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Stationary and oscillatory patterns in a coupled Brusselator model

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Abstract

This paper presents a numerical investigation into the pattern formation mechanism in the Brusselator model focusing on the interplay between the Hopf and Turing bifurcations. The dynamics of a coupled Brusselator model is studied in terms of wavelength and diffusion, thus providing insight into the generation of stationary and oscillatory patterns. The expected asymptotic behavior is confirmed by numerical simulations. The observed patterns include inverse labyrinth oscillations, inverse hexagonal oscillations, dot hexagons and parallel lines.

Keywords: Nonlinear reaction rate; Brusselator model; Coupled system; Turing patterns; Hopf bifurcation

1. Introduction

Models involving termolecular reaction steps exhibit interesting properties and pose challenging mathematical problems regarding the asymptotic behavior of the solutions. It is well-known that models of reaction sequences with two intermediates and only uni- and bimolecular steps do not admit limit cycles [3, Section 7.1]. Therefore, for instability to occur in the thermodynamic branch (the solution in equilibrium) one needs to use cubic reaction rates [1,9,3].

The following reaction sequence was studied by Prigogine and Lefever in 1968 [5]:

$$\mathrm{A} \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} \mathrm{U}$$

$$\mathrm{B} + \mathrm{U} \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} \mathrm{V} + \mathrm{D}$$

$$2\,\mathrm{U} + \mathrm{V} \underset{k_{-3}}{\overset{k_3}{\rightleftharpoons}} 3\,\mathrm{U}$$

$$\mathrm{U} \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} \mathrm{E}\cdot$$

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We note that the third step in the sequence involves a cubic nonlinear reaction term. Under the assumptions that

(i) D and E are removed from the reaction domain the instant they are produced (or equivalently, $k_{-2} = k_{-4} = 0$),
(ii) the nonlinear reaction is irreversible ($k_{-3} = 0$),
(iii) A is in sufficient abundance,

the dynamics of the reaction sequence is represented in [5] by two rate equations:

$$\frac{\partial U}{\partial \hat{t}} = k_1 A - (k_2 B + k_4)U + k_3 U^2 V + \hat{D}_u \nabla^2 U$$
$$\frac{\partial V}{\partial \hat{t}} = k_2 BU - k_3 U^2 V + \hat{D}_v \nabla^2 V. \tag{1}$$

By scaling of the variables,

$$t = k_4 \hat{t} \qquad u = \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} U \qquad v = \left(\frac{k_3}{k_4}\right)^{\frac{1}{2}} V$$
$$a = \left(\frac{k_1^2 k_3}{k_4^3}\right)^{\frac{1}{2}} A \qquad b = \frac{k_2}{k_4} B \qquad D_i = \frac{\hat{D}_i}{k_4} \tag{2}$$

the model (1) is simplified to the following model involving only two parameters.

$$\frac{\partial u}{\partial t} = a - (b+1)u + u^2 v + D_u \nabla^2 u$$
$$\frac{\partial v}{\partial t} = bu - u^2 v + D_v \nabla^2 v. \tag{3}$$

The system (3) of reaction diffusion partial differential equations is known as the trimolecular model or the Brusselator model, the latter term coined by Tyson in 1973 [8]. This model has been widely used to illustrate and study basic features of chemical reaction models involving trimolecular steps. In some sense it plays in the settings of these models a pivotal role similar to the role the harmonic oscillator and the Heisenberg model play in ferromagnetism [3].

This paper presents a numerical investigation into the pattern formation mechanism in the Brusselator model. The next section (Section 2) is devoted to studying the interplay between the two bifurcations in the model, namely the Hopf bifurcation and the Turing bifurcation. This investigation is largely motivated by the observations in [12] that Turing patterns eventually (for sufficiently small ratio of the diffusion coefficients) dominate the Hopf bifurcation induced oscillations. The numerical simulations yield a hyperbola-like shaped boundary between the two regions. Oscillatory patterns are observed only in a small area near the horizontal part of curve. Based on these results, Section 3 deals with pattern formation in a coupled Brusselator model, that is, two systems of the form (3) linked via linear interaction terms. The study of the dynamics of this model in terms of wavelength and diffusion provides insight into generation of stationary and oscillatory patterns. The expected asymptotic behavior is confirmed by numerical simulations. The observed patterns include inverse labyrinth oscillations, inverse hexagonal oscillations, dot hexagons and parallel lines. In Section 4 we provide some concluding remarks and directions for future work. For completeness of the exposition, details on the numerical method used for the simulations are presented in Appendix.

2. Turing and Hopf bifurcations in the Brusselator model

The system (3) has one spatially homogeneous steady state, $u^* = a$, $v^* = \frac{b}{a}$. Its stability is influenced by two factors: the appearance of spatially homogeneous limit cycle (Hopf bifurcation) and the ratio of the diffusion coefficients (Turing instability). We recall them briefly.

The spatially homogeneous solutions of (3) satisfy the system of ODEs

$$\frac{du}{dt} = a - (b+1)u + u^2 v,$$
$$\frac{dv}{dt} = bu - u^2 v. \tag{4}$$