Cumhuriyet Science Journal

e-ISSN: 2587-246X
ISSN: 2587-2680

Cumhuriyet Sci. J., 42(1) (2021) 75-87
http://dx.doi.org/10.17776/csj.695738

Numerical solution of the brusselator model by time splitting method

Sıla Övgü KORKUT [1,*], ***Yeşim ÇİÇEK*** [1]

[1]*İzmir Katip Celebi University, Department of Engineering Sciences, IZMIR/TURKEY*

Abstract

One of the significant models in chemical reactions with oscillations is the Brusselator model. This model essentially describes a nonlinear reaction-diffusion equation. Brusselator system arises in applications of many physical and chemical models. In this study, the Brusselator model is solved numerically with the help of a time-splitting method. Consistency and stability of the method are proved with the help of auxiliary lemmas. Additionally, the positivity preservation of the method is analyzed. The accuracy of the presented method is also tested on numerical examples and all theoretical results are supported by the tables and figures.

Article info

History:
Received:27.02.2020
Accepted:16.12.2020

Keywords:
Local error analysis, Brusselator model, Splitting method, Non-linear partial differential equation, Reaction-Diffusion equation

1. Introduction

Reaction-diffusion models have great importance in the study of chemical and biological systems. One of the main important reaction-diffusion equations is known as the Brusselator system, which is used to describe the mechanism of chemical reaction-diffusion with non-linear oscillations [1-4]. In 1952 Turing [5] showed the importance of oscillations in biochemical systems that leads to the theory of morphogenesis. The Brusselator system occurs in a large number of physical problems such as the formation of ozone by atomic oxygen through a triple collision and enzymatic reactions. In 1968 Prigogine and Lefever proposed the system and the name was coined by Tyson in [6]. In the middle of the last century, Belousov and Zhabotinsky discovered chemical systems exhibiting oscillations.

The non-linear two-dimensional reaction-diffusion Brusselator system is given by [7]

$$\frac{\partial u}{\partial t} = \alpha \Delta u + B + u^2 v - (A+1)u \tag{1}$$

$$\frac{\partial v}{\partial t} = \alpha \Delta v + Au - u^2 v, \tag{2}$$

for $u(x,y,t)$ and $v(x,y,t)$ in the two-dimensional region, $\Omega = [a,b]^2$, with initial condition

$$\big(u(x,y,0), v(x,y,0)\big) = (p(x,y), q(x,y)),$$

and Dirichlet boundary condition

$$\big(u(x,y,t), v(x,y,t)\big) = (M(x,y,t), N(x,y,t)) \quad \text{for } (x,y) \in \partial\Omega, \quad t > 0$$

or subject to Neumann's boundary conditions on the boundary $\partial\Omega$. Here $u(x,y,t)$ and $v(x,y,t)$ represent dimensionless concentrations of two reactants, A and B are constants concentrations of two reactants, α is diffusion coefficient, Δ is Laplace operator, and $p(x,y)$, and $q(x,y)$ are suitably prescribed functions.

The numerical solution of the reaction-diffusion Brusselator system has been an important area of research. There is limited literature on the numerical solution of the Brusselator system. A decomposition method is applied for

*Corresponding author. *email address: silaovgu@gmail.com.*

the numerical solution of the reaction-diffusion Brusselator system in [8]. Twizell et al. [9] developed a second-order (in space and time) finite difference method for a diffusion-free Brusselator system. The modified Adomain decomposition method is applied by Wazwaz in [10]. Ang, in [7] presented the dual-reciprocity boundary element method for the numerical solution of the reaction-diffusion Brusselator system. In [11] the authors proposed a modified cubic B-spline differential quadrature method to show computational modeling of a two-dimensional Brusselator system for Neumann's boundary conditions. A polynomial based differential quadrature method is employed for numerical solutions of two-dimensional nonlinear reaction-diffusion Brusselator system in [12]. A meshless method has been suggested in [13] to obtain a numerical solution of the mentioned system. Another meshfree method based on the radial basis functions has been presented in [14]. Furthermore, more recently, a finite element approach has been applied to several chemical reaction-diffusion equations including the Brusselator system in [15-16] by Yadav and Jiwari. Also, a meshfree algorithm based on radial basis multiquadric functions and differential quadrature (DQ) technique has been developed to approximate the numerical solution of the Brusselator system in [17]. Bhatt and Chowdhury have presented a comparative study of performances of meshfree (radial basis functions) and mesh-based (finite difference) schemes in terms of their accuracy and computational efficiency for solving multi-dimensional Brusselator system in [18]. Moreover, several chemical systems including a two-dimensional Brusselator model have been studied in [19]. All mentioned researches take into account space discretization. Even though the authors in [19] suggest a kind of splitting method, they utilize the method as dimensional splitting to get one-dimensional problems. Unlike their study, we focus on a kind of splitting method for separating the operators concerning their linearity structure. Our purpose is not underestimating that study but considering the problem from a different angle.

The main aim of the present study is that the Lie-Trotter splitting method which is a well-known first-order time splitting method is applied for the numerical solution of Equation 1-2. The essential idea of the splitting methods is that instead of the sum, the operators are considered separately. This means that the original problem is split into sub-problems and the numerical solution of the original problem is obtained from a combination of numerical solutions of these sub-problems. The reader interested in the splitting methods can see [20-23] and the references therein. One of the important advantages of these methods is that the operators with different structures can be solved by different methods. Moreover, employing the splitting idea, some operators can be solved exactly which can increase the reliability of the solution. This is one of our purposes. The other purpose is to preserve some physical behavior such as positivity, stability, and preserving the dynamics of the system.

The paper is organized as follows: Section 2 is devoted to introducing the idea of the time splitting for Equation 1-2. All theoretical results such as consistency and stability are presented in this section. For consistency and stability analyses, the auxiliary lemmas are utilized. Furthermore, the preservation of the positivity of the proposed method has been shown in the current section. In section 3, we apply the proposed scheme to different types of problems related to the reaction-diffusion Brusselator system in both one- and two- dimensional cases. The obtained numerical solutions are tested in both compatibility and accuracy. The theoretical claims are supported by simulations and tables. Finally, Section 4 concludes the study.

2. Materials and Methods

In this section, we introduce the Lie-Trotter splitting method (LSM) for the Brusselator model given in Equation 1-2. For this purpose, we first set up the equations given in Equation 1-2 with the appropriate system form.

$$u_t = \alpha \Delta u + f(u,v) \tag{3}$$
$$v_t = \alpha \Delta v + g(u,v) \tag{4}$$

where $f(u,v) = B + u^2 v - (A+1)u$ and $g(u,v) = Au - u^2$ are scalar functions and the operator Δ corresponds to the spatial derivatives. Equation 3-4 turn into system form as follows:

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \alpha \begin{bmatrix} \Delta & \mathbf{0} \\ \mathbf{0} & \Delta \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} + \begin{bmatrix} f(u,v) \\ g(u,v) \end{bmatrix} \tag{5}$$

Throughout the section, we denote $(u,v)^T$ by the variable Y for the sake of simplicity of the notations. Thus, Equation 5 can be expressed as follows:

$$Y_t = \alpha DY + F(Y), \qquad Y(t): \mathbb{D}(D) \cap \mathbb{D}\big(F(Y)\big) \to X \tag{6}$$

where $\mathbb{D}(D): \mathbb{C}^2(\Omega)$, and $\mathbb{D}\big(F(Y)\big): \mathbb{C}^1(\Omega \times [0, t_{end}])$ and X is a Banach space. As mentioned previously, the essential idea of the time splitting methods is that instead of the sum, the operators are considered separately. To do this, the original problem is divided into sub-problems and they are solved efficiently by an appropriate numerical method. The connections of these sub-problems are via the initial conditions. That is,

$$Y_{t,1} = \alpha DY_1, \quad Y_1(t_n) = Y(t_n) \qquad \forall t \in [t_n, t_{n+1}], \tag{7}$$
$$Y_{t,2} = F(Y_2), \quad Y_2(t_n) = Y_1(t_{n+1}) \quad \forall t \in [t_n, t_{n+1}], \tag{8}$$

where Y_1 and Y_2 denote the sub-problems and t_n denotes the present time whereas t_{n+1} does the future. Moreover, matrix D stands for the matrix consisting of spatial derivative operators. Such splitting leads to two initial value problems which will be solved sequentially. Due to the linearity of Equation 7, the exact solution of this part is already known. However, an efficient solver will be used to obtain a solution of Equation 8, numerically, which will be stored as the approximated one, i. e. $Y(t_{n+1}) = Y_2(t_{n+1})$. By the nonlinearity of Equation 8, a predictor-corrector method is the correct choice to obtain the approximate solution. In the current study, we utilize Heun's method to obtain the approximate solution for the non-linear part. For the sake of simplicity of notations, Heun's method can be expressed on the non-linear part as follows:

$$Y_2(t_{n+1}) = Y_2(t_n) + \frac{\Delta t}{2}\Big(F\big(Y_2(t_n)\big) + F\left(Y_2(t_n) + \Delta t F\big(Y_2(t_n)\big)\right)\Big), \forall t \in [t_n, t_{n+1}] \tag{9}$$

The convergence of the composite of numerical flows should be validated by appropriate analysis. The upcoming subsections present the preservation of positivity and the issue of convergence with the concepts of consistency and stability.

2.1. Positivity preservation of the LSM

Since the solution of the Brusselator system given in Equation 1-2 describes the concentrations of two reactants, the solution is positive naturally. Thus, the approximate solution must satisfy the positivity for each time step. To guarantee the positivity of the LSM we only impose the following assumption:

Assumption 1. Let $Y(x, y, 0) = Y_0 \geq 0$. Assume that

$$F_i\big(Y^i\big) \geq 0, \qquad \forall Y^i \geq 0, \qquad i = 1, 2$$

where F corresponds to the nonlinear part of the Brusselator system, and F_i and Y^i denote the ith components of the F and Y, respectively.

Due to this condition, vector field F pushes the trajectories back to the positive domain whenever the solutions approach the boundary. Moreover, the condition on the nonlinear field is enough to say the LSM preserves the positivity of the solution. Our general reference on positivity preservation is the book given in [24].

Theorem 1. Let Assumption 1 hold for Equation 1-2. The LSM preserves the positivity of the solutions over all the time.

Proof. To prove the positivity we shall first write the approximate solution on $[0, \Delta t]$:

$$\tilde{Y}(\Delta t) = e^{D\Delta t} Y(t_0) + \frac{\Delta t}{2}\Big(F\big(Y_2(t_0)\big) + F\left(Y_2(t_0) + \Delta t F\big(Y_2(t_0)\big)\right)\Big) \tag{10}$$

where $Y_2(t_0) = Y_1(\Delta t) = e^{D\Delta t} Y_1(t_0)$. One can be easily seen that the solution obtained by Equation 7 gives a positive solution when the initial condition is positive, i. e. $Y(t_0) \geq 0$. This provides the positivity of the second term with the help of Assumption 1, which concludes the positivity of $\tilde{Y}(\Delta t) = \tilde{Y}(t_1)$. The solution is stored as

the initial condition for the next interval $[\Delta t, 2\Delta t]$. Inductively, since the scheme preserves the positivity at each one step we guarantee the positivity of the approximate solution $\tilde{Y}(t_{k+1})$ for all $Y(t_k) \geq 0$.

In [25] the author proposed a finite difference scheme preserving the positivity of the reaction-diffusion equation which requires the differentiability of the field. It is crucial to emphasize that the LSM does not need to have any condition on the derivative of the field.

2.2. Local error analysis

The present section aims to analyze the consistency of the method. One can be seen in Table 1 that the eigenvalues of the discretization matrix to approximate to the Laplace operator are negative. Thus, the solutions of Equation 7 remain bounded over all the time. With the help of these results, Remark 1 is given.

Table 1. Several examples of eigenvalues of D for different domains

Domain	$\max_{\Omega} eig(D)$	$\min_{\Omega} eig(D)$
$\Omega = [0,1] \times [0,1]$	-19.7291	-1.2780e+4
$\Omega = [0,10] \times [0,10]$	-0.1973	-127.8027
$\Omega = [0,30] \times [0,30]$	-0.0219	-88.8670

Remark 1. Due to the $\max_{\Omega} eig(D) \leq 0$, where $eig(D)$ represents the eigenvalues of D, the solution of the linear part of the Brusselator system is bounded by the initial condition as follows:

$$\|e^{\alpha D t} Y_0\|_X \leq \gamma \|Y_0\|_X \tag{11}$$

where the constant $\gamma \in [0,1]$ provided that $\alpha \geq 0$.

Moreover, the nonlinear part of the Brusselator system, which is given in Equation 1-2, is bounded, under the well-posedness of the solutions.

Lemma 1. Let the field $F(Y)$: $\mathbb{C}^1(\Omega \times [0, t_{end}]) \to X$ be a nonlinear operator. Suppose that there exists $M, N \in \mathbb{R}^+$ such that

$$\|F(Y)\|_X \leq M \|Y_0\|_X \tag{12}$$
$$\|\partial F(Y)\|_X \leq N \|Y_0\|_X \tag{13}$$

where $\partial F = \frac{\partial(f,g)}{\partial(u,v)} = \begin{bmatrix} 2uv - (A+1) & u^2 \\ A - 2uv & -u^2 \end{bmatrix}$.

Theorem 2 presents the local error analysis of the LSM. To do this, the method is considered on $[0, \Delta t]$.

Theorem 2. Let Remark 1 and Lemma 1 be fulfilled. LSM is the first-order accuracy with error bound

$$\left\|Y(\Delta t) - \tilde{Y}(\Delta t)\right\|_X \leq C\Delta t^2 + \mathcal{O}(\Delta t^3) \tag{14}$$

where C depends on M and $\|Y_0\|_X$.

Proof: To obtain the local error bound of the numerical scheme we employ the standard technique. That is, $\left\|Y(\Delta t) - \tilde{Y}(\Delta t)\right\|_X$ will be calculated.

On one hand, by Picard-Lindelöf theorem the exact solution of Equation 6 is expressed as follows:

$$Y(\Delta t) = e^{D\Delta t} Y_0 + \int_0^{\Delta t} e^{D(\Delta t - s)} F\big(Y(s)\big) ds \tag{15}$$

On the other hand, the numerical solution is defined by

$$\tilde{Y}(\Delta t) = e^{D\Delta t}Y_0 + \frac{\Delta t}{2}\left(F\left(e^{D\Delta t}Y_0\right) + F\left(e^{D\Delta t}Y_0 + \Delta t F\left(e^{D\Delta t}Y_0\right)\right)\right) \tag{16}$$

For the convenience of calculations we restate the exact solution as follows:

$$Y(\Delta t) = e^{D\Delta t}Y_0 + \int_0^{\Delta t} e^{D(\Delta t - s)}F\left(e^{Ds}Y_0 + \int_0^s e^{D(s-\tau)}F\left(Y(\tau)\right)d\tau\right)ds \tag{17}$$

With the help of the Taylor's Expansion Equation 16 and Equation 17 can be rewritten as follows:

$$Y(\Delta t) = e^{D\Delta t}Y_0 + \int_0^{\Delta t} e^{D(\Delta t - s)}F(e^{Ds}Y_0)ds + \int_0^{\Delta t} e^{D(\Delta t - s)}\left(\int_0^s e^{D(s-\tau)}F\left(Y(\tau)\right)d\tau\, \partial F(e^{Ds}Y_0) + \mathcal{O}(s^2)\right)ds \tag{18}$$

and

$$\tilde{Y}(\Delta t) = e^{D\Delta t}Y_0 + \frac{\Delta t}{2}\left(F\left(e^{D\Delta t}Y_0\right) + F\left(e^{D\Delta t}Y_0\right) + \Delta t F\left(e^{D\Delta t}Y_0\right)\partial F\left(e^{D\Delta t}Y_0\right) + \mathcal{O}(\Delta t^2)\right) \tag{19}$$

Subtracting Equation 19 from Equation 18 the residual term is achieved. By virtue of Lemma 1 and Remark 1, the local error bound is attained as follows:

$$\left\|Y(\Delta t) - \tilde{Y}(\Delta t)\right\|_X \leq C\Delta t^2 + \mathcal{O}(\Delta t^3) \tag{20}$$

where C depends on M, N, and $\|Y_0\|_X$.

2.3. Stability analysis

Theorem 3. Let Remark 1 and Lemma 1 be satisfied. The LSM is unconditionally stable.

Proof: To prove the stability of the method we first start with finding a bound of one-step approximate solution given as follows:

$$\tilde{Y}_1 = e^{D\Delta t}Y_0 + \frac{\Delta t}{2}\left(F\left(e^{D\Delta t}Y_0\right) + F\left(e^{D\Delta t}Y_0 + \Delta t F\left(e^{D\Delta t}Y_0\right)\right)\right), \tag{21}$$

where $\tilde{Y}_1 = Y_2(\Delta t)$ in Equation 7-8. Taking the norm of both sides and utilizing from Remark 1 yield

$$\left\|\tilde{Y}_1\right\|_X = \left\|e^{D\Delta t}Y_0 + \frac{\Delta t}{2}\left(F\left(e^{D\Delta t}Y_0\right) + F\left(e^{D\Delta t}Y_0 + \Delta t F\left(e^{D\Delta t}Y_0\right)\right)\right)\right\|_X \tag{22}$$

$$\left\|\tilde{Y}_1\right\|_X \leq \gamma\|Y_0\|_X + \Delta t\left(1 + \frac{\Delta t}{2}\right)M\gamma\|Y_0\|_X \tag{23}$$

Equation 23 represents the boundedness of a one-step solution by the initial condition as $\Delta t \to 0$. If the process is repeated inductively, one can obtain

$$\left\|\tilde{Y}_n\right\|_X \leq \gamma^n\left(1 + M\Delta t + M\frac{\Delta t^2}{2}\right)^n\|Y_0\|_X \tag{24}$$

where the coefficient of $\|Y_0\|_X$ denotes the amplification factor of LSM. As it can be easily seen in Equation 24, the terms consisting of Δt are negligible when n increases. This leads to

$$\left\|\tilde{Y}_n\right\|_X \leq \gamma^n\|Y_0\|_X \tag{25}$$

which concludes the proof. This also guarantees that the LSM is unconditionally stable.

3. Results and Discussion

The current section is dedicated to confirming the theoretical results obtained in the previous section. In this context, it is crucial to state the Brusselator system from both physical and chemical aspects. A chemical process is related to converting reactants into products. One of the most important points for closed systems such as Brusselator is that one can generate an oscillating chemical reaction model using the Belousov-Zhabotinsky reaction which is corresponding to our considered problems. For a more detailed discussion on the Brusselator system and its dynamics we refer the reader to the dissertation about that system, see [26]. An oscillating chemical reaction as the pendulum passes through its equilibrium point while oscillates. The mean of the equilibrium is the equilibrium concentration for all the components. Thus, from a point of mathematical view, as well as its convergence properties it is expected that a numerical scheme to obtain a solution should preserve its dynamics. That is, by the nature of chemical reactions all solutions should be positive. Additionally, due to entropy, the reactants should reach their equilibrium as time increases.

Under the lights of the information above, we consider some test problems both one- and two- dimensional cases to check the accuracy and efficiency of the LSM.

3.1. Example 1

To check the efficiency of the method we first start with a one-dimensional Brusselator system, which is

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + B + u^2 v - (A+1)u$$
$$\frac{\partial v}{\partial t} = \alpha \frac{\partial^2 v}{\partial x^2} + Au - u^2 v,$$

subject to

$$u(0,t) = u(1,t) = B; \quad v(0,t) = v(1,t) = {}^{A}/_{B}$$
$$u(x,0) = B + x(1-x); \qquad v(x,0) = {}^{A}/_{B} + x^2(1-x)$$

By taking parameters given as in [27] we have obtained the approximated solutions which are illustrated in Figure 1.

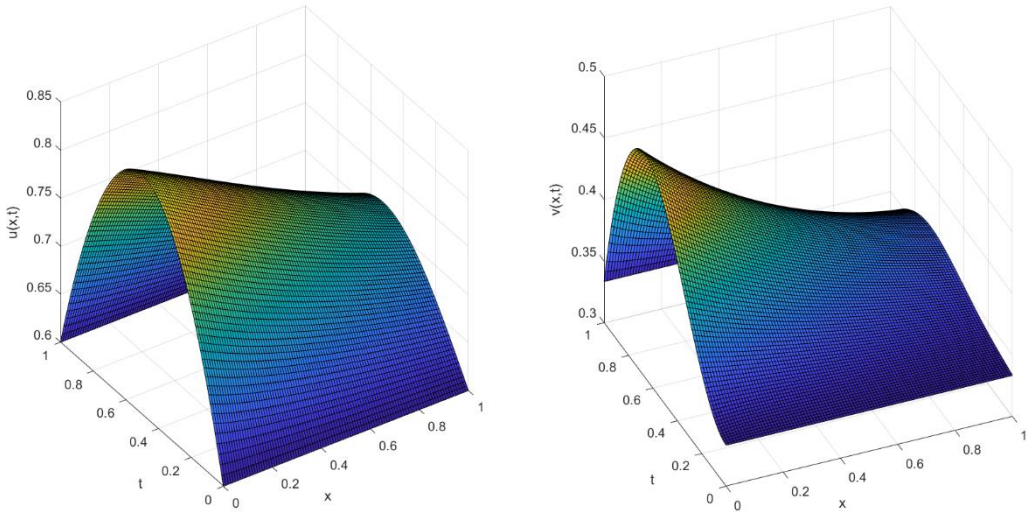


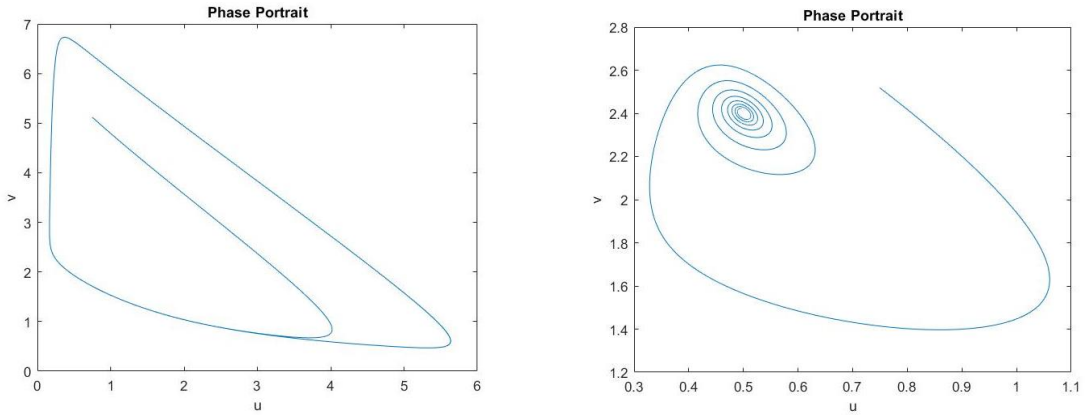
Figure 1. The physical behavior of the approximated solutions for $u(x,t)$ and $v(x,t)$. The numerical solutions are obtained by taking $B = 0.6,\ A = 0.2, \alpha = \frac{1}{40}$, where $x \in [0,1]$ and $t \in [0,1]$.

It is important to say Table 2 emphasizes that the LSM remains stable and preserves the positivity of the solutions for both $u(x,t)$ and $v(x,t)$ for different final times.

Table 2. Maximum and Minimum values of numerical solutions for the parameters $B = 0.6,\ A = 0.2, \alpha = \frac{1}{40}$,

t_{end}	$\max_{x\in[0,1]\ t\in[0,t_{end}]} u(x,t)$	$\min_{x\in[0,1]\ t\in[0,t_{end}]} u(x,t)$	$\max_{x\in[0,1]\ t\in[0,t_{end}]} v(x,t)$	$\min_{x\in[0,1]\ t\in[0,t_{end}]} v(x,t)$
1	0.8500	0.60	0.4812	0.3301
10	0.8500	0.60	0.4812	0.3301
20	0.8500	0.5998	0.4812	0.3302

Furthermore, the theoretical results which are given in [9] state that the limit cycles do not exist for the Brusselator model when $1 - A + B^2 < 0$. Figure 2.a illustrates such a case. However, limit cycles occur for the case of $1 - A + B^2 \geq 0$ and Figure 2.b presents that case. To validate if the proposed method is compatible with the specified system the parameters have been taken from [9].



a. A=2.5, B= 0.5, $1 - A + B^2 = -1.25$ **b.** A=1.2, B= 0.5; $1 - A + B^2 = 0.05$

Figure 2. The limit cycles of the diffusion-free Brusselator system for different choices of parameters.

Figure 2 is evidence that the proposed method preserves the limit cycles which is the physical dynamics of the Brusselator system. The obtained results are consistent with the results that of [9].

3.2. Example 2

As our second test problem, we consider a benchmark problem in the literature. The corresponding equation is the two-dimensional Brusselator system given in Equation 1-2 with parameters $\alpha = 0.25$, $A = 1$ and $B = 0$ in the region $\Omega = [0,1]^2$. By the particular choices of parameters, the exact equations of Equation 1-2 are

$u(x,y,t) = e^{-x-y-0.5t}$,
$v(x,y,t) = e^{x+y+0.5t}$.

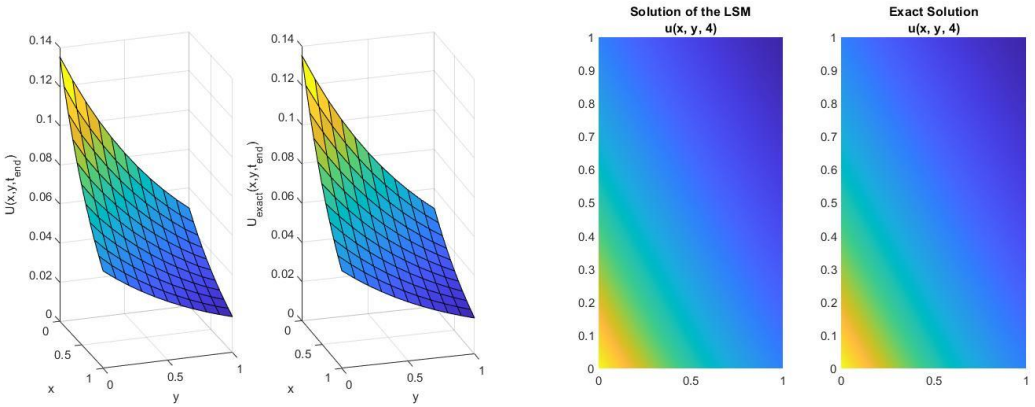
All necessary conditions are extracted from the exact solution. Table 3 lists the numerical solution generated by LSM by comparing it with those in [7] and [14] for the case of M=10 (denotes the notation for the spatial discretization for their studies).

Table 3. Comparison of the results of LSM with the other methods in the literature and exact solution.

	$u(0.4,0.6,t_{end})$				$v(0.4,0.6,t_{end})$			
t_{end}	LSM	[7]	[14]	Exact	LSM	[7]	[14]	Exact
0.3	0.31667	0.3168	0.3174	0.31665	3.15834	3.1530	3.1580	3.15804
0.6	0.27257	0.2724	0.2732	0.27255	3.66956	3.6600	3.6680	3.66911
0.9	0.23459	0.2345	0.2351	0.23457	4.26365	4.2500	4.2620	4.26311
1.2	0.20192	0.2016	0.2024	0.20191	4.95342	4.9390	4.9520	4.95278
1.5	0.17379	0.1739	0.1742	0.17377	5.75535	5.7350	5.7540	5.75460
1.8	0.14958	0.1489	0.1499	0.14957	6.68676	6.6700	6.6850	6.68589

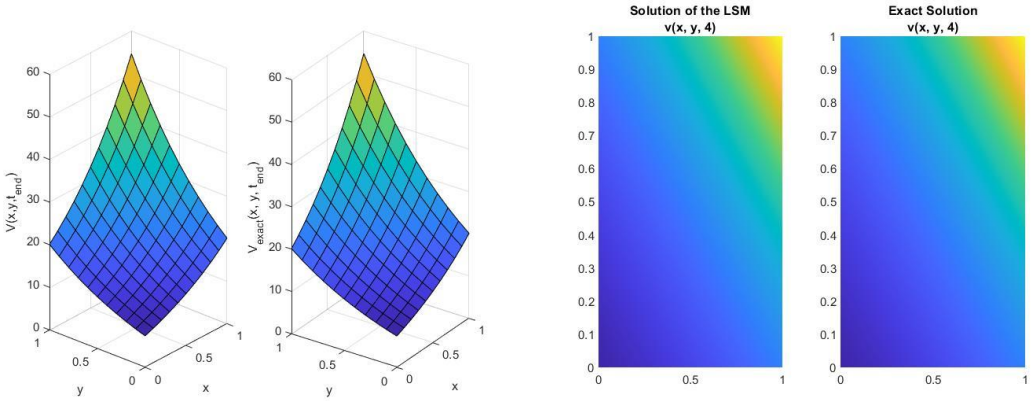
The given table verifies that the proposed method, LSM, in very good agreement with the exact solution for both u and v. Moreover, it can be easily seen that the LSM is better over time.

Furthermore, Figure 3 and Figure 4 depict the comparison of the physical behaviors of the numerical solutions computed by the LSM and the exact solution. The exhibited figures, Figure 3-4, are obtained by taking $\Delta t = 0.01$ over $[0, 4]$ where the spatial domain, $\Omega = [0,1] \times [0,1]$, is divided into 10 equal intervals.



a. Surface plot of $u(x, y, t_{end})$. **b.** Phase plot of $u(x, y, t_{end})$.

Figure 3. The physical behavior of the solutions of $u(x, y, t)$. The parameters are taken as $A = 1, B = 0,\ \alpha = 0.25$ for Equation 1-2.



a. Surface plot of $v(x, y, t_{end})$. **b.** Phase plot of $v(x, y, t_{end})$.

Figure 4. The physical behavior of the solutions of $v(x, y, t)$. The parameters are taken as $A = 1, B = 0, \alpha = 0.25$ for Equation 1-2.

Table 3 and Figure 3-4 are evidence of the validity, compatibility and accuracy of the proposed method for Equation 1-2.

3.3. Example 3

As our final test problem, we consider the two-dimensional Brusselator system which is given in Equation 1-2 for $\alpha = 0.002$, $A = \frac{1}{2}$ and $B = 1$ in the region $\Omega = [0,1]^2$ with the initial and Neumann's boundary conditions are given as follows:

$$u(x,y,0) = \frac{1}{2}x^2 - \frac{1}{3}x^3 \text{ and } v(x,y,0) = \frac{1}{2}y^2 - \frac{1}{3}y^3,$$

$$\frac{\partial u(x,y,0)}{\partial x}|_{x=0} = \frac{\partial u(x,y,0)}{\partial x}|_{x=1} = \frac{\partial u(x,y,0)}{\partial y}|_{y=0} = \frac{\partial u(x,y,0)}{\partial y}|_{y=1} = 0,$$
$$\frac{\partial v(x,y,0)}{\partial x}|_{x=0} = \frac{\partial v(x,y,0)}{\partial x}|_{x=1} = \frac{\partial v(x,y,0)}{\partial y}|_{y=0} = \frac{\partial v(x,y,0)}{\partial y}|_{y=1} = 0,$$

All parameters for this example are taken from the study of [13]. We have checked the convergence of the method to the equilibria point for the two-dimensional Brusselator system. Table 4 guarantees that the numerical solutions converge to their equilibrium points as t increases.

Table 4. The values of $u(x,y,t)$ and $v(x,y,t)$ at the specified x, y and t.

	$(0.2,0.2,t_{end})$		$(0.4,0.6,t_{end})$		$(0.5,0.5,t_{end})$		$(0.8,0.9,t_{end})$	
t_{end}	u	v	u	v	u	v	u	v
1	0.5303	0.1632	0.5602	0.2538	0.5511	0.2278	0.5832	0.3148
2	0.7020	0.3676	0.7312	0.4283	0.7224	0.4113	0.7536	0.4664
3	0.8167	0.4930	0.8474	0.5202	0.8382	0.5129	0.8696	0.5348
4	0.9097	0.5356	0.9342	0.5396	0.9271	0.5389	0.9506	0.5398
5	0.9715	0.5307	0.9849	0.5261	0.9812	0.5275	0.9930	0.5223
6	0.9997	0.5146	1.0041	0.5103	1.0029	0.5115	1.0064	0.5005
7	1.0063	0.5038	1.0065	0.5017	1.0065	0.5023	1.0064	0.5005
8	1.0047	0.4996	1.0039	0.4990	1.0042	0.4992	1.0033	0.4987
9	1.0021	0.4989	1.0015	0.4989	1.0016	0.4989	1.0011	0.4989
10	1.0005	0.4993	1.0002	0.4994	1.0003	0.4993	1.0001	0.4995
↓	↓	↓	↓	↓	↓	↓	↓	↓
∞	1	0.5	1	0.5	1	0.5	1	0.5

The values of Table 4 have been obtained by dividing the spatial domain into 20 equally divided intervals whereas the number of intervals varies for the time domain. That is, $N_x = N_y = 20$ and $\Delta t = 0.01$. The relative errors and the rate of convergence of the LSM method are presented in Table 5 and Table 6. To do this, the relative errors are defined by the following equations,

$$||e_u||_{\boldsymbol{R}} = \frac{||u(\Delta t) - u(\Delta t/2)||_\infty}{||u(\Delta t/2)||_\infty}, \text{ and } ||e_v||_{\boldsymbol{R}} = \frac{||v(\Delta t) - v(\Delta t/2)||_\infty}{||v(\Delta t/2)||_\infty},$$

Table 5. Relative errors and orders at $t_{end} = 1$ with different time step $\Delta \boldsymbol{t}$.

$t_{end} = 1$	Relative Error		Order	
Δt	$\|\|e_u\|\|_R$	$\|\|e_v\|\|_R$	u	v
0.1	$9.1737x10^{-4}$	$3.8232x10^{-4}$	2.0934	2.0969
0.05	$2.1495x10^{-4}$	$8.9365x10^{-5}$	2.0422	2.0164
0.025	$5.2187x10^{-5}$	$2.2087x10^{-5}$	2.0140	1.9490
0.0125	$1.2920x10^{-5}$	$5.7205x10^{-6}$	1.9933	1.8669
0.00625	$3.2449x10^{-6}$	$1.5683x10^{-6}$	1.9701	1.7510

and

Table 6. Relative errors and orders at $t_{end} = 10$ with different time step Δt.

$t_{end} = 10$	Relative Error		Order	
Δt	$\|\|e_u\|\|_R$	$\|\|e_v\|\|_R$	u	v
0.1	$5.4600x10^{-6}$	$5.8788x10^{-6}$	1.9864	2.1264
0.05	$1.3779x10^{-6}$	$1.3463x10^{-6}$	2.0056	2.0652
0.025	$3.4314x10^{-7}$	$3.2171x10^{-7}$	2.0197	2.0355
0.0125	$8.4618x10^{-8}$	$7.8472x10^{-8}$	2.0428	2.0235
0.00625	$2.0536x10^{-8}$	$1.9300x10^{-8}$	2.0903	2.0234

To see the validity of the solutions over time, computations are carried out for a different final time, $t = 1$ and $t = 10$ in Table 5 and Table 6, respectively. For both tables, we take $N_x = N_y = 20$. Even though the proposed method is a first-order method, the results of Table 5 and Table 6 are evidence that the method has second-order accuracy. It is crucial to say that this situation is mainly because of the usage of the exact solution on the diffusion part. Moreover, Table 5 and Table 6 guarantee that the method remains stable which also confirms the theoretical results.

In addition, Table 7 exhibits the comparison of the relative errors obtained by the Meshless Local Petrov-Galerkin (MLPG) method which is studied in [13], and the proposed method, LSM. Although it is a first-order method, it is seen from Table 7 that the LSM achieves good results for a different choice of Δt**.** It is important to note that this study deals with the time splitting algorithms whereas the compared study has mainly focused on the space discretization technique.

Table 7. Comparison of the relative errors at $t_{end} = 4$ with different time step Δt produced by LSM with the results of [13].

$t_{end} = 4$	LSM		MLPG [13]	
Δt	$\|\|e_u\|\|_R$	$\|\|e_v\|\|_R$	$\|\|e_u\|\|_R$	$\|\|e_v\|\|_R$
0.1	$5.4604x10^{-5}$	$1.4324x10^{-4}$	$1.7883x10^{-6}$	$6.0686x10^{-7}$
0.05	$1.7669x10^{-5}$	$4.3478x10^{-5}$	$1.7565x10^{-6}$	$5.5350x10^{-7}$
0.01	$5.2534x10^{-7}$	$1.1857x10^{-6}$	$1.7331x10^{-6}$	$5.2272x10^{-7}$
0.005	$1.4540x10^{-7}$	$2.8553x10^{-7}$	$1.7301x10^{-6}$	$5.1900x10^{-7}$
0.001	$2.2007x10^{-9}$	$1.1446x10^{-8}$	$1.7278x10^{-6}$	$5.1605x10^{-7}$

Furthermore, the exhibited figure, Figure 5, illustrates the numerical solution of u and v for the two-dimensional Brusselator system for the parameters $\alpha = 0.002$, $A = \frac{1}{2}$ and $B = 1$ on $t \in [0,3]$. To show the compatibility of the solution, the proposed method has been compared by a well-known Crank-Nicolson method without applying any splitting process. It can be easily seen that values of u and v approach the values 1 and 0.5 respectively.

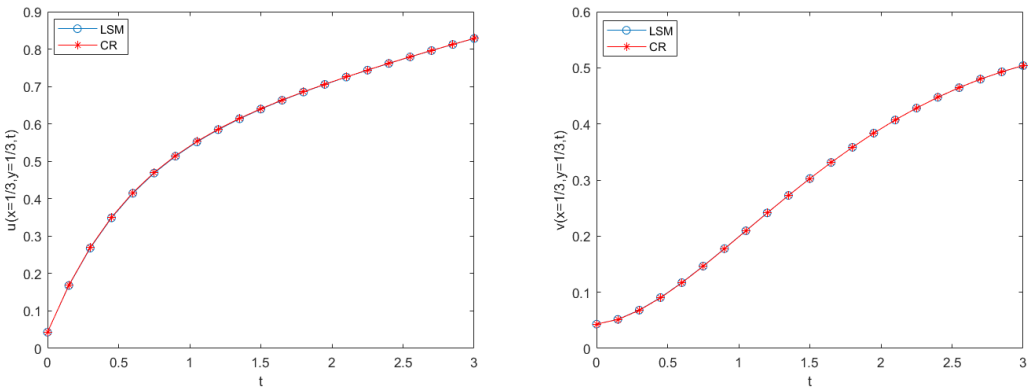


Figure 5. Graphs of $u\left(\frac{1}{3},\frac{1}{3},t\right)$ and $v\left(\frac{1}{3},\frac{1}{3},t\right)$ against time t for Example 3.

The graphs of the numerical solutions obtained for u and v at $t = 10$ with $N_x = N_y = 20$ and $\Delta t = 0.01$ are presented in Figure 6. Initial profiles of u and v are given in Figure 7.

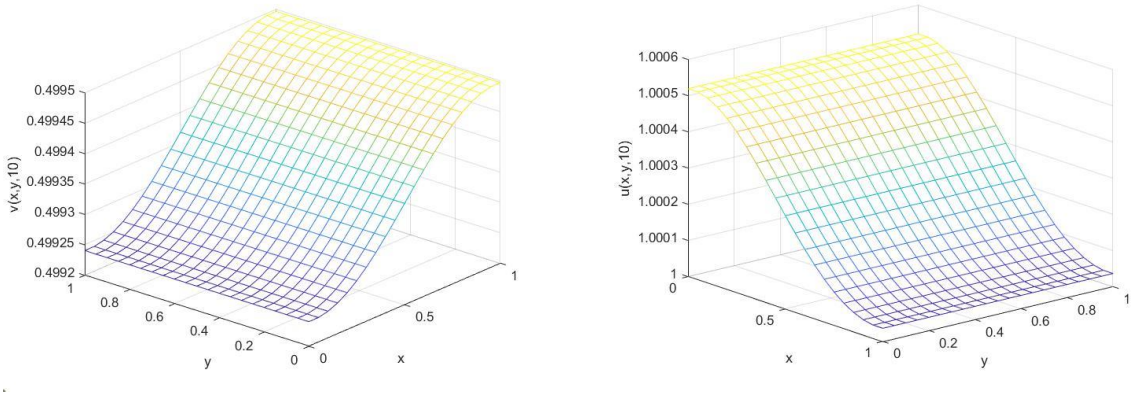


Figure 6. The solutions of u and v at $t = 10$.

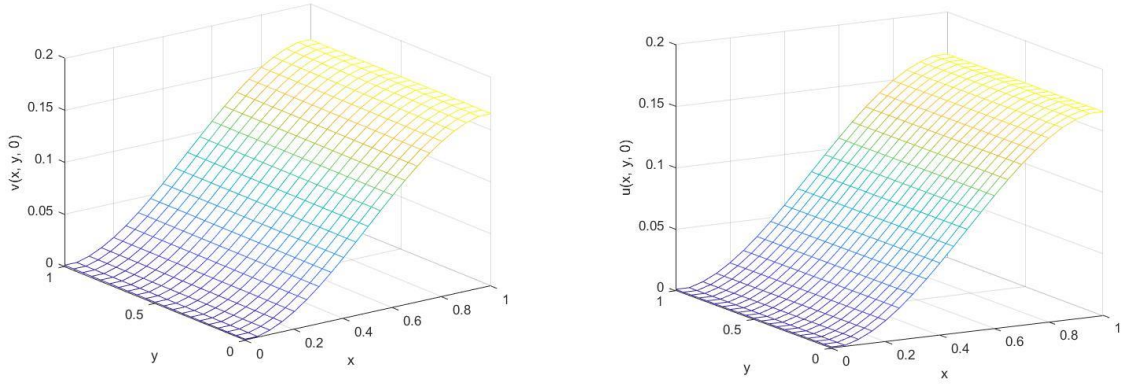


Figure 7. Initial concentration profiles of reactants u and v.

Figure 6 and Figure 7 present that the concentrations tend to approach their equilibrium points. From a mathematical point of view, the proposed method preserves the physical behavior of the initial profiles.

4. Conclusion and Comment

A kind of operator splitting method, the LSM, has been applied to solve the nonlinear reaction-diffusion Brusselator system. The system has been divided into two equations which are solved iteratively. The main contribution of this process is solving the diffusion part exactly which leads to getting high accuracy. Second-order Heun's method has been used for the nonlinear part. By the concepts of stability and consistency analyses, the convergence of the proposed method has been discussed. Additionally, it is shown that the method preserves the positivity of the solutions which plays a key role in chemical reaction-diffusion systems theoretically. In addition to these theoretical results, the current study has been also enriched computationally by applying the proposed method on several Brusselator systems. After generating an accuracy table the convergence rate of the method has been shown. It is important to emphasize that by virtue of the exact solution on the linear part the method performed as a second-order method even though it is a first-order method theoretically. Moreover, one can be seen on the tables and simulations the system reaches its equilibrium point for both one- and two-dimensional versions. All these results are evidence that the method is a very compatible and accurate method both physically and mathematically for the specified system.

Acknowledgment

The authors would like to thank the reviewers and the Editor-in-Chief for their contribution to the progress of the study through constructive, valuable, and insightful comments to this study.

Conflicts of interest

The authors state that there is no conflict of interests.

References

[1] Lefever R., Nicolis G., Chemical instabilities and sustained oscillations, *Journal of Theoretical Biology*, 30 (1971) 267-284.

[2] Nicolis G., Prigogine I., Self-Organization in Non-Equilibrium Systems: From Dissipative Structures to Order through Fluctuations, Wiley/Interscience, New York, London, Sydney, Toronto (1977).

[3] Prigogine I., Lefever R., Symmetries breaking instabilities in dissipative systems II. *The Journal of Chemical Physics*, 48 (1968) 1695-1700.

[4] Tyson J. J., Some further studies of nonlinear oscillations in chemical systems, *The Journal of Chemical Physics*, 58 (1973) 3919-3930.

[5] Turing A., The chemical basis of morphogenesis. *Philosophical Transactions of the Royal Society of London Series B, Biological Sciences*, 237 (1952) 37-72.

[6] Tyson J. J., The Belousov-Zhabotinskii Reaction (Lecture Notes in Biomathematics), 10, Springer-Verlag, Heidelberg, 1976.

[7] Ang W-T., The two-dimensional reaction–diffusion Brusselator system: a dual-reciprocity boundary element solution, *Engineering Analysis with Boundary Elements*, 27 (2003) 897-903.

[8] Adomian G., The diffusion-Brusselator equation, *Computers & Mathematics with Applications*, 29 (5) (1995) 1-3.

[9] Twizell E. H., Gumel A.B., Cao Q., A second-order scheme for the "Brusselator" reaction-diffusion system, *Journal of Mathematical Chemistry*, 26 (1999) 297-316.

[10] Wazwaz A.-M., The decomposition method applied to systems of partial differential equations and to the reaction-diffusion Brusselator model, *Applied Mathematics and Computation*, 110 (2000) 251-264.

[11] Jiwari R., Yuan J., A computational modeling of two dimensional reaction–diffusion Brusselator system arising in chemical processes, *Journal of Mathematical Chemistry*, 52 (2014) 1535-1551.

[12] Mittal R.C., Jiwari R., Numerical solution of two-dimensional reaction-diffusion Brusselator system, *Applied Mathematics and Computation*, 217 (2011) 5404-5415.

[13] Shirzadi A., Sladek V., Sladek J., A Meshless Simulations for 2D Nonlinear Reaction-diffusion Brusselator System, *Computer Modeling in Engineering and Sciences*, 95 (2013) 259-282.

[14] Siraj-ul-Islam Ali A., Haq S., A computational modeling of the behavior of the two-dimensional reaction-diffusion Brusselator system, *Applied Mathematical Modelling*, 34 (2010) 3896-3909.

[15] Yadav O. P., Jiwari R., A finite element approach for analysis and computational modelling of coupled reaction diffusion models, *Numerical Methods for Partial Differential Equations*, 35 (2019) 830-850.

[16] Yadav O. P., Jiwari R., A finite element approach to capture Turing patterns of autocatalytic Brusselator model, *Journal of Mathematical Chemistry*, 57 (2019) 769-789.

[17] Kumar S., Jiwari, R., Mittal R.C., Numerical simulation for computational modelling of reaction-diffusion Brusselator model arising in chemical processes, *Journal of Mathematical Chemistry*, 57 (2019) 149-179.

[18] Bhatt H., Chowdhury A., Comparative analysis of numerical methods for the multidimensional Brusselator system, *Open Journal of Mathematical Sciences*, 3 (2019) 262-272.

[19] Asante-Asamani E. O., Wade B. A., A Dimensional Splitting of ETD Schemes for Reaction-Diffusion Systems, *Communications in Computational Physics*, 19 (2016) 1343-1356.

[20] McLachlan R., Quispel G., Splitting methods, *Acta Numerica*, 11 (2002) 341-434.

[21] Hosseini R., Tatari M., Some splitting methods for hyperbolic PDEs, *Applied Numerical Mathematics*, 146 (2019) 361-378.

[22] Zurnacı F., Gücüyenen-Kaymak N., Seydaoğlu M., Tanoğlu G., Convergence analysis and numerical solution of the Benjamin-Bona-Mahony equation by Lie-Trotter splitting, *Turkish Journal of Mathematics*, 42 (2018) 1471-1483.

[23] Seydaoğlu M., An accurate approximation algorithm for Burgers' equation in the presence of small viscosity, *Journal of Computational and Applied Mathematics*, 344 (2018) 473-481.

[24] Hundsdorfer W., Verwer J., Numerical Solution of Time-Dependent Advection-Diffusion-Reaction Equations. 1st ed. Springer, Berlin, Heidelberg, (2003) 116-121.

[25] Mickens R.E., Nonstandard finite difference schemes for reaction-diffusion equation, *Numerical Methods for Partial Differential Equations*, 15 (1999) 201-214.

[26] Singh R., Brusselator as a Reaction-Diffusion, Master Dissertation, Homi Bhabha National Institute, The Institute of Mathematical Sciences, (2008).

[27] Manaa S. A., Saeed R. K., Easif F. H., Numerical Solution of Brusselator Model by Finite Difference Method, *Journal of Applied Sciences Research*, 6 (11) (2010) 1632-1646.