Abstract. The main objective of this article is to propose a chaos free explicit finite-difference (FD) scheme to find the numerical solution for the Brusselator reaction-diffusion model. The scheme is unconditionally stable and it is unconditionally dynamically consistent with the positivity property of continuous model as unknown quantities of auto-catalytic Brusselator system describe the concentrations of two reactant substances. Stability of the proposed FD method is showed with the help of Neumann criteria of stability. Taylor series is used to validate the consistency of the proposed FD method. Forward Euler explicit FD approach and semi-implicit Crank-Nicolson FD scheme are also applied to solve the Brusselator reaction-diffusion system and to make the comparison with the proposed FD scheme.

Key words: Auto-catalytic chemical reaction; structure preserving scheme; consistency; Von Neumann stability analysis; numerical simulations.

1. INTRODUCTION

The dynamical systems described by ordinary and partial differential equations are used very frequently in different disciplines of science, engineering, and technology. Nonlinearity factor describes the physical phenomena more accurately, but the nonlinear terms involved in the dynamical models make the solutions more difficult to obtain and quite complex ones. Many important quantities such as concentra-
tions, density, pressure, and population sizes, etc. depend on the time variable, hence the structural properties like positivity, boundedness, and convergence towards stable equilibrium point must be kept in mind in the analysis and the computational schemes of such nonlinear dynamical systems. To find the analytical solutions of the dynamical models involving nonlinear evolution equations is either a very difficult task or is not possible, therefore a plethora of numerical methods are frequently used to find the solutions of ordinary differential equations (ODEs) and partial differential equations (PDEs); see, for example, Refs. [1–7].

In this article, we consider a nonlinear autocatalytic Brusselator chemical reaction model, proposed in 1970 by Prigogine. This model is very useful in chemical kinetics for the study of many physical processes. This type of Brusselator model arises in autocatalytic reaction. This is a reaction with nonlinearity in which two reactant species interact with each other to increase the production rate. The Brusselator model also appears in the modeling of some chemical reaction-diffusion processes in various fields of physics such as plasma and laser physics. The Brusselator model consists of two nonlinear partial differential equations, therefore it attracts the researchers working on numerical solutions of these types of problems. Mittal and Rohila [8] have used the cubic B-spline differential quadrature technique for finding the solution of one-dimensional reaction-diffusion systems. Ersoy and Dag [9] have obtained the numerical solutions of the reaction-diffusion system by using exponential cubic B-spline collocation algorithms. Hu et al. [10] have solved the Brusselator and Gray-Scott models with moving finite element method. The homotopy perturbation method has been used to find the approximate closed form solution for Brusselator system by Ajadi et al. [11]. Manna et al. [12] have used the forward Euler explicit and Crank-Nicolson implicit finite difference schemes to solve the Brusselator reaction-diffusion system. Twizell et al. [13] have proposed a second order implicit finite-difference (FD) scheme for the Brusselator reaction-diffusion system. Adomian [14] and Wazwaz [15] have solved this type of system by a decomposition method. Ang [16] has introduced the dual reciprocity boundary element method to obtain the numerical solution of the Brusselator model. Lin et al. [17] have proposed finite volume method for pattern formation of inhomogeneous Brusselator cross diffusion system. Fernandes et al. [18] have introduced an extrapolated alternating direction implicit Crank-Nicolson orthogonal spline colocation method and have applied it on chemical reaction-diffusion systems like Brusselator reaction-diffusion system, Grey-Scot reaction diffusion system, etc. In this work we propose an explicit chaos free FD scheme [19–23] that preserves the positivity property unconditionally. The proposed FD scheme, which is applied to find the numerical solution of reaction-diffusion problems, preserves all important characteristics of the solution of continuous systems.

Let us consider the one-dimensional coupled reaction-diffusion Brusselator model:

\[ \frac{\partial U}{\partial t} = D_1 \frac{\partial^2 U}{\partial x^2} + f(U, V) \]

\[ \frac{\partial V}{\partial t} = D_2 \frac{\partial^2 V}{\partial x^2} + g(U, V) \]

where \( U \) and \( V \) are the concentrations of the reactants, \( D_1 \) and \( D_2 \) are the diffusion coefficients, and \( f(U, V) \) and \( g(U, V) \) are the reaction terms.
model
\begin{align}
\frac{\partial u}{\partial t} &= d_u \frac{\partial^2 u}{\partial x^2} + \rho_2 - (\rho_1 + 1)u + (u)^2 v \\
\frac{\partial v}{\partial t} &= d_v \frac{\partial^2 v}{\partial x^2} + \rho_1 u - (u)^2 v
\end{align}
(1)
\begin{align}
\frac{\partial u}{\partial t} &= d_u \frac{\partial^2 u}{\partial x^2} + \rho_2 - (\rho_1 + 1)u + (u)^2 v \\
\frac{\partial v}{\partial t} &= d_v \frac{\partial^2 v}{\partial x^2} + \rho_1 u - (u)^2 v
\end{align}
(2)
with given initial and homogeneous Neumann boundary conditions. Here \( u = u(x,t) \) and \( v = v(x,t) \), \( u \) describes the concentration of first reactant species and \( v \) describes the concentration of second reactant species, \( \rho_1 \) and \( \rho_2 \) represent the constant concentrations during the reaction process and \( d_u,d_v \) are the diffusion constants. Besides, \( \rho_1, \rho_2, d_u, \) and \( d_v \) are positive. The equilibrium point of system (1)-(2) is \((u^*, v^*) = (\rho_2, \rho_1/\rho_2)\). The solution of the system (1)-(2) describes the positivity property as \( u, v \) are the concentrations of two species [24]. We recall that the non-standard finite difference (NSFD) method was developed by Mickens [25], which gives the idea for designing of structure preserving FD schemes. This method is a very powerful technique to solve mathematical models containing systems of ordinary and partial differential equations, especially the models where positive solutions are necessary because NSFD schemes preserve the positivity property. Over the years, many authors developed different NSFD schemes for different ODEs and PDEs models [26–31]. The Brusselator model contains a system of ODEs, solved numerically by Zain et al. [24] with the help of a nonstandard FD method that preserves the positivity property. We also mention that Mickens [32] has constructed the positivity-preserving nonstandard FD scheme for the Glycolysis Model.

This paper is organized as follows. In Sec. 2, we present two well-known methods and we introduce a positivity preserving method that is employed in this work. Also, we prove mathematically that the proposed method preserves the positive solution unconditionally. Section 3 is devoted to prove the unconditional stability of the proposed method by employing the Neumann stability criteria. The consistency of the proposed method is presented in Sec. 4 by using the Taylor series method. In Sec. 5, we provide numerical simulations in support of the convergent character of our technique. Finally, in Sec. 6 we give our concluding remarks.

2. NUMERICAL TECHNIQUES

In this work, we use FD techniques for the solution of reaction-diffusion systems. For the FD schemes, the domain in \( xt \)-plane is subdivided into a \( M \times N \) matrix with steps \( h = \frac{L}{M} \) and \( \tau = \frac{T}{N} \). The grid points are
\begin{align}
x_i &= ih, \quad i = 1,2,3,\cdots,M \\
t_n &= n\tau, \quad n = 1,2,3,\cdots,N
\end{align}
The FD approximations of $u^n_i$ and $v^n_i$ are denoted by $u(ih,n\tau)$ and $v(ih,n\tau)$, respectively. We get

\[
(1 + \lambda_1)u^{n+1}_i - \frac{\lambda_1}{2}(u^{n+1}_{i-1} + u^{n+1}_{i+1}) = (1 - \lambda_1)u^n_i + \frac{\lambda_1}{2}(u^n_{i-1} + u^n_{i+1}) + \tau \rho_2 - \tau(\rho_1 + 1)u^n_i + \tau(u^n_i)^2v^n_i 
\]

(5)

\[
(1 + \lambda_2)v^{n+1}_i - \frac{\lambda_2}{2}(v^{n+1}_{i-1} + v^{n+1}_{i+1}) = (1 - \lambda_2)v^n_i + \frac{\lambda_2}{2}(v^n_{i-1} + v^n_{i+1}) + \tau \rho_1 u^n_i - \tau(u^n_i)^2v^n_i 
\]

(6)

where $\lambda_1 = \frac{d_1 \tau}{h^2}$ and $\lambda_2 = \frac{d_2 \tau}{h^2}$.

The numerical scheme is unconditionally stable for the system (1)-(2) [33]. Now the forward Euler FD scheme for the system (1)-(2) is

\[
\begin{align}
u^{n+1}_i &= u^n_i + \lambda_1(u^n_{i-1} - 2u^n_i + u^n_{i+1}) + \tau \rho_2 - \tau(\rho_1 + 1)u^n_i + \tau(u^n_i)^2v^n_i \\
v^{n+1}_i &= v^n_i + \lambda_2(v^n_{i-1} - 2v^n_i + v^n_{i+1}) + \tau \rho_1 u^n_i - \tau(u^n_i)^2v^n_i 
\end{align}
\]

(7)

(8)

The numerical scheme is conditionally stable for $\lambda_1 \leq \frac{2-\tau(A+1)}{\tau}$ and $\lambda_2 \leq 1/2$ for the system (1)-(2) [33]. Now we design unconditionally positivity preserving explicit FD scheme [19–21] with the help of rules proposed by Mickens for the NSFD schemes [25]. We thus get

\[
\begin{align}
u^{n+1}_i &= u^n_i + \lambda_1(u^n_{i-1} + u^n_{i+1}) - 2\lambda_1 u_i^{n+1} + \tau(\rho_1 + 1)u^n_i + \tau(u^n_i)^2v^n_i \\
u^n_i &= \frac{u^n_i + \lambda_1(u^n_{i-1} + u^n_{i+1}) + \tau \rho_2 + \tau(u^n_i)^2v^n_i}{1 + 2\lambda_1 + \tau(\rho_1 + 1)} 
\end{align}
\]

(9)

(10)

In a similar way, we have

\[
\begin{align}
v^{n+1}_i &= v^n_i + \lambda_2(v^n_{i-1} + v^n_{i+1}) - 2\lambda_2 v_i^{n+1} + \tau \rho_1 u^n_i - \tau(v^n_i)^2v^n_i \\
v^n_i &= \frac{v^n_i + \lambda_2(v^n_{i-1} + v^n_{i+1}) + \tau \rho_1 u^n_i}{1 + 2\lambda_2 + \tau(v^n_i)^2) 
\end{align}
\]

(11)

(12)

2.1. THEOREM

The numerical scheme demonstrates the positive solution under the supposition of non-negative initial conditions if

\[
u^n_i \geq 0, v^n_i \geq 0 \Rightarrow u^{n+1}_i \geq 0, v^{n+1}_i \geq 0
\]

(13)
2.1.1. Remark

The parameters $\rho_1, \rho_2, d_{u_1}, d_{u_2}$ involved in equations (10) and (12) are all positive. If the initial conditions are non-negative then the equations (10) and (12) show positivity unconditionally because the right hand sides of (10) and (12) have no negative terms.

3. STABILITY OF THE PROPOSED TECHNIQUE

We present the Neumann stability technique to find the stability region of proposed FD scheme. To this aim, we linearize Eq. (9) and then substituting $\Phi(t)e^{i\varpi x}$ for $u_i^n$, we have

$$
\Phi(t + \Delta t)e^{i\varpi x} = \Phi(t)e^{i\varpi x} + \lambda_1(\Phi(t)e^{i(\varpi(x - \Delta x))} + \Phi(t)e^{i(\varpi(x + \Delta x))}) - 2\lambda_1\Phi(t + \Delta t)e^{i(\varpi x)} - \tau(\rho_1 + 1)\Phi(t + \Delta t)e^{i\varpi x} + \tau ab,
$$

where $a$ and $b$ are constants. We get

$$
(1 + 2\lambda_1 + \tau(\rho_1 + 1))\Phi(t + \Delta t) = \Phi(t) + \lambda_1(2\cos(\varpi\Delta x))\Phi(t) + \tau ab
$$

$$
\frac{\Phi(t + \Delta t)}{\Phi(t)} = \frac{1 + \tau ab + 2\lambda_1\cos(\varpi\Delta x)}{1 + 2\lambda_1 + \tau(\rho_1 + 1)} = \frac{1 + \tau ab + 2\lambda_1(1 - 2\sin^2(\varpi\Delta x/2))}{1 + 2\lambda_1 + \tau(\rho_1 + 1)}
$$

$$
\left|\frac{\Phi(t + \Delta t)}{\Phi(t)}\right| = \frac{1 + \tau ab + 2\lambda_1 - 4\lambda_1\sin^2(\varpi\Delta x/2)}{1 + 2\lambda_1 + \tau(\rho_1 + 1)} \leq \frac{1 + \tau ab - 2\lambda_1}{1 + 2\lambda_1 + \tau(\rho_1 + 1)} < 1
$$

A similar procedure is used for (12), and we have

$$
\left|\frac{\Phi(t + \Delta t)}{\Phi(t)}\right| = \frac{1 + \tau \rho_1 + 2\lambda_2 - 4\lambda_2\sin^2(\varpi\Delta x/2)}{1 + 2\lambda_2 + \tau(a)^2} \leq \frac{1 + \tau \rho_1 - 2\lambda_2}{1 + 2\lambda_2 + \tau(a)^2} < 1
$$

From the above result, it is clear that the proposed FD technique is unconditionally stable.

4. CONSISTENCY OF THE PROPOSED TECHNIQUE

To check the consistency [19, 21] of the proposed FD scheme, the Taylor expansion is used for $u_i^{n+1}$, $u_i^{n-1}$, and $u_i^{n}$:

$$u_i^{n+1} = u_i^n + \tau \frac{\partial u}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 u}{\partial t^2} + \frac{\tau^3}{3!} \frac{\partial^3 u}{\partial t^3} + \cdots$$

$$u_i^{n+1} = u_i^n + \tau \frac{\partial u}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 u}{\partial x^2} + \frac{\tau^3}{3!} \frac{\partial^3 u}{\partial x^3} + \cdots$$

$$u_i^{n-1} = u_i^n - \tau \frac{\partial u}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 u}{\partial x^2} - \frac{\tau^3}{3!} \frac{\partial^3 u}{\partial x^3} + \cdots$$

Considering the unconditionally positivity preserving scheme (10) and replacing the values of $u_i^{n+1}$, $u_i^{n-1}$, and $u_i^{n}$ in it, we obtain the following

$$\left( \frac{\partial u}{\partial t} + \tau \frac{\partial^2 u}{\partial t^2} + \frac{\tau^2}{2!} \frac{\partial^3 u}{\partial t^3} + \cdots \right) \left( 1 + 2 \frac{d_u \tau}{h^2} + \tau (\rho_1 + 1) \right)$$

$$= 2d_u \left( \frac{1}{2!} \frac{\partial^2 u}{\partial x^2} + \frac{h^2}{4!} \frac{\partial^4 u}{\partial x^4} + \cdots \right) + u_i^n (-\rho_1 - 1) + \rho_2 + (u_i^n)^2 v_i^n$$

We replace $\tau = h^3$ and $h \to 0$ and we have

$$\frac{\partial u}{\partial t} = d_u \frac{\partial^2 u}{\partial x^2} + \rho_2 - (\rho_1 + 1) u + (u)^2 v$$

$$\left( \frac{\partial u_1}{\partial t} + \tau \frac{\partial^2 u_1}{\partial t^2} + \frac{\tau^2}{2!} \frac{\partial^3 u_1}{\partial t^3} + \cdots \right) \left( 1 + 2 \frac{d_u \tau}{h^2} + \tau (\rho_1 + 1) \right)$$

$$= 2d_{u_1} \left( \frac{1}{2!} \frac{\partial^2 u_1}{\partial x^2} + \frac{h^2}{4!} \frac{\partial^4 u_1}{\partial x^4} + \cdots \right) + u_1^n (-\rho_1 - 1) + \rho_2 + (u_1^n)^2 w_{1,2}^n$$

We replace $\tau = h^3$ and $h \to 0$, and we have

$$\frac{\partial u_1}{\partial t} = d_{u_1} \frac{\partial^2 u_1}{\partial x^2} + \rho_2 - (\rho_1 + 1) u_1 + (u_1)^2 u_2$$

In a similar way, the formulas for $v_i^{n+1}$, $v_i^{n-1}$, and $v_i^{n}$ are as follows

$$v_i^{n+1} = v_i^n + \tau \frac{\partial v}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 v}{\partial t^2} + \frac{\tau^3}{3!} \frac{\partial^3 v}{\partial t^3} + \cdots$$

$$v_i^{n+1} = v_i^n + \tau \frac{\partial v}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 v}{\partial x^2} + \frac{\tau^3}{3!} \frac{\partial^3 v}{\partial x^3} + \cdots$$

$$v_i^{n-1} = v_i^n - \tau \frac{\partial v}{\partial t} + \frac{\tau^2}{2!} \frac{\partial^2 v}{\partial x^2} - \frac{\tau^3}{3!} \frac{\partial^3 v}{\partial x^3} + \cdots$$

We consider the proposed FD scheme (12) for equation (2)

\[ v_{n+1}^i = v_i^n + \lambda_2 (v_{i-1}^n + v_{i+1}^n) - 2\lambda_2 u_i^n + \tau \rho_1 u_i^n - \tau (u_i^n)^2 v_{n+1}^i \]  

(19)

We put the values of \( v_{n+1}^i, v_i^n, \) and \( v_{i-1}^n \) in Eq. (19) and after some computations, we have

\[
\left( \frac{\partial v}{\partial t} + \frac{\tau}{2} \frac{\partial^2 v}{\partial t^2} + \frac{\tau^2}{3!} \frac{\partial^3 v}{\partial t^3} + \cdots \right) \left( 1 + 2 \frac{\partial u}{\partial x} + \frac{\tau (u_i^n)^2}{h^2} \right) = 2 \frac{\partial^2 v}{\partial x^2} + \frac{\partial^4 v}{4! \partial x^4} + \cdots + \rho_1 u_i^n - (u_i^n)^2 v_i^n
\]

We replace \( \tau = h^3 \) and \( h \to 0 \), and we have

\[
\frac{\partial v}{\partial t} = d_v \frac{\partial^2 v}{\partial x^2} + \rho_1 u - (u)^2 v
\]

5. EXAMPLE

We consider the auto-catalytic chemical reaction Brusselator system in one dimension [8] as

\[
\begin{align*}
\frac{\partial u}{\partial t} &= d_u \frac{\partial^2 u}{\partial x^2} + \rho_2 - (\rho_1 + 1)u + (u)^2 v \\
\frac{\partial v}{\partial t} &= d_v \frac{\partial^2 v}{\partial x^2} + \rho_1 u - (u)^2 v
\end{align*}
\]

(20)  

(21)

subject to the initial data

\[
\begin{align*}
u(x, 0) &= 1/2 \\
v(x, 0) &= 1 + 5x
\end{align*}
\]

(22)  

(23)

and the derivatives of the solution pair are prescribed on the boundary as follows

\[
\begin{align*}
u_x(0, t) &= u_x(1, t) = 0 \\
v_x(0, t) &= v_x(1, t) = 0
\end{align*}
\]

(24)  

(25)

Now we will present the numerical simulations of all FD schemes at different step sizes to see to behavior of all these schemes under consideration.
In Figs. 1-3, we take the values $h = 0.05$, $\tau = 0.06$, $\rho_1 = 1$, $\rho_2 = 3.4$, $d_u = d_v = 10^{-4}$, which implies that $\lambda_1 = \lambda_2 = 0.0024$. If we consider these values, then the stability conditions of $\lambda_1$ and $\lambda_2$ for the forward Euler FD scheme are $\lambda_1 \leq 0.434$ and $\lambda_2 \leq 0.5$. This verifies that the values under consideration of this numerical experiment are within the stability criteria of forward Euler FD scheme.

Now from Fig. 2 and Fig. 3 we see that the graph of $v$ clearly shows that the forward Euler scheme violates the positivity property and gives negative values. The negative values for the concentration of reactant species are meaningless. Note that Twizell et al. [13] concluded that the system (1)-(2) is attracted to the equilibrium point $(u^*, v^*)$ if $1 - \rho_1 + \rho_2^2 \geq 0$. But the forward Euler FD scheme does not converge to the equilibrium point and diverges at $\lambda_1 = \lambda_2 = 0.0036$ as shown in Fig. 4.
Figures 5-8 present the solutions of concentrations $u$ and $v$ using the Crank-Nicolson FD scheme. We apply the semi-implicit Crank-Nicolson FD scheme that is unconditionally stable. The graphs in Figs. 5-8 are plotted with the same values as taken for the forward Euler FD scheme in Figs. 1-4. The behaviors of the Crank-Nicolson semi-implicit FD scheme and the forward Euler scheme are similar. The Crank-Nicolson scheme is also showing negative values of concentration. The Crank-Nicolson FD scheme overflows and fails to show the convergence towards the equilibrium point $(u^*, v^*)$.

Figure 9-11 are the graphs of concentration $u(x, t)$ and $v(x, t)$ using the proposed FD scheme at $h = 0.05$, $\tau = 0.06$, $\rho_1 = 1$, $\rho_2 = 3.4$, $d_u = d_v = 10^{-4}$, which implies that $\lambda_1 = \lambda_2 = 0.0024$. These values are the same as given for the forward Euler method and the Crank-Nicolson method. Figures 12-14 are the graphs for $u$ and $v$ of the proposed FD scheme at $\lambda_1 = \lambda_2 = 0.0036$. It can be observed that the proposed scheme not only preserves the positivity but also converges to the equilibrium points of the Brusselator reaction-diffusion system under the condition $1 - \rho_1 + \rho_2^2 \geq 0$. 
Fig. 9 – Mesh graph of $u$.

Fig. 10 – Mesh graph of $v$.

Fig. 11 – Combined plot of $u$ and $v$. 

Fig. 12 – Mesh graph of u.

Fig. 13 – Mesh graph of v.

Fig. 14 – Combined plot of u and v.

Fig. 15 – Mesh graph of u.

Fig. 16 – Mesh graph of v.
The properties possessed by the Brusselator one-dimensional reaction-diffusion system are preserved by the proposed FD scheme. Figures 15-16 demonstrate that the proposed method preserves the positive solution of the continuous Brusselator model even at large values \( \lambda_1 = \lambda_2 = 100 \). Also, the FD scheme converges to the equilibrium point of the Brusselator one-dimensional reaction-diffusion system, which shows the novelty and efficacy of the proposed FD scheme.

As discussed above, the equilibrium point \((u^*, v^*)\) of the system (1)-(2) is stable for \(1 - \rho_1 + \rho_2^2 \geq 0\) and unstable for \(1 - \rho_1 + \rho_2^2 < 0\). In Figs. 17-20, the values of \(\rho_1\) and \(\rho_2\) are taken in such a way that \(1 - \rho_1 + \rho_2^2 < 0\). Here we take \(\rho_1 = 3.4\), \(\rho_2 = 1\), \(h = 0.1\), \(\lambda_1 = \lambda_2 = 0.004\). All the graphs in Figs. 17-20 validate the conclusion made by Twizell et al. [13] and show that the equilibrium point \((u^*, v^*)\) of the system (1)-(2) becomes unstable when \(1 - \rho_1 + \rho_2^2 < 0\).
6. CONCLUSION

In this article, the auto-catalytic chemical reaction Brusselator system in one dimension is solved by three different finite-difference numerical schemes, the forward Euler scheme, the Crank-Nicolson semi-implicit scheme, and the proposed finite-difference scheme. Remember that for every numerical method, any property possessed by a continuous system must be preserved by that numerical method. In nonlinear problems, many well-known numerical methods fail to preserve the properties possessed by the continuous reaction-diffusion system. To overcome these issues, we have proposed a novel FD scheme that is designed for the numerical approximation of reaction-diffusion problems. The proposed method preserves the positive solution of a continuous system unconditionally. This novel method is an explicit FD scheme, which is computationally efficient. This numerical scheme is unconditionally stable and unconditionally consistent with respect to the positivity property. These attributes are verified by numerical simulations. The graphs obtained using the proposed FD scheme show the convergence, consistency, and positivity of the numerical scheme. On the other hand, the graphs show the divergence of the forward Euler and Crank-Nicolson schemes for different values of the parameters. These two numerical schemes also failed to preserve the positivity property for different values of step sizes.

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