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Self-Segregation of Competitive Chaotic Populations

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The dynamical behavior of species competing for a common resource is studied with a reaction-diffusion system based on cubic autocatalysis. Randomly seeded populations self-segregate to form a complex network of domains separated by distinct interfaces. For chaotic populations in one-dimensional media, the interfaces exhibit irregular motions on long time scales. In two-dimensional media, the interface motions are governed by curvature-induced drift.

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Pattern formation in competitive environments has been the subject of numerous studies in chemistry, ecology, sociology, and genetics [1–5]. Nonclassical phenomena, such as spontaneous cluster formation, reactant segregation, and depletion-zone formation, have been investigated in diffusion-controlled chemical reactions [1]. Another class of systems, in which two populations compete for a common sustaining resource, has yielded the ecologically motivated and controversially discussed “competitive exclusion principle” [2], where two species with similar characteristics are unable to coexist. In this context, closed reaction-diffusion systems exhibit exclusive product selectivity when the species have different diffusivities or different rates of autocatalysis [4], or, in the case of open Lotka-Volterra kinetics (with equal diffusivities), segregation of steady-state populations [5].

In this Letter, we present a reaction-diffusion system with chaotic dynamics that exhibits complex interface patterns arising from self-segregation behavior. We study the evolution of coupled reactions, each governed by cubic autocatalysis [6], which compete for a common resource [7,8]. Self-segregating domains of uncorrelated chaotic populations, separated by interfaces that exhibit irregular motions on long time scales, spontaneously arise in one-dimensional configurations with random initial conditions. Localized interfaces are exhibited for steady state populations or for correlated chaotic populations arising from symmetric initial conditions. Curvature-induced interface drift governs the pattern evolution in two-dimensional configurations, which develops on a time scale much longer than that of the population dynamics and yields complex reorganizations at interface junctions in the case of three or more autocatalytic species.

Competitive spatiotemporal chaos.—We begin by examining the dynamics of two autocatalytic species, B and C , which compete for a common sustaining resource, A , and then decay to products, P and Q : $A + 2B \rightarrow 3B$, $B \rightarrow P$, $A + 2C \rightarrow 3C$, $C \rightarrow Q$. Dimensionless reaction-diffusion equations for this system in an open spatial reactor are derived following previous studies of the

two-variable Gray-Scott model [8,9], where a , b , and c represent the dimensionless concentrations:

$$\begin{aligned}\partial_t a &= \Delta a + 1 - a - \mu a(b^2 + c^2), \\ \partial_t b &= \delta_b \Delta b + b_0 - \Phi b + \mu a b^2, \\ \partial_t c &= \delta_c \Delta c + c_0 - \Phi c + \mu a c^2.\end{aligned}\quad (1)$$

Δ is the Laplacian operator, and Φ and μ are bifurcation parameters of the system, determined by the flow rate and concentrations of the species in the reservoir. Throughout this study, we assume equal diffusivities, $\delta_b = D_B/D_A = 1$ and $\delta_c = D_C/D_A = 1$, and equal growth rates for autocatalysis in B and C , in order to focus on behavior arising from competitive species with similar characteristics. For simplicity, we also assume that there is no supply of the autocatalysts from the reservoir, $b_0 = c_0 = 0$.

Within the parameter range of interest, where the dynamics of the single-autocatalyst system [$c \equiv 0$ in Eqs. (1)] exhibits chaotic behavior [8,9], the coupled system is characterized by the steady states $S^A = (1, 0, 0)$, $S_{\pm}^B = (a_{\pm}, h_{\pm}, 0)$, and $S_{\pm}^C = (a_{\pm}, 0, h_{\pm})$, where $a_{\pm} = (1 \pm \sqrt{1 - 4\Phi^2/\mu})/2$ and $h_{\pm} = \Phi/(\mu a_{\pm})$ correspond to the two unstable steady states $(a_{\pm}, h_{\pm})$ of the single autocatalyst system. $S_{\pm}^{B,C}$ exist for μ above the saddle node bifurcation, $\mu_{sn} = 4\Phi^2$. (Another pair of steady states, arising for $\mu > 8\Phi^2$, is not relevant to this study.) A stability analysis of the spatially homogeneous system shows that S^A is a stable node for all parameter values, $S_{+}^{B,C}$ are saddle points, and $S_{-}^{B,C}$ are unstable (saddle) foci that become stable for $\mu > \mu_H$ at the Hopf bifurcation point, $\mu_H = \Phi^4/(\Phi - 1)$. We note that the additional, third eigenvalue of Eqs. (1)—compared to the single autocatalyst system—is negative ($-\Phi$) for each steady state. The particular symmetry and stability of these states imply that the system is characterized by either an extinct state, S^A , or an exclusive state, $S_{\pm}^{B,C}$, where one competing species survives and the other becomes extinct. From the analysis of the bifurcation structure of the single-autocatalyst system presented in [9], it follows that a traveling wave solution with a positive velocity

exists only for μ above a critical value, $\mu_c \approx 33$ for $\Phi = 2.8$, which restricts the parameter space of interest to $[\mu_c, \mu_H]$ in our study.

Self-segregation in one-dimensional media.—The spatiotemporal evolution of Eqs. (1) is shown in Fig. 1. After a brief transient period, spatially localized domains develop from randomly distributed perturbations initiating autocatalysis in B and C . Species B is restricted to domains where species C is extinct, while species C exists only in domains where species B is extinct. The relative location of the interfaces between the domains is robust with respect to changes in the parameters, as long as traveling wave solutions exist and both autocatalytic species have the same growth rates and diffusivities. The particular location of the interfaces, however, is a consequence of the

FIG. 1. Spatiotemporal pattern of reactant concentration a (top), and autocatalyst concentrations b (middle) and c (bottom) of Eqs. (1) for $\delta_b = \delta_c = 1$, $\Phi = 2.8$, and $\mu = 33.15$. A concentration of 1 (0) is represented in white (black). The reactant A is initially distributed homogeneously, $a = 1$, over the entire domain. Species B and C are randomly seeded, indicated by the white ($b = 1$) and gray ($c = 1$) rectangles at the top of the figure, with the following constraints: the seeds are each 20 grid points, they are separated by a minimum of 60 grid points, and there is a total of 200 occupied grid points per species. An explicit Euler method, with a three-point approximation of the Laplacian operator and periodic boundary conditions, was used for the numerical integration ($\delta t = 0.0003$) of the one-dimensional array of length $L = 600$ (2400 grid points). Each panel consists of 5000 layers, with each layer plotted every $200\delta t$. Time increases from top to bottom in each panel.

initial perturbation distribution. The chaotic populations in each of the domains are uncorrelated except when symmetric initial conditions give rise to reflecting symmetries between domains. The local perturbations must exceed a concentration threshold to initiate autocatalysis, as well as cover a sufficiently large region. Once autocatalysis is initiated, the local trajectory approaches the extinct state, S^A . Such transient activity appears in the spatiotemporal pattern as triangular white zones below the initial seeds, where the reactant concentration $a = 1$. Waves propagating into the nonreaction zones give rise to domain interfaces when two different autocatalytic species collide. There is, however, a minimum domain size below which a species cannot survive, which depends on the particular parameter values. With these considerations, it is possible to predict the location of the segregation interfaces for different initial seed configurations (for example, as in Fig. 1).

Figure 2(a) shows representative concentration profiles of reactant A and autocatalysts B and C from Fig. 1. We see the transitions between domains as well as excursions away from the unstable focus $S_{-}^{B,C}$ within the domains. The domain interfaces are characterized by a high concentration of A and low concentrations of B and C as the wave fronts of each species intersect. While the exact profile at the interface depends on the system parameters and the behavior in adjacent domains, small fluctuations are typically observed around a state determined by continuity constraints of the neighboring steady states $S_{-}^{B,C}$ [Fig. 2(b)]. Within a domain, the dynamical behavior can range from regular to chaotic, depending on the domain size and configuration of the initial local perturbations. For example, limit cycle behavior is exhibited for a periodic distribution of the initial perturbations and a relatively small domain size (65 grid points and $\mu = 33.15$). In contrast, the behavior in Fig. 1, arising from random initial perturbations, yields the chaotic trajectory shown in Fig. 2(b), which displays frequent excursions from the unstable focus $S_{-}^{B,C}$ to approach the S^A state. This spatiotemporal chaos is much like that observed in the two-variable, single-autocatalyst system [8].

Even though the domain boundaries appear to be completely localized on the time scale of the local dynamics within a domain, Fig. 1, the long-time behavior reveals irregular motions of these interfaces, as shown in Fig. 3. These motions, which occur only for chaotic populations, are most pronounced when the system is close to the wave propagation threshold where large-scale pulse structures are exhibited, such as in Figs. 1 and 3. The interfaces are characterized by a state that moves closer to the S^A state as the parameter μ is decreased. Concentration fluctuations at the interface are larger for smaller μ and, consequently, injections of the trajectory to the neighborhood of the unstable focus are more likely. In contrast, steady-state behavior above the Hopf bifurcation point, $\mu > \mu_H$, is accompanied by interfaces that are completely localized (spatially stationary) with constant concentrations (a, b, c)

FIG. 2. (a) Representative concentration profile from Fig. 1 for reactant A (upper full line) and autocatalysts B (lower full line) and C (dotted line) taken at the final time step of Fig. 1. Horizontal lines show the concentrations a (upper), b , c (lower) at the unstable focus $S_{-}^{B,C}$. Domains with $B(C)$ activity are indicated by white (black) bars at top. (b) Characteristic phase portraits of the dynamics at a domain interface (full line localized near $a = 0.9$) and within a chaotic domain (dotted line) of Fig. 1.

for any random initial seeding. We also note that interface boundaries are always localized for symmetrical initial perturbations, even for chaotic populations, when the neighboring populations are dynamically in phase. Randomly seeded autocatalyst populations, on the other hand, yield domains of neighboring populations with out-of-phase oscillations that generate spatially asymmetric perturbations to the interface.

The qualitative features of the self-segregation and domain interfaces are not dependent on the boundary conditions or the numerical method, although quantitative differences appear for no-flux and periodic boundary conditions. Furthermore, the qualitative behavior is preserved when inputs of each autocatalyst are provided from outside reservoirs ($b_0 \neq 0, c_0 \neq 0$). In this case, however, a very low concentration of the “minor” species is present in the domains. Additional considerations arise for predicting the appearance of segregation interfaces if we abandon the requirement of nonoverlapping perturbations initiating autocatalysis. In this case, the autocatalytic species with the larger concentration survives at sites where overlapping perturbations have different concentrations. For equal initial concentrations, however, the reaction-diffusion waves of both species die out (even when $b + c < 1$). These results point to the existence of a planar separatrix in the phase space, defined by $b = c$, which partitions

the orthogonal manifolds of the competing autocatalysis subsystems. Trajectories starting on this separatrix move to the stable steady state S^A . When the autocatalytic species have different diffusivities ($D_B \neq D_C, D_i \leq D_A$), the interfaces become less irregular and domains with the faster diffusing autocatalyst shrink, with the interfacial motion dependent on the difference in the diffusivities. An increase of the parameter μ for the inferior species, however, can compensate for the disadvantage in the diffusivity. Finally, we note that a significant qualitative change in behavior occurs when the reaction kinetics in Eqs. (1) is modified from cubic to quadratic autocatalysis [4]. The self-segregation is replaced by a coexistence of the two species (when they are governed by the same kinetics and diffusivities) throughout the medium.

Self-segregation in two-dimensional media.—The competitive autocatalysis system can be readily generalized to two-dimensional media with two, three, or more species. As shown in Fig. 4, self-segregating populations are also found in two-dimensional media for the case of three competing autocatalytic species. The appearance of chaotic behavior and more ordered behavior in smaller domains, as well as the local concentration profiles at interfacial boundaries, are similar to those observed in the one-dimensional case, Fig. 2. A new feature appearing in two-dimensional media is the drift of domain boundaries such that convex curvature is reduced, following the curve-shortening mechanism discussed in [5,10]. For a closed interface, this yields the collapse of a convex domain. Approximately circular domains obey a paraboliclike decrease in radius with time for chaotic as well as steady-state ($\mu > \mu_H$) behavior. The interface drift occurs on a much slower time scale than that of the chaotic behavior within a domain.

Interface junctions, which occur with three or more competing species, as well as isolated interface loops and domains connected to the medium boundaries, can be seen in the segregation patterns shown in Fig. 4. The evolution shown in successive panels reveals curvature-induced shrinking and ultimate extinction of domains, giving rise to the local breakup and reorganization of interface junctions. Domains of the same species merge (sometimes only

FIG. 3. Long-term spatiotemporal dynamics of reactant concentration a for the dynamical system in Fig. 1. The panel consists of 2500 layers with each layer plotted every $2 \times 10^4 \delta t$. Other parameters are the same as in Fig. 1.

FIG. 4. Spatiotemporal evolution of concentration a when three autocatalytic species compete for the reactant. From upper left: $t = 41, 176, 239, 364, 655$, and 1154 . The white patches within the domains correspond to local reaction dynamics close to the extinct state S^A . Initial conditions: 20 seeds of each species (B, C, D) with a cell size of 20×20 grid points were randomly distributed on the array of $L \times L = 200 \times 200$ (800×800 grid points) with a uniform reactant concentration $a = 1$. A five-point approximation of the Laplacian operator, no-flux boundary conditions, and an integration time step of $\delta t = 0.0052$ were used. Other parameters are the same as in Fig. 1.

after a long and complex transient period) and small domains diminish in number during such reorganizations. At the same time, irregular interfaces tend to straighten and the angles at the interface junctions tend to equalize. The counterpart to the irregular interface motions for chaotic populations in one-dimensional media is not readily apparent in two-dimensional media, although slight motions in nearly linear interfaces are observed. For interfaces with significant curvature, however, interfacial drift dominates the behavior and the irregular interface motions are suppressed. Although the evolution of the interface reorganization varies with the parameter μ , the qualitative features of the asymptotic states are very similar. We note that a similar interface evolution has been found for competitive steady-state populations [5].

In summary, the n species of reaction-diffusion systems such as Eqs. (1) compete for a common sustaining resource and segregate into domains of uncorrelated, chaotic populations over a range of parameter values. Irregular motions of the interfaces occur due to the influence of out-of-phase oscillatory behavior of neighboring populations, while completely localized interfaces are ob-

served for adjacent steady-state populations or in-phase oscillatory populations arising from symmetrical initial perturbations. In two-dimensional media, curvature-induced interface drift gives rise to shrinking and, ultimately, extinction of domains as well as domain reorganizations arising from the breakup of interface junctions.

The self-segregation behavior found in this study is relevant to systems composed of species with similar characteristics, and we have focused on the case of identical diffusivities and growth rates of autocatalysis. Examples of such systems include competing populations in biological ecologies as well as isomers or isotopically labeled species in competing chemical reactions. As the diffusivities and rate constants are allowed to differ, the self-segregation behavior is retained only transiently, with the lifetime of the transient dependent on the similarity of the competing species.

Ever more complicated self-segregation behavior, with topological features determined by domain interface motions and the stability of interface junctions, should be found in the generalization of Eqs. (1) to $n > 3$ chaotic populations.

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- [1] S. Havlin, M. Araujo, H. Larralde, H.E. Stanley, and P. Trunfio, *Physica* (Amsterdam) **191A**, 143 (1992); A. Yen and R. Kopelman, *Phys. Rev. E* **56**, 3694 (1997); R. Reigada, F. Sagués, I.M. Sokolov, J.M. Sancho, and A. Blumen, *J. Chem. Phys.* **107**, 843 (1997).
- [2] G. Hardin, *Science* **131**, 1292 (1961).
- [3] J. Huisman and F.J. Weissing, *Nature* (London) **402**, 407 (1999).
- [4] J.H. Merkin, A.J. Poole, S.K. Scott, J. Masere, and K. Showalter, *J. Chem. Soc. Faraday Trans.* **94**, 53 (1998).
- [5] S.-I. Ei, R. Ikota, and M. Mimura (to be published).
- [6] P. Gray and S.K. Scott, *Chem. Eng. Sci.* **39**, 1087 (1984).
- [7] J.E. Pearson, *Science* **261**, 189 (1993); K.J. Lee, W.D. McCormick, J.E. Pearson, and H.L. Swinney, *Nature* (London) **369**, 215 (1994).
- [8] J.H. Merkin, V. Petrov, S.K. Scott, and K. Showalter, *Phys. Rev. Lett.* **76**, 546 (1996); *J. Chem. Soc. Faraday Trans.* **92**, 2911 (1996).
- [9] J.H. Merkin and M.A. Sadiq, *IMA J. Appl. Math.* **57**, 273 (1996).
- [10] M. Gage and R.S. Hamilton, *J. Differ. Geom.* **23**, 69 (1986).