Transition from Self-Replicating Behavior to Stationary Patterns Induced by Concentration-Dependent Diffusivities

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In this Letter, we report the observation of a transition from self-replicating behavior to stationary spatial structures induced by concentration-dependent diffusivities in the excitable Gray-Scott medium. Notably, the transition occurs even though there is no change in the relative diffusivities between the activator and the inhibitor. In contrast to the well-known Turing patterns, the obtained time-independent spatial structure has no intrinsic wavelength and the asymptotic state depends exclusively on the initial perturbations. This study illustrates that variable diffusivities can also have profound effects on pattern formation and selection in excitable media.

Pattern formation in inhomogeneous reaction-diffusion media has attracted increasing attention in the past decade [1–13]. In the majority of these studies, the inhomogeneity appears in the kinetic terms rather than the transport coefficients [1–8]. For instance, the ruthenium catalyzed Belousov-Zhabotinsky (BZ) reaction has been modulated by projecting an illumination pattern of varying intensity onto the reaction medium, where light stimulates the production of bromide, an inhibitor of the BZ reaction [1,2]. A variety of phenomena that are not found in homogeneous media are obtained in systems subjected to spatiotemporal modulation of the kinetics [1–8]. In nature, the inhomogeneity may also arise from the gel or porous medium in which the studies of pattern formation are often performed, i.e., in the transport processes [14,15].

In this Letter, we investigate the impact of concentration-dependent diffusion processes on pattern formation. The local diffusion coefficients are assumed to have functional relationships with the local concentration of a chemical reactant. The inclusion of concentration-dependent diffusivities has been found to be essential to the modeling of ionic reaction-diffusion systems, among other physical, chemical, and biological systems [9–13]. In living cells, the metabolites frequently modulate the function of transporters. Density-dependent migration and its effect on spatial segregation in population models has also been the subject of intensive study [11–13]. The present study shows that concentration-dependent diffusivities can induce a transition from self-replicating behavior to stationary patterns, even though there is no change in the relative diffusivity between the activator and the inhibitor. These results thus suggest that transport gradients in excitable media can also be used to manipulate pattern formation and selection.

This study is carried out with a two-variable Gray-Scott model [16,17] in one spatial dimension. In dimensionless form the equations are

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D_u\frac{\partial u}{\partial x}\right) + \frac{(1-u)}{\tau} - uv^2, \quad (1)$$

$$\frac{\partial v}{\partial t} = \frac{\partial}{\partial x}\left(D_v\frac{\partial v}{\partial x}\right) - \frac{v}{\tau} + uv^2 - \alpha v, \quad (2)$$

where u and v are the dimensionless concentrations of the reactant and the autocatalyst, respectively; α and τ are parameters related to the residence time and autocatalyst decay rate. D_u and D_v are the diffusion coefficients of the reactant and the autocatalyst, respectively. The diffusion coefficients are assumed to depend linearly on the concentration v: $D_u(x) = D_u^0(1 + k_u v(x))$ and $D_v(x) = D_v^0(1 + k_v v(x))$, where k_v and k_u are the coefficients regulating the relationships between the diffusivity and the local concentration $v(x)$ [18]. Earlier studies have shown that the relative diffusivity D_u/D_v is an important parameter in controlling pattern formation [19–26]. To exclude the influence of changing this ratio, we focus here on the situation $k_v = k_u$ such that there is no variation in the value of D_u/D_v when v changes.

The parameter values used throughout this study are $\alpha = 0.07$, $\tau = 20$. At the above dynamical condition, the system has one trivial steady state solution $u = 1$ and $v = 0$, which is linearly stable and globally attracting. Small perturbations decay exponentially but larger perturbations result in a long excursion in the phase space before returning to the steady state. Figure 1a presents a space-time plot of solutions to the classical model in which the diffusion coefficients are constant, i.e., $k_u = k_v = 0$ so that D_u and D_v are independent of the concentration of v. Gray levels represent the concentration of v, with white corresponding to maximum and black to minimum. An initial perturbation on v with spatial size of 20 grid points is applied to the center of the medium. The initial perturbation initiates two traveling waves, one traveling to the left and one to the right, which split repeatedly (replicate) until the medium is filled with pulses [27–31]. Then, the pattern becomes time independent. The final pattern is largely independent of the initial conditions. For instance, if we change the width of the initial perturbation, the replication sequence is slightly modified but the final pattern still displays eight stable pulses because these
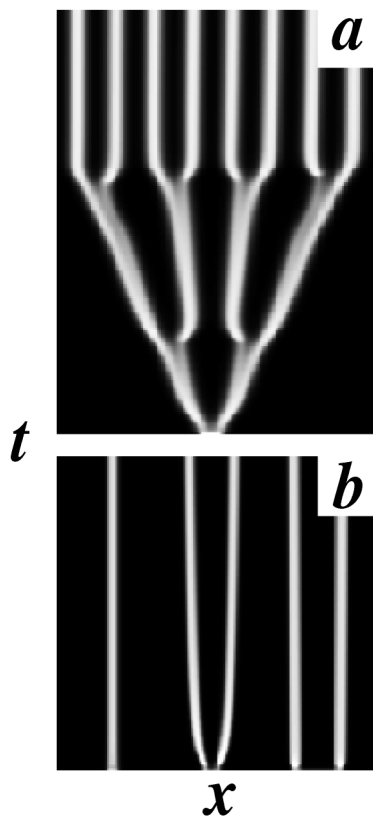
FIG. 1.   (a) Space-time plot of a one-dimensional medium with a local perturbation of size 20 grid points applied to the middle of the system. The (constant) diffusion coefficients are $D_u^0 = 2 \times 10^{-5}$ and $D_v^0 = 3.3 \times 10^{-6}$. Other parameter values are given in the text. Gray levels represent the concentration of v, with white corresponding to maximum and black to minimum. Regardless of the initial conditions, the pulses replicate until they fill the medium with a characteristic wavelength (pulse-to-pulse distance). (b) Space-time plot showing the formation of time-independent spatial structures induced by concentration-dependent diffusivities. All parameters are as in panel (a) except $k_u = k_v = 0.4$. The medium was perturbed by three initial perturbations with different spatial sizes: 8 grid points (left), 20 grid points (middle), and 70 grid points (right). While there is a minimum separation between pulses, there is no replication leading to a pattern of fixed wavelength. In both sets of simulations, the unit grid length is 0.002 dimensionless units. The spatial extents of the simulations are, respectively, 300 grid points in panel (a) and 600 grid points in (b). Nonflux boundaries and the first-order Euler method were employed in these calculations. Qualitatively, the same results were obtained when smaller unit grid lengths and integration step sizes were used.

patterns, similar to many others studied recently, have an intrinsic chemical wavelength [19–25]. However, the stable pulses do not emerge from the amplification of small inhomogeneities near a linearly unstable homogeneous steady state as in a Turing bifurcation. Indeed, the medium is excitable and the initial perturbations required to create these patterns are localized, above threshold perturbations from the stable state.

Calculation results with the concentration-dependent diffusivities are presented in Fig. 1b, in which three initial perturbations on v with different spatial sizes (8,

20, and 40 grid points, respectively) were applied to the medium. Instead of traveling waves that split, the stable solutions here are time-independent pulses. The perturbation with the smallest spatial size remains static at its initial location and there is no replication at all. The perturbation of moderate spatial size (the middle one in Fig. 1b) first breaks into two pulses which repel each other to propagate outward. When the space between the two pulses is large enough, they become time independent. Further increase of the spatial size of the perturbation shows similar behavior in that two pulses are formed from the ends of the perturbation. However, the pulses do not propagate in space, given that their initial distance is large enough. Unlike the pattern shown in Fig. 1a, here the space between pulses (the "wavelength") depends strongly on the initial perturbations, suggesting that the stable pattern obtained here has no intrinsic wavelength. This is an essential difference from the Turing and other recently reported stable patterns [19–25].

The existence of single-pulse and single-spot solutions in excitable Gray-Scott media has been studied recently by several groups [32–34]. Doelman and co-workers reported that, by varying the kinetics and chemical transport, the excitable Gray-Scott medium might undergo a transition from self-replicating behavior to the globally uniform stable state ($u = 1$, $v = 0$). Near the transition there exists a narrow parameter window for existence of single-pulse solutions. Results shown in Fig. 1b illustrate that variable transportation properties in the excitable medium can also cause a bifurcation from self-replicating to stable patterns. More significantly, the transition occurs even at constant D_u/D_v, whereas in classical models of pattern formation this ratio is critical to the eventual behavior of the system.

In Fig. 2 the threshold value of k_u (or k_v) for inducing a transition from self-replicating to stable pulses is characterized with respect to the ratio D_u/D_v at different values of the kinetic parameter α. Stable pulses are achieved in the region above each curve, whereas self-replication behavior can be seen for parameter values below each curve. A saddle-node bifurcation occurs when $\alpha = 0.062$. The positive k_u implies that the local diffusion coefficients increase with v. As shown in the figure, with the same D_u/D_v ratio the threshold value of k_u (and k_v) increases when the dynamics of the system is close to the saddle-node bifurcation. Also, the increase of the threshold k_u is faster at smaller values of D_u/D_v and eventually approaches a constant value.

To qualitatively analyze the formation of these stable pulses, Fig. 3 presents the nullclines of the system in the (u, v) concentration space and the projection of the spatiotemporal profiles of the stable pulses shown in Fig. 1. As shown in this figure, the two nullclines have no intersection [35] and the system has only one trivial stable steady state. In general, the system will evolve to this globally attracting state after being perturbed away from it. Plots of the stable pulses in the concentration space appear as
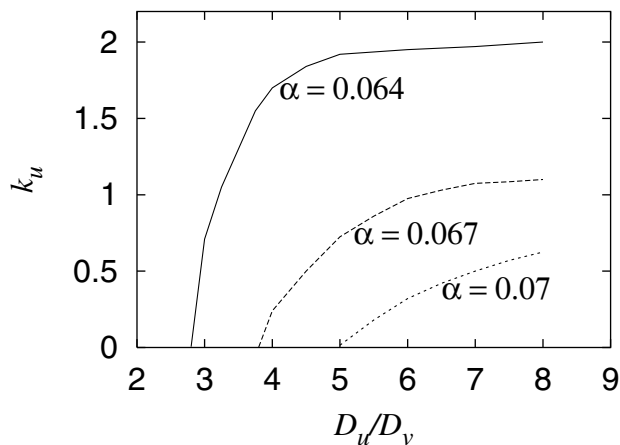
FIG. 2. Phase diagram showing the influence of D_u/D_v on the threshold values of $k_u = k_v$ for stable pattern formation at different values of α. Stable pulses exist for parameter values above the curve, whereas the self-replication phenomena can be achieved for values below these curves.

curves of bounded extent because of the roughly bell-shaped appearance of the pulses. The free ends of these curves represent the centers of the corresponding pulses. For the case $k_u = k_v = 0.4$ corresponding to Fig. 1b, all five stable pulses are plotted but only one curve can be distinguished here, indicating that the pulses are identical. However, the $k_u = k_v = 0$ pulses are not identical to each other. Stable pulses are eventually obtained in both cases due to a similar balance of kinetics and diffusion: The center of the pulse lies above the u and v nullclines. In this region, the chemical kinetics tend to increase v and to decrease u. However, the diffusion terms have the opposite effect: Since v is high in the middle, diffusion tends
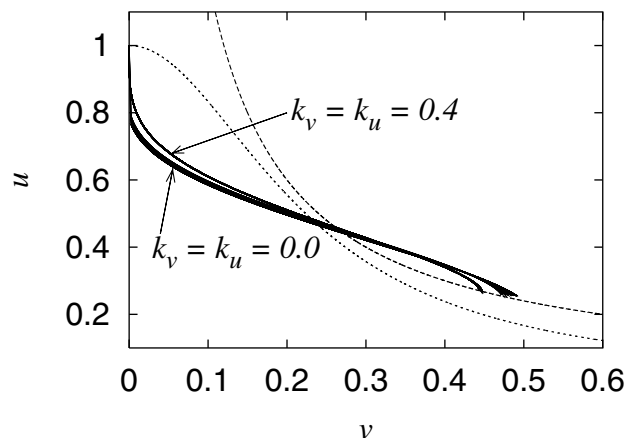

FIG. 3. Nullclines and projections of the stable pulses in the (u, v) phase space. The projections are represented by the solid lines. The dotted line is the nullcline $\frac{du}{dt} = 0$, the kinetics of u being negative above the curve and positive below. The $\frac{dv}{dt} = 0$ nullcline is the dashed line; the kinetic term for v is positive above the dashed line and negative below. There is no intersection between the two nullclines inside the positive quadrant [35].

to decrease its concentration while the low concentration of u in the middle of the pulse implies a net inward diffusion. The situation is reversed in the tail. A stable pulse results when diffusion and kinetics exactly balance each other in every region of the pulse. In the case with constant diffusion coefficients, a single pulse is not stable: It replicates due to the very high value of v which is reached in the middle of the pulse. This causes the concentration of the reactant u to drop to such an extent that the value of v in the center of the pulse collapses. It is only the interaction between several closely packed pulses which eventually stabilizes them, thus leading to a well-defined wavelength for the pattern. Conversely, in the case with concentration-dependent diffusivities, the removal of v by diffusion is specifically enhanced in the center of the pulse. (Compare the profiles of the pulses in Fig. 3.) The resultant stabilization of the center of the pulse allows it to reach a stable profile without interacting with other pulses.

In summary, the above results illustrate that inhomogeneous transport can play an important role in pattern formation, even when the relative diffusivity of the activator and inhibitor is constant. It has been well documented that the relative diffusivity in activator-inhibitor systems is crucial in inducing transitions in spatiotemporal dynamics [19–26]. The results presented here complement these earlier studies by showing that a self-organized gradient in diffusivity can also be a bifurcation control parameter in pattern formation and selection. In contrast to the well-studied Turing patterns, the stable pulses observed here have no intrinsic wavelength but do have a characteristic spatial extent, and above-threshold perturbations are required to initiate the pattern formation. Our analysis shows that the emergence of these stable pulses is due to a fine balance between the kinetics and transport terms.

The transition from self-replication to stable pulses induced by concentration-dependent diffusivities presents a new approach to achieving stable spatial structures lacking an intrinsic wavelength. This mechanism may play an important role in the development and the evolution of stable patterns in nature. The transport of chemicals through cells in biological systems, for instance, is known to be affected by the local concentrations of chemical species. Recently, Yoshida *et al.* also reported the volume change of a gel with respect to the variation of the local concentrations of chemicals [14]. We considered one, and perhaps the simplest, way in which the local diffusion process can depend on the concentration of chemical species. Nevertheless, the results clearly demonstrate the new features which can be expected to be observed in these pattern forming systems.

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