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Sufficient conditions for wave instability in three-component reaction-diffusion systems

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Sufficient conditions for the wave instability in general three-component reaction-diffusion systems are derived. These conditions are expressed in terms of the Jacobian matrix of the uniform steady state of the system, and enable us to determine whether the wave instability can be observed as the mobility of one of the species is gradually increased. It is found that the instability can also occur if one of the three species does not diffuse. Our results provide a useful criterion for searching wave instabilities in reaction-diffusion systems of various origins.
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1. Introduction

The wave instability provides an important mechanism for oscillatory pattern formation in nonequilibrium chemical systems. When it takes place, a critical mode corresponding to a traveling wave with a certain wavenumber and oscillation frequency begins to grow, destabilizing the uniform steady state. Although being less known, the wave instability has already been considered in 1952 by A. Turing in his pioneering publication [1], where the classical (i.e. static) Turing instability, leading to the establishment of a periodic stationary pattern, has also been introduced. Therefore, it may also be appropriate to describe it as the oscillatory Turing bifurcation. Moreover, it was noticed by A. Turing [1] that at least three interacting species are needed for this instability to occur.

Because of the spatial reflection symmetry, waves traveling in the left and right directions have the same growth rates, and both of them begin to spontaneously develop above the instability threshold. Nonlinear interactions between such modes determine whether one of the modes gets suppressed, so that a wave traveling in a certain direction is established, or standing waves, representing superpositions of left- and right-traveling waves, are formed instead [2,3]. The wave patterns resulting from such instability can also exhibit secondary instabilities, and wave turbulence may set on.

In contrast to the classical Turing bifurcation, which has been extensively discussed for both biological and chemical systems [1,4–10], the wave bifurcation has so far attracted less attention. It has been considered for special chemical models [11,12], and its existence was suggested in the experiments with Belousov-Zhabotinsky microemulsions [13]. There are also publications in which this instability was discussed for special ecological models [14].

Because at least three species are needed for the wave instability to occur, the linear stability analysis is more complex in this case, as compared with the classical Turing bifurcation in two-component activator-inhibitor systems. The complexity of the stability analysis, which was performed separately for individual chemical systems, has probably also been responsible for the fact that the wave instability was not broadly investigated for reaction-diffusion media. In a recent study, sufficient conditions for the wave instability in general three-component reaction-diffusion systems have been derived [15]. These conditions have been formulated in terms of the elements of the Jacobian matrix and the diffusion constants of the reacting species.

By using an essentially different method, in this article we derive another set of sufficient conditions for the wave bifurcation in general three-component reaction–diffusion models. As we show, the derived sufficient conditions are complementary to those obtained in Ref. [15]. Indeed, there are systems where our conditions can be used to predict the wave instability, whereas the other set of sufficient conditions does not apply. On the other hand, our conditions do not work for some systems while the conditions from Ref. [15] hold.

The conditions derived in the present paper tell whether the wave bifurcation is possible when the mobility of any chosen species is gradually increased, while diffusion coefficients of other species are kept constant. The instability may take place even if one of the three species is immobile.

2. Three-component reaction–diffusion systems

We consider reaction–diffusion systems with three chemical reactants U , V , and W . Local densities of the reactants are denoted as $u = [U]$, $v = [V]$, and $w = [W]$. All reactants diffuse over the space and undergo local chemical reactions. Generally, such systems are described by the equations

$$\begin{cases} \frac{du}{dt} = f(u, v, w) + D_u \nabla^2 u, \\ \frac{dv}{dt} = g(u, v, w) + D_v \nabla^2 v, \\ \frac{dw}{dt} = h(u, v, w) + D_w \nabla^2 w, \end{cases} \quad (1)$$

where functions f , g , and h represent the local reactions. Diffusion coefficients of the reactants are D_u , D_v , and D_w . We assume that a uniform steady state $(u, v, w) = (\bar{u}, \bar{v}, \bar{w})$ determined by $f(\bar{u}, \bar{v}, \bar{w}) = g(\bar{u}, \bar{v}, \bar{w}) = h(\bar{u}, \bar{v}, \bar{w}) = 0$ exists and that this state is stable in the absence of diffusion.

3. Linear stability analysis with rescaled variables

We introduce small perturbations to the steady state as $(u, v, w) = (\bar{u}, \bar{v}, \bar{w}) + (\delta u, \delta v, \delta w)$. Substituting this into Eqs. (1), the following linearized differential equations for the perturbations are obtained:

$$\begin{cases} \frac{d}{dt} \delta u = f_u \delta u + f_v \delta v + f_w \delta w + D_u \nabla^2 \delta u, \\ \frac{d}{dt} \delta v = g_u \delta u + g_v \delta v + g_w \delta w + D_v \nabla^2 \delta v, \\ \frac{d}{dt} \delta w = h_u \delta u + h_v \delta v + h_w \delta w + D_w \nabla^2 \delta w, \end{cases} \quad (2)$$

where $f_u = \partial f / \partial u|_{(\bar{u}, \bar{v}, \bar{w})}$, $f_v = \partial f / \partial v|_{(\bar{u}, \bar{v}, \bar{w})}$, $f_w = \partial f / \partial w|_{(\bar{u}, \bar{v}, \bar{w})}$, ... are partial derivatives at the steady state. The following rescaled variables are introduced for convenience:

$$\delta \tilde{u} = \delta u, \quad \delta \tilde{v} = \sqrt{\left| \frac{f_v}{g_u} \right|} \delta v, \quad \delta \tilde{w} = \left| \frac{f_v}{h_v} \right| \delta w, \quad \tilde{t} = \sqrt{|f_v g_u|} t. \quad (3)$$

We substitute these variables into Eqs. (2) to obtain the set of equations

$$\begin{cases} \frac{d}{d\tilde{t}} \delta \tilde{u} = m_0 \delta \tilde{u} + \alpha \delta \tilde{v} + n \delta \tilde{w} + D_u \mu \nabla^2 \delta \tilde{u}, \\ \frac{d}{d\tilde{t}} \delta \tilde{v} = \beta \delta \tilde{u} + p_0 \delta \tilde{v} + q \delta \tilde{w} + D_v \mu \nabla^2 \delta \tilde{v}, \\ \frac{d}{d\tilde{t}} \delta \tilde{w} = r \delta \tilde{u} + \gamma \delta \tilde{v} + s_0 \delta \tilde{w} + D_w \mu \nabla^2 \delta \tilde{w}, \end{cases} \quad (4)$$

where

$$\begin{aligned} m_0 &= \frac{f_u}{\sqrt{|f_v g_u|}}, & n &= \frac{f_w |h_v|}{\sqrt{|f_v^3 g_u|}}, \\ p_0 &= \frac{g_v}{\sqrt{|f_v g_u|}}, & q &= g_w \left| \frac{h_v}{f_v g_u} \right|, \\ r &= \frac{h_u}{|h_v|} \sqrt{\left| \frac{f_v}{g_u} \right|}, & s_0 &= \frac{h_w}{\sqrt{|f_v g_u|}}, \\ \mu &= \frac{1}{\sqrt{|f_v g_u|}}. \end{aligned} \quad (5)$$

The coefficients α , β , γ are determined by the signs of f_v , g_u , h_v , $\alpha = \text{sign}(f_v)$, $\beta = \text{sign}(g_u)$, $\gamma = \text{sign}(h_v)$. The perturbations $(\delta \tilde{u}, \delta \tilde{v}, \delta \tilde{w})$ are expanded over plane waves as

$$\begin{aligned} \delta \tilde{u} &= \int d\vec{k} \tilde{U}^{(\vec{k})} \exp \left[\lambda^{(\vec{k})} \tilde{t} - i\vec{k} \cdot \vec{x} \right], \\ \delta \tilde{v} &= \int d\vec{k} \tilde{V}^{(\vec{k})} \exp \left[\lambda^{(\vec{k})} \tilde{t} - i\vec{k} \cdot \vec{x} \right], \\ \delta \tilde{w} &= \int d\vec{k} \tilde{W}^{(\vec{k})} \exp \left[\lambda^{(\vec{k})} \tilde{t} - i\vec{k} \cdot \vec{x} \right], \end{aligned} \quad (6)$$

where $\vec{k} = (k_1, k_2, \dots)$ is the wave vector, and $\lambda^{(\vec{k})}$ is the growth rate of the plane wave with wave vector \vec{k} . Thus, we obtain the following equations for each wave vector \vec{k} :

$$\lambda^{(k)} \begin{pmatrix} \tilde{U}^{(k)} \\ \tilde{V}^{(k)} \\ \tilde{W}^{(k)} \end{pmatrix} = \begin{pmatrix} m_0 - D_u \mu k^2 & \alpha & n \\ \beta & p_0 - D_v \mu k^2 & q \\ r & \gamma & s_0 - D_w \mu k^2 \end{pmatrix} \begin{pmatrix} \tilde{U}^{(k)} \\ \tilde{V}^{(k)} \\ \tilde{W}^{(k)} \end{pmatrix}, \quad (7)$$

where $k = |\vec{k}|$ is the wave number, the magnitude of the wave vector \vec{k} . Because only the magnitude of the wave vector is important, we drop the vector symbols from here on.

The condition

$$\det \begin{pmatrix} m_0 - D_u \mu k^2 - \lambda^{(k)} & \alpha & n \\ \beta & p_0 - D_v \mu k^2 - \lambda^{(k)} & q \\ r & \gamma & s_0 - D_w \mu k^2 - \lambda^{(k)} \end{pmatrix} = 0 \quad (8)$$

should be satisfied for Eq. (7) to have non-trivial solutions. Thus, the linear growth rate $\lambda^{(k)}$ is determined by the characteristic equation

$$\begin{aligned} \lambda^3 - (m + p + s)\lambda^2 + (mp + ps + sm - nr - \gamma q - \alpha\beta)\lambda \\ - (mps - npr + \alpha qr - \gamma mq + \beta\gamma n - \alpha\beta s) = 0, \end{aligned} \quad (9)$$

where

$$\begin{aligned} m &= m(k) = m_0 - k^2 \mu D_u, \\ p &= p(k) = p_0 - k^2 \mu D_v, \\ s &= s(k) = s_0 - k^2 \mu D_w. \end{aligned} \quad (10)$$

The growth of each plane-wave mode is determined by the real part of $\lambda^{(k)}$. The uniform steady state is stable if $\text{Re}(\lambda^{(k)})$ is negative for all k . The instability occurs if $\text{Re}(\lambda^{(k)})$ becomes positive for at least one wave number $k = k_c$. Then the uniform steady state is destabilized, leading to spontaneous development of wave patterns with critical wave number k_c . If the imaginary part $\text{Im}(\lambda^{(k_c)})$ of the unstable mode is zero, the first critical mode represents a stationary plane wave and the Turing instability occurs. On the other hand, if $\text{Im}(\lambda^{(k_c)}) \neq 0$, the critical mode is oscillatory in time and periodic in space, so that the critical mode represents a traveling wave and the wave instability takes place.

4. Critical condition for the instabilities

The *complex conjugate root theorem* holds that a characteristic equation with real coefficients

$$\lambda^3 + a\lambda^2 + b\lambda + c = 0 \quad (11)$$

has either three real roots or one real root and a pair of complex conjugate roots. In the latter case, the three roots can be written as

$$\lambda_{1,2} = \psi \pm i\omega, \quad \lambda_3 = \phi, \quad (12)$$

so that the coefficients are represented as

$$a = -(2\psi + \phi), \quad b = \psi^2 + \omega^2 + 2\psi\phi, \quad c = -(\psi^2 + \omega^2)\phi. \quad (13)$$

Combining these three equations, we obtain

$$\begin{aligned} c - ab &= -(\psi^2 + \omega^2)\phi + (2\psi + \phi)(\psi^2 + \omega^2 + 2\psi\phi) \\ &= 2\psi \left[(\psi + \phi)^2 + \omega^2 \right]. \end{aligned} \quad (14)$$

At the threshold of the wave instability, we have $\psi = 0$, so that $c - ab = 0$. At the threshold of the Turing instability, we would have $\phi = 0$, and therefore $c = 0$. Note that the Turing instability is also possible when the characteristic equation has three real roots and one of them becomes positive. It can be easily checked that, also in this case, the instability threshold corresponds to $c = 0$.

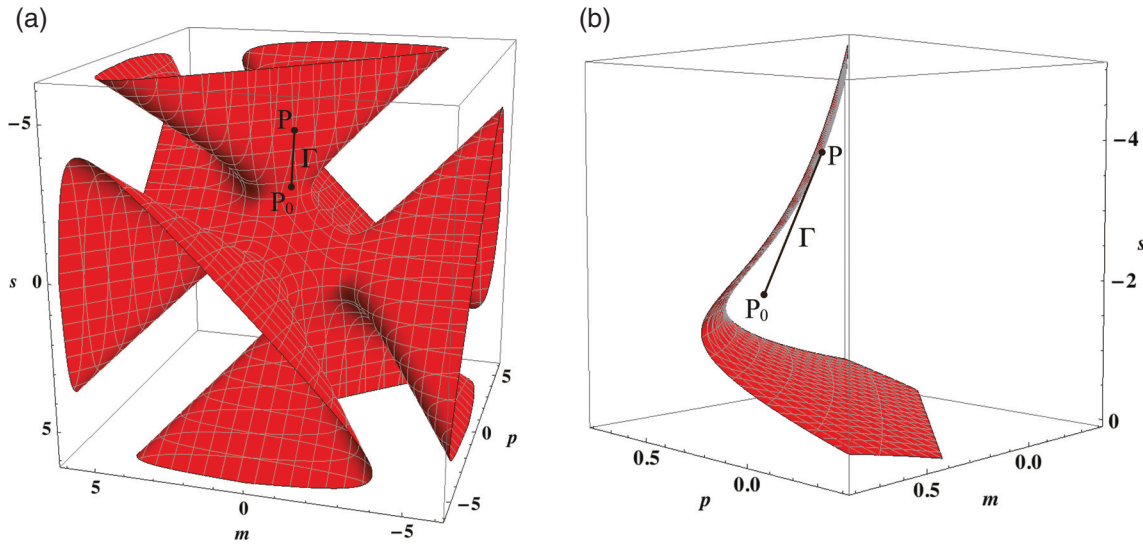


Fig. 1. Boundary surface for the wave instability $I_{\text{wav}}(m, p, s) = 0$. The line Γ touches the surface at a point P . Panel (b) is a close-up of (a). The parameters are fixed at $n = q = r = \alpha = \beta = \gamma = 1$, $m_0 = 0.4$, $p_0 = 0.4$, and $s_0 = -1.8$. The diffusion constants are $D_u = 1$, $D_v = 1$, and $D_w = 14.521$.

Thus, the wave instability first takes place when, for one wave number $k = k_c$, the equation

$$I_{\text{wav}} = (mps - npr + \alpha qr - \gamma mq + \beta \gamma n - \alpha \beta s) + (m + p + s)(mp + ps + sm - nr - \gamma q - \alpha \beta) = 0 \tag{15}$$

becomes satisfied, where m , p , and s are given by Eqs. (10) with $k = k_c$.

The Turing instability first takes place when, for one wave number $k = k_c$, the equation

$$I_{\text{st}} = -(mps - npr + \alpha qr - \gamma mq + \beta \gamma n - \alpha \beta s) = 0 \tag{16}$$

becomes satisfied, where the coefficients m , p , and s are again given by Eqs. (10) with wave number k_c .

It is convenient to introduce the three-dimensional m - p - s space in order to represent these conditions graphically. As illustrated in Figs. 1 and 2, each of the conditions (15) and (16) defines a boundary surface and Eqs. (10) determine a straight line Γ which is parameterized by the wave number k . If the line Γ touches the boundary surface $I_{\text{wav}}(m, p, s) = 0$ or $I_{\text{st}}(m, p, s) = 0$, then condition (15) or (16) is satisfied and the corresponding instability takes place.

5. Sufficient conditions for wave instability

The uniform steady state $(\bar{u}, \bar{v}, \bar{w})$, corresponding to the plane-wave mode of wave number $k = 0$, should be stable if diffusion is absent. In terms of the coefficients of the characteristic equation (11), this implies that

$$a > 0, b > 0, c > 0 \quad \text{and} \quad c - ab < 0, \tag{17}$$

which is known as the Routh-Hurwitz criteria [5]. Note that the third and fourth criteria in (17) are equivalent to the conditions $I_{\text{st}} < 0$ and $I_{\text{wav}} < 0$, respectively. Thus, the initial point P_0 with coordinates (m_0, p_0, s_0) on the line (10) should lie inside the stable region in the m - p - s space.

The wave instability takes place if the first critical mode is oscillatory. At the threshold of the wave instability, the line Γ defined by Eq. (10) should touch the boundary surface $I_{\text{wav}} = 0$ without having intersections with the surface $I_{\text{st}} = 0$.

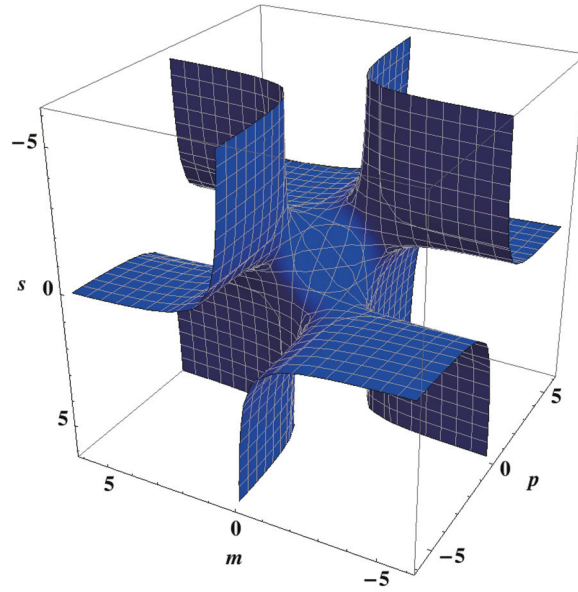


Fig. 2. Boundary surface for the Turing instability $I_{st}(m, p, s) = 0$. The parameters are fixed at $n = q = r = \alpha = \beta = \gamma = 1$.

Suppose that we want to check whether the wave instability can occur when the diffusion constant D_w is varied. Let us denote $A = D_v/D_u$ and $B = p_0 - m_0 D_v/D_u$, and consider a plane $p = Am + B$ parallel to the s -axis. The line Γ always lies on this plane irrespective of D_w , because the conditions $p_0 = Am_0 + B$ and $D_v/D_u = A$ are satisfied. A coordinate

$$x = \frac{m + p}{A + 1} \tag{18}$$

is introduced on the plane in such a way that we have $x = 0$ when $m + p = 0$ holds. From the conditions $p = Am + B$ and (18), variables m and p are represented as $m = x - B/(A + 1)$ and $p = Ax + B/(A + 1)$ on the plane. The slope of the line Γ in the x - s space is $D_u D_w / \sqrt{D_u^2 + D_v^2}$ and is nonnegative. The initial point P_0 of the line Γ is at (x_0, s_0) on the plane, where $x_0 = (m_0 + p_0)/(A + 1)$. The point (x_0, s_0) is in the stable region of the x - s space. Thus, two surfaces $I_{wav} = 0$ and $I_{st} = 0$ intersect the plane along the boundary curves $\hat{I}_{wav} = 0$ and $\hat{I}_{st} = 0$, that is

$$\hat{I}_{wav}(x, s; A, B) = I_{wav}\left(x - \frac{B}{A + 1}, Ax + \frac{B}{A + 1}, s\right) = 0, \tag{19}$$

$$\hat{I}_{st}(x, s; A, B) = I_{st}\left(x - \frac{B}{A + 1}, Ax + \frac{B}{A + 1}, s\right) = 0. \tag{20}$$

Below, we examine the dependences of the boundary curves $\hat{I}_{wav} = 0$ and $\hat{I}_{st} = 0$ on the parameters $m_0, p_0, s_0, n, q, r, \alpha, \beta$, and γ . This allows us to obtain the parameter conditions under which the wave instability can occur.

5.1. Conditions to satisfy $I_{wav} = 0$

Let us examine the shape of the boundary curve $\hat{I}_{wav} = 0$ at large values of $|s|$. If $|s| \gg 1$, we can neglect $\mathcal{O}(s^0)$ terms and obtain

$$\hat{I}_{wav}(x, s; A, B) \approx s \left[(1 + A)^2 x^2 + s(1 + A)x - nr - \gamma q \right]. \tag{21}$$

Then the boundary curve $\hat{I}_{\text{wav}} = 0$ is given by the equation

$$(1 + A)^2 x^2 + s(1 + A)x - nr - \gamma q = 0, \tag{22}$$

and we have

$$\begin{aligned} x &= \frac{1}{2} \left[-\frac{s}{A + 1} \pm \sqrt{\left(\frac{s}{A + 1}\right)^2 + 4\frac{nr + \gamma q}{(A + 1)^2}} \right] \\ &\simeq \frac{s}{2(A + 1)} \left[-1 \pm \left(1 + 2\frac{nr + \gamma q}{s^2} \right) \right]. \end{aligned} \tag{23}$$

From Eq. (21), the boundary curve approaches $x = 0$ in the limit of large $|s|$ as

$$(A + 1)xs^2 = 0. \tag{24}$$

Then the plus sign should be chosen in Eq. (23). Thus, the asymptotic boundary curve in the limit $s \gg 1$ is the hyperbola

$$xs = \frac{nr + \gamma q}{A + 1}. \tag{25}$$

If the coefficient of this hyperbola is negative, i.e. $nr + \gamma q < 0$, the boundary curve lies in the region of $x > 0$ and $s < 0$. In such cases, given that $x_0 > 0$, the line Γ always touches the boundary curve when increasing the diffusion constant D_w , as shown in Figs. 3 and 4. Therefore, we require $nr + \gamma q < 0$ and $x_0 > 0$ as a part of the sufficient conditions. Using the definitions of the model parameters (4), these requirements can be written in terms of the Jacobian matrix as

$$f_w h_u + g_w h_v < 0, \tag{26}$$

$$f_u + g_v > 0. \tag{27}$$

5.2. Conditions not to satisfy $I_{\text{st}} = 0$

The boundary curve for the Turing instability $\hat{I}_{\text{st}}(x, s; A, B) = 0$ is given by

$$s(x) = -\frac{(A + 1)^2(Anr + \gamma q)x - (A + 1)^2(\beta\gamma n + \alpha q r) + (A + 1)B(nr - \gamma q)}{A(A + 1)^2 x^2 - (A^2 - 1)Bx - \alpha\beta(A + 1)^2 - B^2}, \tag{28}$$

which is a single-valued function of x .

Let us assume that all three reactants diffuse over the space, $D_u \neq 0$, $D_v \neq 0$, and $D_w \neq 0$, which leads to $A \neq 0$. If the denominator on the right-hand side of Eq. (28) is not zero for all values of x , then $s(x)$ is a continuous function. Figure 3(a) illustrates the qualitative shape of the boundary curves $\hat{I}_{\text{wav}} = 0$ and $\hat{I}_{\text{st}} = 0$ in such a situation. In this case, the line Γ touches the boundary curve $\hat{I}_{\text{wav}} = 0$ without intersecting $\hat{I}_{\text{st}} = 0$ as D_w is increased. As a consequence, the wave instability takes place. The condition is given by

$$(A^2 - 1)^2 B^2 + 4A(A + 1)^2 \left[\alpha\beta(A + 1)^2 + B^2 \right] < 0, \tag{29}$$

which implies

$$f_u g_v - f_v g_u > \frac{(f_u D_v + g_v D_u)^2}{4D_u D_v}. \tag{30}$$

If the denominator on the right-hand side of Eq. (28) vanishes at x_- and x_+ , the boundary curve $\hat{I}_{\text{st}} = 0$ diverges in two ways depending on the values of n, q, r, α, β , and γ [Fig. 3(b) and (c)].

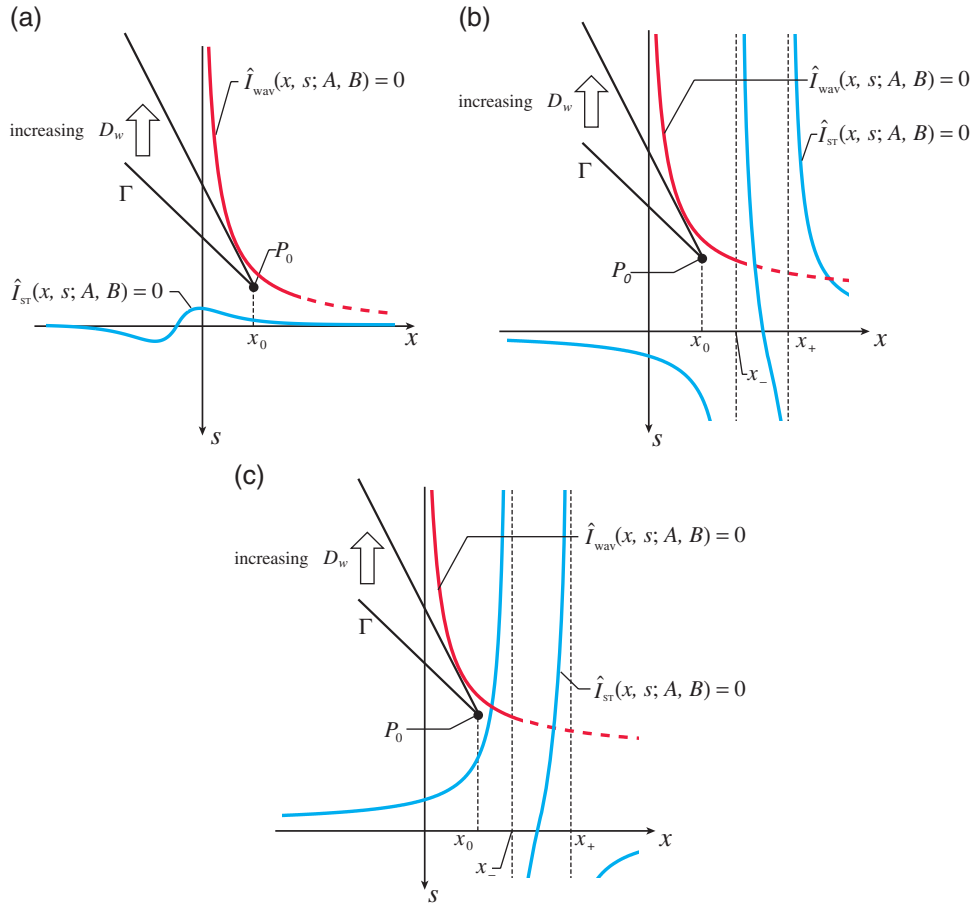


Fig. 3. Boundary curves $\hat{I}_{\text{wav}} = 0$ (red) and $\hat{I}_{\text{st}} = 0$ (blue) when (a) the condition (30) and (b, c) the condition (34) are satisfied. All species are mobile. The positions of the line Γ defined by (10) are shown for two different values of D_w . The boundary curve $\hat{I}_{\text{st}} = 0$ can behave as shown in (b) or (c), depending on the model parameters.

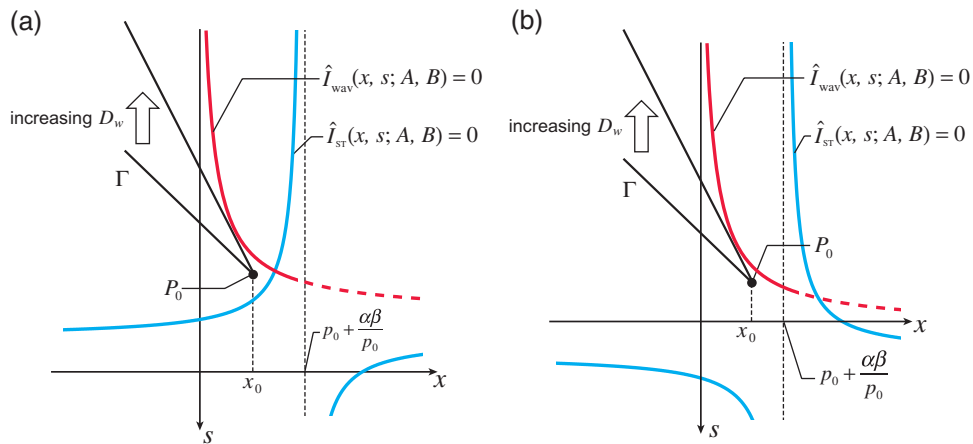


Fig. 4. Boundary curves $\hat{I}_{\text{wav}} = 0$ (red) and $\hat{I}_{\text{st}} = 0$ (blue). The reactant V does not diffuse ($D_v = 0$). The line Γ defined by (10) is shown as black lines for two different values of D_w . The boundary curve $\hat{I}_{\text{st}} = 0$ can behave as shown in (a) or (b), depending on the parameters n, q, r, α, β , and γ .

In both cases, if $x_0 \leq x_-$, the line Γ touches $\hat{I}_{\text{wav}} = 0$ first. Thus, if the condition

$$x_0 \leq x_- = \frac{(A^2 - 1)B - (A + 1)^2 \sqrt{B^2 + 4\alpha\beta A}}{2A(A + 1)^2}, \quad (31)$$

which is equivalent to

$$f_u g_v - f_v g_u > 0 \quad (32)$$

and

$$f_u D_v + g_v D_u \leq 0 \quad (33)$$

is satisfied, the wave instability takes place as D_w is increased.

Next, we assume that the reactant V does not diffuse, that is $D_v = 0$, leading to $A = 0$. In this case, the boundary curve $\hat{I}_{\text{st}} = 0$ is given by

$$s(x)|_{A=0} = -\frac{\gamma q x + \beta \gamma n + \alpha q r + B(nr - \gamma q)}{Bx - \alpha\beta - B^2}, \quad (34)$$

which diverges at $x = B + \alpha\beta/B = p_0 + \alpha\beta/p_0$ [Figs. 4(a) and (b)]. In this case, if $x_0 \leq p_0 + \alpha\beta/p_0$, the line Γ touches $\hat{I}_{\text{wav}} = 0$ without intersecting $\hat{I}_{\text{st}} = 0$ when D_w is increased. Thus, the instability condition for a system with two diffusible reactants is given by

$$x_0 \leq p_0 + \frac{\alpha\beta}{p_0}, \quad (35)$$

which implies

$$g_v(f_u g_v - f_v g_u) \leq 0. \quad (36)$$

On the other hand, if the reactant U does not diffuse, $D_u = 0$, one can choose a plane $m = A'p + B'$ where $A' = D_u/D_v$ and $B' = m_0 - p_0 D_u/D_v$, and derive the condition

$$f_u(f_u g_v - f_v g_u) \leq 0. \quad (37)$$

Thus, sufficient conditions for the wave instability under increasing diffusion constant D_w of the reactant W has been derived for the four cases depending on the diffusion constants. The first two conditions (26) and (27) are common to all cases. The last condition depends on the diffusion constants, i.e. we have

$$\begin{cases} f_u g_v - f_v g_u > \frac{(f_u D_v + g_v D_u)^2}{4D_u D_v} & (D_u \neq 0, D_v \neq 0), & (38) \\ f_u g_v - f_v g_u > 0 \quad \text{and} \quad f_u D_v + g_v D_u \leq 0 & (D_u \neq 0, D_v \neq 0), & (39) \\ f_u(f_u g_v - f_v g_u) < 0 & (D_u = 0, D_v \neq 0), & (40) \\ g_v(f_u g_v - f_v g_u) < 0 & (D_u \neq 0, D_v = 0). & (41) \end{cases}$$

These different requirements can, however, be expressed in a single equation:

$$\det \begin{pmatrix} f_u + D_u \Lambda & f_v \\ g_u & g_v + D_v \Lambda \end{pmatrix} \neq 0 \text{ for any } \Lambda < 0, \quad (42)$$

when at least two diffusion constants are non-vanishing.

The wave instability may take place also under the variation of the other two diffusion constants D_u or D_v . The corresponding sufficient conditions for each case can be obtained by permutating the three variables u , v , and w .

In summary, the wave instability occurs under increasing diffusion constants D_u , D_v , or D_w if the conditions

$$\begin{aligned} g_v + h_w > 0 \quad \text{and} \quad g_u f_v + h_u f_w < 0 \\ \text{and} \quad \det \begin{pmatrix} g_v + D_v \Lambda & g_w \\ h_v & h_w + D_w \Lambda \end{pmatrix} \neq 0 \text{ for any } \Lambda < 0, \end{aligned} \quad (43)$$

$$\begin{aligned} h_w + f_u > 0 \quad \text{and} \quad h_v g_w + f_v g_u < 0 \\ \text{and} \quad \det \begin{pmatrix} h_w + D_w \Lambda & h_u \\ f_w & f_u + D_u \Lambda \end{pmatrix} \neq 0 \text{ for any } \Lambda < 0, \end{aligned} \quad (44)$$

or

$$\begin{aligned} f_u + g_v > 0 \quad \text{and} \quad f_w h_u + g_w h_v < 0 \\ \text{and} \quad \det \begin{pmatrix} f_u + D_u \Lambda & f_v \\ g_u & g_v + D_v \Lambda \end{pmatrix} \neq 0 \text{ for any } \Lambda < 0, \end{aligned} \quad (45)$$

are respectively satisfied.

6. Numerical examples

In order to illustrate the results, we examine several three-component reaction-diffusion systems. The first example is a chemical reaction-diffusion system introduced by Meinhardt [16], where self-enhancement of an activator U is antagonized by two inhibitors V and W . The system is described by the equations

$$\begin{cases} \frac{du}{dt} = -r_u u + \frac{s(u^2 + b_u)}{v(1 + s_u u^2)(1 + s_w w)} + D_u \nabla^2 u, \\ \frac{dv}{dt} = -r_v v + s u^2 + b_v + D_v \nabla^2 v, \\ \frac{dw}{dt} = -r_w w + r_w u + D_w \nabla^2 w. \end{cases} \quad (46)$$

We fix the parameters at $r_u = 1.0$, $r_v = 1.0$, $r_w = 0.01$, $b_u = 0.2$, $b_v = 0$, $s_u = 0$, $s_w = 2.0$, and $s = 1.0$, yielding the uniform steady state $(\bar{u}, \bar{v}, \bar{w}) \simeq (0.646, 0.417, 0.646)$. The Jacobian matrix at the uniform steady state is

$$J \simeq \begin{pmatrix} 0.352 & -1.548 & -0.564 \\ 1,291 & -1 & 0 \\ 0.01 & 0 & -0.01 \end{pmatrix}. \quad (47)$$

This satisfies the conditions (17), so that the uniform steady state is stable when diffusion is absent. Below, we demonstrate numerically wave instability in the system (46) to check the validity of the derived conditions (43)–(45).

Suppose that the inhibitor W does not diffuse, i.e. $D_w = 0$. In this case, the conditions (44) are always satisfied irrespective of the diffusion mobility D_u of the activator U . Thus, the wave instability will be found when D_v is gradually increased.

Figure 5 illustrates the linear stability analysis in this case, and also presents the results of numerical simulations which were performed for a one-dimensional system under periodic boundary conditions. The boundary surfaces $I_{\text{wav}} = 0$ and $I_{\text{st}} = 0$ and the x - p plane in the m - p - s space are shown

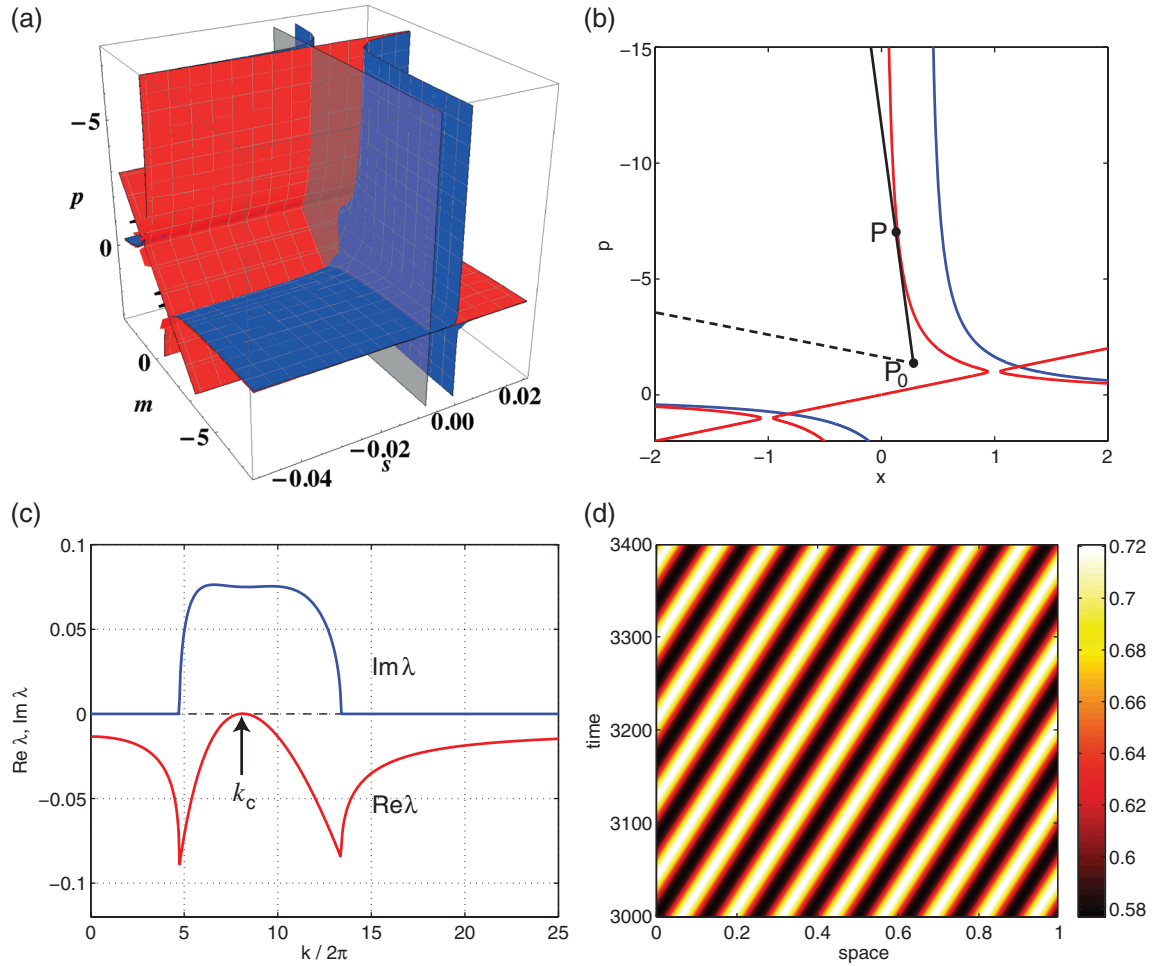


Fig. 5. Wave instability in the model (46). (a) Boundary surfaces $I_{\text{wav}}(m, p, s) = 0$ (red surface), $I_{\text{st}}(m, p, s) = 0$ (blue surface), and the x - p plane (gray transparent plane) in the three-dimensional m - p - s space. (b) Boundaries $\hat{I}_{\text{wav}}(x, p) = 0$ (red curve) and $\hat{I}_{\text{st}}(x, p) = 0$ (blue curve) on the x - p plane. The lines Γ for two different diffusion constants, $D_v = 2.5$ (black dashed line) and $D_v = 156$ (black solid line), are shown. (c) The real part (red curve) and the imaginary part (blue curve) of the linear growth rate λ as functions of wave number k . (d) The space-time plot of the final established patterns at $D_v = 157.5$. The diffusion constants of two species U and W are fixed at $D_u = 2.5$ and $D_w = 0$ in this figure.

in Fig. 5(a). Note that, while the variable x was introduced by using the variables m and p in Eq. (18), here it depends on the variables s and m , so that the line Γ lies on the x - p plane irrespective of the value of D_v . The boundary curves $\hat{I}_{\text{wav}} = 0$ and $\hat{I}_{\text{st}} = 0$ in the x - p plane are shown in Fig. 5(b). Figure 5(c) plots the linear growth rate λ for the instability threshold. The emerging wave pattern is shown in Fig. 5(d).

Starting from equal mobilities of the species U and V , $D_u = D_v = 2.5$, we gradually increase the mobility D_v . When it reaches a certain threshold, the line Γ touches the boundary curve $\hat{I}_{\text{wav}} = 0$ at P_0 without having intersections with $\hat{I}_{\text{st}} = 0$, as shown in Fig. 5(b). At the instability threshold, the real part of the linear growth rate vanishes, $\text{Re}\lambda^{(k)} = 0$, for the critical wave number $k_c \simeq 8$, whereas the imaginary part remains finite [Fig. 5(c)]. Thus, the wave instability takes place and the uniform steady state becomes unstable. When the instability occurs, traveling waves with wave number $k = 8$ spontaneously develop, as can be seen in Fig. 5(d).

As another example, we apply our theory to an ecological reaction-diffusion (dispersal predator-prey) system with three species U , V , and W , where the top predator W feeds on intermediate species V , which is in turn a predator for prey U . All species are able to diffuse, and their diffusion constants are different. Such a system can be modelled by the equations

$$\begin{cases} \frac{du}{dt} = \left[a_u - b_u u - c_u \frac{w}{u + \mu} \right] u + D_u \nabla^2 u, \\ \frac{dv}{dt} = \left[a_v \left(1 - c_v \frac{v}{u} \right) - d_v \frac{w}{v + \nu} \right] v + D_v \nabla^2 v, \\ \frac{dw}{dt} = \left[a_w \left(1 - d_w \frac{w}{v} \right) \right] w + D_w \nabla^2 w, \end{cases} \quad (48)$$

where the Holling type II dependence and a linear function are employed to describe the predator-prey interactions [5,17]. The parameters are fixed at $a_u = 3$, $b_u = 1$, $c_u = 1$, $a_v = 6$, $c_v = 1$, $d_v = 1$, $a_w = 4$, $d_w = 0.25$, and $\mu = \nu = 0.25$, which give a uniform steady state $(\bar{u}, \bar{v}, \bar{w}) \simeq (1.084, 2.557, 10.23)$. If all species have the same mobilities, $D_u = D_v = D_w$, the steady state is stable. The Jacobian matrix at the steady state is

$$J \simeq \begin{pmatrix} 0.471 & -0.813 & 0 \\ 5.552 & 0.962 & -0.911 \\ 0 & 16 & -4 \end{pmatrix}. \quad (49)$$

By substituting this into the inequalities (45), one can directly verify that the system satisfies the sufficient conditions. Then, our theory tells us that the wave instability will take place when the diffusion constant D_w of the predator W is increased.

Figure 6(a) shows the boundary surfaces $I_{\text{wav}} = 0$ and $I_{\text{st}} = 0$ and the x - s plane in m - p - s space. The boundary curves $\hat{I}_{\text{wav}} = 0$ and $\hat{I}_{\text{st}} = 0$ in the x - s plane are displayed in Fig. 6(b). Figure 6(c) gives the linear growth rate λ as a function of the wave number k at the instability threshold. The developed wave pattern is shown in Fig. 6(d).

Starting from equal mobilities of all three species, $D_u = D_v = D_w = 20$, the mobility D_w of the top predator W is gradually increased. When it comes up to a threshold $D_w = 892$, the line Γ touches the boundary curve $\hat{I}_{\text{wav}} = 0$ without having intersections with $\hat{I}_{\text{st}} = 0$ [Fig. 6(b)]. Correspondingly, the real part of the linear growth rate vanishes at the threshold, $\text{Re}\lambda^{(k)} = 0$, for the critical wave number $k_c \simeq 4$, whereas the imaginary part remains finite [Fig. 6(c)]. As a result, the wave instability takes place and the uniform steady state becomes unstable. After the instability, spontaneous development of traveling wave patterns with wave number $k = 4$ is observed [Fig. 6(d)]. Thus, as illustrated by the above examples, the derived sufficient conditions (43)–(45) indeed provide a useful criterion when searching for the wave instabilities in specific reaction-diffusion systems.

It should be emphasized that the derived conditions (43)–(45) are sufficient, but not necessary. This means that systems may exist where such conditions do not hold, but the wave instability is observed nonetheless.

An example of such a situation is provided by the extended Brusselator system [12]:

$$\begin{cases} \frac{du}{dt} = a - (1 + b)u + u^2 v - cu + dw + D_u \nabla^2 u, \\ \frac{dv}{dt} = bu - u^2 v + D_v \nabla^2 v, \\ \frac{dw}{dt} = cu - dw + D_w \nabla^2 w, \end{cases} \quad (50)$$

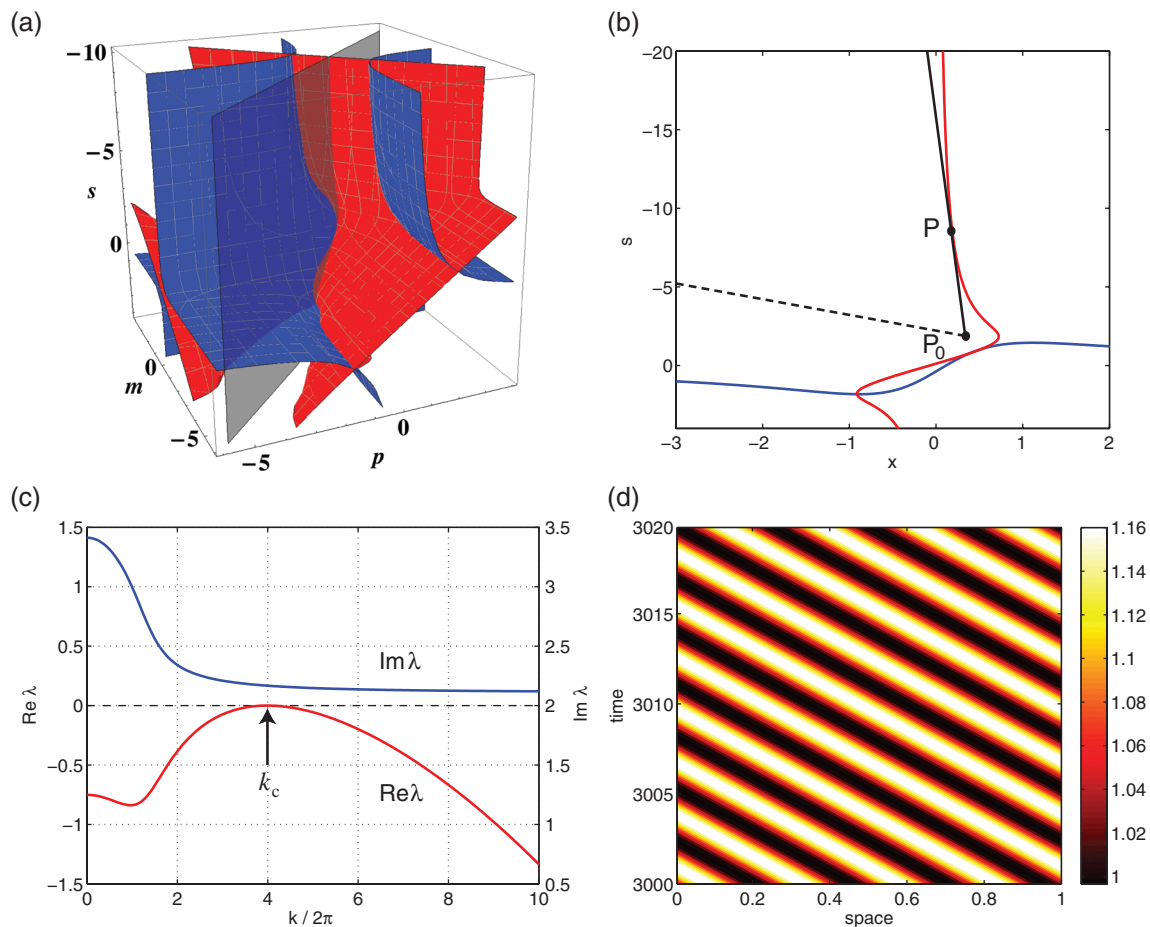


Fig. 6. Wave instability in the ecological model (48). (a) Boundary surfaces $I_{\text{wav}}(m, p, s) = 0$ (red surface), $I_{\text{st}}(m, p, s) = 0$ (blue surface), and the x - s plane (gray transparent plane) in the three-dimensional m - p - s space. (b) Boundaries $\hat{I}_{\text{wav}}(x, s) = 0$ (red curve) and $\hat{I}_{\text{st}}(x, s) = 0$ (blue curve) on the x - s plane. The lines Γ for two different diffusion constants, $D_w = 20$ (black dashed line) and $D_w = 892$ (black solid line), are shown. (c) The real part (red curve) and the imaginary part (blue curve) of the linear growth rate λ as functions of the wave number k . (d) The space-time plot of the final established patterns at $D_w = 900$. The diffusion constants of the two species U and V are fixed at $D_u = D_v = 20$ in this figure.

where activator U and inhibitor V react chemically, and the activator U reversibly transforms into non-reacting species W . The parameters are fixed at $a = 1, b = 2.9, c = 1,$ and $d = 1,$ which yield the uniform steady state $(\bar{u}, \bar{v}, \bar{w}) = (1, 2.9, 1)$. The steady state is stable if all three species have the same mobility, $D_u = D_v = D_w$.

The Jacobian matrix at the steady state is

$$J \simeq \begin{pmatrix} 0.9 & 1 & 1 \\ -2.9 & -1 & 0 \\ 1 & 0 & -1 \end{pmatrix}, \quad (51)$$

which gives $f_u + g_v < 0$ and $f_w h_u + g_w h_g > 0$. Thus, the system does not satisfy the conditions (45).

However, numerical simulations show that the wave instability takes place in this model when the nonreactive species W diffuses sufficiently faster than the other two species (Fig. 7). The linear

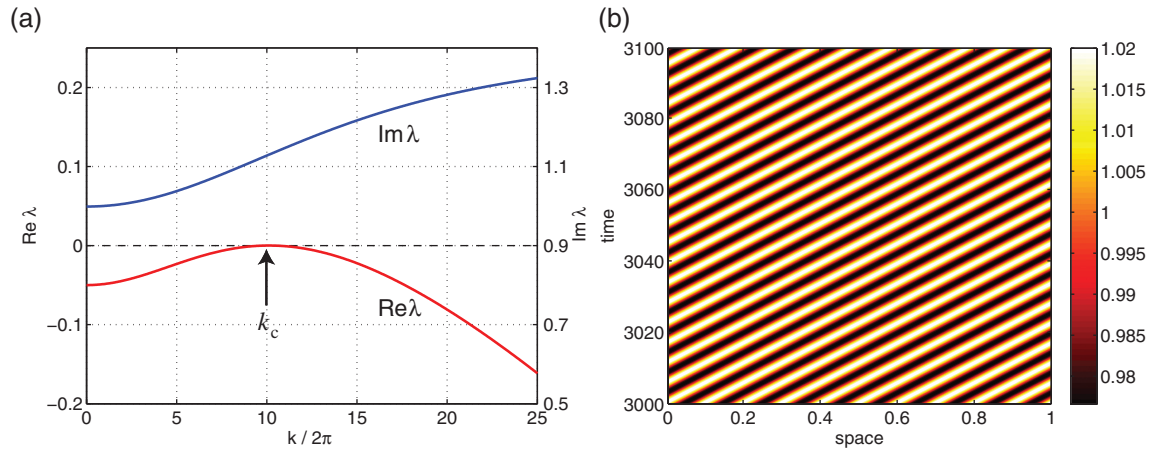


Fig. 7. Wave instability in the extended Brusselator system (50). (a) The real part (red curve) and the imaginary part (blue curve) of the linear growth rate λ at the instability threshold as functions of wave number k . (b) The space-time plot of the final established pattern at $D_u = D_v = 0.3$ and $D_w = 6.95$.

growth rate as a function of wave number is shown in Fig. 7(a). The established traveling wave pattern is displayed in Fig. 7(b).

7. Discussion and conclusions

We have constructed alternative sufficient conditions for the wave instability in general three-component reaction-diffusion systems. The conditions are formulated in terms of the Jacobian matrix elements at a steady state and of the diffusion constants. They do not depend on model details. Once these conditions are satisfied, wave instability occurs as we increase the diffusion mobility of one of the reacting species.

Our general results are applicable for systems of various origins, including biological, chemical, physical, and ecological systems. Our analysis has revealed that the wave instability may occur even if one of three reactants is immobile. This result can be important in a variety of applications involving both diffusible and non-diffusible reactants.

In contrast to necessary and sufficient conditions, different sets of merely sufficient conditions may be derived and hold for the same system. In fact, another set of sufficient conditions for the wave instability in general three-species reaction-diffusion systems has recently been constructed in Ref. [15].

In Ref. [15], the authors focused particularly on how the stability of a three-species system is affected by instabilities of its two-species subsystems. They classified the instabilities of the subsystems into several types and analyzed their effect on the complete three-species system in detail. Their investigation was based on linear stability analysis, and the sufficient conditions were formulated in terms of the elements of the Jacobian matrix and the diffusion constants of the three species. They also derived sufficient conditions for the classical (stationary) Turing instability in three-component reaction-diffusion systems.

In our study, we have constructed the sufficient conditions using a different method, based on linear stability analysis and inspection of the instability threshold in the parameter space. Once the Jacobian matrix is obtained, the boundary surfaces of the instabilities and the line whose slope corresponds to the diffusion constants of the three species can be drawn as in Figs. 1 and 2. If the line touches the boundary surface as its slope is varied, the instability occurs. By considering the situation where

the line always touches the boundary surfaces of the wave instability when one of the three diffusion constants is increased, we have derived sufficient conditions that are different from those in Ref. [15].

We stress that these two sets of sufficient conditions are complementary. There is an overlap between them, but neither set of sufficient conditions includes the other one. For example, our conditions can predict the wave instability in the ecological model (48); however, this model does not satisfy the conditions [(iv)–(1) and (2) in Corollary 1.1] derived in Ref. [15]. On the other hand, our conditions cannot predict the wave instability in the extended Brusselator system (50), while the conditions in Ref. [15, Sect. 3.2] can do this.

Although our conditions have been derived for continuous media, they are also applicable for reaction-diffusion networks where reactants diffuse over links and undergo local reactions on each node [18–21]. In such systems, diffusion processes are described by the Laplacian matrix instead of the Laplacian differential operator in Eqs. (1) and (2). Expanding small perturbations over eigenvectors of the Laplacian matrix, we obtain the same characteristic equation as that for continuous media (9), where (m, p, s) are parameterized by the Laplacian eigenvalues Λ instead of $-k^2$ in Eq. (10)—see Appendix A. Thus, the critical conditions $I_{\text{wav}} = 0$ and $I_{\text{st}} = 0$ are valid, so that we also obtain the sufficient conditions (43)–(45) in networks. This may be useful for finding the oscillatory Turing bifurcation in networks of coupled reactors or biological cells [22,23].

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Appendix A. Linear stability analysis on reaction–diffusion networks

We consider three reactant species U , V , and W on a network of size N . The local densities of the reactants on the network node i are denoted as $u_i = [U]_i$, $v_i = [V]_i$, and $w_i = [W]_i$. The network architecture is determined by the adjacent matrix \mathbf{A} whose elements A_{ij} are 1 if the nodes i and j are connected, and 0 otherwise. All reactants diffuse over network links and undergo local reactions in each node. Such dynamics are described by the equations

$$\begin{cases} \dot{u}_i = f(u_i, v_i, w_i) + D_u \sum_{j=1}^N L_{ij} u_j, \\ \dot{v}_i = g(u_i, v_i, w_i) + D_v \sum_{j=1}^N L_{ij} v_j, \\ \dot{w}_i = h(u_i, v_i, w_i) + D_w \sum_{j=1}^N L_{ij} w_j, \end{cases} \quad (\text{A1})$$

for $i = 1, \dots, N$, where the functions f , g , and h specify the local reactions, D_u , D_v , and D_w are the diffusion constants of the three reactants, and $L_{ij} = A_{ij} - \delta_{ij} \sum_j A_{ij}$ is the Laplacian matrix.

The linear stability analysis is performed on the system in an analogous way to continuous media (See Sect. 3). The system is assumed to have a uniform steady state $(\bar{u}, \bar{v}, \bar{w})$ which is determined by $f(\bar{u}, \bar{v}, \bar{w}) = g(\bar{u}, \bar{v}, \bar{w}) = h(\bar{u}, \bar{v}, \bar{w}) = 0$. Small perturbations are introduced on the steady state as $(u_i, v_i, w_i) = (\bar{u}, \bar{v}, \bar{w}) + (\delta u_i, \delta v_i, \delta w_i)$. We substitute this into Eq. (A1) to obtain linearized differential equations. Introducing the rescaled variables in the same way as in Eq. (3), the linearized

differential equations are rewritten as

$$\begin{cases} \frac{d}{dt}\delta\tilde{u}_i = m_0\delta\tilde{u}_i + \alpha\delta\tilde{v}_i + n\delta\tilde{w}_i + D_u\mu \sum_{j=1}^N L_{ij}\delta\tilde{u}_j, \\ \frac{d}{dt}\delta\tilde{v}_i = \beta\delta\tilde{u}_i + p_0\delta\tilde{v}_i + q\delta\tilde{w}_i + D_v\mu \sum_{j=1}^N L_{ij}\delta\tilde{v}_j, \\ \frac{d}{dt}\delta\tilde{w}_i = r\delta\tilde{u}_i + \gamma\delta\tilde{v}_i + s_0\delta\tilde{w}_i + D_w\mu \sum_{j=1}^N L_{ij}\delta\tilde{w}_j, \end{cases} \quad (\text{A2})$$

where $m_0, p_0, s_0, n, q, r,$ and μ are given in Eq. (5). Perturbations are expanded over a set of Laplacian eigenvectors $\{\phi_i^{(\kappa)}\}$ as

$$\begin{aligned} \delta\tilde{u}_i(t) &= \sum_{\kappa=1}^N \tilde{U}^{(\kappa)} \exp[\lambda^{(\kappa)}t]\phi_i^{(\kappa)}, \\ \delta\tilde{v}_i(t) &= \sum_{\kappa=1}^N \tilde{V}^{(\kappa)} \exp[\lambda^{(\kappa)}t]\phi_i^{(\kappa)}, \\ \delta\tilde{w}_i(t) &= \sum_{\kappa=1}^N \tilde{W}^{(\kappa)} \exp[\lambda^{(\kappa)}t]\phi_i^{(\kappa)}, \end{aligned} \quad (\text{A3})$$

where $\lambda^{(\kappa)}$ is the linear growth rate of the κ th eigenmode. Substituting into Eq. (A2), we obtain the following matrix equation for each eigenmode:

$$\lambda^{(\kappa)} \begin{pmatrix} \tilde{U}^{(\kappa)} \\ \tilde{V}^{(\kappa)} \\ \tilde{W}^{(\kappa)} \end{pmatrix} = \begin{pmatrix} m_0 + D_u\mu\Lambda^{(\kappa)} & \alpha & n \\ \beta & p_0 + D_v\mu\Lambda^{(\kappa)} & q \\ r & \gamma & s_0 + D_w\mu\Lambda^{(\kappa)} \end{pmatrix} \begin{pmatrix} \tilde{U}^{(\kappa)} \\ \tilde{V}^{(\kappa)} \\ \tilde{W}^{(\kappa)} \end{pmatrix}, \quad (\text{A4})$$

where $\Lambda^{(\kappa)}$ is the Laplacian eigenvalue, which is defined by $\sum_j L_{ij}\phi_j^{(\kappa)} = \Lambda^{(\kappa)}\phi_i^{(\kappa)}$. Assuming that the equations (A4) have non-trivial solutions, we obtain the same characteristic equation as Eq. (9) with

$$\begin{aligned} m &= m(\kappa) = m_0 + \Lambda^{(\kappa)}\mu D_u, \\ p &= p(\kappa) = p_0 + \Lambda^{(\kappa)}\mu D_v, \\ s &= s(\kappa) = s_0 + \Lambda^{(\kappa)}\mu D_w. \end{aligned} \quad (\text{A5})$$

Thus, the critical conditions for the instabilities (15) and (16) are valid, and therefore the sufficient conditions (43)–(45) are also applicable for reaction-diffusion networks.

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