the two dimensional DQM, the n -th and m -th partial derivatives of a dependent function $u(x,y,t)$ can be approximated the formula given in [16]

$$u_x^{(n)}(x_i, y_j, t) \cong \sum_{k=1}^N a_{ik}^{(n)} u(x_k, y_j, t), \tag{5}$$

$$u_y^{(m)}(x_i, y_j, t) \cong \sum_{k=1}^M b_{jk}^{(m)} u(x_i, y_k, t), \tag{6}$$

$$\text{for } i = 1, 2, \dots, N; j = 1, 2, \dots, M; n = 1, 2, \dots, N-1; m = 1, 2, \dots, M-1,$$

where $u_x^{(n)}(x_i, y_j, t)$ and $u_y^{(m)}(x_i, y_j, t)$ indicate the n -th and m -th order partial derivatives of $u(x,y,t)$ with respect to x and y at grid points (x_i, y_j) and $a_{ij}^{(n)}$ and $b_{ij}^{(m)}$ are the weighting coefficients related to $u_x^{(n)}(x_i, y_j, t)$ and $u_y^{(m)}(x_i, y_j, t)$ at (x_i, y_j) . Bellman et al. [6] proposed two approaches to compute the weighting coefficients. To improve Bellman's approaches in computing the weighting coefficients, many attempts have been made by researchers. One of the most useful approaches is the one introduced by Quan and Chang [17,18]. After that, Shu's [16] general approach which was inspired from Bellman's approach was made available in the literature. Shu's recurrence formulation for higher order derivatives is given by

$$a_{ij}^{(n)} = n \left[a_{ij}^x a_{ii}^{(n-1)} - \frac{a_{ij}^{(n-1)}}{x_i - x_j} \right] \quad \text{for } i \neq j, \tag{7}$$

$$a_{ii}^{(n)} = - \sum_{j=1, j \neq i}^N a_{ij}^{(n)} \quad \text{for } i = j, \tag{8}$$

$$n = 2, 3, \dots, N-1; i, j = 1, 2, \dots, N,$$

$$b_{ij}^{(m)} = m \left[b_{ij}^y b_{ii}^{(m-1)} - \frac{b_{ij}^{(m-1)}}{y_i - y_j} \right] \quad \text{for } i \neq j, \tag{9}$$

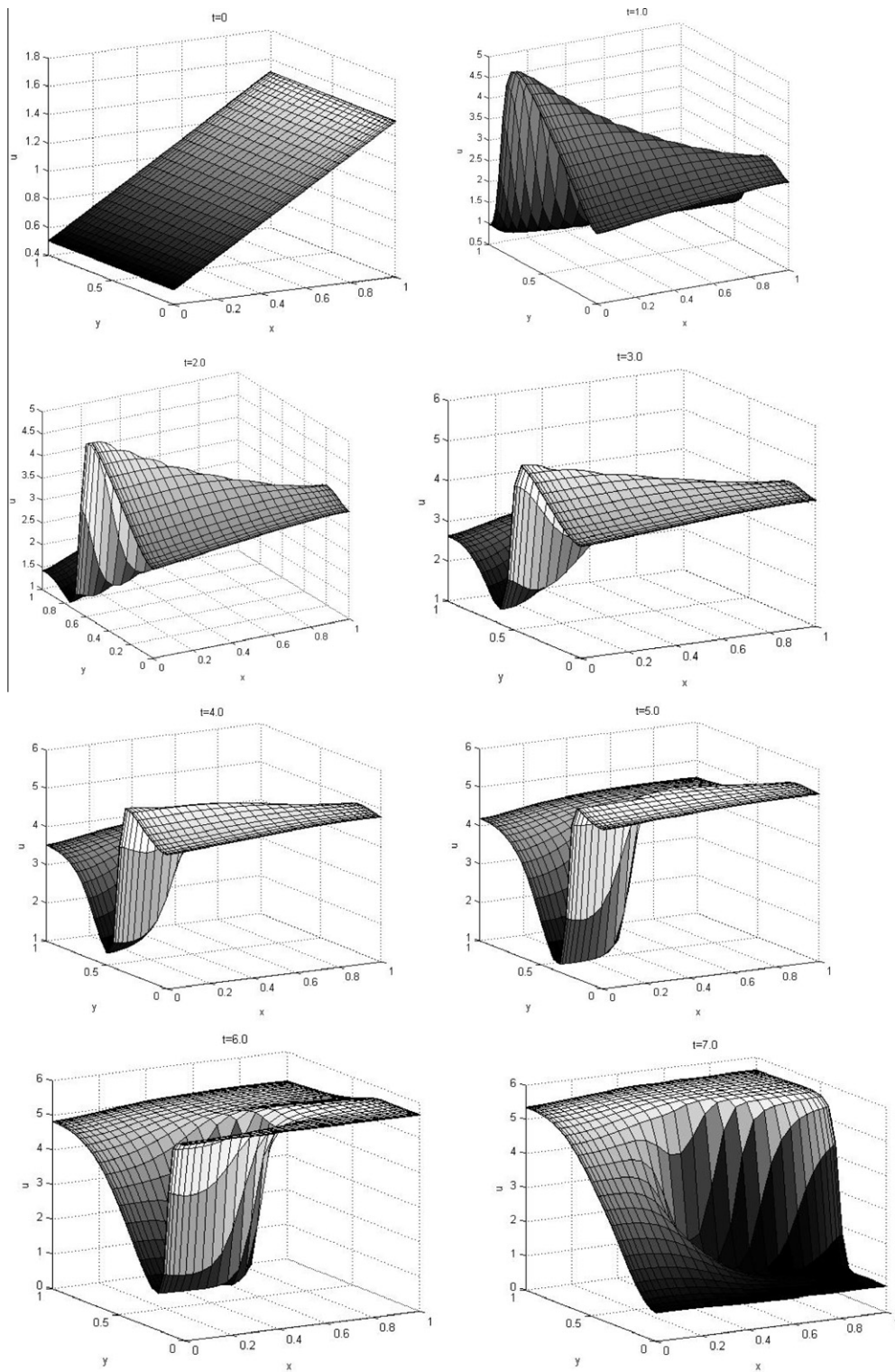


Fig. 1. Concentration profiles of u of Problem 1 at different time $t = 0, 1.0, \dots, 50.0$.

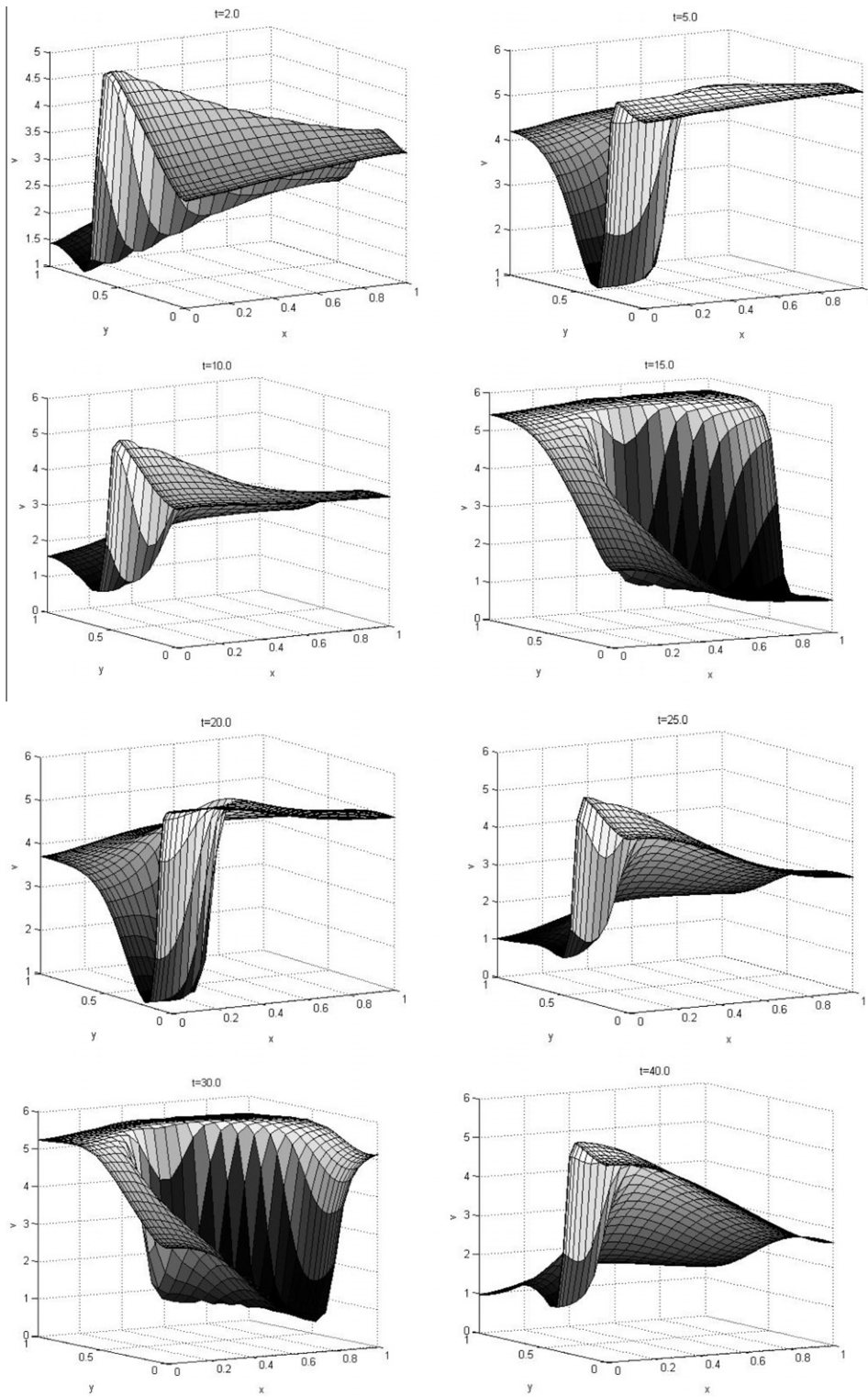


Fig. 2. Concentration profiles of ν of Example 7.1 at different time t .

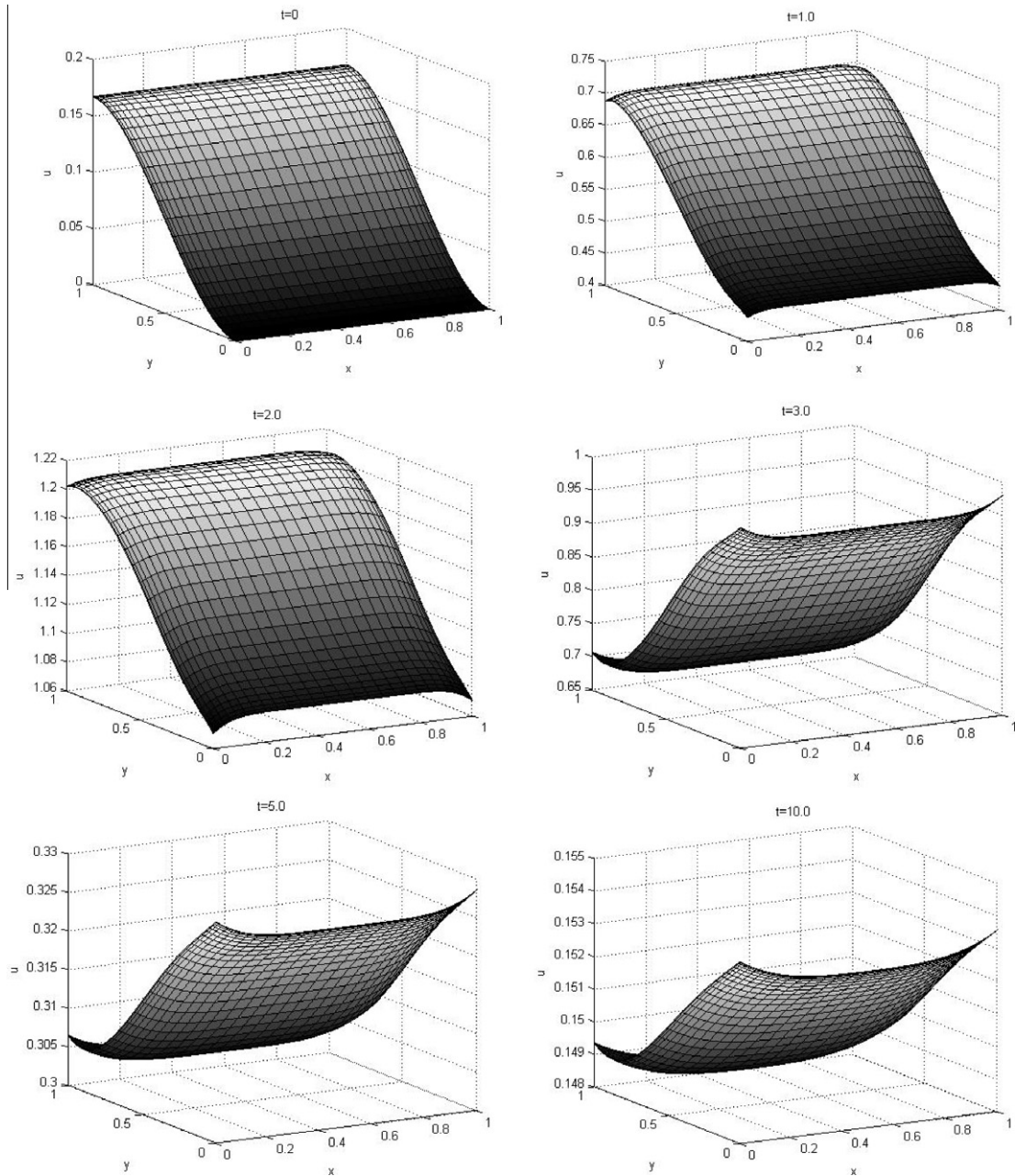


Fig. 3. Concentration profiles of u of Problem 2 at different times $t = 0, 1.0, \dots, 40.0$.

$$b_{ii}^{(m)} = - \sum_{j=1, j \neq i}^M b_{ij}^{(m)} \quad \text{for } i = j, \quad (10)$$

$$n = 2, 3, \dots, M-1; \quad i, j = 1, 2, \dots, M,$$

where a_{ij}^x and b_{ij}^y are the weighting coefficients of the first order partial derivatives of $u(x, y, t)$ with respect to x and y mention in [16].

Obviously, Eqs. (7)–(10) offer an easy way to compute the weighting coefficients.

3. Numerical solution of two-dimensional reaction–diffusion Brusselator system

The system of Eqs. (1)–(4) has been reduced into the following system of non linear ordinary differential equations after applying the differential quadrature method

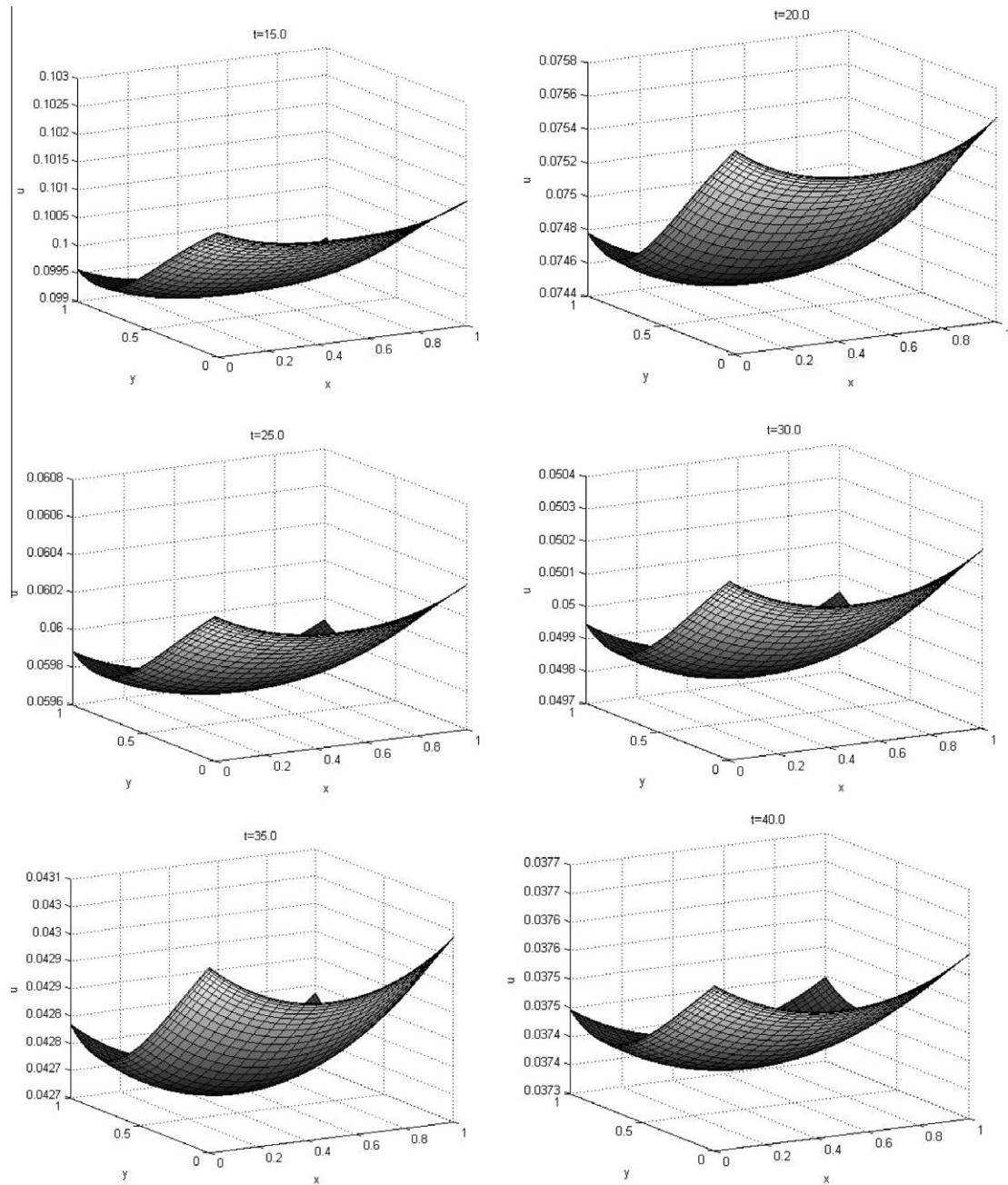


Fig. 3 (continued)

Table 1

Convergence and accuracy of numerical solution of Example-1 at (0.1, 0.9) at different grid points.

t	Number of grid points in x and y direction							
	15×15		17×17		23×23		25×25	
	u	v	u	v	u	v	u	v
0.5	0.65942	2.25341	0.65923	2.25387	0.65904	2.25393	0.65897	2.25402
1.0	0.38609	2.78468	0.38449	2.78649	0.38811	2.78206	0.38838	2.78161
5.0	0.43055	5.41028	0.42925	5.40827	0.42915	5.40555	0.42936	5.40376

Table 2

Convergence and accuracy of numerical solution of Example-2 at (0.1,0.9) at different grid points.

t	Number of grid points in x and y direction							
	11×11		21×21		23×23		25×25	
	u	v	u	v	u	v	u	v
0.5	0.35640	0.15449	0.35635	0.15446	0.35632	0.15443	0.35633	0.15443
1.0	0.54724	0.46505	0.54705	0.464634	0.54698	0.46650	0.54697	0.46651
5.0	4.69927	0.32267	4.69060	0.32328	4.68809	0.32346	4.68815	0.32366

Table 3

Convergence and accuracy of numerical solution of Example-3 at (0.3,0.7) at different grid points.

t	Number of grid points in x and y direction							
	15×15		17×17		23×23		25×25	
	u	v	u	v	u	v	u	v
0.5	2.70500	0.39520	2.70560	0.39533	2.70618	0.39547	2.70618	0.39548
1.0	2.42060	0.40038	2.42072	0.40047	2.42088	0.40048	2.42088	0.40048
5.0	2.09934	0.49932	2.09982	0.49946	2.00104	0.49955	2.00105	0.49954

$$\frac{du_{ij}}{dt} = B + u_{ij}^2 v_{ij} - (A + 1)u_{ij} + \alpha \left(\sum_{k=1}^N a_{i,k}^{(2)} u_{k,j} + \sum_{k=1}^M b_{j,k}^{(2)} u_{i,k} \right), \quad (11)$$

$$\frac{dv_{ij}}{dt} = Au_{ij} - u_{ij}^2 v_{ij} + \alpha \left(\sum_{k=1}^N a_{i,k}^{(2)} v_{k,j} + \sum_{k=1}^M b_{j,k}^{(2)} v_{i,k} \right) \quad (12)$$

with initial conditions

$$\begin{aligned} u(x_i, y_j, 0) &= f(x_i, y_j), \quad (x_i, y_j) \in R, \\ v(x_i, y_j, 0) &= g(x_i, y_j), \quad (x_i, y_j) \in R \end{aligned} \quad (13)$$

boundary conditions on the boundary ∂C of the square C can be discretized as below

$$\sum_{k=1}^N a_{1,k}^{(1)} u_{k,j} = \sum_{k=1}^N a_{N,k}^{(1)} u_{k,j} = 0, \quad j = 1, 2, \dots, M, \quad (14)$$

$$\sum_{k=1}^M b_{1,k}^{(1)} u_{i,k} = \sum_{k=1}^M b_{M,k}^{(1)} u_{i,k} = 0 \quad i = 1, 2, \dots, N, \quad (15)$$

$$\sum_{k=1}^N a_{1,k}^{(1)} v_{k,j} = \sum_{k=1}^N a_{N,k}^{(1)} v_{k,j} = 0, \quad j = 1, 2, \dots, M, \quad (16)$$

$$\sum_{k=1}^M b_{1,k}^{(1)} v_{i,k} = \sum_{k=1}^M b_{M,k}^{(1)} v_{i,k} = 0 \quad i = 1, 2, \dots, N. \quad (17)$$

Eq. (14) can written as

$$a_{1,1}^{(1)} u_{1,j} + a_{1,N}^{(1)} u_{N,j} = - \sum_{k=2}^{N-1} a_{1,k}^{(1)} u_{k,j}, \quad (18)$$

$$a_{N,1}^{(1)} u_{1,j} + a_{N,N}^{(1)} u_{N,j} = - \sum_{k=2}^{N-1} a_{N,k}^{(1)} u_{k,j}. \quad (19)$$

Solving the Eqs. (18) and (19), we have

$$u_{1,j} = \frac{1}{AXU} \sum_{k=2}^{N-1} \left(a_{N,N}^{(1)} a_{1,k}^{(1)} - a_{1,N}^{(1)} a_{N,k}^{(1)} \right) u_{k,j}, \quad (20)$$

$$u_{Nj} = \frac{1}{AXU} \sum_{k=2}^{N-1} \left(a_{1,1}^{(1)} a_{N,k}^{(1)} - a_{N,1}^{(1)} a_{1,k}^{(1)} \right) u_{kj}, \quad (21)$$

for $j = 1, 2, \dots, M$, where $AXU = a_{1,N}^{(1)} a_{N,1}^{(1)} - a_{1,1}^{(1)} a_{N,N}^{(1)}$.

Similarly, from Eq. (16), we have

$$v_{1j} = \frac{1}{AXV} \sum_{k=2}^{N-1} \left(a_{N,N}^{(1)} a_{1,k}^{(1)} - a_{1,N}^{(1)} a_{N,k}^{(1)} \right) v_{kj}, \quad (22)$$

$$v_{Nj} = \frac{1}{AXV} \sum_{k=2}^{N-1} \left(a_{1,1}^{(1)} a_{N,k}^{(1)} - a_{N,1}^{(1)} a_{1,k}^{(1)} \right) v_{kj}, \quad (23)$$

for $j = 1, 2, \dots, M$, where $AXV = a_{1,N}^{(1)} a_{N,1}^{(1)} - a_{1,1}^{(1)} a_{N,N}^{(1)}$.

In the similar way solve the Eqs. (15) and (17), we have

$$u_{i,1} = \frac{1}{AYU} \sum_{k=2}^{M-1} \left(b_{M,M}^{(1)} b_{1,k}^{(1)} - b_{1,M}^{(1)} b_{M,k}^{(1)} \right) u_{ik}, \quad (24)$$

$$u_{i,M} = \frac{1}{AYU} \sum_{k=2}^{M-1} \left(b_{1,1}^{(1)} b_{M,k}^{(1)} - b_{M,1}^{(1)} b_{1,k}^{(1)} \right) u_{ik}, \quad (25)$$

$$v_{i,1} = \frac{1}{AYV} \sum_{k=2}^{M-1} \left(b_{M,M}^{(1)} b_{1,k}^{(1)} - b_{1,M}^{(1)} b_{M,k}^{(1)} \right) v_{ik}, \quad (26)$$

$$v_{i,M} = \frac{1}{AYV} \sum_{k=2}^{M-1} \left(b_{1,1}^{(1)} b_{M,k}^{(1)} - b_{M,1}^{(1)} b_{1,k}^{(1)} \right) v_{ik}, \quad (27)$$

for $i = 1, 2, \dots, N$, where $AYU = b_{1,M}^{(1)} b_{M,1}^{(1)} - b_{1,1}^{(1)} b_{M,M}^{(1)}$.

where $u(x_i, y_j, t)$ and $v(x_i, y_j, t)$ is referred as u_{ij} and v_{ij} and $a_{ij}^{(1)}$, $a_{ij}^{(2)}$, $b_{ij}^{(1)}$ and $b_{ij}^{(2)}$ are the weighting coefficients of first and second order partial derivatives of u , v with respect to x and y .

The system of ordinary differential Eqs. (11)–(13), (18)–(25) are solved by Pike and Roe's fourth-stage RK4 scheme [14] for the event that function f contains no explicit dependent on t .

4. Selection of grid points

The stability of the DQM depends on the eigen-values of differential quadrature discretization matrices. These eigen-values in turn very much depend on the distribution of grid points. It has been shown by Shu [16] in his book that the uniform grid points distribution does not give stable solution which we have also notice in our numerical experiments. According to Shu the stable solution can be obtained when Chebyshev–Gauss–Lobatto grid points are chosen. The Chebyshev–Gauss–Lobatto grid points are given by

$$\begin{aligned} x_i &= \frac{1}{2} \left(1 - \cos \frac{((i-1)\pi)}{N-1} \right) L_x, \\ y_j &= \frac{1}{2} \left(1 - \cos \frac{((j-1)\pi)}{M-1} \right) L_y \quad i = 1, 2, \dots, N; \quad j = 1, 2, \dots, M, \end{aligned} \quad (28)$$

where L_x and L_y are the rectangular domain length along x -axis and y -axis respectively.

The convergence of the present approach is demonstrated by the Tables 1–3. These Tables show that as soon as grid points increase, we get stable solutions. The Figures also show the stable solutions.

5. Numerical experiments and discussions

In this Section, we apply DQM on three test problems which are taken from literature by different researchers to show its applicability. In the whole numerical experiment done in all the three Examples, we have used the time step $\Delta t = 0.001$.

Problem 1 [19]. Consider the Brusselator system (1) and (2) subject to Neumann boundary conditions (4) and with the initial conditions

$$u(x, y, 0) = 0.5 + y \quad v(x, y, 0) = 1 + 5x. \quad (29)$$

The constants A , B and α are taken 1, 3.4 and 0.002 respectively similar to [19]. Table 1 shows that the numerical solutions are converging as the grid points are increased. The concentration profiles of u and v computed at time from $t = 1$ to $t = 50$ are

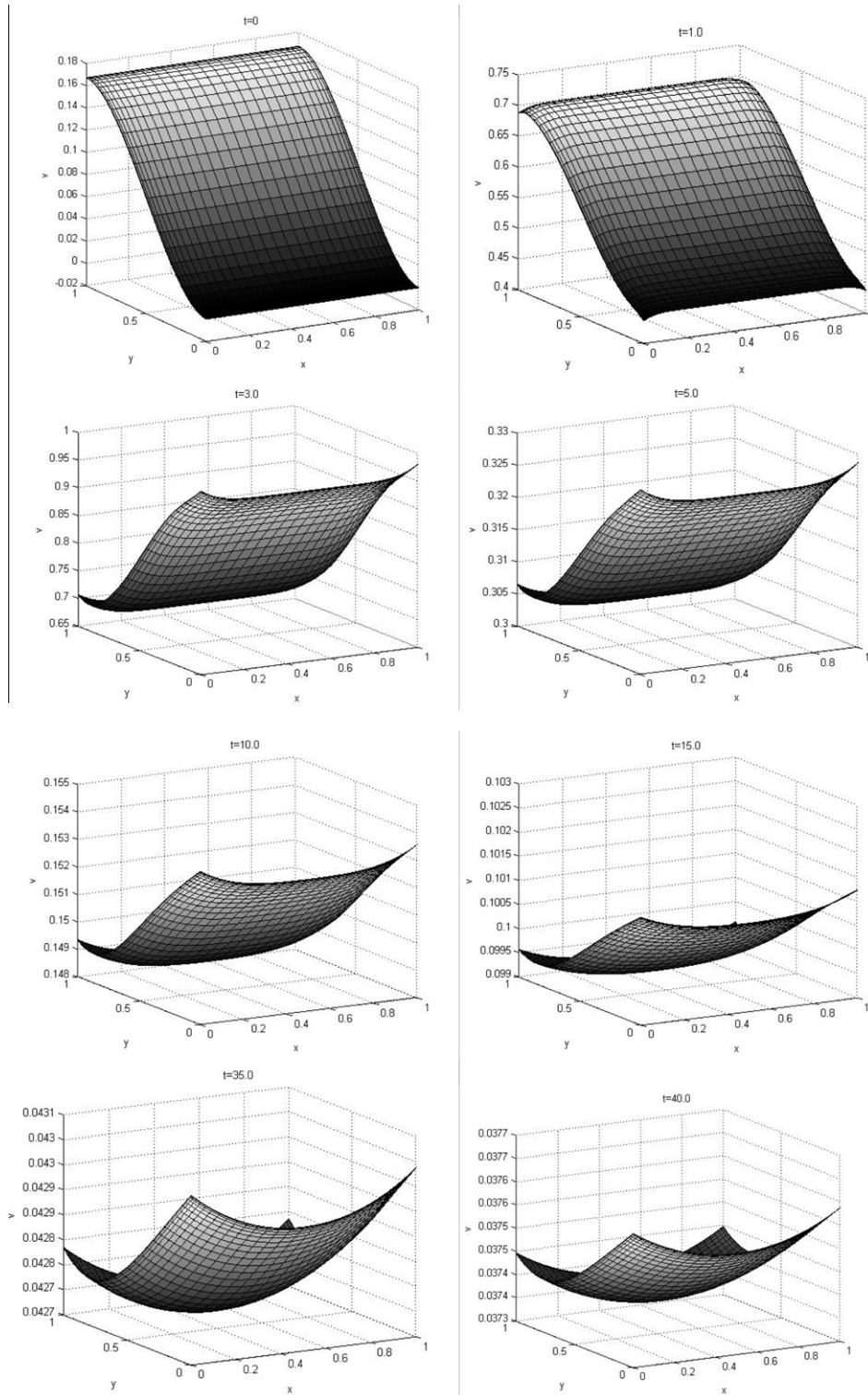


Fig. 4. Concentration profiles of ν of Example 2 at different time $t = 0, 1.0, \dots, 40.0$.

depicted in the Figs. 1 and 2. It is clear from the Figs. 1 and 2 that for these values of α and time step, the numerical method is stable with the combination of $A = 1$ and $B = 3.4$. It is found that the concentration profiles of u and ν are similar to [19].

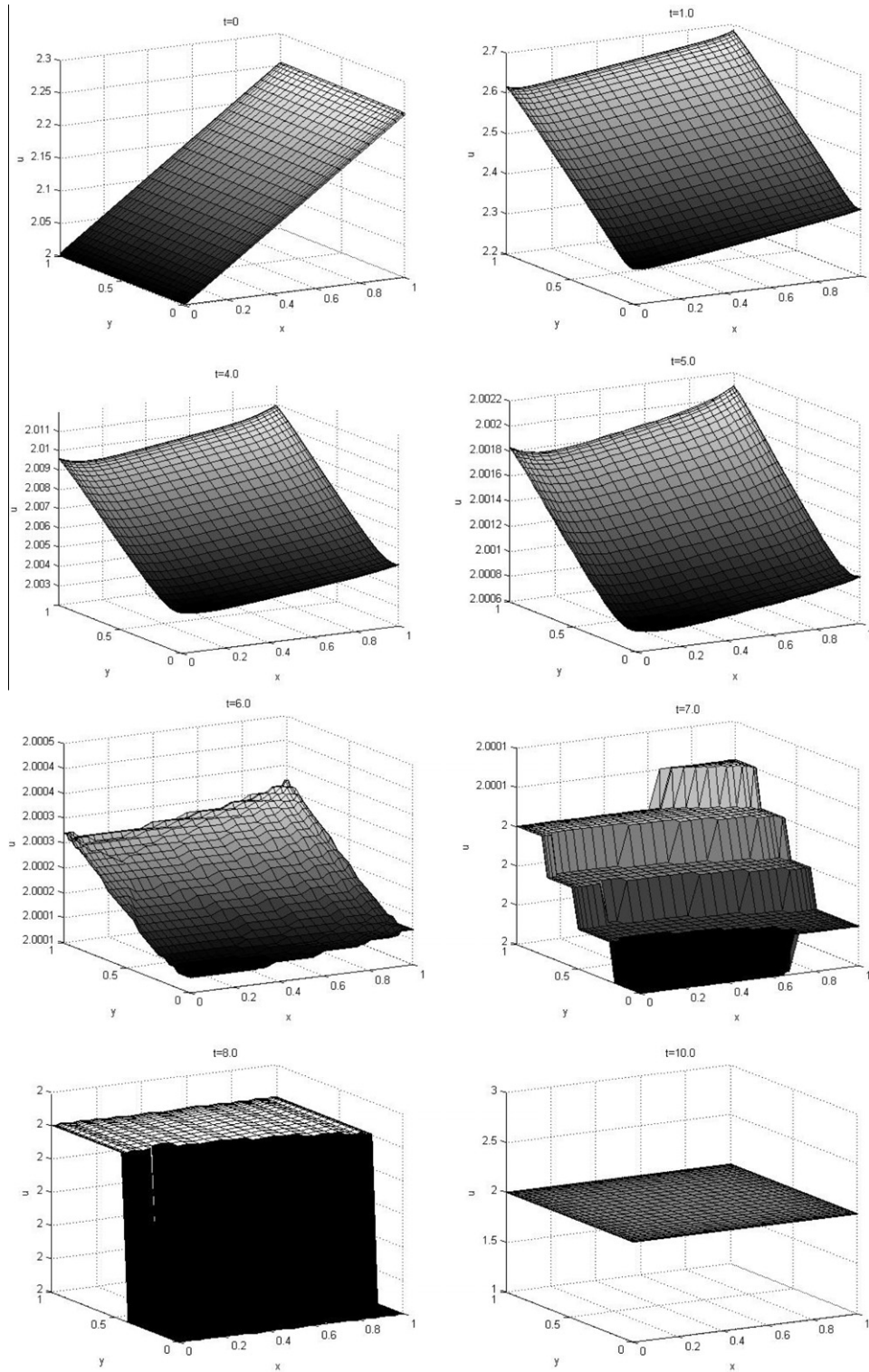


Fig. 5. Concentration profiles of u of Problem 3 at different time $t = 0, 1.0, \dots, 10.0$.

Problem 2 [13]. In this Example, we have considered the non linear PDEs of Brusselator system (1) and (2) subject to Neumann boundary conditions (4) and with the initial conditions

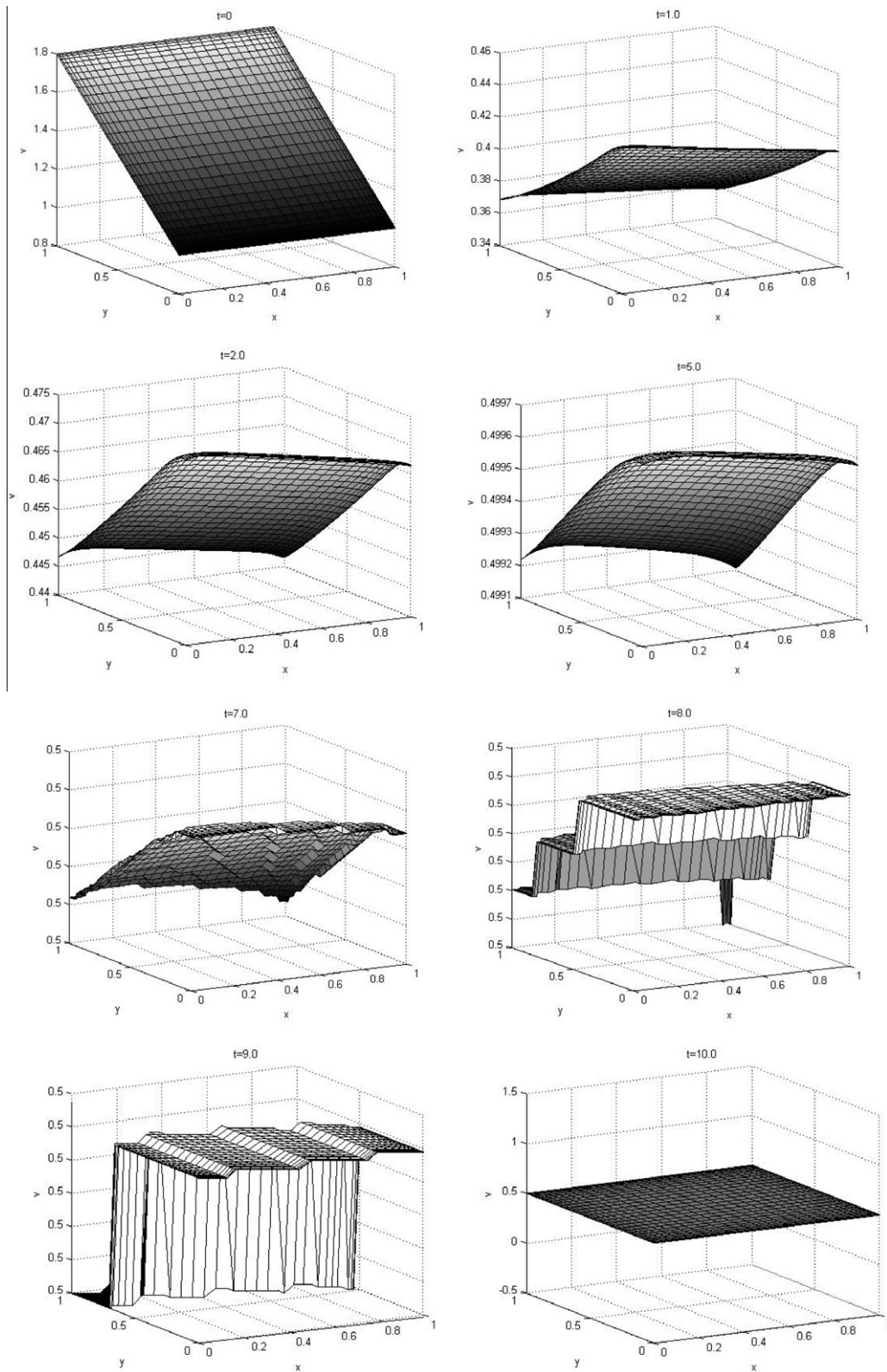


Fig. 6. Concentration profiles of v of Example 3 at different time $t = 0, 1.0, \dots, 10.0$.

$$u(x, y, 0) = 0.5x^2 - \frac{1}{3}x^3 \quad v(x, y, 0) = 0.5y^2 - \frac{1}{3}y^3. \quad (30)$$

The constants A , B and α are taken 0.5, 1 and 0.002 respectively similar to [13]. The Figs. 3 and 4 show the concentration profiles of u and v at time from $t = 1$ to $t = 40$. It is clear from Figs. 3 and 4 that for these values of α and time step, the numerical method is stable with the combination of $A = 0.5$ and $B = 1$. Table 2 shows the convergence and accuracy of the numerical solutions.

Problem 3 [10]. Consider the Brusselator system (1) and (2) with Neumann boundary conditions (4) and with the initial conditions

$$u(x, y, 0) = 2.0 + 0.25y \quad v(x, y, 0) = 1.0 + 0.8x. \quad (31)$$

The constants A , B and α are taken 1, 2 and 0.002 respectively considered in [10]. Table 3 shows the convergence of numerical solutions at different grid points. The concentration profiles of u and v computed at time from $t = 1$ to $t = 10$, are depicted in Figs. 5 and 6. It is clear from Figs. 5 and 6 that for these values of α and time step; the numerical method is stable with the combination of $A = 1$ and $B = 2$.

6. Conclusion

In this paper, a polynomial based differential quadrature method (DQM) is employed for numerical solutions of two-dimensional non linear reaction–diffusion Brusselator system. The method is simple and straight forward which gives a system of ordinary differential equations. The resulting system of ordinary differential equations is solved by a four-stage RK4 method. The method is applied on three test problems given in the literature. Convergence and stability of the method is also examined numerically. It is shown in the Tables that the accuracy of the method depends on the number of grid points chosen for DQM. The strength of the method lies in its easiness to apply.

Acknowledgements

The author Ram Jiwari thankfully acknowledges the financial assistance provided by UGC India.

References

- [1] G. Nicolis, I. Prigogine, *Self-Organization in Nonequilibrium Systems*, Wiley-Interscience, 1977.
- [2] I. Prigogine, R. Lefever, Symmetry breaking instabilities in dissipative systems, *J. Chem. Phys.* 48 (1968) 1695.
- [3] J. Tyson, Some further studies of nonlinear oscillations in chemical systems, *J. Chem. Phys.* 58 (1973) 3919.
- [4] A. Mohebbi, M. Dehghan, High-order compact solution of the one-dimensional heat and advection-diffusion equations, *Appl. Math. Model.* 34 (2010) 3071–3084.
- [5] M. Dehghan, Weighted finite difference techniques for the one-dimensional advection-diffusion equation, *Appl. Math. Comput.* 147 (2004) 307–319.
- [6] M. Dehghan, On the numerical solution of the one-dimensional convection-diffusion equation, *Math. Prob. Eng.* (2005) 61–74.
- [7] M. Dehghan, Time-splitting procedures for the solution of the two-dimensional transport equation, *Kybernetes* 36 (2007) 791–805.
- [8] M. Dehghan, Numerical solution of the three-dimensional advection-equation, *Appl. Math. Comput.* 150 (2004) 5–19.
- [9] M. Dehghan, A. Hamidi, M. Shakourifar, The solution of coupled Burgers' equation using Adomain-Pade technique, *Appl. Math. Comput.* 189 (2007) 1034–1047.
- [10] E.H. Twizell, A.B. Gumel, Q. Cao, A second-order scheme for the 'Brusselator' reaction–diffusion system, *J. Math. Chem.* 26 (1999) 297–316.
- [11] G. Adomian, The diffusion-Brusselator equation, *Comput. Math. Appl.* 29 (1995) 1–3.
- [12] A.M. Wazwaz, The decomposition method applied to systems of partial differential equations and to the reaction–diffusion Brusselator model, *Appl. Math. Comput.* 110 (2000) 251–264.
- [13] W.T. Ang, The two-dimensional reaction-diffusion Brusselator system: a dual-reciprocity boundary element solution, *Eng. Anal. Bound Elem.* 27 (2003) 897–903.
- [14] J. Pike, P.L. Roe, Accelerated convergence of Jameson's finite volume Euler scheme using Van Der Houwen integrators, *Comput. Fluids* 13 (1985) 223–236.
- [15] R. Bellman, B.G. Kashef, J. Casti, Differential quadrature: a technique for the rapid solution of nonlinear partial differential equations, *J. Comput. Phys* 10 (1972) 40–52.
- [16] Chang, Shu, *Differential Quadrature and its Application in Engineering*, Springer-Verlag London Ltd., Great Britain, 2000.
- [17] J.R. Quan, C.T. Chang, New insights in solving distributed system equations by the quadrature methods-I, *Comput. Chem. Eng.* 13 (1989) 779–788.
- [18] J.R. Quan, C.T. Chang, New insights in solving distributed system equations by the quadrature methods-II, *Comput. Chem. Eng.* 13 (1989) 1017–1024.
- [19] J.G. Verwer, W.H. Hundsdorfer, B.P. Sommeijer, Convergence properties of the Runge–Kutta–Chebyshev method, *Numer. Math.* 57 (1990) 157–178.