Arm splitting and backfiring of spiral waves in media displaying local mixed-mode oscillations

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Spiral waves are ubiquitous in nonlinear science, appearing in a wide range of biological, chemical, and physical systems. In many systems, simple spirals evolve into more complex structures, and several scenarios have been identified by which this process can take place. Often, formation of complex spiral structures leads to spiral breakup and spiral turbulence. Again, generic scenarios by which this behavior emerges have been studied. In this paper, we identify through the numerical investigation of a model of two coupled allosteric enzymes a novel mechanism, characterized by the splitting of spiral arms, that produces complex spiral waves, which can subsequently evolve into spiral turbulence via a distinctive breakup process involving collision of waves with backfired segments expelled by their neighbors.

I. INTRODUCTION

Spiral waves are perhaps the most common dissipative structures1–5 and have been observed in diverse systems such as galaxies,6 populations of a unicellular slime mold,7 premixed flames,8 the Belousov–Zhabotinsky chemical reaction,9 intracellular Ca2+ release from Xenopus laevis oocytes,10 and chicken retina.11 Because of their ubiquity in nature and significance in human health,12 spiral waves have attracted attention from both experimental and theoretical researchers seeking generic principles that govern the various spiral-generating systems. Earlier studies focused mainly on simple spiral waves, but these shed little light on the more complex structures in natural spiral patterns such as galaxies, typhoons, seashells, and lichens. Recently, attention has shifted to investigations of complex spiral waves, and four classes of mechanisms responsible for their generation have been identified: (1) tip meandering, which induces the formation of superspiral structures;13 (2) period-doubling bifurcation of the local dynamics, which leads to the formation of line defects on the period-2n spiral waves;14,15 (3) transverse wave instability, which results in the formation of rippling spiral arms16 or segmentation of spiral segments in the presence of a fast-diffusing inhibitor;17 (4) interaction of two steady states, one excitable and the other pseudo-Turing unstable, which also induces the formation of segmented spiral waves.18

The formation of complex spiral structures usually portends the onset of spiral turbulence, which occurs via spiral breakup. To date, two principal mechanisms for the breakup of spirals have been described: (1) approach of two neighboring spiral fronts until the local wavelength is below the critical value allowed by the dispersion relation;19–21 (2) transverse instability of line defects in period-2 spiral waves.22

In this paper, using a three-variable reaction-diffusion (RD) model, we elucidate a new mechanism that generates complex spiral waves, which can evolve to spiral turbulence via a distinctive breakup process, in which waves break on collision with backfiring wave segments of nearby waves.

II. MODEL

The Decroly–Goldbeter model is based on a homogeneous model23 of two coupled allosteric enzymes, which was developed to investigate systems in which two instability-generating mechanisms are coupled. In the original system, the instabilities arise from the positive feedback of reaction products on the two enzymes phosphofructokinase and adenylyl cyclase.24

The RD version of the model has been applied to the study of spiral waves with superimposed target waves.25 The model equations are
\[
\frac{d\alpha}{dt} = (uK_{m1}) - \sigma_1 \Phi + D\nabla^2 \alpha,
\]
\[
\frac{d\beta}{dt} = q_1\sigma_1 \Phi - \sigma_2 \eta + D\nabla^2 \beta,
\]
\[
\frac{d\gamma}{dt} = q_2\sigma_2 \eta - k_r \gamma + D\nabla^2 \gamma,
\]
with
\[
\Phi = \alpha(1 + \alpha)(1 + \beta)^2/[L_1 + (1 + \alpha)^2(1 + \beta)^2]
\]
and
\[
\eta = \beta(1 + d\beta)(1 + \gamma)^2/[L_2 + (1 + d\beta)^2(1 + \gamma)^2],
\]
where the variables \(\alpha\), \(\beta\), and \(\gamma\) represent three biochemical species. The parameters \(u\), \(K_{m1}\), \(\sigma_1\), \(\sigma_2\), \(q_1\), \(q_2\), \(L_1\), \(L_2\), \(d\), and \(k_r\) are determined by the reaction conditions. Detailed discussions of the model can be found in Ref. 23. We set the diffusion coefficients of all three species, denoted by \(D\), equal to \(1.0 \times 10^{-6}\) cm\(^2\) s\(^{-1}\) in this study.

The simulations were carried out with the Euler integration method using a spatial grid \(dx=dy=0.002\) cm and an integration time step \(dt=0.02\) s. With smaller spatial grids and time steps, the results were essentially unchanged. As in earlier studies, \(^23\) we took \(k_r\) as the control parameter and fixed the other parameters. Zero-flux boundary conditions were used.

III. RESULTS

The model supports simple spiral waves [see Figs. 1(a) and 1(b)] over a wide range of parameters. When we decrease \(k_r\) from 1.0 to 0.84 s\(^{-1}\) as shown in Figs. 1(d) and 1(e), the uniform arm [Fig. 1(b)] spawns a second, adjacent arm [Figs. 1(e)]. In Figs. 1(c) and 1(f) we plot the oscillation maxima of the species \(\beta\) against the distance \(r\) from the spiral core \((r=0)\) at \(k_r=1.0\) and 0.84 s\(^{-1}\), respectively. We define the symbol \(M^N\) to represent an oscillation with \(M\) large and \(N\) small peaks per cycle. We see that the local dynamics in the radial direction consists of (simple) \(1^0\) oscillations at \(k_r=1.0\) s\(^{-1}\), but for \(k_r=0.84\) s\(^{-1}\), beyond \(r=66.26\) the local dynamics bifurcates to \(1^1\) oscillations. This transformation of the local behavior coincides with the minimum distance at which splitting of a spiral arm takes place.

If we continue to decrease the control parameter \(k_r\), the spiral arms begin to split beyond a critical distance from the spiral core [Figs. 2(a) and 2(b)]. The split waves rejoin a small distance away from the splitting point, producing a nodal structure within the spiral arm, and a new split can occur near the new node [see Fig. 2(b)], where we use the term node to refer to a point at which an arm begins to divide. Accompanying the formation of the nodal structure within the spiral arm is a series of bifurcations of the local dynamics as we move out from the spiral core. As shown in Fig. 2(c), the local dynamics transforms from \(1^0\) to \(1^1\) oscillations at \(r=15\) and then to a regime of \(1^2\) [Fig. 2(d)] and \(1^3\) [Fig. 2(e)] mixed-mode oscillations at \(r=142\). The spatial bifurcation points where the local dynamics bifurcates from \(1^5\) to \(1^{5+1}\) mixed-mode oscillations move inward as \(k_r\) is lowered.

At \(k_r=0.6\) s\(^{-1}\), the nodal structure some distance away from the spiral core loses stability and becomes more irregular [see Figs. 3(a) and 3(b)]. As this complex spatial structure emerges with decreasing \(k_r\), the bifurcation radii continue to move inward, so that at \(k_r=0.6\) s\(^{-1}\), \(1^0\) oscillations transform to \(1^1\) at \(r=10\), and the regime of \(1^1\) oscillations gives way to \(1^2\), \(1^3\), and newly emerging \(1^4\) oscillations at \(r=77\) [Fig. 3(c)]. Figures 3(d) and 3(e), respectively, show \(1^4\) and \(1^5\) mixed-mode oscillations at two representative spatial points.

When \(k_r\) reaches 0.57 s\(^{-1}\), the irregular nodes dominate the entire spiral wave, except very near the spiral core [Fig. 4(a)], and the radial dynamics [see Fig. 4(b)] displays not only periodic \(1^N\) mixed-mode oscillations [see Fig. 4(c), showing \(1^3\) oscillations], as found at higher \(k_r\), but more complex mixed-mode oscillations [Figs. 4(d)–4(f)] as well.

At \(k_r=0.56\) s\(^{-1}\), the spiral wave begins to break up, as shown in Fig. 5(a). The breakup first occurs near the spiral core, resulting in a central small spiral fragment surrounded...
by a much larger spiral fragment. Later, the large fragment starts to split at the lower left corner of the medium. Further decreases in the control parameter cause the central and surrounding spiral fragments to rupture into still more fragments [Figs. 5(b)–5(d)]. The central spiral fragment disappears when $k_s$ is decreased to 0.5 s$^{-1}$, as shown in Fig. 5(c).

As long as $k_s > 0.5$ s$^{-1}$, each spiral fragment retains the arm splitting and nodal structures of the spiral arms [see Figs. 5(a) and 5(b)] as well as a sense of rotation, and the medium still supports local 1$^0$, 1$^1$, and more complex mixed-mode oscillations in different regions. At $k_s = 0.50$ s$^{-1}$, the density of nodes significantly increases, and each spiral fragment contains multiple nodes [Fig. 5(c)]. Although the spiral waves have dissociated in Figs. 5(a)–5(c), the fragments maintain their integrity, and the patterns are not yet turbulent. At still lower $k_s$, e.g., 0.46 s$^{-1}$ as in Fig. 5(d), the pattern is dominated by continuously generated and annihilated fragments and evolves into turbulence, while the local dynamics becomes aperiodic.

A detailed view of the onset of spiral breakup is shown in Fig. 6, which shows the evolution of the system when $k_s$ is switched from 0.57 to 0.56 s$^{-1}$. After $k_s$ is decreased, a section near the spiral core soon becomes quite complex [Fig. 6(a)], and 40 s later three wave segments are backfired from this section of the wave [white arrows in Fig. 6(b)]. These segments propagate inward and collide with the neighboring outwardly propagating wave, as shown in Figs. 6(c) and 6(d), causing the wave to rupture at the collision sites. The spiral fragments formed due to these breaks propagate outward and continue rotating, growing, and colliding, as shown in Fig. 6(e), where a new backfired wave segment, indicated by the white arrow, can be observed. This segment collides with the central spiral fragment to create a crack, from which the spiral arm recovers without rupturing [see Fig. 6(f)].
Note that the wave segments indicated by white arrows in Fig. 6(f) are generated by collision of spiral fragments rather than by backfiring, which cannot increase the number of spiral fragments [see Fig. 6(g)]. About 800 s later, a new wave segment [indicated by the white arrow in Fig. 6(h)] is backfired from an arm near the lower left corner of the medium and leads to the wave fracture seen in Fig. 6(i). Figure 6(j) presents a time series $\beta(t)$ at the point marked by the white square in Fig. 6(f). We note a long quiescent period, denoted by the black arrow, which results from the annihilation of the wave in that region by a large backfired wave segment.

![FIG. 4. (Color) Spiral waves at $k_s=0.57$ s$^{-1}$. (a) Snapshot of the spatial distribution of $\beta$. (b) Plot of the oscillation maxima of $\beta$ vs $r$. (c)–(f) Time series at points with $r=96$, 176, 296, and 446, respectively. Other parameters are as in Fig. 1.](image1)

![FIG. 5. (Color) Snapshots of the spatial distribution of $\beta$. $k_s=$ (a) 0.56 s$^{-1}$, (b) 0.54 s$^{-1}$, (c) 0.5 s$^{-1}$, and (d) 0.46 s$^{-1}$. Other parameters are as in Fig. 1.](image2)

### IV. DISCUSSION

Our investigation of the mixed-mode spiral waves has been performed in a parameter region that supports only simple $1^0$ oscillations in the homogeneous system. At all parameters where a definable core exists, the trajectory of the spiral tip is a small regular circle. How then does the instability of the simple spiral waves occur? To answer this question, we studied a one-dimensional (1D) analog of the spiral waves: a 1D system with Dirichlet boundary conditions at one end and the usual zero-flux boundary conditions at the opposite end. The values of the variables at the fixed Dirichlet source were set at the unstable steady state, corresponding to the values in the spiral tip. This “1D spiral” approximates the radial dynamics of the two-dimensional (2D) spiral waves. Figure 7 shows the variation of the maxima of the $\beta$ oscillations as a function of $k_s$ at spatial point 301 in the 1D spiral. As $k_s$ decreases, the temporal dynamics at this point undergoes a series of bifurcations: the oscillations transform from $1^0$ to $1^1$, $1^2$, $1^3$, and more complex mixed-mode oscillations, mirroring the evolution of the temporal dynamics in the 2D spiral waves. Hence we conclude that the formation of spiral waves with mixed-mode local dynamics is due to the bifurcations of the radial dynamics of the simple spiral waves. Quantitative differences in the values of the bifurcation parameters and, more importantly, the generation of complex spatial behavior, result from 2D, notably curvature, effects.

We have described here a new scenario of spiral breakup, which proceeds from spiral arm splitting, nodes, adjunct arms, and backfiring through turbulence. Although the full scenario has not yet been clearly demonstrated experimentally, some reported experiments and simulations
show indications of the phenomena described here. Spiral waves with adjunct arms have been observed in aggregating populations of the amoeba Dictyostelium discoideum and in simulations of a FitzHugh–Nagumo model, but the further evolution of these structures has not been described. Spontaneous backfiring of traveling waves has been seen in a numerical simulation of an excitable Bär–Eiswirth model, and in another two-variable model with three fixed points in the mixed-mode oscillations that give rise to arm splitting, nodes, and even backfiring breakup of a spiral. In the Decroly–Goldbeter RD model, the mixed-mode oscillations result from a homoclinic connection via collision of a saddle point and a limit cycle to form the spiral-type attractor. The local mixed-mode dynamics is critical in determining the fine structure of the spiral arm. It is well known that the properties of the spiral tip, which is the source (or in less common antispirlars, the sink) of the spiral wave plays a key role in the spiral dynamics. In most models studied to date, the tip of the spiral is an unstable focus, but here the spiral tip is a saddle point, which may be the underlying cause of the bifurcations found in the radial dynamics.

Studies of complex chemical oscillations in homogeneous systems have revealed several bifurcation scenarios starting from simple oscillations: quasiperiodicity, period doubling, and mixed-mode oscillations, all of which can ultimately lose stability and give way to chaos as a control parameter is varied. Bifurcations of spiral dynamics in RD systems are found to mirror the behavior of the corresponding homogeneous systems: simple spiral waves with simple local dynamics can evolve to complex spiral waves with quasiperiodic local dynamics and then to spiral turbulence or can proceed via period-doubling local dynamics to complex spiral waves and then to spiral turbulence. Here we have studied a new route from simple to complex spiral waves containing such features as adjunct arms and nodes via bifurcation of the local dynamics into mixed-mode oscillations and then to spiral breakup through arm splitting and backfiring. The radial distance from the spiral core and the model parameters decide the complexity of the local oscillations.

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All positions $r$ and distances are measured in grid points, which are separated by 0.002 cm, with $r=0$ located at the center of the spiral core.