Breaking of translational symmetry of a traveling planar impulse in a two-dimensional two-variable reaction-diffusion model

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The stability of a planar impulse in rectangular spatial domains for a two-variable excitable reaction-diffusion system is numerically studied. The dependence of the stability on the size of the domain perpendicular to the direction of the propagation of the impulse is shown. The instability results in asymptotic stable curved impulses or an asymptotic spatiotemporal structure, which is generated similarly to the one-dimensional backfiring phenomenon.

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I. INTRODUCTION

Each solution to a one-dimensional (1D) reaction-diffusion system is also the solution to a two-dimensional (2D) system, if initial conditions depend only on one coordinate. However, the stability of the solution to the 1D reaction-diffusion system does not imply the stability of this solution in the 2D system. In one- and two-variable reaction-diffusion systems with one stable and one unstable stationary state, 1D (planar or circular) traveling fronts connecting these states are unstable if the diffusion coefficient for the reactant is greater than that for the autocatalyst [1–3]. Instabilities of such fronts have been observed in experiments with iodate—arsenous acid [4] and chlorite-tetrathionate [5] systems, performed in the conditions for which the autocatalysts (iodide and hydrogen ions, respectively) are immobilized. If the autocatalysts are not immobilized, the planar fronts are stable [4,5].

Unlike traveling fronts, which can exist in one variable as well as in multivariable systems, traveling impulses can appear in at least two-variable reaction-diffusion systems because the necessary condition of their existence is the excitability. Planar traveling impulses in two-variable excitable activator-inhibitor systems are stable if the diffusion coefficients for the activator and the inhibitor are equal or close to each other. However, if the diffusion coefficient of the inhibitor is sufficiently greater than the diffusion coefficient of the activator, then the planar or circular impulses in two-variable systems may be unstable. The instability of the planar and the circular impulses in 2D systems has been reported by numerical calculations in a model of an excitable thermochemical system [6].

In the present paper, the stability of the planar impulse in a 2D two-variable excitable activator-inhibitor model is considered in detail. The asymptotic solution for this model has the form of a traveling impulse and is stable in the 1D system for appropriate values of the parameters. We show that the stability of the planar traveling impulse depends on the size of the space domain perpendicular to the direction of propagation of the impulse for the diffusion coefficient of the inhibitor greater than the diffusion coefficient of the activator. For narrow space domains, the planar impulse is stable; but if the size of the domain becomes greater than some critical value, the planar impulse becomes unstable. Other asymptotic solutions appear in the 2D system. We show that two types of stable asymptotic solutions may coexist in semi-infinite systems for the same vertical system size. One of them is a single curved traveling impulse and the other is an infinite series of curved traveling impulses that leaves behind a stationary periodical structure. In the next section, we present a model of the reaction-diffusion system. The main results are presented in the subsequent section, and the conclusions are presented in the last section.

II. MODEL

The model describes an open chemical system, in which two catalytic (enzymatic) reactions occur.

$$S_0 \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} S, \tag{1}$$

$$S + E \underset{k_{-2}}{\overset{k_2}{\rightleftharpoons}} SE, \tag{2}$$

$$SE \overset{k_3}{\rightarrow} P + E, \tag{3}$$

$$S + SE \underset{k_{-4}}{\overset{k_4}{\rightleftharpoons}} S_2E, \tag{4}$$

$$P + E \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} EP, \tag{5}$$

$$P + SE \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} SEP, \tag{6}$$

$$P + S_2E \underset{k_{-5}}{\overset{k_5}{\rightleftharpoons}} S_2EP, \tag{7}$$

$$P + E' \underset{k_{-6}}{\overset{k_6}{\rightleftharpoons}} PE', \tag{8}$$

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$$PE' \xrightarrow{k_7} R + E', \tag{9}$$

$$P \xrightarrow{k_8} Q. \tag{10}$$

An excess of the reactant S (activator) inhibits its transformation to the product P (inhibitor). The inhibitor reversibly reacts with the free catalyst (enzyme) E, as well as with its complexes SE and S_2E, which causes the inhibition of the transformation of the reactant to the product. We assume that this inhibition has an allosteric character that allows us to assume that the rate constants for Reactions (5)–(7) are identical. These Reactions describe the influence of the product on the rate of its formation. The other catalytic (enzymatic) reactions (8) and (9) occur in its saturation regime and therefore, its rate is assumed to be constant. The system is open due to Reaction (1), in which S_0 plays the role of the reservoir variable for the reactant S, and Reaction (10), in which the product P is irreversibly transformed to inactive reagent Q. It is noteworthy that the chemical scheme consists only of elementary, mono-molecular, and bimolecular chemical reactions (excluding autocatalysis).

We assume that the total concentrations of catalysts (enzymes) E and E' are much smaller than the concentrations of the reactant S and the product P. On the basis of the Tikhonov theorem [7], the concentrations of both catalysts (enzymes) and their complexes may be eliminated as fast variables, and the dynamics of the system may be described by the two kinetic equations for the reactant S and the product P only.

We consider the initial-boundary value problem for a 2D system in which Reactions (1)–(10) occur. Its space-time behavior in dimensionless variables is described by the following equations:

$$\frac{\partial s(x,y,t)}{\partial t} - \frac{\partial^2 s(x,y,t)}{\partial x^2} - \frac{\partial^2 s(x,y,t)}{\partial y^2} = A_1 - A_2 s - \frac{s}{(1+s+A_3 s^2)(1+p)}, \tag{11a}$$

$$\frac{\partial p(x,y,t)}{\partial t} - D\left(\frac{\partial^2 p(x,y,t)}{\partial x^2} + \frac{\partial^2 p(x,y,t)}{\partial y^2}\right) = B\left(\frac{s}{(1+s+A_3 s^2)(1+p)} - B_1 - B_2 p\right), \tag{11b}$$

where $x=\sqrt{k_3E_0/(D_S K_m)}x'$ and $y=\sqrt{k_3E_0/(D_S K_m)}y'$ are dimensionless space coordinates, $t=k_3E_0/K_m t'$ is dimensionless time, $s=S/K_m$ and $p=K_5P$ are dimensionless concentrations of the reactant S and the product P, $D=D_p/D_s$ is the ratio of the diffusion coefficients for the product D_p and the reactant D_s, $K_5=k_5/k_{-5}$, $K_m=(k_{-2}+k_3)/k_2$, and $K'_m=(k_{-6}+k_7)/k_6$ are the Michaelis constants. $A_1=k_1S_0/(k_3E_0)$, $A_2=k_{-1}K_m/(k_3E_0)$, $A_3=k_4/k_{-4}K_m$, $B=K_mK_5$, $B_1=k_7E'_0/(k_3E_0)$, and $B_2=k_8/(k_3E_0K_5)$ are dimensionless parameters. The assumption that Reactions (8) and (9) occur in its saturation regime means that K'_m is much smaller than p. Therefore, the rate of this reaction is constant and equal to B_1.

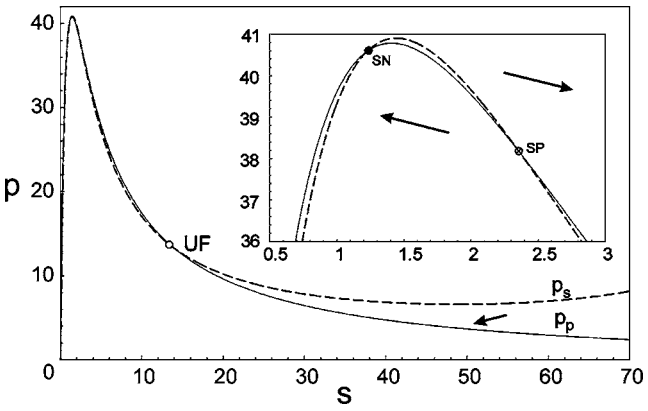

FIG. 1. The nullclines for the activator (p_s) and the inhibitor (p_p). Arrows schematically show directions of the vector field.

In order to define the problem, we assume the following initial conditions:

$$s(x,y,0) = s(x,t_0) + \text{delta}(x,y), \quad p(x,y,0) = p(x,t_0) \quad (x,y) \in [0,L_x] \times [0,L_y], \tag{12}$$

where $s(x,t_0)$ and $p(x,t_0)$ are profiles of the 1D impulses at $t=t_0$, and the boundary conditions:

$$\frac{\partial s}{\partial x}(0,y,t) = \frac{\partial s}{\partial x}(L_x,y,t) = \frac{\partial s}{\partial y}(x,0,t) = \frac{\partial s}{\partial y}(x,L_y,t) = 0,$$

$$\frac{\partial p}{\partial x}(0,y,t) = \frac{\partial p}{\partial x}(L_x,y,t) = \frac{\partial p}{\partial y}(x,0,t) = \frac{\partial p}{\partial y}(0,L_y,t) = 0. \tag{13}$$

We assume the following values of the parameters: $A_1=0.01$, $A_2=0.0001$, $A_3=0.505$, $B_1=7.99\times10^{-3}$, $B_2=4.65\times10^{-5}$, $B=0.3$, and $D=D_p/D_s=3.9$. At these values of the parameters, System (11) without the diffusion terms has three stationary states: the stable node, the saddle point, and the unstable focus (see Fig. 1).

III. RESULTS

We solve Eqs. (11)–(13) numerically using the Cranck-Nicholson scheme with the spatial step equal to 2×10^{-2} for diffusion terms, and the Runge-Kutta algorithm of the fourth order with respect to the time step equal to 4.0 for the kinetics terms. The 2D rectangular domain $((x,y)\in[0,L_x]\times[0,L_y])$ is considered, but the nontrivial asymptotic behavior of the system can be observed for infinite size in one dimension that is $((x,y)\in[0,\infty]\times[0,L_y])$. The asymptotic solution to Eqs. (11)–(13) in a 1D infinite system has the form of a traveling impulse $s(\xi)$ and $p(\xi)$ where $\xi=x-ct$ and c is its velocity. In a finite 1D system, the traveling impulse reflects from the boundaries and spreads periodically from one wall to the other. An example of the traveling impulse

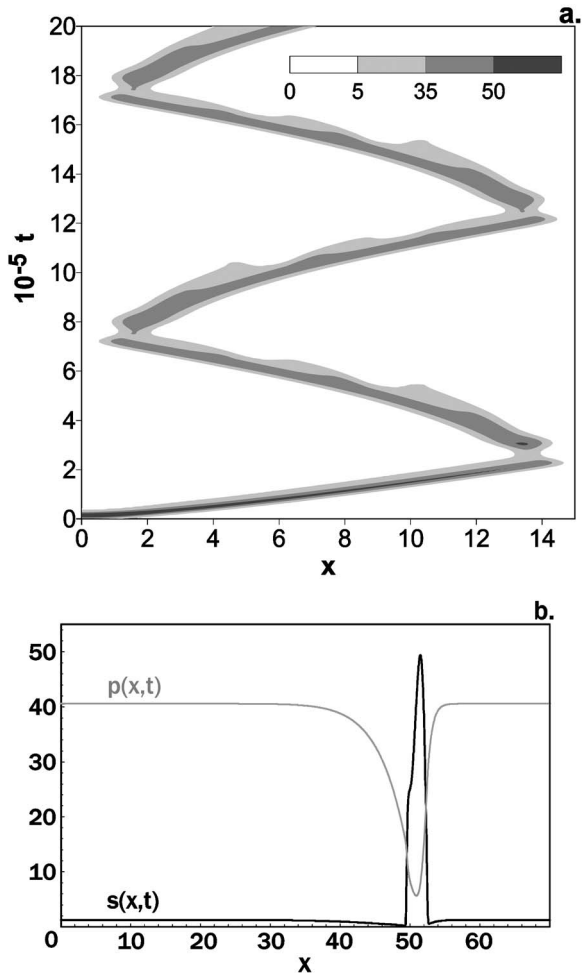

FIG. 2. 1D solution to Eqs. (11)–(13) in the form of an impulse for $A_1=0.01$, $A_2=0.0001$, $A_3=0.505$, $B_1=7.99\times10^{-3}$, $B_2=4.65\times10^{-5}$, $B=0.3$, and $D=3.9$. The profiles of reagents for $t=10^6$ are shown below.

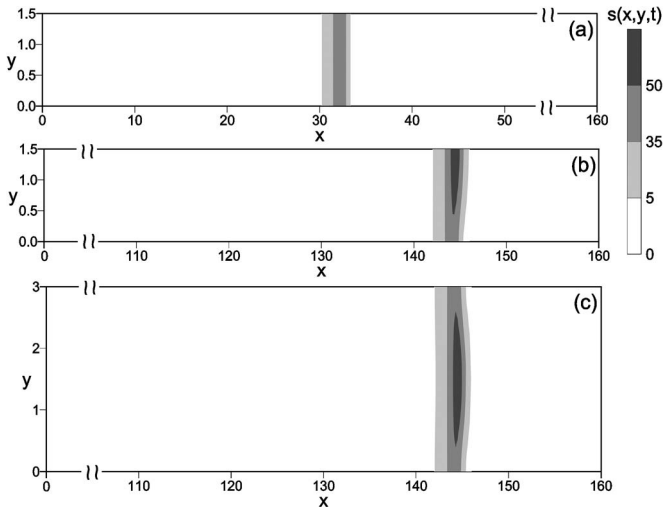

FIG. 3. Solutions to Eqs. (11)–(13) for delta(x,y)={5 if $(x,y)=(32.18,1.49)$ and 0 for all other points} (a,b) and delta(x,y)={5 if $(x,y)=(32.18,1.49)$, $(32.18,1.51)$ and 0 for all other points} (c) at $t=0$ (a) and $t=2\times10^6$ (b),(c).

is shown in Fig. 2. Figure 2(b) shows the solution at time $t=10^6$ for which the traveling impulse is very close to its asymptotic form. The reflection of the impulse from impermeable boundaries was reported in other two-variable 1D reaction-diffusion models, such as the Gray-Scott model [8] and the model of an exothermic reaction whose rate constant obeys Arrhenius formula [9]. It should be stressed that for $B=0.3$, the 1D traveling impulse is the structurally stable asymptotic solution for $D\in(1.0,4.2)$. For values of $D>4.2$, the backfiring phenomenon [10,11] is observed.

The planar traveling impulse is the stable asymptotic solution in the 2D system for L_y, smaller than some critical value $L_{y,\mathrm{cr}}\cong1.4$. Perturbations of the system by delta(x,y) at one or many grid points decay in time and the perturbed solution approaches its asymptotic form. However, if L_y grows above the critical value $L_{y,\mathrm{cr}}$, the planar traveling impulse loses its stability and the curved traveling impulse becomes the stable asymptotic solution. This situation is shown in Figs. 3(a) and 3(b) for $L_y=1.5$. Note that in this case, the system is perturbed only at one grid point. The velocity of the curved traveling impulse equal to 6.920×10^{-5} is greater than the velocity of the planar traveling impulse equal to 4.793×10^{-5}. Moreover, the curved traveling impulse vanishes at the wall, whereas the planar traveling impulse reflects from the boundaries. The maximum value of the concentrations of the reactant is greater than the amplitude of the 1D impulse [compare Figs. 3(a) and 3(b)]. Due to the zero-flux boundary conditions the traveling impulse, which is a mirror reflection of the impulse shown in Fig. 3(b), is the asymptotic solution for $L_y=3.0$ [see Fig. 3(c)]. This solution is obtained for the perturbation of the system at two grid points being a mirror reflection of the perturbation for $L_y=1.5$. Numerical perturbations of the solution at one, as well as at many grid points decay in time, and therefore the curved traveling impulse shown in Fig. 3(c) is stable. The mirror symmetry conditions allow one to obtain the general form of the asymptotic solutions for a system with the size along y being a multiple of $L_y=\lambda/2$. Such curved traveling impulses have the following form:

$$S=S(x-c(\lambda)t,|(y+\lambda/2)\mathrm{mod}\,\lambda-\lambda/2|),$$

where λ is the spatial period in the y direction and $c(\lambda)$ is the velocity of the impulse which depends on the spatial period λ.

The curved traveling impulse shown in Fig. 3(c) may coexist with the solution whose evolution is shown in Fig. 4. In this case, the planar impulse has been perturbed only at one grid point. After perturbation, the planar traveling impulse splits into a curved impulse leaving behind it a small excited region [see Fig. 4(b)]. In further evolution, a curved traveling impulse spreading in the opposite direction is generated [see Figs. 4(c) and 4(d)], leaving behind the excited region. This region splits, producing a pair of next-generation curved traveling impulses behind which a periodic pattern is generated [see Figs. 4(e) and 4(f)]. The creation of the stationary

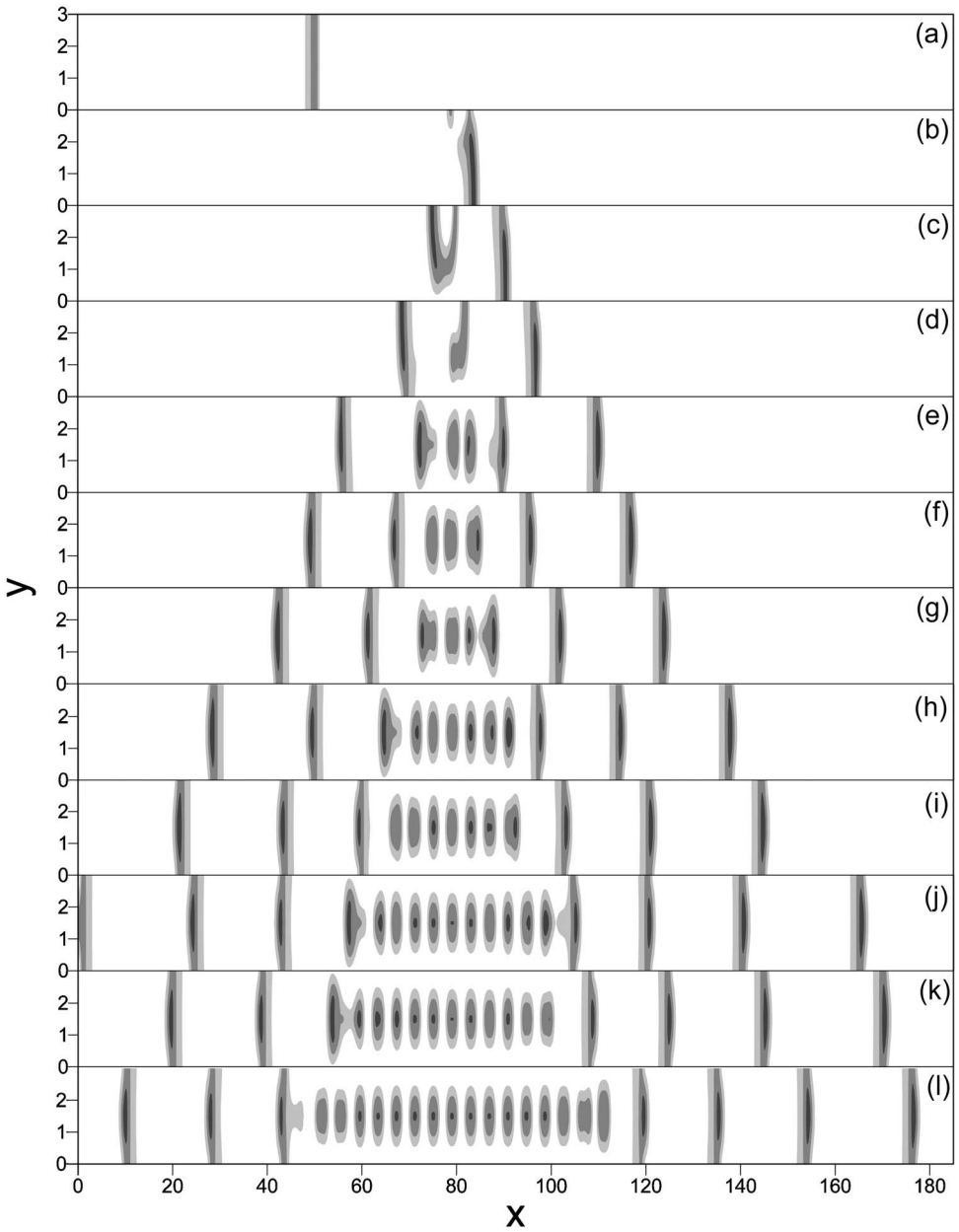

FIG. 4. Solutions to Eqs. (11)–(13) for delta(x,y)={5 at $(x,y)=(32.18,1.49)$ and 0 on all other points) for $t=:0$ (a), 0.67×10^6 (b), 0.77×10^6 (c), 0.87×10^6 (d), 1.07×10^6 (e), 1.17×10^6 (f), 1.3×10^6 (g), 1.47×10^6 (h), 1.57×10^6 (i), 1.87×10^6 (j), 1.94×10^6 (k), and 2.41×10^6 (l).

periodic pattern is similar to the backfiring phenomenon observed in the 1D systems [10,11] [see Figs. 4(g)–4(l)]. In a finite system, the subsequent curved traveling impulses vanish at the boundaries and, finally, the stationary periodic structure occupies the whole system. In an infinite system, an infinite series of curved traveling impulses is produced, leaving behind the stationary periodical structure, which is generated step by step.

We want to stress that if the diffusion coefficient of the inhibitor is equal or close to the diffusion coefficient of the activator ($D\cong1$), then the planar traveling impulse is stable for all values of the size perpendicular to the direction of its propagation.

IV. CONCLUSIONS

The chemical model consisting of mono- and bimolecular reactions without autocatalysis is presented. We have shown that in the 1D reaction-diffusion system, the traveling impulse reflects from the boundary. We have shown that the planar traveling impulse is stable in the 2D systems with a small size (L_y) perpendicular to the direction of the propagation. If L_y exceeds some critical value, then the planar traveling impulse becomes unstable. Two types of stable asymptotic solutions appear for sufficiently large values of L_y. One of them is a single curved traveling impulse. The other one consists of an infinite series of curved traveling

impulses that leaves behind the stationary periodical structure. The selection of one of these asymptotic solutions depends on the initial conditions.

The instability of planar fronts observed in real chemical systems was explained as a result of the nonequilibrium Ising-Bloch bifurcation [12] in which a standing front splits into two counterpropagating fronts. In our model, the instability of the traveling impulse seems to be the consequence of a mechanism similar to the Mullins-Sekerka-Kuramoto or Sivashinsky instabilities found in investigations of the stability of phase interfaces in crystal growing [13,14] and in the propagation of flames [15], respectively.

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