

Global existence and numerical simulations of a coupled two-cell activator-inhibitor reaction-diffusion system

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Abstract

A coupled two-cell Brusselator system subject to Neumann boundary conditions is considered. Firstly, we obtain the global existence of classical solutions for the system. Then, with the aim of showing the model dynamics, we develop a positivity preserving splitting technique to find the numerical solution of the proposed model. The numerical scheme leads to the convergence of the solution to a steady-state or to the equilibrium point.

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1 Introduction

Since the revolutionary research published by A. Turing in the early 1950s [1] regarding the chemical basis of formation, the model proposed by him received great interest from the research community in the fields of mathematics, biology, chemistry and many others [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13]. The Brusselator system is a simple system of reaction-diffusion equations occurring in biochemical reactions, chemical kinetics and biological processes. It was first proposed by Prigogine and Lefever in 1968 (cf. [14]) and was given its current name by Tyson in 1973 (cf. [15]). The Brusselator chemical reaction can be represented by the following mechanism:



where X and Y are intermediates, A and B are input chemicals with a constant concentration, and D and E are output chemicals. The steps in (1.1) yield the nondimensionalized Brusselator reaction-diffusion system

$$\begin{cases} \frac{\partial u}{\partial t} = d_1 \frac{\partial^2 u}{\partial x^2} + a - (b+1)u + u^2v, & x \in (0, l), t > 0 \\ \frac{\partial v}{\partial t} = d_2 \frac{\partial^2 v}{\partial x^2} + bu - u^2v, & x \in (0, l), t > 0 \end{cases} \tag{1.2}$$

subject to the homogeneous Dirichlet or Neumann boundary conditions and initial data. In this system, the reactions occur in an interval $(0, l)$, $l > 0$, $u := u(x, t)$ and $v := v(x, t)$ are the chemical

concentrations of an activator and an inhibitor, respectively, and d_1, d_2, a, b are positive numbers. The Brusselator system (1.2) has drawn the attention of various researchers who have obtained interesting analytical and numerical results [16, 17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29]. In general, numerous numerical schemes have been proposed for solving evolutionary partial differential equations [30, 31, 32, 33, 34, 35, 36, 37, 38].

In the present work, we consider the coupled two-cell Brusselator model

$$\begin{cases} u_t - d_1 \Delta u = a - (b+1)u + u^2 v + c(w-u) & \text{in } \Omega \times (0, T) \\ v_t - d_2 \Delta v = bu - u^2 v & \text{in } \Omega \times (0, T) \\ w_t - d_3 \Delta w = a - (b+1)w + w^2 z + c(u-w) & \text{in } \Omega \times (0, T) \\ z_t - d_4 \Delta z = bw - w^2 z & \text{in } \Omega \times (0, T) \\ \partial_\nu u = \partial_\nu v = \partial_\nu w = \partial_\nu z = 0 & \text{on } \partial\Omega \times (0, T) \\ u(x, 0) = u_0(x), v(x, 0) = v_0(x) & \text{on } \bar{\Omega} \\ w(x, 0) = w_0(x), z(x, 0) = z_0(x) & \text{on } \bar{\Omega} \end{cases} \quad (1.3)$$

where $u := u(x, t)$, $v := v(x, t)$, $w := w(x, t)$, $z := z(x, t)$, $\Omega := (L_{in}, L_{end})$, $L_{in} \geq 0$, $d_1, d_2, d_3, d_4, a, b, c, L_{end}$ and T are positive numbers, Δ is the Laplacian operator on Ω , and ν is the unit outer normal to $\partial\Omega$. Some results have been reported regarding the dynamics of the coupled two-cell Brusselator model (1.3) with/without modifications on the system [39, 40, 41]. R.D. Parshad *et al.* [42] proved the global existence for system (1.3) subject to the homogeneous Dirichlet boundary conditions.

In this paper, we are primarily interested in continuing the work on the two-cell Brusselator model (activator-inhibitor system), in which we demonstrate the global existence of classical solution for system (1.3) by using a suitable Lyapunov-type function (cf. J. Morgan [19]). In addition, we develop an efficient explicit unconditionally numerical scheme which preserves positivity of the solution for system (1.3). To affirm our findings, numerical examples will be presented.

2 Global existence of solutions

The main step toward the result is to establish a so called Lyapunov-type function $H \in C^2(\mathbb{R}_+^4; \mathbb{R})$ with $h_i \in C^2(\mathbb{R}_+; \mathbb{R})$ for $i = 1, \dots, 4$ such that

$$H(z) = \sum_{i=1}^4 h_i(z_i), \quad z = (z_i)_{i=1}^4 \in \mathbb{R}_+^4, \quad (2.1)$$

with

$$h_i(z_i), h_i''(z_i) \geq 0, \quad z_i \in \mathbb{R}_+, \quad i = 1, \dots, 4, \quad (2.2)$$

and

$$H(z) \rightarrow \infty, \quad \text{if and only if } |z| \rightarrow \infty \text{ in } \mathbb{R}_+^4, \quad (2.3)$$

Assume there exists a lower triangular matrix $A = (a_{ij})_{1 \leq i, j \leq 4} \in \mathbb{R}^4 \times \mathbb{R}^4$ which satisfies $a_{ij} \geq 0$, $a_{ii} > 0$ for $1 \leq i, j, \leq 4$ such that for all $1 \leq l \leq 4$ there exist $K_1, K_2 \geq 0$ independent of l , in which

$$\sum_{j=1}^l a_{jl} h_j'(z_j) f_j(z) \leq K_1 H(z) + K_2, \quad z \in \mathbb{R}_+^4. \quad (2.4)$$

Also, assume that there exist $q, K_3, K_4 \geq 0$ such that for $1 \leq i \leq 4$,

$$h'_i(z_i)f_i(z) \leq K_3(H(z))^q + K_4, \quad z \in \mathbb{R}_+^4. \quad (2.5)$$

Furthermore, assume that there exist $K_5, K_6 \geq 0$ such that

$$\nabla H(z) \cdot f(z) \leq K_5 H(z) + K_6, \quad z \in \mathbb{R}_+^4. \quad (2.6)$$

Based on J. Morgan's method (cf. [19]), we get the following result

Theorem 2.1. Consider the initial conditions $u_0, v_0, w_0, z_0 \in L^\infty(\Omega; (0, +\infty))$. Then, there exists a unique positive global (i.e. $T = \infty$) classical solution for the coupled two-cell Brusselator system (1.3).

Proof. At the outset, we swap variables u and v as well as w and z in the coupled two-cell Brusselator system (1.3), which yields the equivalent system

$$\begin{cases} u_t - d_1 \Delta u = f_1(U) & \text{in } \Omega \times (0, T) \\ v_t - d_2 \Delta v = f_2(U) & \text{in } \Omega \times (0, T) \\ w_t - d_3 \Delta w = f_3(U) & \text{in } \Omega \times (0, T) \\ z_t - d_4 \Delta z = f_4(U) & \text{in } \Omega \times (0, T) \\ \partial_\nu u = \partial_\nu v = \partial_\nu w = \partial_\nu z = 0 & \text{on } \partial\Omega \times (0, T) \\ u(x, 0) = u_0(x), v(x, 0) = v_0(x) & \text{on } \bar{\Omega} \\ w(x, 0) = w_0(x), z(x, 0) = z_0(x) & \text{on } \bar{\Omega} \end{cases} \quad (2.7)$$

where $U := (u, v, w, z)$ and

$$\begin{aligned} f_1(U) &:= bv - uv^2, \\ f_2(U) &:= a - (b+1)v + uv^2 + c(z-v), \\ f_3(U) &:= bz - wz^2, \\ f_4(U) &:= a - (b+1)z + wz^2 + c(v-z). \end{aligned}$$

The local existence of a solution for system (1.3) results from the well-known semigroup theory (cf. [43, 44]). We choose $h_i(z_i) = z_i$ for $i = 1, \dots, 4$, and $A = (a_{ij})_{1 \leq i, j \leq 4}$ such that

$$a_{ij} := \begin{cases} 1 & \text{if } i \geq j \\ 0 & \text{else} \end{cases}$$

Then, conditions (2.1)-(2.6) are fulfilled.

Q.E.D.

Remark 2.2. The proof of Theorem 2.1 remains effective when Ω is an open subset of \mathbb{R}^n ($n \in \mathbb{N}$) that is both smooth and bounded (cf. [19]). The same results can also be obtained with a wider class of boundary conditions by using the method of S. Abdelmalek and S. Kouachi (cf. [45]).

3 Numerical method

3.1 Discretization of domain

We aim to show the approximate solutions of system (1.3) by applying the finite difference method. We consider the numerical approximation in the time domain $[0, T]$ and the space domain $[L_{in}, L_{end}]$. Let $t_k = k\Delta t$ ($0 \leq t_k \leq T$), $k = 0, \dots, M$, $x_i = L_{in} + i\Delta x$ ($L_{in} \leq x_i \leq L_{end}$), and $i = 0, \dots, N$, where the time step is $\Delta t = \frac{T}{M}$ and the space step is $\Delta x = \frac{L_{end} - L_{in}}{N}$ ($M, N \in \mathbb{N}$). We use the following notations $u_i^k = u(x_i, t_k)$, $v_i^k = v(x_i, t_k)$, $w_i^k = w(x_i, t_k)$, $z_i^k = z(x_i, t_k)$.

3.2 Numerical scheme

Based on Mickens' rules for the nonstandard finite difference schemes (cf. [46]), we obtain the following new scheme for system (1.3):

$$u_i^{k+1} = u_i^k + \alpha_1 (u_{i-1}^k + u_{i+1}^k) + a\Delta t - \Delta t(b+1)u_i^{k+1} + \Delta t(u_i^k)^2 v_i^k + c\Delta t w_i^k - c\Delta t u_i^{k+1} - 2\alpha_1 u_i^{k+1}, \quad (3.1)$$

$$v_i^{k+1} = v_i^k + \alpha_2 (v_{i-1}^k + v_{i+1}^k) - 2\alpha_2 v_i^{k+1} + b\Delta t u_i^k - \Delta t(u_i^k)^2 v_i^{k+1}, \quad (3.2)$$

$$w_i^{k+1} = w_i^k + \alpha_3 (w_{i-1}^k + w_{i+1}^k) + a\Delta t - \Delta t(b+1)w_i^{k+1} + \Delta t(w_i^k)^2 z_i^k + c\Delta t u_i^k - c\Delta t w_i^{k+1} - 2\alpha_3 w_i^{k+1}, \quad (3.3)$$

$$z_i^{k+1} = z_i^k + \alpha_4 (z_{i-1}^k + z_{i+1}^k) - 2\alpha_4 z_i^{k+1} + b\Delta t w_i^k - \Delta t(w_i^k)^2 z_i^{k+1}, \quad (3.4)$$

$$(3.5)$$

where $\alpha_j = \frac{d_j \Delta t}{(\Delta x)^2}$ for $j = 1, \dots, 4$. Thus, the explicit formula is

$$u_i^{k+1} = \frac{u_i^k + \alpha_1 (u_{i-1}^k + u_{i+1}^k) + a\Delta t + \Delta t(u_i^k)^2 v_i^k + c\Delta t w_i^k}{1 + 2\alpha_1 + \Delta t(b+1) + c\Delta t}, \quad (3.6)$$

$$v_i^{k+1} = \frac{v_i^k + \alpha_2 (v_{i-1}^k + v_{i+1}^k) + b\Delta t u_i^k}{1 + 2\alpha_2 + \Delta t(u_i^k)^2}, \quad (3.7)$$

$$w_i^{k+1} = \frac{w_i^k + \alpha_3 (w_{i-1}^k + w_{i+1}^k) + a\Delta t + \Delta t(w_i^k)^2 z_i^k + c\Delta t u_i^k}{1 + 2\alpha_3 + \Delta t(b+1) + c\Delta t}, \quad (3.8)$$

$$z_i^{k+1} = \frac{z_i^k + \alpha_4 (z_{i-1}^k + z_{i+1}^k) + b\Delta t w_i^k}{1 + 2\alpha_4 + \Delta t(w_i^k)^2}. \quad (3.9)$$

3.3 Positivity, stability and consistency of the proposed scheme

By following the arguments in [29] it is not difficult to obtain the following results:

Theorem 3.1. Subject to the initial conditions of system (1.3) being non-negative, the numerical scheme (3.6)-(3.9) demonstrates positive solutions.

Theorem 3.2. Subject to the initial conditions of system (1.3) being non-negative, the numerical scheme (3.6)-(3.9) is stable.

Theorem 3.3. Subject to the initial conditions of system (1.3) being non-negative, the numerical scheme (3.6)-(3.9) is consistent.

4 Numerical experiments

Let us now show the approximate solution of the coupled two-cell Brusselator system (1.3) in order to demonstrate the changes in solution behaviour that arise when the parameters are varied. The computer algorithm for numerical scheme (3.6)-(3.9) was written in Matlab. Throughout the

simulations we considered the following initial conditions:

$$\begin{aligned} u_0(x) &= a + \frac{\cos(10\pi x)}{2}, \\ v_0(x) &= a + 1 + \frac{\sin(10\pi x)}{2}, \\ w_0(x) &= \frac{a+b}{4} + \frac{\cos(5\pi x)}{2}, \\ z_0(x) &= \frac{a+b+1}{6} + \frac{\sin(5\pi x)}{2}. \end{aligned}$$

The following sets of system parameters are considered for each simulation:

1. $a = 2$, $b = 3.4$, $c = 2$, $L_{in} = 0$, $L_{end} = 2$, $T = 50$, $d_1 = 0.01$, $d_2 = 0.02$, $d_3 = 0.001$ and $d_4 = 0.003$.
2. $a = 1$, $b = 3.4$, $c = 2$, $L_{in} = 0$, $L_{end} = 4$, $T = 50$, $d_1 = 0.01$, $d_2 = 0.02$, $d_3 = 0.001$ and $d_4 = 0.003$.
3. $a = 2.3$, $b = 1.7$, $c = 3.4$, $L_{in} = 0$, $L_{end} = 5$, $T = 50$, $d_1 = 0.03$, $d_2 = 0.05$, $d_3 = 0.03$ and $d_4 = 0.05$.
4. $a = 1.5$, $b = 2.78$, $c = 3.4$, $L_{in} = 0$, $L_{end} = 5$, $T = 150$, $d_1 = 0.03$, $d_2 = 0.05$, $d_3 = 0.03$ and $d_4 = 0.05$.

Remark 4.1. The approximate solutions depicted in Figure 3 and Figure 4 agree with the theoretical results obtained in [40] regarding the dynamics of such a system.

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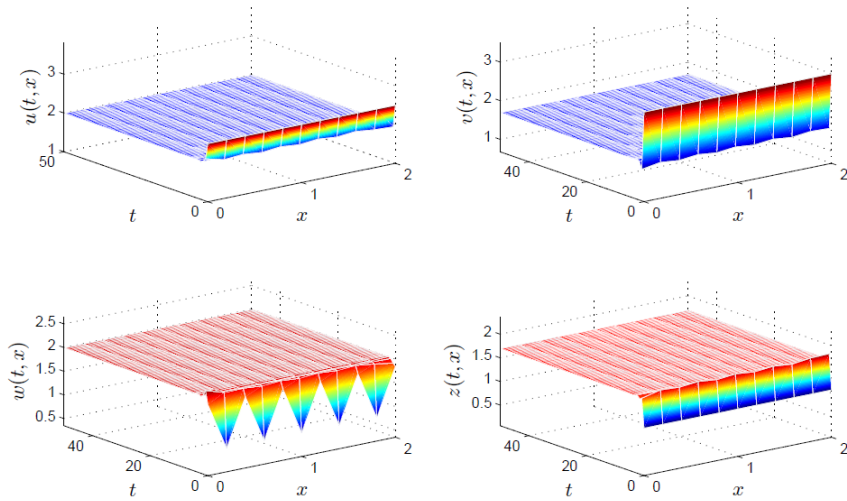


FIGURE 1. Numerical simulation of a coupled two-cell Brusselator system (1.3) subject to the first set of parameters.

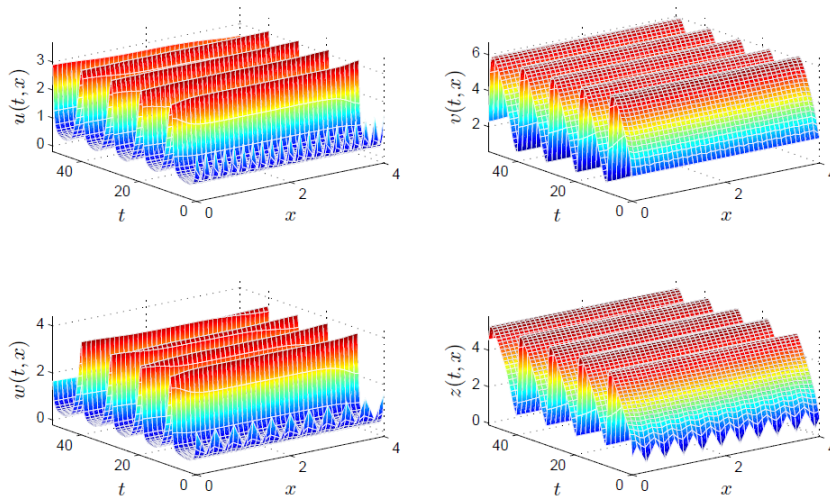


FIGURE 2. Numerical simulation of a coupled two-cell Brusselator system (1.3) subject to the second set of parameters.

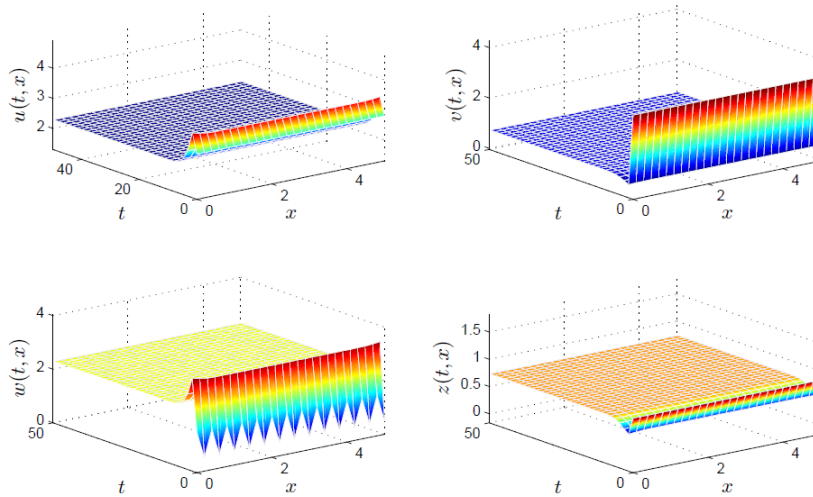


FIGURE 3. Numerical simulation of a coupled two-cell Brusselator system (1.3) subject to the third set of parameters.

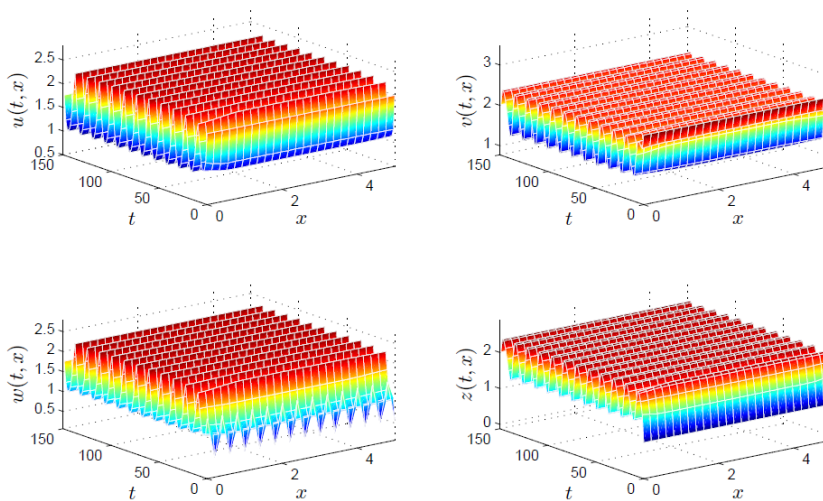


FIGURE 4. Numerical simulation of a coupled two-cell Brusselator system (1.3) subject to the fourth set of parameters.

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