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Pattern Formation in the Brusselator Model Using Numerical Bifurcation Analysis

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Abstract. Pattern formation is one of the most surprising natural phenomena in real life. Analysis of spatiotemporal reaction-diffusion system can lead to understanding the pattern dynamics. However, the periodic traveling wave solutions resulting from the reaction-diffusion system can play an important role to explain the pattern dynamics. In this study, we analyze a system of nonlinear reaction-diffusion equations called the Brusselator model. We establish a parameter plane to investigate the existence of periodic traveling waves as well as stability results of the model using the method of continuation. We also find an Eckhaus type stability boundary where we confirm the stability change by calculating the essential spectra of the solutions of the model. As a result, we obtain a pattern transition from stripe pattern to spot pattern of the model in the two spatial dimensions numerically.

AMS (MOS) Subject Classification Codes: 92C15; 37G15; 65P40
Key Words: Brusselator model, Pattern formation, Periodic traveling wave, Stability.

1. Introduction

In excitable media [8], spatiotemporal periodic traveling wave (PTW) solutions are significant for many partial differential equations (PDEs) to recognize the pattern formation. The PTW solutions were more mentioned in ecological [1, 10, 16], chemical [2, 5, 23], physical [17, 21, 22] and biological systems [3, 15]. In this paper, we numerically examine the stability of the PTW solutions of the reaction-diffusion (R-D) model. The method of continuation [13] is a powerful and standard procedure to analyze the PTW solutions of the system of PDEs.

This paper presents the mechanism of the pattern formation through the numerical investigation with the R-D Brusselator model which is also known as the trimolecular model. This chemical R-D model involves rich spatiotemporal patterns. When two or more interacting chemical diffuses then spatial patterns arise due to the instability [18]. Since the concept about the pattern selection, pigmentation process of an activation and inhibition in any natural system has no clear evidence [7]. Therefore the pattern formation of any activator-inhibitor model is an interesting and challenging phenomenon for many researchers. The Brusselator model with pattern formations are studied in [4, 6, 20, 24]. A numerical solution technique of the model named second-order method is developed in [19].

In this article, we discuss the R-D Brusselator model in Section 2. In Section 3, We employ the method of continuation through a package WAVETRAIN [13] to analyze the PTW solutions of the R-D model. Also, numerical simulations in one dimension and two dimensions are discussed in this section. Finally, some conclusions regarding the obtained results are given in Section 4.

2. MODEL

The autocatalytic chemical reactions for the standard R-D Brusselator model [9] is given by

$$\begin{aligned} \frac{\partial u}{\partial t} &= d_1 \nabla u + a - (b+1)u + u^2 v, \\ \frac{\partial v}{\partial t} &= d_2 \nabla v + bu - u^2 v, \end{aligned} \tag{2. 1}$$

where the dimensionless concentrations u and v represents activator and inhibitor, respectively and d_1 and d_2 are the corresponding diffusion coefficients. Also, $f(u,v) = a - (b+1)u + u^2 v$ and $g(u,v) = bu - u^2 v$ are the reaction kinetics for the activator and inhibitor, respectively where a and b represents the kinetic parameters. The steady state solution of (2. 1) is $(u^*, v^*) = (a, \frac{b}{a})$.

3. METHODOLOGY, RESULTS AND DISCUSSIONS

3.1. **Existence and Stability Analysis Through Continuation Package.** In this part, we demonstrate the existence and stability of the PTW solutions of (2. 1) by the method of continuation through a software package WAVETRAIN. The continuation package WAVETRAIN needs some specific settings as input files. We consider $z = x - ct$ as the traveling wave coordinate with the space variable x, time variable t and the wave speed c. Now, we use $u(x,t) = U(z)$ and $v(x,t) = V(z)$ and put in (2. 1) and hence, we get a system of ordinary differential equations (ODEs) as following:

TABLE 1. Considered parameter values of (2. 1)

Parameters	a	b	d_1	d_2
Values	3.0	$\cdots$	3.0	10.0

$$\begin{aligned} \frac{dU}{dz} &= P, \\ \frac{dP}{dz} &= (-cP - a + (b+1)U - U^2V)/d_1, \\ \frac{dV}{dz} &= Q, \\ \frac{dQ}{dz} &= (-cQ - bU + U^2V)/d_2. \end{aligned} \tag{3. 2}$$

In order to solve the set of traveling wave equations (3. 2), WAVETRAIN requires an initial PTW solution and we use an initial solution from the simulation of the model (2. 1) for a pair of free parameter b and wave speed c values. The system (3. 2) represents the limit cycle solution indicates that, the existence of PTW solutions of the model (2. 1). In order to calculate the stability results of the model (2. 1) in WAVETRAIN, we need to perform some necessary calculations. By putting $u_{lin}(x,t) = u(x,t) - U(z)$ and $v_{lin}(x,t) = v(x,t) - V(z)$, we form a set of linearized equations from (2. 1) on traveling wave solution. By substituting $u_{lin}(x,t) = e^{\lambda t}U(z)$ and $v_{lin}(x,t) = e^{\lambda t}V(z)$ in the linearized equations, we find the eigenvalue equations as follows:

$$\begin{aligned} \lambda U_{lin} &= c\frac{dU_{lin}}{dz} + d_1\frac{d^2U_{lin}}{dz^2} + U_{lin}(-b - 1 + 2UV) + V_{lin}(U^2), \\ \lambda V_{lin} &= c\frac{dV_{lin}}{dz} + d_2\frac{d^2V_{lin}}{dz^2} + U_{lin}(b - 2UV) + V_{lin}(-U^2). \end{aligned} \tag{3. 3}$$

where the boundary conditions are as follows:

$$\begin{aligned} U_{lin}(P) &= U_{lin}(0)\,\exp(i\gamma),\ \text{for some } \gamma \in \mathbb{R}, \\ V_{lin}(P) &= V_{lin}(0)\,\exp(i\gamma),\ \text{for some } \gamma \in \mathbb{R}, \end{aligned} \tag{3. 4}$$

where P is the period of the PTW, γ is the wave phase shift for the one period, U_{lin} and V_{lin} are the eigenfunctions and λ is the eigenvalue.

Now, using the method employed in [11], WAVETRAIN calculates the stability of PTW solutions of the model (2. 1) by determining the essential spectrum. In the large domain of the PTW solution spectrum, there exists only the essential spectrum [12]. Eckhaus type stability change occurs if the spectrum curvature changes the sign near the origin and Hopf type stability change occurs if the spectrum curvature changes the sign away from the origin. [14]. 1 shows the PTW solutions of (2. 1) with the existence as well as the stability results. We determine a two dimensional parameter plane as a function of the bifurcation parameter b, where we use 8×8 grid elements. In the numerical computations, we use the parameter values of (2. 1) as mentioned in 1 and the parameter b is considered as a bifurcation parameter. We find a locus of Hopf bifurcation points which is represented by the orange color. Also, the green triangle represents that there is no PTW solution.

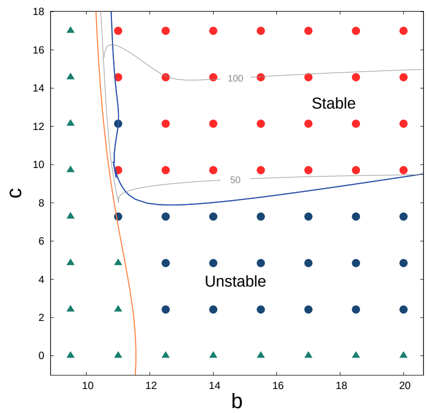

FIGURE 1. An illustration of the existence and stability of PTW solutions of (2. 1) as a function of b and c. Here 8×8 grid elements is used to generate this two dimensional parameter plane. The other parameter values of (2. 1) are same as in 1. The symbol 115 refers that there is no periodic traveling wave at that point, the symbol 108 refers the stable PTW solutions and the symbol 108 refers the unstable PTW solutions. The orange line refers to the locus of Hopf bifurcation points. The gray line represents the iso-period lines. Also, The blue line indicates the Eckhaus type stability boundary of the PTW solutions.

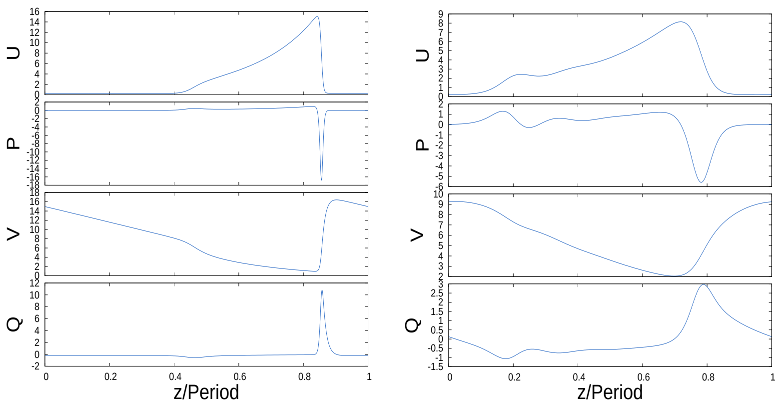

FIGURE 2. PTW solution profiles of (2. 1)(a) A stable PTW solution profile for $b = 14.0$ and $c = 12.14$ with period= 75.40.(b) A unstable PTW solution profile for $b = 15.5$ and $c = 2.42$ with period= 18.95.

Moreover, the red and blue circle on the parameter plane represents the stable and unstable PTW solutions, respectively. After that, we determine a Eckhaus type stability boundary between these stable and unstable PTW solution regions.

3.1 shows a stable PTW solution where $b = 14.0$ and $c = 12.14$ where the period for this particular stable PTW solution is 75.40 and 3.1 shows an unstable PTW solution profile where $b = 15.50, c = 2.42$ and in this case, the calculated period is 18.95. In 2, the remaining values of the parameters in (2. 1) are same as in 1.

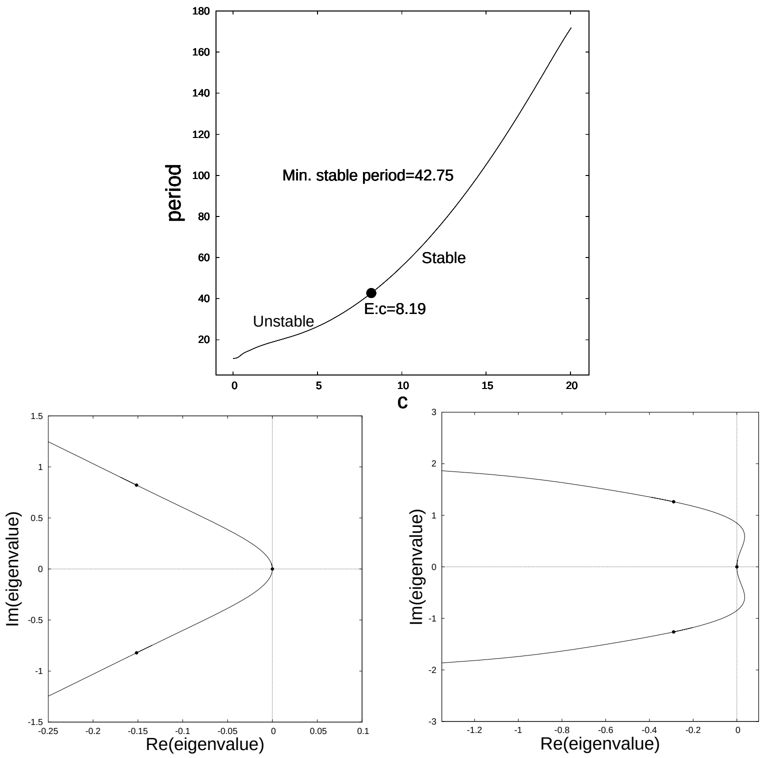

FIGURE 3. (a)A dispersion diagram of the period and wave speed c for $b = 15.0$. (b) a stable PTW solution behavior using essential spectrum when c=11.0 (c) an unstable PTW solution behavior using essential spectrum when c=5.0.

3.1 shows the bifurcation diagram of the period of the PTW solutions and the corresponding wave speeds. This bifurcation diagram is calculated at $b = 15.0$ where the other parameter values are same as in 1.Our analysis shows that, the stability change occurs at $c = 8.19$ when $b = 15.0$ and which is Eckhaus type. For $b = 15.0$ and $c = 8.19$, the period of the PTW solution is 42.75 (approximately) which is the minimum stable period. An illustration of the bifurcation diagram in 3.1 by using essential spectra is given by 3.1

and 3.1. 3.1 is plotted for $c = 11.0$ $(c > 8.19)$ where we see that the spectrum curvature changes the sign near the origin and does not cross the imaginary axis indicate that stable PTW solution exists. In 3.1, we use $c = 5.0$ $(c < 8.19)$ where we see that spectrum curvature changes the sign near the origin but imaginary axis crosses indicate that unstable PTW solution exists.

3.2. **Pulse Increment of PTW Solutions.** In this subsection, we verify our result obtained in 3.1 with the direct numerical simulations of (2. 1) in one dimensional space. We apply the periodic boundary conditions over the domain $[0, D_x]$ with an implicit scheme. Here D_x is the system size and can be represented by $D_x = n \times p$ with the number of periodic pulses n and the spatial period of the pulse p. Also we use 1305 grid elements with $dx = 0.006$ and $dt = 0.01$. In 4, the parameter values of (2. 1) are same as in 3.1. In 3.1, the

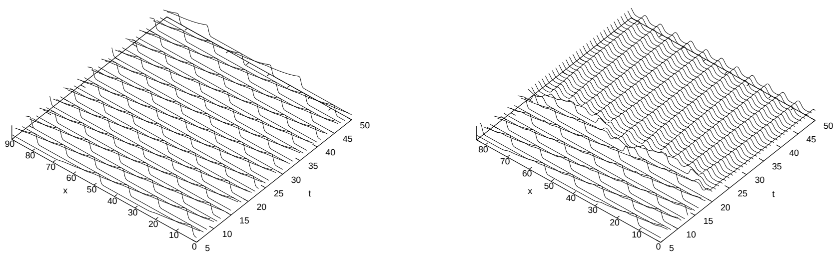

FIGURE 4. Space-time plots of the PTW solutions of (2. 1) based on the bifurcation diagram. (a) A stable two pulses PTW solution for the period$= 45$. (b) A PTW solution where pulse increases from two pulses to eleven pulses for the period$= 42$.

minimum stable period is $P = 42.75$ approximately at the Eckhaus bifurcation point. First, we use $D_x = 90$ as the system size with two periodic pulses that means, the spatial period of each pulse is $p_1 = 45$ which is higher value than minimum stable period value 42.75. Then we perform the numerical simulation with the above settings for $5 < t < 50$ and we obtain a stable PTW solution as 3.2. Next, we use $D_x = 84$ as the system size with two periodic pulses that means, the spatial period of each pulse is $p_2 = 42$ which is lower value than the minimum stable period value 42.75. After that, we perform the numerical simulation with $5 < t < 50$ and we get a PTW transformation from two pulses to eleven pulses. Since 3.1 represents a dispersion diagram which comes from 1 where 1 shows the continuation results of the system (3. 2) that means existence as well as the stability of PTW solutions of the model (2.1), hence we get a satisfactory correspondence between the continuation results and the results from the direct numerical simulations of the model (2. 1).

3.3. **Pattern Formation Phenomenon.** In this subsection, we verify our result obtained in 1 with the direct PDE numerical simulations of (2. 1) in two dimensional space. We apply Neumann boundary conditions in (2. 1) with the alternating direction implicit method

(ADI). We use $dx = dy = 0.5$ as space step and $dt = 0.001$ as time step on a grid of 220×220 elements. We also consider b as a bifurcation parameter and the other values

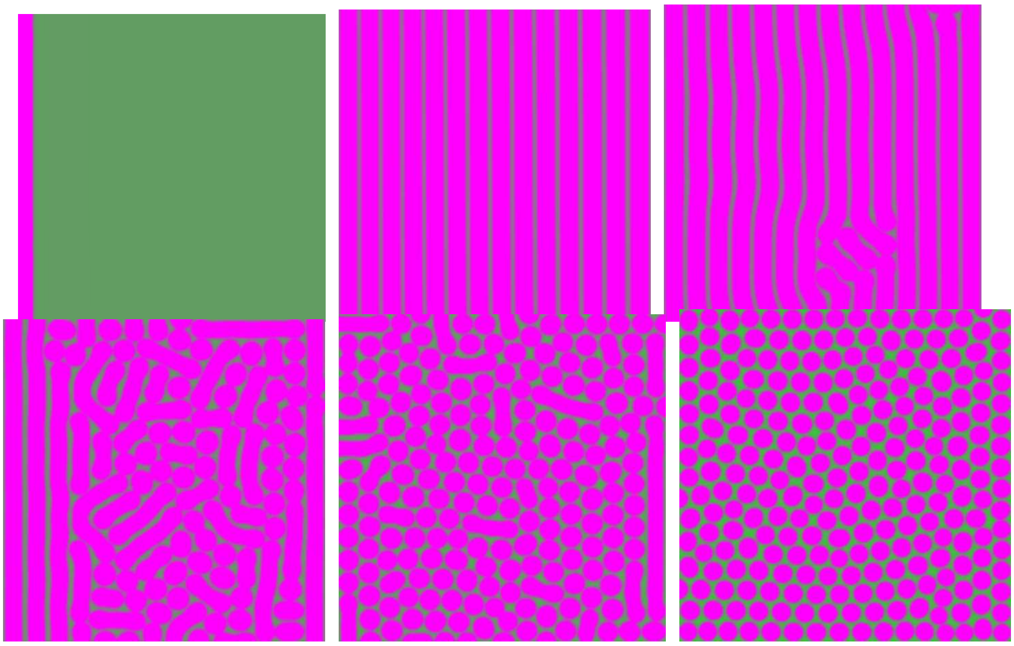

FIGURE 5. An illutration of the pattern evolution from stripe to spot in two-dimensional space as we vary a parameter b in (1) and the other parameter settings are same as those in Table I. Numerical results with space step $dx = dy = 0.5$ and time step $dt = 0.001$ on grid of 220×220 elements with (a) initial data (b) $b = 10.5$ (c) $b = 10.8$ (d) $b = 12.0$ (e) $b = 14.0$ (f) $b = 15.5$.

of the parameters of (2. 1) are the same as in 1. We assume a bar initial data to perform the whole simulation process. We continue our simulation process for a long time until we reach a steady state pattern. The dynamics of the transformation of pattern formation for the R-D model (2. 1) as a function of b is observed in 5. 3.3 shows bar data as an initial guess. We obtain a regular stripe pattern for $b = 10.5$ shows in 3.3. We find the breakup of the stripe pattern near the stability boundary for $b = 10.8$ which shows in 3.3. When we cross the stability boundary by increasing the value of b, breakup also increases which shows in 3.3 and 3.3. In 3.3, we get a fully spot pattern for $b = 15.5$. That means the transformations from the stripe pattern to the spot pattern occurs for the PTW transformations via the Eckhaus type stability boundary. Consequently, we get a good agreement between the continuation result obtained in reffig:wavetrain and the numerical result in two dimensions.

4. Conclusion

Regular spatial pattern formation is a central feature of natural phenomenon in a wide range of biological and chemical systems. Recent evidence shows that spatial patterns become an important indicator to explain the dynamical behavior of any R-D models. Nowadays, numerical analysis is a major way to understand the pattern solutions of the PDE models. For such reasons, we studied the dynamics of pattern formation represented by the nonlinear R-D Brusselator model. We showed the existence as well as the stability result analysis of the model through a continuation package WAVETRAIN. We obtained an Eckhaus type stability boundary where we confirmed our stability results by determining the essential spectra curvature. The stability result of the direct PDE simulations in one dimension agreed with the continuation result of the system of ODEs. Also, the numerical simulations in two dimensions showed that the transformation of the pattern formation occurred as a consequence of the PTW transformation due to the Eckhaus type stability boundary. Hence, we get a fine correspondence of the system of ODEs continuation result with the direct numerical simulations of the PDE system.

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