The Numerical Study Of Reaction-Diffusion Equation Systems Using Trigonometric Cubic B-Spline Differential Quadrature Method

Nithin Thomas Aji, Varun Joshi*

Department of Mathematics, School of Chemical Engineering and Physical Sciences, Lovely Professional University, Phagwara 144411, Punjab, India.
**E mail: varunjoshi20@yahoo.com*

Abstract : The trigonometric differential quadrature method has been utilized to compute the numerical solution of the reaction-diffusion equation system. To compute the approximate space derivatives in this method we use trigonometric b-spline basis function. Under the considered equation different forms of the linear and non-linear model are considered for the numerical solution and obtained results are presented at different time levels.

1. Introduction

In mathematics many incidents can be modeled by using a reaction-diffusion equation system. RDS are significant nonlinear wave conditions that have gotten expanding consideration from scientists as of late [1]. There are many applications for RDS in physics, chemistry, biology and in engineering such as gene propagation [2, 3]. Both forms and some indications of nature are labeled RDS. Berestycki and Hamel introduced a generalized concept of the traveling wave, named the transition wave, which is still a special kind of the entire solution and describes a general class of wave-like solutions for RDE in general heterogeneous media. Another researcher Onarcan has used the same system to find numerical solutions with collocation method with TCB basis. Mittal and Rohila have solved RDS by improved CB-spline DQM [4]. Ruan and Feng found the traveling wave solution this system [5]. Homogenization results for this system is computed in the doctoral work of Cardone and Preugia [6]. Karl used the first passage Monte Carlo algorithms to solve the equations [7]. Functional separable solutions of these equations with the variable coefficient in the research paper of Polyanin [8]. The DQM constructed on the spline function is required for two causes for the differential equations' numerical solution. Firstly in the overall region, it will be easy to implement and secondly it approximate the derivative of the function is given at any particular point as summation of function values**.** DQM had been studied globally and its adaptability had been recognized in various applications. Sine and cosine expansion and Lagrange interpolation related quadrature methods are mostly used nowadays. By using DQM we should be able to estimate the functional derivatives in space at each point with the weighted summation functional values. To compute the weighting coefficients there are plenty of ways possible in literature. Quan and Chang's methodology, Shu's methodology are a good example of that [9, 10]. Recently researchers like O.H. Muhammed and M.A Saeed [11] has used the same method to solve thin plate problems. For several nonlinear partial differential equations Korkmaz and Dag [12, 13] implimented DQ based on cosine expansion and sine expansion process. For non-linear PDE, Mittal [14] recommended the polynomial based DQM. It has started to obtain the differential equation using TB-splines for the numerical methods. The trigonometric B-spline is not well-known while many polynomial B-spline procedures have been established to find its solution.

Nikolis and Seimenis [15] in the regular form, learned the technique of quadratic and CTB to find solution of the ODE. Arora and Joshi [16] studied the Hyperbolic Telegraph and Fisher's equation with B-spline and TB-spline by DQM. Same equation by using cubic TB-spline with DQM was elucidated by Tamsir and Dhimam [17]. The wave equation by CTB is studied numerically by Mat Zin and Majid [18]. Hamid et al [19]. Gupta and Kumar [20] have solved linear second-order two-point and single two-point boundary value problems by using CTB collocation method.

2. Reaction Diffusion Equation System

The non-linear RDS is categorized arithmetically as the semi-linear parabolic PDE which comprises Gray–Scott models, Schnakenberg, Brusselato and more. A transition wave can also be viewed as a spatial the transition between the two different limiting states here we analysis the RDE with bistable nonlinearity, includes the following system of equation with free boundaries

$$U_t = a_1 U_{xx} + b_1 U + c_1 V + d_1 U^2 V + e_1 UV + m_1 UV^2 + n_1 \quad (1)$$

$$V_t = a_2 U_{xx} + b_2 U + c_2 V + d_2 U^2 V + e_2 UV + m_2 UV^2 + n_2. \quad (2)$$

The spatial realm is limited to a finite interval for computational purposes $[x_0, x_n]$.The conditions are

$$U(x,0) = U_0(x), \ \ V(x,0) = V_0(x), x \in \Omega \quad (3)$$

3. Cubic Trigonometric B-Spline

The word "B-spline" was created by Schoenberg. For this function of the same order specified on one knot, B-Spline functions are simple, i.e. all potential spline functions that be generated by a linear B-Splines combination and there can be only one distinctive combination for each spline function. The significance of trigonometric polynomials in different areas, such as electronics or medicine has increased. The intermission [a, b] is separated into equal subintervals with points $x_i, i = 0,1, \dots N$ with step length $l = \frac{b-a}{N}$ and $a = x_0, b = x_N$. Trigonometric cubic B-spline $TCB_i(x), i = -1, N+1$ are distinct at these points at the intermission [a, b] with points $x_{N-2}, x_{N-1}, x_{N+1}, x_{N+2}$ external to the problems are as follows:

$$TCB_i = \frac{1}{\theta}\begin{cases} \delta^3(x_{i-2}), & x \in [x_{i-2}, x_{i-1}] \\ \delta(x_{i-2})\begin{pmatrix}\delta(x_{i-2})\phi(x_i) + \\ \phi(x_{i+1})\delta(x_{i-1})\end{pmatrix} + \phi(x_{i+2})\delta^2(x_{i-1}), & x \in [x_{i-1}, x_i] \\ \delta(x_{i-2})\phi^2(x_{i+1}) + \phi(x_{i+2})\begin{pmatrix}\delta(x_{i-1})\phi(x_{i+1}) + \\ \phi(x_{i+2})\delta(x_i)\end{pmatrix}, & x \in [x_i, x_{i+1}] \\ \phi^3(x_{i+2}), & x \in [x_{i+1}, x_{i+2}] \\ 0, & otherwise \end{cases} \quad (4)$$

Tables: 1.1: The values of basis function and their derivatives at different node points

x	$TCB_i(x_k)$	$TCB_i'(x_k)$	$TCB_i''(x_k)$
x_{i-2}	0	0	0

x_{i-1}	$\sin^2\left(\frac{l}{2}\right)\csc(l)\csc\left(\frac{3l}{2}\right)$	$-\frac{3}{4}\csc\left(\frac{3l}{2}\right)$	$\frac{3(1+3\cos(l))\csc^2\left(\frac{l}{2}\right)}{16\left(2\cos\left(\frac{l}{2}\right)+\cos\left(\frac{3l}{2}\right)\right)}$
x_i	$\frac{2}{1+2\cos(l)}$	0	$\frac{-3\cot^2\left(\frac{3l}{2}\right)}{2+4\cos(l)}$
x_{i+1}	$\sin^2\left(\frac{l}{2}\right)\csc(l)\ \csc\left(\frac{3l}{2}\right)$	$\frac{3}{4}\csc\left(\frac{3l}{2}\right)$	$\frac{3\left(1+3\cos l\ \csc^2\left(\frac{l}{2}\right)\right)}{16\left(2\cos\left(\frac{l}{2}\right)+\cos\left(\frac{3l}{2}\right)\right)}$
x_{i+2}	0	0	0

Where $\delta(x_i) = \sin\frac{(x-x_i)}{2}, \phi(x_i = \sin\frac{x_i-x}{2}, \theta = \sin\frac{l}{2}\sin l \sin\frac{3l}{2}$. All of them is non-negative on the sub elements $[x_{i-2}, x_{i+2}]$. The values of $TCB_i(x), TCB_i'(x), TCB_i''(x)$ at knots x_i's can be calculated from Eq. 3 as in Table.1.1

4. Proposed Scheme

It is a scheme for fairly accurate the solutions of ODE and PDE numerically. It approximate the functional derivatives at any specified distinct points as the linear summation. Considering that the leading coefficient depend on the spacing by spatial grid, we consider M mesh points on the real plane with step length l. The following equations give the DQ discretization of the first and second derivatives at x_i:

$$u_x(x_i,t) = \sum_{J=1}^{k} w_{ij}^{(1)} u(x_j,t),\ i = 1,2,\dots,M \qquad (5)$$

$$u_{xx}(x_i,t\ ) = \sum_{j=1}^{N} w_{ij}^{(2)} u\left(x_j,t\right),\quad j = 1,2,\dots,M \qquad (6)$$

Where $w_{ij}^{(1)}$ and $w_{ij}^{(2)}$ are first and second derivatives coefficients.

5. Numerical Solutions and Discussion

This section compares the efficacy and accuracy proposed on the given equation method for RDS. The findings acquired for each model would be related with the reference studies. The scheme's consistency is calculated as per the following differential error:

$$L_2 = \sqrt{h \times \sum (numerical\ value - exact\ value)^2}$$

$$L_\infty = max|numerical\ value - exact\ value|$$

5.1 Linear Problem

The problem was solved in linear form to measure error levels to check the process:

$$U_t = d_1 U_{xx} - a_1 U + V \qquad (7)$$

$$V_t = d_1 V_{xx} - b_1 V \qquad (8)$$

Which has the following analytical solution given:

$$U(x,t) = \left(e^{(a_1+d_1)t} + e^{-(b_1+d_1)t}\right)\cos(x), \qquad (9)$$

$V(x,t) = (a_1 - b_1)\left(e^{-(b_1+d_1)t}\right)\cos(x).$ (10)

In computational estimation three separate cases were considered in terms of predominance of reaction or diffusion. As $t = 0$ in [21] solutions, the initial conditions can be obtained. The boundary conditions are defined as follows when the solution area is selected as $(0, \frac{\pi}{2})$ interval:

$U_x(0,t) = 0 \qquad U\left(\frac{\pi}{2}, t\right) = 0$ (11)

$V_x(0,t) = 0 \qquad V_x\left(\frac{\pi}{2}, t\right) = 0$ (12)

In the numerical calculation the program will be ran up to $t = 1, 2, 3, 4$. For $N = 81$ and Δt, RDS is observed for diverse constants a_1, b_1, d_1. The error value L_∞ and L_2 are obtainable in the tables. The system (1) is calculated for constraints $a_1 = 100, b_1 = 1, d_1 = 0.001$ which is reaction subjugated with result of RDS is obtained. Again the recommended technique offers the same degree of the errors as shown in Table 1.2

Table 1.2 Error norm L_2 & L_∞ for dominant diffusion case for $a_1 = 100, b_1 = 1, d_1 = 0.001$ and $N = 81$

Error/Time	t=1	t=2	t=3	t=4
$L_2(u)$	5.6108e-06	2.1656e-06	8.2438e-07	3.1158e-07
$L_\infty(u)$	3.6790e-05	1.3521e-05	4.9690e-06	1.8262e-06
$L_2(V)$	5.5547e-04	2.1440e-04	8.1613e-05	3.8047e-05
$L_\infty(V)$	0.0036	0.0013	4.9193e-04	1.8079e-04

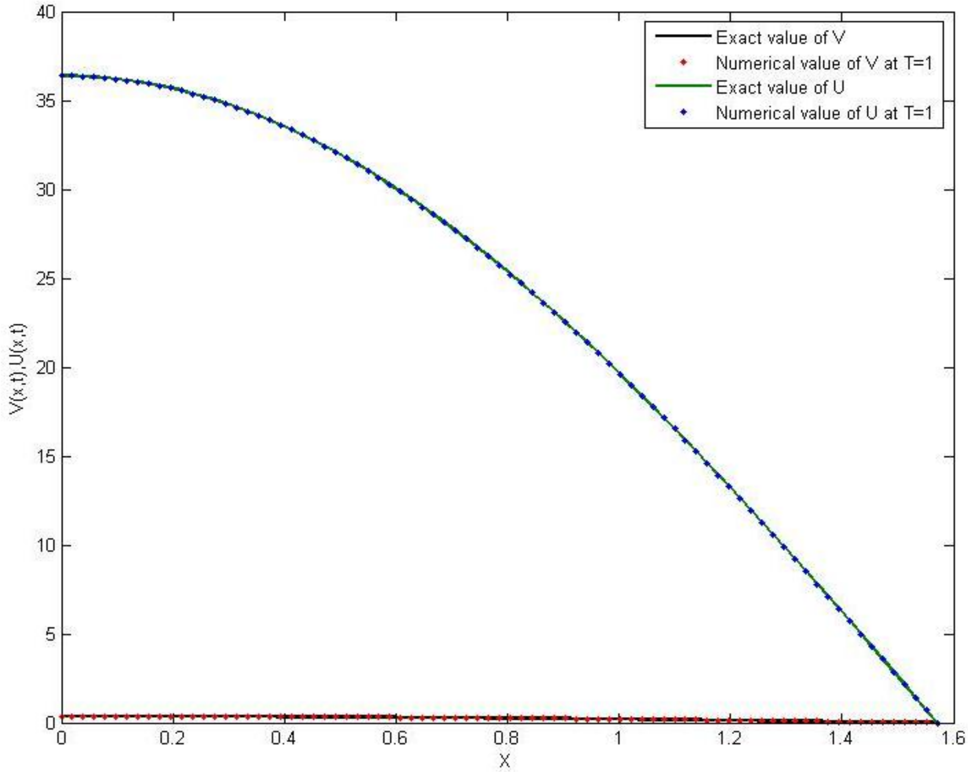

Figure 1: Exact and numerical solution of U and V at $t = 1$.

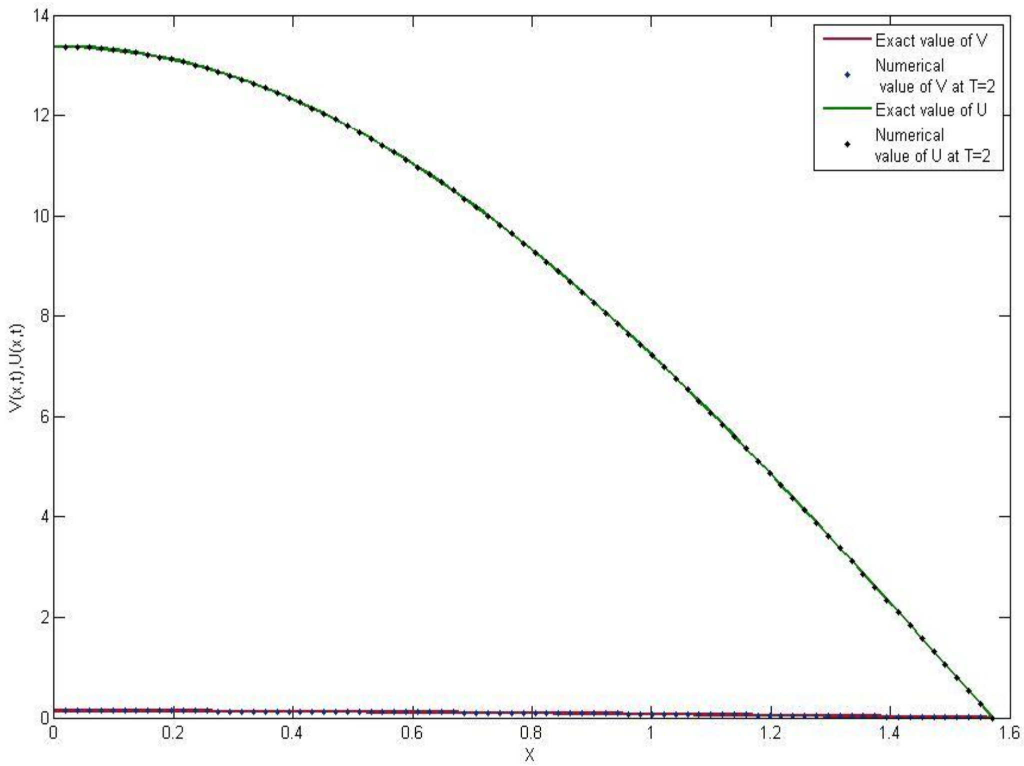

Figure 2: Exact and numerical solution of U and V at $t = 2$.

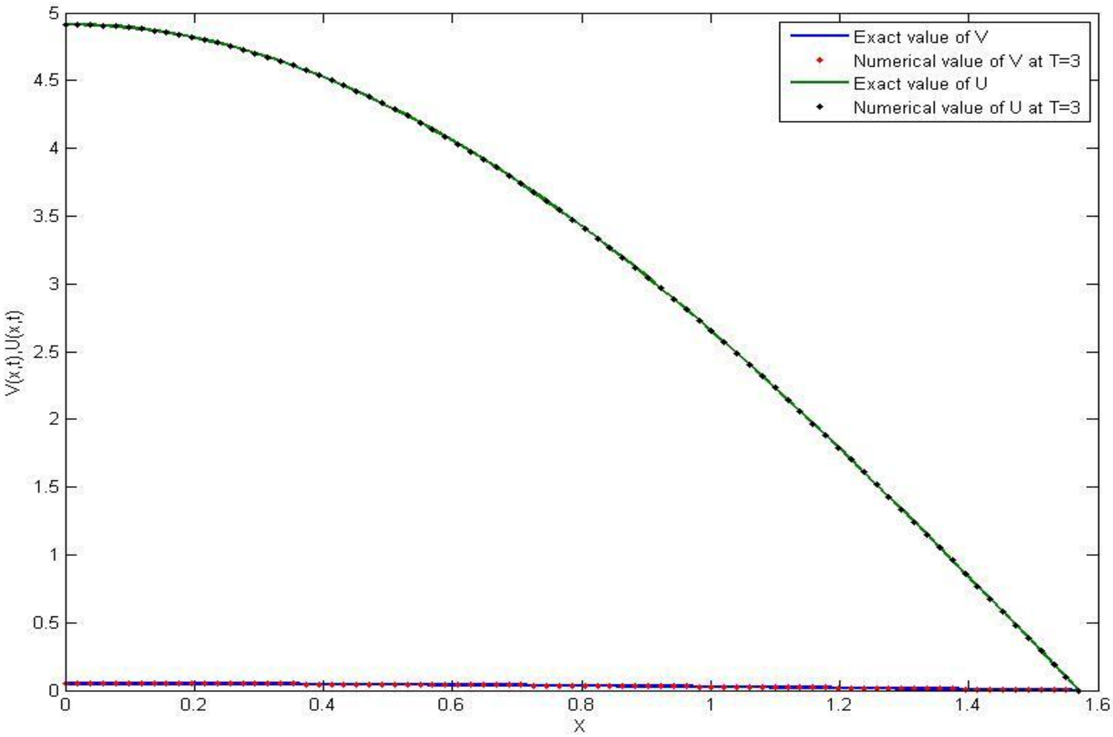

Figure 3: Exact and numerical solution of U and V at $t = 3$.

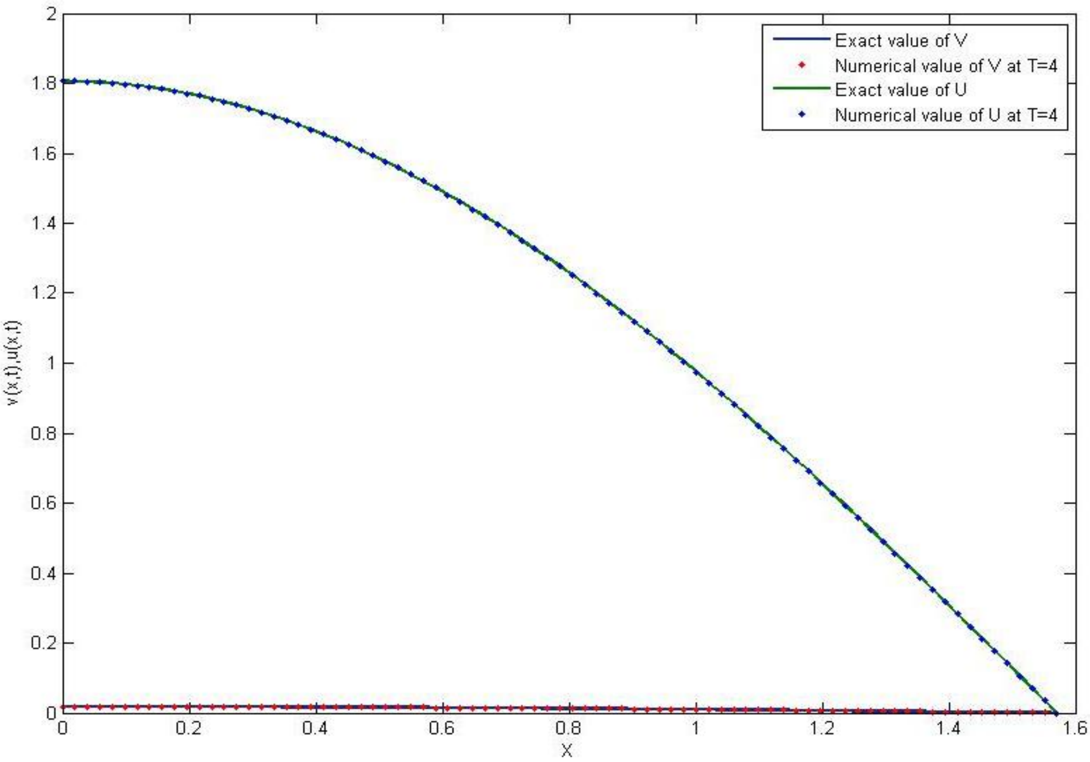

Figure 3: Exact and numerical solution of U and V at $t = 4$.

5.2 Non-linear problem (Brussellator model)

Another different forms of non-linear RDS is the Brusselator model that predicts oscillations in the chemical reaction. Prigogine and Lefever [21] build the basis for the chemical reactions with two components:

$$U_t = e_1 U_{xx} + A + U^2 V - (B+1)U, \qquad (13)$$
$$V_t = e_2 V_{xx} + BU - U^2 V. \qquad (14)$$

Where $e_1 \& e_2$ are constants of diffusion, x is the spatial coordinate and U, V is the concentration-representing x and t variables. Initial conditions are

$$U(x,0) = 0.5, \quad V(x,0) = 1 + 5x\ . \qquad (15)$$

And the second derivative initial boundary conditions for this test problem replaces the first derivative initial boundary condition as follows:

$$U_{xx}(x_0,t) = 0 \quad U_{xx}(x_N,t) = 0, \qquad (16)$$
$$V_{xx}(x_0,t) = 0 \quad V_{xx}(x_N,t) = 0. \qquad (17)$$

In the system (4) the coefficients $e_1 = e_2 = 10^{-4}$, $A = 1$ and $B = 3.4$. The solutions are obtained in region [0, 1] with step length $N = 101$, at time $\Delta t = 0.01$ and the program is run by $t = 1,2,3,4,50,60,100$ .The smaller e_1, e_2 is generated with selected steeper wave. Therefore the algorithm gives waves which are equally moving [22-24].

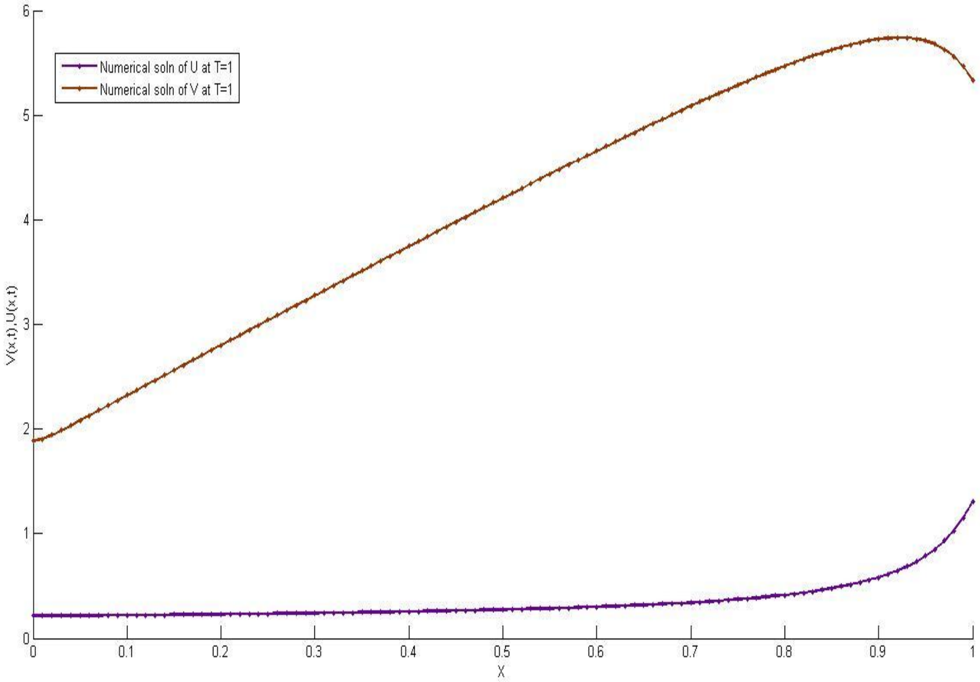

Figure: 4: Exact and numerical solution of U and V at $t = 1$.

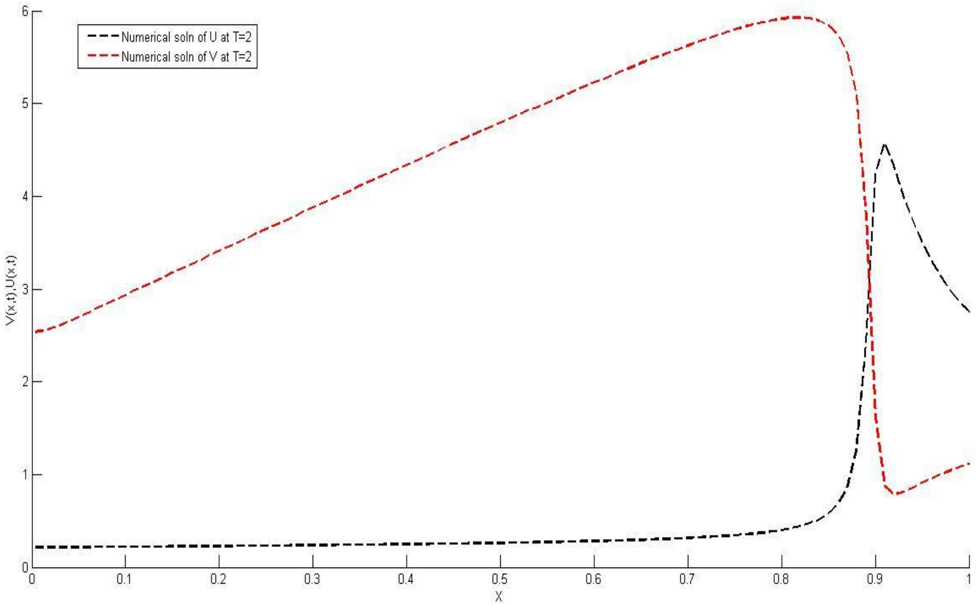

Figure: 5: Exact and numerical solution of U and V at $t = 2$.

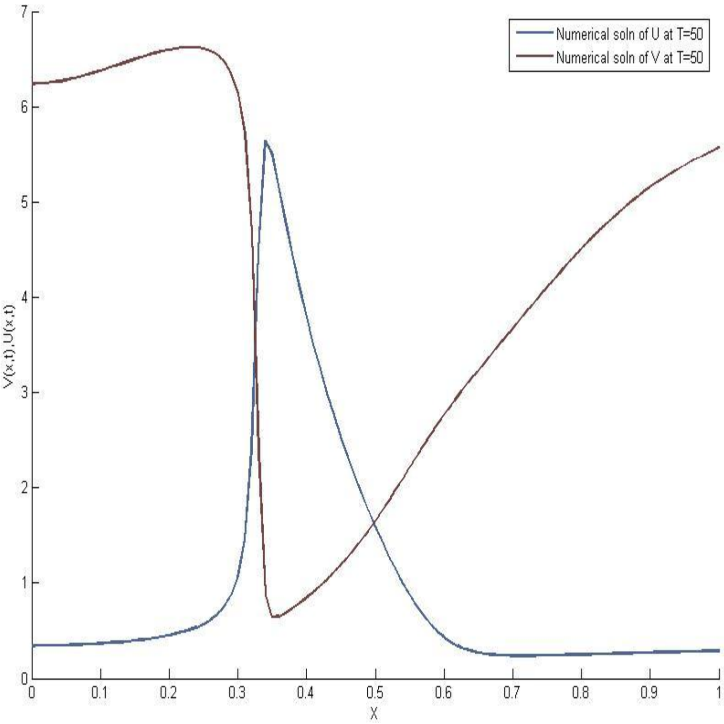

Figure: 6: Exact and numerical solution of U and V at $t = 50$.

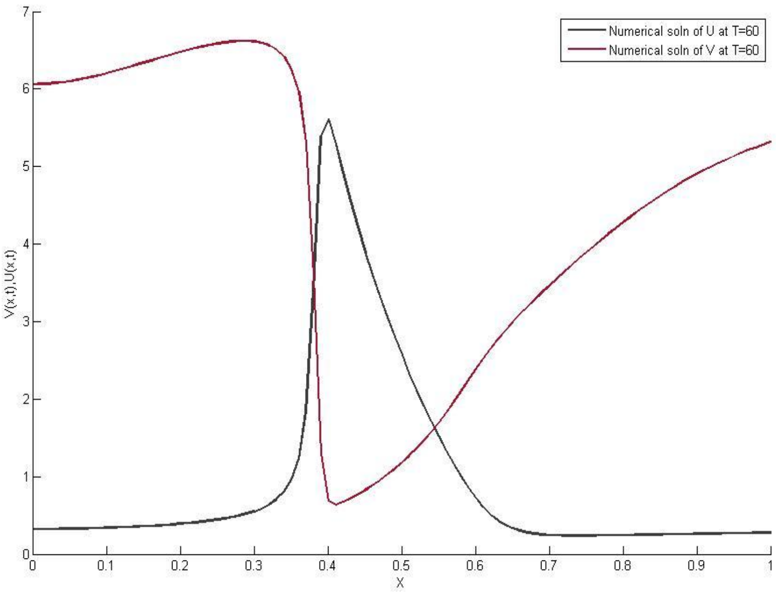

Figure 7: Exact and numerical solution of U and V at $t = 60$.

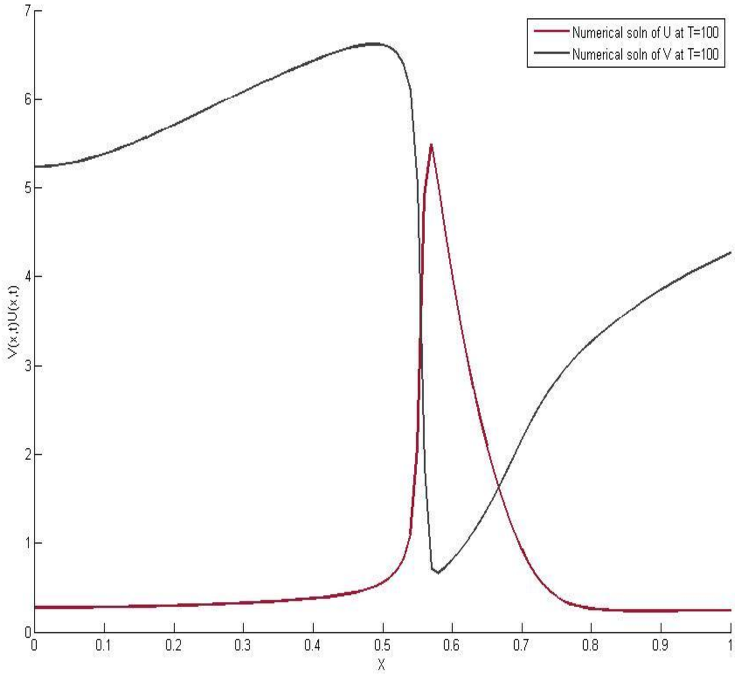

Figure 8: Exact and numerical solution of U and V at $t = 100$.

6. Conclusion

The outcome of the trigonometric cubic B-Spline for the DQM has been sought on getting numerical solutions of the RD equation system. The approach's efficacy and reliability are evaluated for different research problems under consideration. Specific error rates are determined at various periods, or the results in the literature are matched with the numerical solutions achieved using the approach. Solutions of the nonlinear reaction-diffusion equation known as the Linear and nonlinear (Brusselator model) system are simulated suitably by use of the TCB DQM.

References

[1] G. Cardone, Homogenization results for a coupled system of reaction–diffusion Equations. Elsevier (2019).

[2] R.A. Fisher, The wave of advance of advantageous genes. Ann Eugen (1937)

[3] J. Canosa, On a nonlinear diffusion equation describing population growth. IBM J Res Dev (1973).

[4] R.C. Mittal, R. Rohila, Numerical simulation of reaction–diffusion systems by modified cubic B-spline differential quadrature method. Chaos Solitons Fractals (2016).

[5] W. Ruan, W Feng, On traveling wave solutions in general reaction–diffusion systems with time delays. Elsevier (2016).

[6] G. Cardone, C. Perugia, C. Timofte, Homogenization results for a coupled system of reaction–diffusion equations. Elsevier (2019).

[7] S. Karl, First passage Monte Carlo algorithms for solving coupled systems of diffusion-reaction equations Applied Mathematics Lett. ttps://doi.org/10.1016/j.aml.2018.08.018 (2018).

[8] A. D. Polyanin, Functional separable solutions of nonlinear convection–diffusion equations with variable coefficients doi.org/10.1016/j.cnsns.2019.02.022 (2019).

[9] J.R. Quan, C.T. Chang, Newinsights in solving distributed system equations by the quadrature methods- II, Comput. Chem. Eng. 13 Prgamon Press plc (1989)

[10] C. Shu, Differential Quadrature and its Application in Engineering, Athenaeum Press Ltd., Great Britain, (2000).
[11] A. Korkmaz, I. Dag, Shock wave simulations using Sinc differential quadrature method, Eng. Comput. 28 (6) 654–674, (2011).
[12] A. Korkmaz, I. Dag, A differential quadrature algorithm for nonlinear Schrödinger equation, Nonlinear Dynam. 56 (1–2) (2009) 69–83.
[13] R.C. Mittal, R. Jiwari, Numerical study of two-dimensional reaction–diffusion Brusselator system, Appl. Math. Comput. 217 (12) 5404–5415, (2011).
[14] R.C. Mittal, R. Jiwari, A differential quadrature method for solving Burgers'-type equation, Internat. J. Numer. Methods Heat Fluid Flow 22 (7) 880–895, (2012).
[15] A. Nikolis, I. Seimenis, Solving dynamical systems with cubic trigonometric splines. Appl Math E Notes 5:116–123, (2005).
[16] G. Arora, V. Joshi, Comparison of numerical solution of 1Dhyperbolic telegraph equation using B-Spline and trigonometric B-Spline by differential quadrature method. Indian J. Sci. Technol. 9(45). https://doi.org/10.17485/ijst/2016/v9i45/106356 (2016)
[17] M. Tmasir, N.Dhimam, Cubic trigonometric B-spline differential quadrature method for numerical treatment of Fisher's reaction-diffusion equations, Production and hosting by Elsevier B.V. doi.org/10.1016/j.aej.2017.05.007, (2017).
[18] S. M. Zin, Majid, Cubic Trigonometric B-spline Approach to Numerical Solution of Wave Equation World Academy of Science, Engineering and Technology International Journal of Mathematical and Computational Sciences Vol:8, No:10, (2014).
[19] N. N. A. Hamid, A.A. Majid, A.I.M. Ismail, Cubic trigonometric B-spline applied to linear two-point boundary value problems of order two. World Acad. Sci. Eng. Technol 47:478–803 (2010).
[20] Y. Gupta, M. Kumar, A computer based numerical method for singular boundary value problems. Int J Comput Appl 1:0975–8887 (2011).
[21] I.Prigogine, R.Lefever, Symmetry breaking instabilities in dissipative systems. J. Chem. Phys. 48:1695–1700 (1968).
[22] R.C. Mittal and R. Jiwari, Numerical study of two-dimensional reaction-diffusion Brusselator system by differential quadrature method, Taylor and Francis group,(2011)
[23] Farooq, R., & Shankar, R. (2016). Role of structural equation modeling in scale development. *J*ournal of Advances in Management Research.
[24] A.H.D. Cheng, M.A. Goldberg, E.J. Kansa, G. Zammito, Exponential convergence and H-C multiquadric collocation method for partial differential equations, Numerical Methods Partial Differential Equitation 19 (2003) 571–594.