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LETTER TO THE EDITOR

Bounds on steady states for a non-systemically autocatalysed reaction–diffusion system

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Abstract. Bounds on parameter values that lead to different types of solutions for a non-systemically autocatalysed reaction-diffusion system are derived and show the existence of a critical concentration beyond which the stability properties undergo change. Additionally, bifurcating solutions at the zero eigenvalue are obtained.

This letter considers an alternative form of autocatalysis where the product formed affects its own rate through interactions with the rate constant as against the normal autocatalysis where the rate is affected directly by the concentration of the product. This form of the rate has wide applications in several biochemical systems as well as in explaining the phenomena in diverse chemical and combustion-type reactions (Ravi Kumar *et al* 1984). The exponential autocatalysis has received acceptance as a general model for a class of reaction-diffusion systems (Bar-Eli 1984a, b, c, 1985) and results obtained by using the conventional autocatalysis, such as the one used in Brusselator-type models, compare well with this model system. The exponential autocatalysis has revealed the existence of multiplicity and oscillatory behaviour under homogeneous conditions (Ravi Kumar *et al* 1984). This letter begins with this reaction scheme to derive bounds on the values of the parameters that lead to the existence of different types of solutions in presence of diffusion gradients.

More specifically the conditions under which the governing system would have real eigenvalues with positive real part, the conditions when eigenvalues are complex and the conditions when the complex eigenvalues have real positive parts have been derived. In addition to this, bifucating solutions for a simple case of zero eigenvalue are obtained. The mathematical aspects of reacting and diffusing systems are well documented (see, for example, Sattinger 1973, Auchmuty and Nicolis 1975a, b, Fife 1979, Kuramoto 1984), but the present scheme provides an example where the functions involved are transcendental in nature.

The reaction-diffusion system is represented by following coupled nonlinear parabolic partial differential equations:

$$\begin{aligned}\frac{\partial x}{\partial t} &= D_1 \frac{\partial^2 x}{\partial r^2} + x_0 - x - Da_1 x \exp(\alpha y)\\ \frac{\partial y}{\partial t} &= D_2 \frac{\partial^2 y}{\partial r^2} + y_0 - y + Da_1 x \exp(\alpha y) - Da_2 y.\end{aligned} \tag{1}$$

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At steady state, the values of x and y, denoted as x_s and θ respectively, are given by

$$\exp(\alpha\theta) = \frac{(x_0 - x_s)}{x_s Da_1} \qquad \theta = \frac{x_0 + y_0 - x_s}{1 + Da_2}. \tag{2}$$

Defining deviations from steady state as u and v

$$x = u + x_s \qquad y = v + \theta \tag{3}$$

and with linearisation of the nonlinear term $\exp(\alpha v) = (1 + \alpha v)$, equation (1) can be rewritten as

$$\frac{\partial u}{\partial t} = D_1 \frac{\partial^2 u}{\partial r^2} - (1 + Da_1\, e^{\alpha\theta})u - (\alpha Da_1 x_s\, e^{\alpha\theta} v) - \alpha Da_1\, e^{\alpha\theta} uv \tag{4a}$$

$$\frac{\partial v}{\partial t} = D_2 \frac{\partial^2 v}{\partial r^2} + Da_1\, e^{\alpha\theta} u + (\alpha Da_1 x_s\, e^{\alpha\theta} - (1 + Da_2))v + \alpha Da_1\, e^{\alpha\theta} uv. \tag{4b}$$

The eigenvalue problem for equations (4*a*) and (4*b*) can be formulated as:

$$D_1 u'' - (1 + Da_1\, e^{\alpha\theta})u - \alpha Da_1 x_s\, e^{\alpha\theta} v = \lambda u \tag{5a}$$

$$D_2 v'' + Da_1\, e^{\alpha\theta} u + (\alpha Da_1 x_s\, e^{\alpha\theta} - (1 + Da_2))v = \lambda v. \tag{5b}$$

Using equations (5*a*) and (5*b*), and defining constants k_1, k_2, k_3, k_4 for the sake of simplification as,

$$k_1 = -(1 + Da_1\, e^{\alpha\theta}) \qquad k_2 = -\alpha Da_1 x_s\, e^{\alpha\theta} \tag{6}$$

$$k_3 = \alpha x_s Da_1\, e^{\alpha\theta} - (1 + Da_2) \qquad k_4 = Da_1\, e^{\alpha\theta} \tag{7}$$

the solution to the eigenvalue problem can be given as

$$\begin{pmatrix} u_m(r) \\ v_m(r) \end{pmatrix} = \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} \sin m\pi r. \tag{8}$$

From equations (5)-(8) we obtain

$$c_1^2 + c_2^2 = 2 \tag{9}$$

$$\delta_m = \frac{c_2}{c_1} = \frac{-m^2\pi^2 D_1 + k_1}{k_2} \tag{10}$$

giving us c_1 and c_2 as

$$c_1 = \frac{\sqrt{2}}{\sqrt{1 + \delta_m^2}} \qquad c_2 = \frac{\sqrt{2}\,\delta_m}{\sqrt{1 + \delta_m^2}}. \tag{11}$$

The system of linear equations possesses the following characteristic equation:

$$\lambda^2 + (\beta_m - \alpha_m)\lambda + \alpha x_s (Da_1\, e^{\alpha\theta})^2 - \alpha_m \beta_m = 0. \tag{12}$$

The eigenvalues are the roots of the characteristic equation given by

$$\lambda^{\pm} = \tfrac{1}{2}\{(\alpha_m - \beta_m) \pm [(\alpha_m + \beta_m)^2 - 4\alpha x_s (Da_1\, e^{\alpha\theta})^2]^{1/2}\}. \tag{13}$$

Analysis of equation (13) helps us to fix the following conditions for different stability behaviour of steady state solutions.

(1) λ^+ has positive real part whenever

$$y_0 > (x_s - x_0) + \frac{(1 + Da_2)}{\alpha} \ln\left\{\frac{m^4\pi^4 D_1 D_2 + m^2\pi^2[D_1(1 + Da_2) + D_2] + (1 + Da_2)}{Da_1[m^2\pi^2(\alpha x_s D_1 - D_2) + (\alpha x_s - Da_2 - 1)]}\right\}. \tag{14}$$

(2) The eigenvalues are complex whenever the discriminant in equation (12) obeys the condition $\Delta<0$. The resulting inequality is

$$(x_s-x_0)+\frac{(1+Da_2)}{\alpha}\ln\left\{\frac{(\alpha x_s+1)(1+Da_2-\delta)-\psi}{Da_1(\alpha x_s-1)^2}\right\}<y_0$$
$$<(x_s-x_0)+\frac{(1+Da_2)}{\alpha}\ln\left\{\frac{(\alpha x_s+1)(1+Da_2-\delta)+\psi}{Da_1(\alpha x_s-1)^2}\right\} \tag{15}$$

where

$$\psi=\{4[\alpha x_s(\delta-1)^2-Da_2(\delta-1)(\alpha^2x_s^2+1)+\alpha x_s Da_2^2]+(\alpha x_s-1)^2\}^{1/2} \tag{16}$$

and

$$\delta=1+m^2\pi^2(D_1-D_2). \tag{17}$$

(3) A complex value will have positive real part provided

$$y_0>(x_s-x_0)+\frac{(1+Da_2)}{\alpha}\ln\left\{\frac{\delta'+Da_2+1}{Da_1(\alpha x_s-1)}\right\} \tag{18}$$

where

$$\delta'=1+m^2\pi^2(D_1+D_2). \tag{19}$$

Combining the two inequalities given by equations (15) and (18), one sees that

$$(x_s-x_0)+\frac{(1+Da_2)}{\alpha}\ln\left\{\frac{\delta'+Da_2+1}{Da_1(\alpha x_s-1)}\right\}$$
$$<y_0<(x_s-x_0)+\frac{(1+Da_2)}{\alpha}\ln\left\{\frac{(\alpha x_s+1)(1+Da_2-\delta)-\psi}{Da_1(\alpha x_s-1)^2}\right\}. \tag{20}$$

The equations (15) and (16) can be rewritten as:

$$m^4\pi^4(D_1-D_2)^2+2m^2\pi^2\{(D_1-D_2)[Da_1\,e^{\alpha\theta}(\alpha x_s+1)-Da_2]\}$$
$$+\{(\alpha x_s-1)^2(Da_1\,e^{\alpha\theta})^2-2Da_2(\alpha x_s+1)Da_1\,e^{\alpha\theta}+Da_2^2-1\}=0. \tag{21}$$

Now, to obtain the critical value of the wavenumber m_c or μ we shall minimise the function in equation (14). If $f=m^2\pi^2$, then we have the following quadratic equation:

$$f^2\{D_1D_2(\alpha x_sD_1-D_2)\}+f\{2D_1D_2(\alpha x_s-Da_2-1)\}$$
$$+(\alpha x_s-Da_2-1)[(1+Da_2)D_1+D_2]-(1+Da_2)(\alpha x_sD_1-D_2)=0 \tag{22}$$

giving

$$f=\frac{(1+Da_2-\alpha x_s)D_1D_2\pm q}{D_1D_2(\alpha x_sD_1-D_2)} \tag{23a}$$

where

$$q=[\![[D_1D_2(\alpha x_s-Da_2-1)]^2-(\alpha x_sD_1-D_2)$$
$$\times\{D_1D_2(\alpha x_s-Da_2-1)[(1+Da_2)D_1+D_2]+\tfrac{1}{4}(1+Da_2)\}]\!]^{1/2}. \tag{23b}$$

From equations (14), (22) and (23), we obtain the expression for critical value of bifurcating parameter as:

$$y_{0c} \geqslant (x_s - x_0) + \frac{(1+Da_2)}{\alpha} \ln\left\{ \pm \frac{D_1 D_2}{q} \left[2(1+Da_2) - \frac{(\alpha x_s - Da_2 - 1)[(1+Da_2)D_1 + D_2]}{(\alpha x_s D_1 - D_2)} + \frac{(1+Da_2 - \alpha x_s)D_1 D_2 \pm q}{(\alpha x_s D_1 - D_2)} \left(\frac{2(1+Da_2 - \alpha x_s)}{(\alpha x_s D_1 - D_2)} + \frac{D_1(1+Da_2)+D_2}{D_1 D_2} \right) \right] \right\}. \tag{24}$$

From equation (18), one gets

$$y_{01} = (x_s - x_0) + \frac{(1+Da_2)}{\alpha} \ln\left\{ \frac{1+\pi^2(D_1+D_2)+(1+Da_2)}{(\alpha x_s - 1)Da_1} \right\}. \tag{25}$$

Then combining inequalities (20) and (25),

$$D_2 < 2(Da_2 + 2 + \pi^2 D_1) - \{4[\alpha x_s(\delta_0 - 1)^2 - Da_2(\delta_0 - 1)(\alpha^2 x_s^2 + 1) + \alpha x_s Da_2^2] + (\alpha x_s - 1)^2\}^{1/2} \tag{26}$$

where

$$\delta_0 = 1 + \pi^2(D_1 - D_2). \tag{27}$$

In particular, if $D_1 = D_2 = D$, equation (26) becomes

$$D < \frac{2(Da_2+2) - [4\alpha x_s Da_2^2 + (\alpha x_s - 1)^2]^{1/2}}{1 - 2\pi^2}. \tag{28}$$

For a simple zero eigenvalue, the eigenfunction has a condition for the wavenumber as

$$\alpha_m \beta_m = \alpha x_s (Da_1 \, e^{\alpha\theta})^2.$$

This produces the following quadratic equation:

$$m^4 D_1 D_2 + \frac{m^2}{\pi^2} \{D_1[\alpha x_s Da_1 \, e^{\alpha\theta} - (1+Da_2)] - D_2(1 + Da_1 \, e^{\sigma\theta})\} + \frac{1}{\pi^4} \{\alpha x_s Da_1 \, e^{\alpha\theta} - (1+Da_2)(1+Da_1 \, e^{\alpha\theta})\} = 0 \tag{29}$$

or for y_{0m} we can rewrite equation (29) using the critical value of m as

$$y_{0m} \geqslant (x_s - x_0) + \frac{(1+Da_2)}{\alpha} \ln\left\{ \pm \frac{D_1 D_2}{q} \left[2(1+Da_2) - \frac{(\alpha x_s - Da_2 - 1)[(1+Da_2)D_1 + D_2]}{(\alpha x_s D_1 - D_2)} + \frac{(1+Da_2 - \alpha x_s)D_1 D_2 \pm q}{(\alpha x_s D_1 - D_2)} \left(\frac{2(1+Da_2 - \alpha x_s)}{(\alpha x_s D_1 - D_2)} + \frac{D_1(1+Da_2)+D_2}{D_1 D_2} \right) \right] \right\}. \tag{30}$$

In a similar fashion, we can substitute the value of m_c into equation (30), and obtain another relationship, which confirms that $y_0 = 0$ can never be a bifurcation point.

Now for the quadratic equation (29) in m^2, there exist two positive integers m_1 and m_2 such that,

$$D_1 D_2 (m^2 - m_1^2)(m^2 - m_2^2) = 0.$$

When m_1 is an integer solution, this yields a condition,

$$\nu = \frac{(1 + Da_2) - \alpha x_s Da_1 \, e^{\alpha\theta}}{D_2} + \frac{1 + Da_1 \, e^{\alpha\theta}}{D_1} - m_1^2 \tag{31}$$

which is not a square.

For the normalised eigenvector given in equation (8), using equations (9)-(11), the constants c_1 and c_2 can be computed. Similarly, putting the critical value of wavenumber m_c, we can see that

$$c_2 / c_1 < 0. \tag{32}$$

The adjoint $L_{y_0}^*$ of L_{y_0} is given as

$$L_{y_0}^* \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} D_1 \nabla_r + k_1 & k_4 \\ k_2 & D_2 \nabla_r + k_3 \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} \tag{33}$$

with the condition

$$u = v = 0. \tag{34}$$

The eigenvalues of the adjoint operator $L_{y_0}^*$ are the same as that of L_{y_0}, and the eigenfunction for simple zero eigenvalue is given as

$$\begin{pmatrix} u_m(r) \\ v_m(r) \end{pmatrix} = \begin{pmatrix} d_1 \\ d_2 \end{pmatrix} \sin m\pi r. \tag{35}$$

Using equations (5) and (35) we obtain

$$d_1^2 + d_2^2 = 2 \tag{36}$$

$$\varepsilon_m = \frac{d_1}{d_2} = \frac{-m^2 \pi^2 D_2 + k_3}{k_2} \tag{37}$$

which produces expressions for d_1 and d_2 as

$$d_1 = \frac{\sqrt{2}\,\varepsilon_m}{\sqrt{1 + \varepsilon_m^2}} \qquad d_2 = \frac{\sqrt{2}}{\sqrt{1 + \varepsilon_m^2}}. \tag{38}$$

This letter presents the analysis of the steady state solutions of the system of nonlinear equations which describe an exponentially autocatalysed reaction with diffusion. The stability of steady state solutions of the system has been derived using a linear stability analysis. In particular, criteria in terms of the bounds on the values of a parameter appearing in the equations are developed. The analysis reveals the existence of the critical value y_{0c} of a component y beyond which the uniform steady state solutions undergo a change in stability properties. It is possible to have additional steady state solutions of the system of equations, which may be stable for the various ranges of y_0. These solutions, however, are inhomogeneous and possess several well defined maxima or minima. The results here form a basis for obtaining the so-called dissipative structures.

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