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ORIGINAL ARTICLE

Bifurcation in the Lengyel–Epstein system for the coupled reactors with diffusion

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Abstract The main goal of this paper is to continue the investigations of the important system of Fengqi et al. (2008). The occurrence of Turing and Hopf bifurcations in small homogeneous arrays of two coupled reactors via diffusion-linked mass transfer which described by a system of ordinary differential equations is considered. I study the conditions of the existence as well as stability properties of the equilibrium solutions and derive the precise conditions on the parameters to show that the Hopf bifurcation occurs. Analytically I show that a diffusion driven instability occurs at a certain critical value, when the system undergoes a Turing bifurcation, patterns emerge. The spatially homogeneous equilibrium loses its stability and two new spatially non-constant stable equilibria emerge which are asymptotically stable. Numerically, at a certain critical value of diffusion the periodic solution gets destabilized and two new spatially nonconstant periodic solutions arise by Turing bifurcation.

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1. Introduction

Alan Turing (cf. [1]) showed mathematically that a system of coupled reaction-diffusion equations could give rise to spatial concentration patterns of a fixed characteristic length from an arbitrary initial configuration due to the so-called diffusion-driven instability, that is, diffusion could destabilize an otherwise stable equilibrium of the reaction-diffusion system and lead to nonuniform spatial patterns. Over the years, Turing's idea has attracted the attention of a great number of investigators and was successfully developed on the theoretical backgrounds (cf. [2–5]). Not only it has been studied in biological and chemical fields, some investigations range as far as economics, semiconductor physics, ecology, embryology and star formation (cf. [6–9,12]). However, the research for Turing patterns in real chemical or biological systems turned out to be difficult. The first experimental observation of a Turing pattern in a chemical reactor was due to De Keppers group, who observed a spotty pattern in a chlorite-iodide-malonic acid (CIMA) reaction (cf. [10]). The experiment on

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the CIMA reaction has revealed the existence of stationary space periodic concentration patterns, the so-called Turing structures, in open gel reactors. Later, Lengyel and Epstein suggested (cf. [3,11]) that these patterns could arise because the iodine activator species forms a reversible complex of low mobility with the starch molecules used as color indicator for this reaction. The difference between our results and the results pointed out by Fengqi et al. [4] is that, here we investigate the occurrence of Turing and Hopf bifurcations in small homogeneous arrays of two coupled reactors via diffusion-linked mass transfer which described by a system of ordinary differential equations. This is not the case in [4].

This paper is organized as follows: In Section 2 the model is built; in Section 3 we study the asymptotical behavior of the equilibrium of the local system and show that for the local system Hopf bifurcation occurs; in Section 4 its linearization is treated and the conditions for the Turing bifurcation are established (these are the main results of this paper); in Section 5 we illustrate our results with numerical simulations; in Section 6 we summarize the main conclusions of the study.

2. The model

We investigate the occurrence of Turing and Hopf bifurcations in small homogeneous arrays of coupled reactors. We consider a general two-variable model that represents an activator-inhibitor scheme with a substrate that can form an inert complex with the activator. We use the Lengyel–Epstein model for the kinetics as a specific example of such a scheme. The Lengyel–Epstein model is in the form of

$$\dot{u} = a - u - \frac{4uv}{1+u^2} := f(u,v), \quad \dot{v} = \sigma b\left(u - \frac{uv}{1+u^2}\right) := g(u,v), \tag{1}$$

where u, v denote the chemical concentrations of the activator iodide (I^-) and the inhibitor chlorite (ClO_2^-), respectively; a and b are parameters related to the feed concentrations, σ is a re-scaling parameter depending on the concentration of the starch. We shall assume accordingly that all constants a, b and σ are positive. In laboratory conditions, a sample of parameters is taken in the range $0 < a < 35$, $0 < b < 8$ and $\sigma = 8$. For the reaction-diffusion Lengyel–Epstein model, let $u(t,i), v(t,i)$ denote the chemical concentrations of the activator iodide and the inhibitor chlorite, respectively, at time t, in patch $i, i = 1,2; t \in R$. Homogeneous two coupled reactors via diffusion-linked mass transfer are described by the following system of ordinary differential equations:

$$\begin{aligned}
\dot{u}(t,1) &= a - u(t,1) - \frac{4u(t,1)v(t,1)}{1+u^2(t,1)} + d_1(u(t,2) - u(t,1)),\\
\dot{v}(t,1) &= \sigma b\left(u(t,1) - \frac{u(t,1)v(t,1)}{1+u^2(t,1)}\right) + d_2(v(t,2) - v(t,1)),\\
\dot{u}(t,2) &= a - u(t,2) - \frac{4u(t,2)v(t,2)}{1+u^2(t,2)} + d_1(u(t,1) - u(t,2)),\\
\dot{v}(t,2) &= \sigma b\left(u(t,2) - \frac{u(t,2)v(t,2)}{1+u^2(t,2)}\right) + d_2(v(t,1) - v(t,2)),
\end{aligned} \tag{2}$$

where $d_i > 0, (i = 1,2)$ are the diffusion coefficients of mass transfer.

We will focus on the existence of equilibria and their local stability. This information will be crucial in the next section where we study the effect of the diffusion parameters on the stability of the steady states.

3. Stability and Hopf bifurcation

The interaction is described as a system of differential equations as follows:

$$\begin{aligned}
\dot{u}(t,1) &= a - u(t,1) - \frac{4u(t,1)v(t,1)}{1+u^2(t,1)},\\
\dot{v}(t,1) &= \sigma b\left(u(t,1) - \frac{u(t,1)v(t,1)}{1+u^2(t,1)}\right),\\
\dot{u}(t,2) &= a - u(t,2) - \frac{4u(t,2)v(t,2)}{1+u^2(t,2)},\\
\dot{v}(t,2) &= \sigma b\left(u(t,2) - \frac{u(t,2)v(t,2)}{1+u^2(t,2)}\right).
\end{aligned} \tag{3}$$

We see that $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2) := (\alpha, 1+\alpha^2, \alpha, 1+\alpha^2)$ is a unique spatially homogeneous equilibrium of the system without diffusion, where $\alpha = a/5$.

The Jacobian matrix of system (3) at $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ can be written as:

$$J_{kinetic} = \begin{pmatrix} \frac{3\alpha^2-5}{1+\alpha^2} & -\frac{4\alpha}{1+\alpha^2} & 0 & 0 \\ \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} & 0 & 0 \\ 0 & 0 & \frac{3\alpha^2-5}{1+\alpha^2} & -\frac{4\alpha}{1+\alpha^2} \\ 0 & 0 & \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} \end{pmatrix}. \tag{4}$$

The characteristic polynomial is

$$D_{kinetic}(\lambda) = (D_2(\lambda))^2, D_2(\lambda) = \lambda^2 - \frac{3\alpha^2 - 5 - \sigma\alpha b}{1+\alpha^2}\lambda + \frac{5\sigma\alpha b}{1+\alpha^2}. \tag{5}$$

Under condition $3\alpha^2 - 5 > 0$, system (3) is an activator-inhibition system.

If

$$0 < 3\alpha^2 - 5 < \sigma\alpha b, \tag{6}$$

holds, then the equilibrium $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ of system (3) is locally asymptotically stable.

Next we analyze the Hopf bifurcation occurring at $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ by choosing b as the bifurcation parameter. Denote

$$b_{crit} := \frac{3\alpha^2 - 5}{\sigma\alpha}, \tag{7}$$

then when $b = b_{crit}$, the Jacobian matrix $J_{kinetic}$ has a pair of imaginary eigenvalues $\lambda = \pm i\sqrt{\frac{5\sigma\alpha b_{crit}}{1+\alpha^2}}$. let $\lambda = \beta(b) \pm i\omega(b)$ be the roots of $D_2(\lambda)$, then

$$\begin{aligned}
\beta(b) &= \frac{3\alpha^2 - 5 - \sigma\alpha b}{2(1+\alpha^2)},\\
\omega(b) &= \frac{1}{2}\sqrt{\frac{20\sigma\alpha b}{1+\alpha^2} - \left(\frac{3\alpha^2 - 5 - \sigma\alpha b}{1+\alpha^2}\right)^2},
\end{aligned} \tag{8}$$

and

$$\beta'(b)_{b=b_{crit}} = -\frac{\sigma\alpha}{2(1+\alpha^2)} < 0. \tag{9}$$

By the *Poincare Andronov Hopf* Bifurcation Theorem (cf. [12], Theorem 3.1.3), we know that system (3) undergoes a Hopf bifurcation at $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ when $b = b_{crit}$.

4. Turing instability with diffusion

For two coupled reactors, we will derive conditions for the diffusion-driven instability with respect to the equilibrium solution, the spatially homogenous solution of the reaction-diffusion Lengyel–Epstein system. We see that $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ is also a spatially homogeneous equilibrium of the system with diffusion. The Jacobian matrix of system (2) with diffusion at $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ can be written as:

$$J_T = \begin{pmatrix} \frac{3\alpha^2-5}{1+\alpha^2} - d_1 & -\frac{4\alpha}{1+\alpha^2} & d_1 & 0 \\ \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} - d_2 & 0 & d_2 \\ d_1 & 0 & \frac{3\alpha^2-5}{1+\alpha^2} - d_1 & -\frac{4\alpha}{1+\alpha^2} \\ 0 & d_2 & \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} - d_2 \end{pmatrix}, \tag{10}$$

$$\det(J_T - \lambda I) = \begin{vmatrix} \frac{3\alpha^2-5}{1+\alpha^2} - d_1 - \lambda & -\frac{4\alpha}{1+\alpha^2} & d_1 & 0 \\ \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} - d_2 - \lambda & 0 & d_2 \\ d_1 & 0 & \frac{3\alpha^2-5}{1+\alpha^2} - d_1 - \lambda & -\frac{4\alpha}{1+\alpha^2} \\ 0 & d_2 & \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2} - d_2 - \lambda \end{vmatrix}. \tag{11}$$

Using the properties of determinant we get

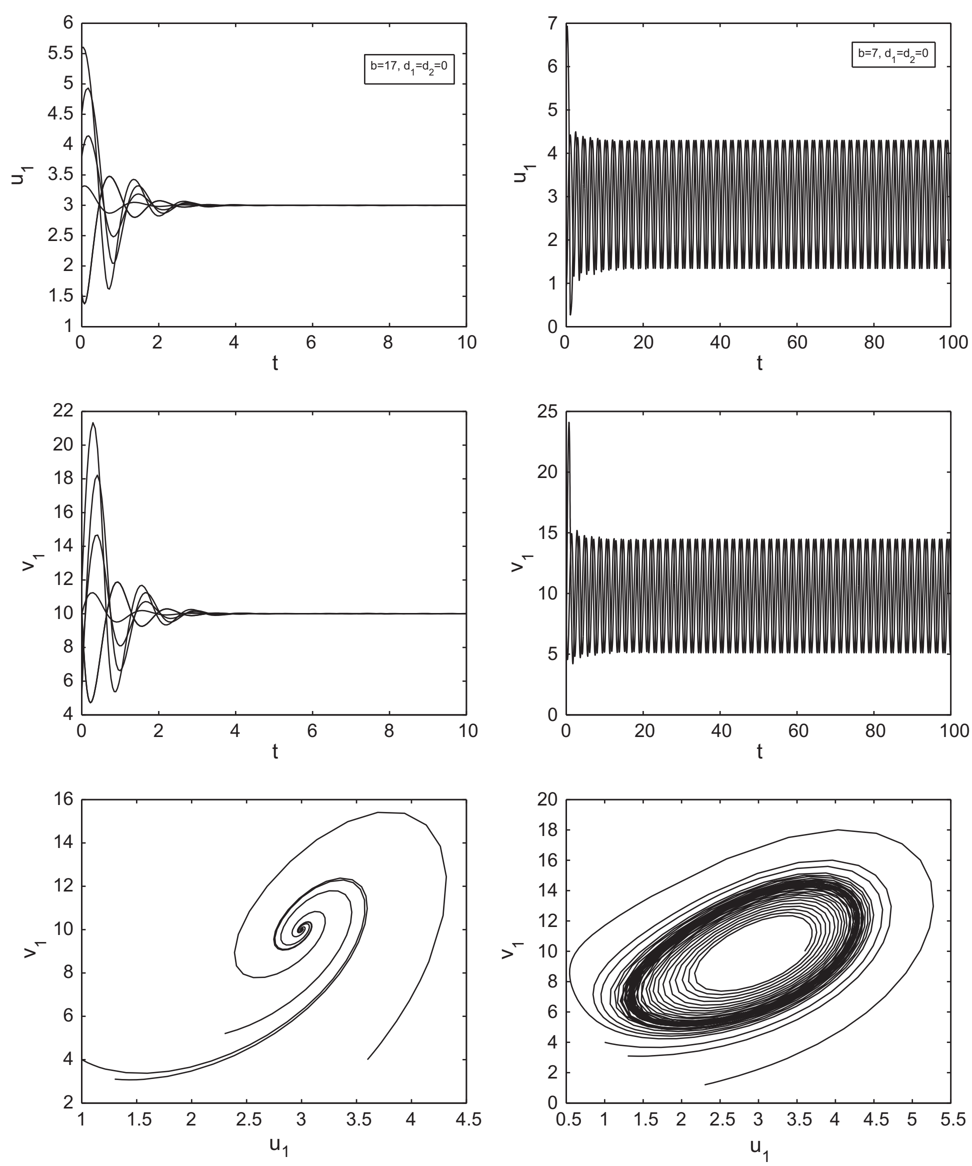

Fig. 1 Left figures: The solutions u_1 and v_1 before bifurcation at $b = 17$; the solution is stable. Right figures: The solutions u_1 and v_1 after bifurcation at $b = 7$; the solutions loss its stability by Turing bifurcation (Figure produced by applying MATLAB).

$$\begin{vmatrix} \frac{3\alpha^2-5}{1+\alpha^2}-\lambda & -\frac{4\alpha}{1+\alpha^2} & d_1 & 0 \\ \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2}-\lambda & 0 & d_2 \\ 0 & 0 & \frac{3\alpha^2-5}{1+\alpha^2}-2d_1-\lambda & -\frac{4\alpha}{1+\alpha^2} \\ 0 & 0 & \frac{2\sigma\alpha^2 b}{1+\alpha^2} & -\frac{\sigma\alpha b}{1+\alpha^2}-2d_2-\lambda \end{vmatrix}. \tag{12}$$

In order to have Turing instability of the system (2), the characteristic polynomial

$$D_4(\lambda, d_1, d_2) = D_2(\lambda)D_2(\lambda, d_1, d_2), \tag{13}$$

$$D_2(\lambda, d_1, d_2) = \lambda^2 - \lambda\left[\frac{3\alpha^2-5-\sigma\alpha b}{1+\alpha^2} - 2(d_1+d_2)\right] + \frac{5\sigma\alpha b}{1+\alpha^2} + 2d_1\frac{\sigma\alpha b}{1+\alpha^2} - 2d_2\left(\frac{3\alpha^2-5}{1+\alpha^2} - 2d_1\right),$$

must have at least one eigenvalue with positive real part.

We know that $D_2(\lambda)$ has two roots with negative real parts. By (6), clearly,

$$\frac{3\alpha^2-5-\sigma\alpha b}{1+\alpha^2} - 2(d_1+d_2) < 0,$$

the other polynomial will have a negative and a positive root if the constant term is negative. By the properties of the model the first two terms are positive.

Suppose that the parameters have been chosen so that

$$d_1 < \frac{3\alpha^2-5}{2(1+\alpha^2)}. \tag{14}$$

If we have achieved this we may increase $d_2(b)$ and the constant term becomes negative. The calculations lead to the following Theorem.

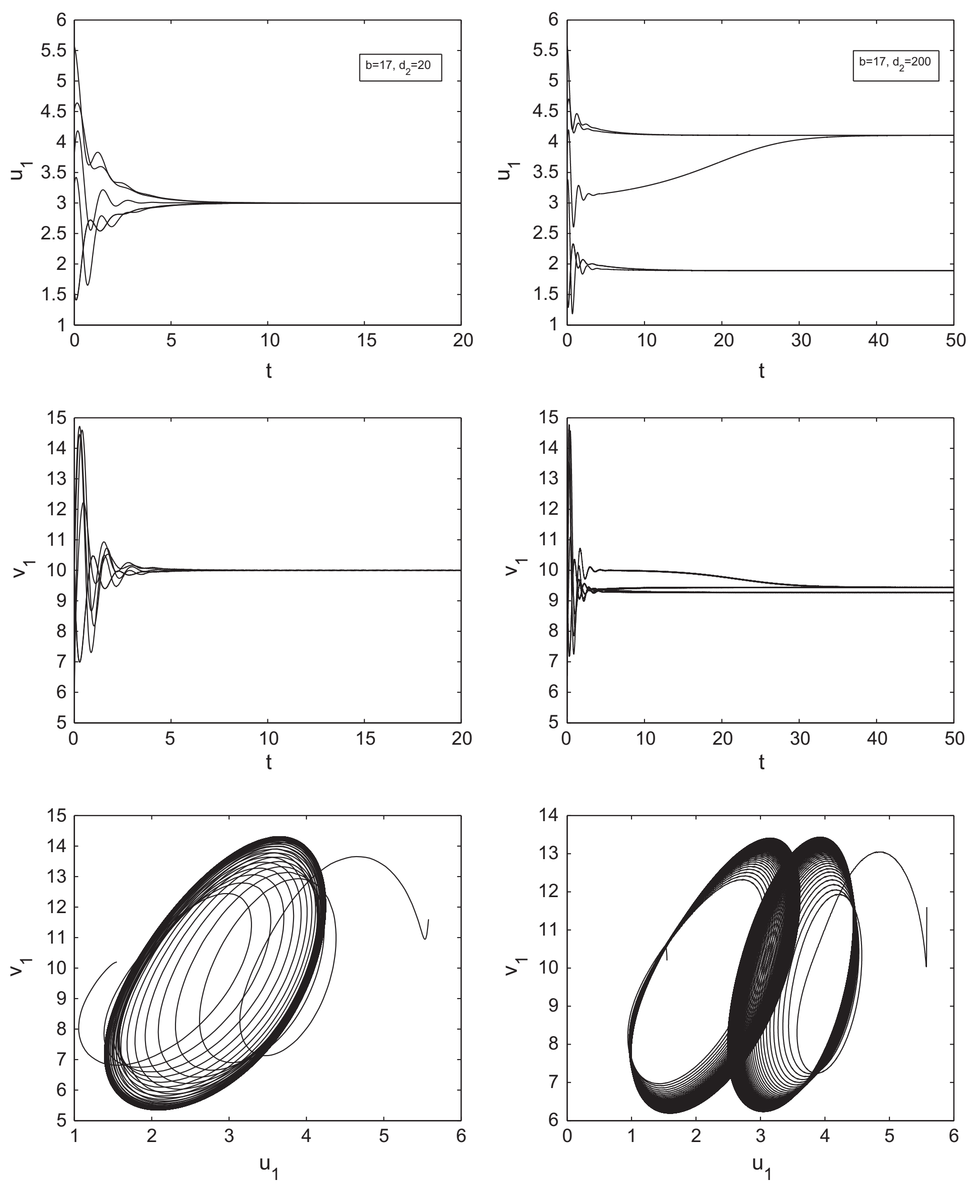

Fig. 2 Left figures: The solutions u_1 and v_1 before bifurcation at $d_2 = 20$; the solution is stable. Right figures: The solutions u_1 and v_v after bifurcation at $d_2 = 200$; the solutions loss its stability by Turing bifurcation (Figure produced by applying MATLAB).

Theorem 1. *If (6) and (14) hold and if*

$$d_2(b) > d_{2crit}(b) := \frac{\sigma\alpha b(5+2d_1)}{2(3\alpha^2 - 5 - 2d_1(1+\alpha^2))}, \quad (15)$$

then Turing instability occurs.

Notes: At $d_{2crit}(b)$ we have four eigenvalues $\lambda_i(i=1,2,3,4)$ such that $\lambda_i < 0(i=1,2,3)$ and $\lambda_4 = 0$.

If $d_2(b) < d_{2crit}(b)) \Rightarrow \lambda_i < 0 \ \ (i=1,2,3,4)$, then, $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ is asymptotically stable.

If $d_2(b) > d_{2crit}(b) \Rightarrow \lambda_i < 0 \ \ (i=1,2,3)$ and $\lambda_4 > 0$, then, $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ is unstable.

Thus if $d_2(b)$ is increased through $d_2(b) = d_{2crit}(b)$ then the spatially homogeneous equilibrium loses its stability.

Remark 1. If (6) holds and the parameters have been chosen so that

$$d_1 > \frac{3\alpha^2 - 5}{2(1+\alpha^2)}, \quad (16)$$

then self-diffusion never destabilizes the equilibrium $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ which is asymptotically stable for the kinetic system, i.e. the equilibrium $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ is diffusively stable for all values of d_2.

5. Numerical Investigations

In this section, we present some numerical simulations to illustrate our theoretical analysis.

First we choose parameters: $a = 15, \ \sigma = 8, \ d_1 = 1$, then we have $b_{crit} = 0.9166$ and $d_{2crit}(b) = 21b$.

In the absence of diffusion, we show that the equilibrium $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ is asymptotically stable if $b > b_{crit}$ and a Hopf bifurcation occurs at $b = b_{crit}$, the direction of the bifurcation is subcritical and the bifurcating periodic solutions are asymptotically stable. This is shown in Fig. 1.

For the model with diffusion: If $d_2 > d_{2crit}(b) = 21b$ and $b > b_{crit}$, then by (6), (14) and (15) the spatially homogenous equilibrium $(\overline{u}_1, \overline{v}_1, \overline{u}_2, \overline{v}_2)$ loss its stability by Turing bifurcation. If $d_2 > d_{2crit}(b) = 21b$ and $b < b_{crit}$. By (7), Hopf bifurcation occurs at b_{crit}, the direction of the bifurcation is subcritical, and the bifurcating periodic solutions are locally asymptotically stable. This is shown in Fig. 2.

6. Discussions

The main purpose of this article is to identify the parameter ranges of stability/instability of spatial homogeneous equilibrium solution and periodic solutions. The equilibrium and periodic solution of the ODE system (3) are spatial homogeneous solutions of the reaction-diffusion system (2). The stability of the solution can change because of the diffusion. We show that analytically a diffusion driven instability occurs at a certain critical value, that is, the system undergoes a Turing bifurcation, patterns emerge, the spatially homogeneous equilibrium loses its stability and two new spatially non-constant stable equilibria emerge which are asymptotically stable. Numerically, for the periodic solution, at a certain critical value of diffusion this periodic solution gets destabilized and a two new spatially nonconstant periodic solution arises by Turing bifurcation.

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