# Turing instability for a two dimensional semi-discrete Oregonator model

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*Abstract:* - In this paper, a semi-discrete (time continuous but two-dimensional spatially discrete) Oregonator model has been given in the microscopic domain, and Turing instability theory analysis is discussed in detail. Turing instability conditions have been deduced by combining linearization method and inner product technique. Various patterns such as spiral wave, target wave, stripes and spotlike patterns are selectively obtained from numerical simulations in the Turing instability region. In particular, the effect of both system parameters and initial value on pattern formation is numerically proved.

*Key-Words:* - semi-discrete Oregonator model; Turing instability; pattern formation; initial value; linearization method; inner product

## **1** Introduction

In the last few years, the problem of pattern formation has become one of the most studied topics in the field of modern science. Patterns are observed in a wide range of physical systems, chemical and biological systems, magnetic and optical media, gas and electron hole plasmas, semiconductor and gas discharge structures [1-2]. From the experimental point of view, pattern formation can be easily reproduced for chemical systems, such as the Belousov Zhabotinsky (briefly, B-Z) reaction, which has been found to be the most simple and prototypical example of pattern forming in chemical reactions.

Experiments about B-Z reaction in thin layers have exhibited such generic two dimensional wave patterns as pacemakers or spiral waves, and the transition to chemical turbulence due to spiral breakup has also been observed [3-5]. Turing patterns, such as labyrinthine, hexagonal and spotlike standing waves, have been reported by Vanag and Epstein [6-9] when the B-Z reaction is carried out in the aqueous domain of water in oil microemulsions. Twinkling eyes, where oscillating Turing spots are arranged as a hexagonal lattice, have also been observed in the work of Vanag and Epstein [10]. In short, the B-Z system exhibits an extremely rich variety of dynamical concentration patterns, which can be stable only far from equilibrium.

The Oregonator model, regarded as a successful time-honored mathematical model in the macroscopic domain, was proposed to capture the main qualitative and quantitative features of the B-Z reaction [2]. In dimensionless units a simplified version of the model is given by the following reaction--diffusion equations of the form

$$\begin{cases} \frac{du}{dt} = F(u, v) + D_1 \nabla^2 u\\ \frac{dv}{dt} = G(u, v) + D_2 \nabla^2 v \end{cases}$$
(1)

where t is time, u and v denote the concentrations of the activator and the inhibitor,  $D_1$  and  $D_2$  are the constant diffusion coefficients of u and v , respectively

$$F(u,v) = \frac{1}{\varepsilon}(u-u^2 - fv\frac{u-q}{u+q}), \quad G(u,v) = u-v.$$

The small  $\epsilon > 0$  parameter represents the ratio of time scales of the fast variable over that of the slow one, f is the stoichiometric parameter which is positive, and q > 0 is another chemical parameter.

Recently, the dynamic of the model has been widely studied by numerical experiments and theoretical analysis to understand those mechanisms by a number of authors, for example, see [11-15] and the listed references. The negative-tension instability of scroll waves is been shown and the Winfree turbulence as well. Further, and a relationship between the negative-tension instability and the meandering behavior of spiral waves is also found [13]. In [14], the occurrence of the Turing pattern generated by the two-variable Oregonator model has been proved when  $\varepsilon$ =1.

Note that the model (1) includes a basic assumption that the cells or units always live in a continuous patch environment. However, this may not be the case in reality, since the motion of individuals of given cells is random and isotropic, i.e., without any preferred direction. The cells or units are also absolute individuals in microscopic sense, and each isolated cell exchanges materials by diffusion with its neighbors [16-17]. Thus, it is reasonable to consider a one-dimensional (1D) or twodimensional (2D) spatially discrete reaction-diffusion system to describe the B-Z system. In [18], the author gives a continuous time but 1D discrete space model for Belousov-Zhabotinsky medium. Similarly, it is sound to consider the following time continuous but 2D spatially discrete reaction--diffusion system to make a mathematical description of spatiotemporal dynamics:

$$\begin{cases} u'_{i,j} = F(u_{i,j}(t), v_{i,j}(t)) + D_1 \nabla^2 u_{i,j}(t) \\ v'_{i,j} = G(u_{i,j}(t), v_{i,j}(t)) + D_2 \nabla^2 v_{i,j}(t) \end{cases}$$
(2)

where

$$F(u_{i,j}(t), v_{i,j}(t)) = \frac{1}{\varepsilon} (u_{i,j}(t) - u_{i,j}^{2}(t) - fv \frac{u_{i,j}(t) - q}{u_{i,j}(t) + q}),$$
  

$$G(u_{i,j}(t), v_{i,j}(t)) = u_{i,j}(t) - v_{i,j}(t) , i, j \text{ is mesh}$$
  
point, and  $i = 1, 2, ..., m, j = 1, 2, ..., n . \nabla^{2}$  is a  
discrete Laplace operator

$$\nabla^2 u_{i,j}^t = u_{i+1,j}^t + u_{i,j+1}^t + u_{i-1,j}^t + u_{i,j-1}^t - 4u_{i,j}^t$$

and

$$\nabla^2 v_{i,j}^t = v_{i+1,j}^t + v_{i,j+1}^t + v_{i-1,j}^t + v_{i,j-1}^t - 4v_{i,j}^t.$$

It also indicates each cell or unit exchanges materials by diffusion with the left (i, j-1) and right (i, j+1), top (i+1, j) and bottom (i-1, j) cell respectively.

Although the solution of (2) may be justified by considering the limiting case of the solution of (1), So far, to our knowledge, there have been very few works on dynamical behavior of the 2D semi-discrete Oregonator system.

In this paper, we will mainly discuss Turing instability, namely diffusion-driven instability and pattern formation for above 2D semidiscrete Oregonator system.

This paper is organized as follows. After a brief presentation of the model without diffusion, the Turing instability theory analysis will be given for the semi-discrete Oregonator system, then Turing instability conditions can be deduced combining linearization method and inner product technique in Section 2. Based on the results of Section 2, a series of numerical simulations are performed and different patterns, including spiral wave and target wave but also honeycombs, stripes and spots, have been exhibited. The final Section is the conclusion.

### **2** Turing Instability

In this section, first of all, we shall show some properties of the system as follows

$$\begin{cases} u'_{i,j} = \frac{1}{\varepsilon} (u_{i,j}(t) - u_{i,j}^{2}(t) - fv \frac{u_{i,j}(t) - q}{u_{i,j}(t) + q}) \\ v'_{i,j} = u_{i,j}(t) - v_{i,j}(t) \end{cases}$$
(3)

In the sense of chemistry, only nonnegative steady state of (3) is really of interests. It is obvious that (3) has a unique positive constant solution  $(u^*, v^*)$ , which is explicitly determined by

$$u^* = v^* = \frac{1 - f - q + \sqrt{(1 - f - q)^2 + 4q(1 + f)}}{2}$$

Linear stability analysis around this steady state yields the characteristic equation for the eigenvalue problem

$$A = \begin{bmatrix} \frac{\partial f}{\partial u} & \frac{\partial f}{\partial v} \\ \frac{\partial g}{\partial u} & \frac{\partial g}{\partial v} \end{bmatrix}_{(u^*, v^*)}$$
$$= \begin{bmatrix} \frac{1}{\varepsilon} p(f, q) & \frac{f(q - u^*)}{\varepsilon(q + u^*)} \\ 1 & -1 \end{bmatrix}$$

where

$$p(f,q) = 1 - 2u^* - \frac{2fqu^*}{(u^*+q)^2}$$

From the Jacobian matrix we observe that

det 
$$A = -\frac{1}{\varepsilon} (p(f,q) + \frac{f(q-u^*)}{q+u^*})$$
  
=  $\frac{u^*}{\varepsilon} [1 + \frac{2qu^*}{(u^*+q)^2}] > 0.$ 

Thus the positive steady state  $(u^*, v^*)$  is stable against homogeneous perturbations if

$$trA = p(f,q) - 1 < 0.$$
(4)

So we can get the following fact.

**Proposition 1.** The system (3) at the positive steady state ( $u^*, v^*$ ) is local asymptotically stable when the condition (4) holds.

Now we consider the reaction diffusion system as following

$$\begin{cases} u'_{i,j} = F(u_{i,j}(t), v_{i,j}(t)) + D_1 \nabla^2 u_{i,j}(t) \\ v'_{i,j} = G(u_{i,j}(t), v_{i,j}(t)) + D_2 \nabla^2 v_{i,j}(t) \end{cases}$$
(5)

with the periodic boundary conditions

$$\begin{cases} u_{i,0}^{t} = u_{i,m}^{t}, & u_{i,1}^{t} = u_{i,m+1}^{t} \\ u_{0,j}^{t} = u_{m,j}^{t}, & u_{1,j}^{t} = u_{m+1,j}^{t} \end{cases}$$
(6)

and

$$\begin{cases} v_{i,0}^{t} = v_{i,m}^{t}, v_{i,1}^{t} = v_{i,m+1}^{t} \\ v_{0,j}^{t} = v_{m,j}^{t}, v_{1,j}^{t} = v_{m+1,j}^{t} \end{cases}$$
(7)

 $i, j \in \{1, 2, 3, \dots, m\} = [1, m], t \in R^+ = [0, +\infty),$ where *m* is a positive integer. For the above reaction diffusion system, again linearize about the steady state  $(u^*, v^*)$ , to get

$$w_{ij}(t) = Aw_{ij}(t) + D\nabla^2 w_{ij}(t)$$

$$D = \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix}$$
(8)

with the periodic boundary conditions

$$\begin{cases} w_{i,0}^{t} = w_{i,m}^{t}, w_{i,1}^{t} = w_{i,m+1}^{t} \\ w_{0,j}^{t} = w_{m,j}^{t}, w_{1,j}^{t} = w_{m+1,j}^{t} \end{cases}$$
(9)

where

$$w_{ij}(t) = \begin{pmatrix} u_{i,j}(t) - u^* \\ v_{i,j}(t) - v^* \end{pmatrix} = \begin{pmatrix} x_{ij}(t) \\ y_{ij}(t) \end{pmatrix}.$$

In order to study instability of (5)-(7), we firstly think over eigenvalues of the following equations

$$\nabla^2 X^{ij} + \lambda X^{ij} = 0 \tag{10}$$

with the periodic boundary conditions

$$X^{i,0} = X^{i,m}, \quad X^{i,1} = X^{i,m+1}$$
$$X^{0,j} = X^{m,j}, X^{1,j} = X^{m+1,j}$$
(11)

In view of [19], the eigenvalue problem (10)-(11) has the eigenvalues as

$$\lambda_{l,s} = 4(\sin^2 \frac{(l-1)\pi}{m} + \sin^2 \frac{(s-1)\pi}{m}) = k_{ls}^2$$
  
k, l \in [1,m]

Then respectively taking the inner product of (8) with the corresponding eigenfunction  $X_{ls}^{ij}$  of the eigenvalue  $\lambda_{ls}$ , we get

$$\begin{split} \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij}^{'} &= f_{u} \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij}^{} + f_{v} \sum_{i,j=1}^{m} X_{ls}^{ij} y_{ij}^{} + D_{1} \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^{2} x_{ij} \\ \sum_{i,j=1}^{m} X_{kj}^{ij} y_{ij}^{'} &= g_{u} \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij}^{} + g_{v} \sum_{i,j=1}^{m} X_{ls}^{ij} y_{ij}^{} + D_{2} \sum_{i,j=1}^{m} X_{ls}^{ij} \nabla^{2} y_{ij} \end{split}$$

Let  $U(t) = \sum_{i,j=1}^{m} X_{ls}^{ij} x_{ij}(t)$ ,  $V(t) = \sum_{i,j=1}^{m} X_{ls}^{ij} y_{ij}(t)$ and use the periodic boundary conditions (11), then we have

$$\begin{cases} U'(t) = f_{u}U(t) + f_{v}V(t) - D_{1}k_{ls}^{2}U(t) \\ V'(t) = g_{u}U(t) + g_{v}V(t) - D_{2}k_{ls}^{2}V(t) \end{cases}$$

$$\begin{cases} U'(t) = (f_u - D_1 k_{ls}^2)U(t) + f_v V(t) \\ V'(t) = g_u U(t) + (g_v - D_2 k_{ls}^2)V(t) \end{cases}$$

The eigenvalue equation is

$$\lambda^{2} - [-k_{ls}^{2}(D_{1} + D_{2}) + (f_{u} + g_{v})]\lambda + h(k_{ls}^{2}) = 0$$

where

or

$$h(k_{ls}^{2}) = D_{1}D_{2}k_{ls}^{4} - (D_{2}f_{u} + D_{1}g_{v})k_{ls}^{2} + |A|$$
  
=  $D_{1}D_{2}k_{ls}^{4} - (D_{2}p(f,q) - D_{1})k_{ls}^{2} + \frac{u^{*}}{\varepsilon}[1 + \frac{2qu^{*}}{(u^{*}+q)^{2}}]$ 

Then the homogeneous steady state will be unstable for an inhomogeneous perturbation when

$$h(k_{ls}^{2}) = D_{1}D_{2}k_{ls}^{4} - (D_{2}f_{u} + D_{1}g_{v})k_{ls}^{2} + |A| < 0$$
(12)
or

$$-k_{ls}^{2}(D_{1}+D_{2})+(f_{u}+g_{v})>0$$
(13)

holds, where  $k_{ls}^2 \in [0, 8]$ .

Thus, in the view of Proposition 1, we can obtain the fact as follows.

**Proposition 2.** There exist positive numbers  $D_1$ ,  $D_2$  and the eigenvalues of  $k_{ls}^2$  such that the conditions (12) or (13) holds, then the system (5)-(7) at the positive homogeneous steady state  $(u^*, v^*)$  is unstable.

Proposition 1 and 2 imply the system (5)-(7) is diffusion-driven unstable or Turing unstable.

#### **3** Numerical simulation

To provide some numerical evidence for the qualitative dynamic behavior of the time continuous but spatial discrete system (1), the simulations were performed with periodic boundary conditions in a square domain of 128×128). size:128×128 (grid: To solve differential equations by computers, the time evolution should be discrete, i.e., the time goes in steps of  $\Delta t$ . The time evolution can be solved by the Euler method, approximating the value of the concentration at the next time step based on the change rate of the concentration at the previous time step. The initial value function  $u^0$  and  $v^0$  are choose by

$$\begin{cases} u^0 = u^* + \zeta \\ v^0 = v^* + \eta \end{cases}$$

If there is no special note in the following,  $\zeta$  and  $\eta$  are always small amplitude random perturbations 1% around the steady state, and spatial-temporal plots will be the ones about u.

The value of  $\varepsilon$  influences the concentration in the system mainly. When the value of  $\varepsilon$ , which can control the excitability of the system, is in the range of 0-1, spiral and target patterns can be observed (see, Fig. 1).

An interesting phenomena is observed when the value is taken as  $\varepsilon = 1$ , the system undergoing a Turing instability exhibits an extremely rich variety of dynamical concentration patterns, which can be stable only far from equilibrium. There are three types of honeycombs typical Turing structures, stripes, and (hexagons), spots (reentrant hexagons), as shown in Fig. 2.

It is plausible to argue that patterns observed in natural phenomena may be modeled as a combination of two complementary procedures, (i) fluctuations of system parameters; (ii) variation of the initial conditions. In order to show what changes the system parameters bring into the pattern formation, as a example, Fig. 3 exhibit the impact of the parameter f on patterns, by keeping all the other parameters of the system fixed. On varying the control parameter f the sequence hexagons(Fig. 3(a))  $\rightarrow$  hexagon-stripe mixtures(Fig. 3(b))  $\rightarrow$  stripes(Fig. 3(c))  $\rightarrow$ reentrant hexagon--stripe mixtures(Fig. 3(d)) $\rightarrow$ reentrant hexagons(Fig. 3(e)) is observed. With the further increase of f, the number of reentrant hexagons will increasingly decrease, seen in Fig. 3(f).

Likewise, we have considered the effect of initial value by keeping the system parameters of the system fixed, and some different patterns are depicted in Fig. 4.

Since the time continuous but 2D spatially discrete reaction--diffusion system is derived from converting the elementary reactions of the BZ reaction system into reaction rate equations, it can reproduce the behavior of the reaction [15]. The patterns from above simulations can be found in laboratory experiment by given conditions. But only to the Oregonator model, complex dynamics will exist because of nonlinear term. In this paper, of course, we focus on the numerical simulations not theory analysis. So, next in Fig. 5, we show some different patterns by simulations.

The above simulations show that the dynamics of a lattice site changes from the fixed point, with the change of parameters in the Turing instability region or different initial value by keeping the system parameters of the system fixed. We have seen various patterns such as spiral wave, target wave, stripes and spotlike patterns and so on.

## **4** Conclusion

In this paper, a semi-discrete Oregonator system is modeled, and Turing instability conditions have been illustrated by linearization method and inner product technique. Based on numerical simulations, we have found various spatial patterns including spiral wave, target wave, stripes and spotlike patterns in the parameter region of Turing instability. Simulations also show that the patterns are sensitive to initial values, which may render us to pay more attention to the effect of initial values on pattern formation. The further study along this line may lead to better prediction for patterns formation, and better control of pattern

formation may be possible when the initial values are well characterized.

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# **Appendix Figures:**



(a)



(b)

Fig. 1: Selective pattern in the Turing instability region for model (5)-(7). (a) Spiral pattern when  $\mathcal{E} = 0.25$ , f = 0.7, q = 0.0008,  $D_1 = 3$ ,  $D_2 = 0.03$ ,  $\Delta t = 0.002$ . (b)Target (circular) pattern when  $\mathcal{E} = 0.4$ , f = 1, q = 0.0008,  $D_1 = 1$ ,  $D_2 = 0.03$ ,  $\Delta t = 0.002$  and initial circular perturbation is made at the center of the 2D domain.









Fig. 2: Turing patterns in the Turing instability region for model (5)-(7) when  $\varepsilon = 1$ . (a) Honeycombs (Hexagons). f = 0.60, q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ .  $\Box$ (b) Stripes. f = 0.75, q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ . (c) Spots (Reentrant hexagons). f = 1.60, q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ .

















Fig. 3: A series of patterns obtained by increasing the strength of the parameter f. The other parameters are the same, namely:  $\mathcal{E} = 1$ , q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ . (a) Hexagonal pattern (f=0.60). (b) Hexagon-tripe mixtures (f=0.65). (c) Stripe pattern (f=0.75). (d) Reentrant hexagon-tripe mixtures (f=0.90). (e) Reentrant hexagons (f=1.2). (f) Reentrant hexagons (f=1.6).









when initial vertical perturbation is made in the 2D domain (c) Spotlike pattern when initial vertical and horizontal perturbation is made in the 2D domain.



(a)





(c)



(d)

Fig. 5: Some different from simulations in the parameter space. (a)  $\mathcal{E} = 0.3$ , f = 1, q = 0.0008,  $D_1 = 3$ ,  $D_2 = 0.03$ ,  $\Delta t = 0.0025$ . (b)  $\mathcal{E} = 0.4$ , f = 0.1, q = 0.0008,  $D_1 = 1$ ,  $D_2 = 0.03$ ,  $\Delta t = 0.0025$ . (c)  $\mathcal{E} = 1$ , f = 0.57, q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ . Localized initial perturbation in the centre domain. (d)  $\mathcal{E} = 1$ , f = 0.59, q = 0.002,  $D_1 = 1$ ,  $D_2 = 75$ ,  $\Delta t = 0.0025$ . Circle initial perturbation in the 2D domain.