Coexistence of stationary and traveling waves in reaction-diffusion-advection systems

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The flow- and diffusion-distributed structures (FDS) and the differential-flow instability (DIFI) are mechanisms that give rise to static and traveling waves in reactive flows with general, species-dependent transport terms. Here we consider a general framework which supports the simultaneous existence of FDS and DIFI patterns. We study the necessary conditions for each instability in general and compare them in order to derive their connection. The interaction between FDS and DIFI patterns gives rise to interesting wave behavior including stationary, upstream, and downstream traveling waves as well as an interesting regime where stationary and traveling waves coexist.

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I. INTRODUCTION

Over the last decade a wide variety of spatiotemporal structures have been documented in systems of reaction-diffusion-advection (RDA) equations. Prominent examples, such as traveling and stationary waves are known to occur via the flow- and diffusion-distributed structures (FDS) [1] and differential-flow instability (DIFI) scenarios [2,11]. We recently extended the theory to open reactive flows with a fixed inflow boundary condition and proposed a general scenario that gives rise to stable stationary, space periodic patterns [1,3]. The mechanism of flow- and diffusion-distributed structures (FDS) is robust [3] and has none of the limitations of the Turing scenario [4]. Furthermore, in the limit of vanishing flow it recovers the Turing mechanism. The interaction of FDS and Turing instabilities was studied in [3]. The particular case of stationary waves in an oscillatory medium with equal flow and diffusion rates was proposed theoretically in [5] and was subsequently demonstrated experimentally in [6]. Other recent theoretical studies modeling the FDS waves have been reported using the classical model for a cross-flow reactor [7] and the Oregonator [8] and Brusselator [9] models. Those papers have presented scenarios for complex spatiotemporal patterns in such systems.

Similarly, it was recently shown that traveling waves arise when the boundary condition at the inflow region is time periodic [10]. It was shown that the gene-expression waves that precede the formation of somites (the precursors of vertebrae) in chick and mouse embryos arise by a FDS mechanism that involves axial growth, coupled with periodic forcing at the growth zone. The connection between developmental biology and open flows comes from the recognition of the equivalence of axial growth and open flow [10].

In this Brief Report we discuss the link between DIFI and FDS and observe an interesting wave behavior arising from the interaction of the two. The analytical results are derived in Sec. II. In Sec. III the results are illustrated numerically for the cubic autocatalator scheme [11]. A subsequent study of the Oregonator system [12], FitzHugh-Nagumo [13], and the chlorine iodide malonic acid (CIMA) reaction [14] models suggests that the present scenario is quite universal. These results will be presented elsewhere [15].

II. REACTION-DIFFUSION-ADVECTION SYSTEMS WITH GENERAL DIFFUSION AND FLOW RATES

We consider a general reaction-diffusion-advection model that allows for arbitrary differential rates of flow and diffusive transport of the key reactive species. This RDA system admits a variety of instabilities, among them FDS [1,3,5,6], DIFI (or differential-flow) [2,11], and Turing [4] instabilities. Here we are interested in the possible coexistence and interacting behavior of FDS and DIFI patterns. The general equations for a one-dimensional spatial domain are

\[
\frac{\partial a}{\partial t} = \delta \frac{\partial^2 a}{\partial x^2} - \phi \frac{\partial a}{\partial x} + f(a,b), \quad (2.1)
\]

\[
\frac{\partial b}{\partial t} = \frac{\partial^2 b}{\partial x^2} - r \frac{\partial b}{\partial x} + g(a,b), \quad (2.2)
\]

where \(a, b, t, x\) and \(a\) are the dimensionless concentrations, time, and distance along the reactor \((t>0, 0<x<\infty)\). As the domain is semi-infinite the effects of the outflow boundary are negligible. \(\delta = D_a/D_b\) is the ratio of diffusion coefficients of species \(a\) and \(b\). \(r = \text{advection rate of the two species, or the differential-flow parameter.} \phi \) is the dimensionless flow velocity of \(b\). Without any loss of generality we assume that \(\phi > 0\). From now on we shall consider that the parameters \(r\) and \(\delta\) are independent and take the advection rate \(\phi\) as our bifurcation parameter. For the reaction terms we chose the cubic autocatalator model \[11\]

\[
f(a,b) = \mu - ab^2, \quad g(a,b) = ab^2 - b. \quad (2.3)
\]

This ordinary differential equation (ODE) system has a single steady state \(S = \{a_s = 1/\mu, b_s = \mu\}\), for all \(\mu > 0\). \(S\) is temporally unstable (for the ODE system) for any \(\mu \leq 1\) and temporally stable for \(\mu > 1\) [3,11]. At \(\mu = 1\) there is a supercritical Hopf bifurcation with solutions existing in the region \(\mu_0 = 0.99033 \leq \mu \leq 1 = \mu_1\). We now analyze the conditions for forming uniform solutions brought out from small perturbations to the temporally stable uniform steady state \(S\). To do so put

\[
a = a_s + A, \quad b = b_s + B, \quad (2.4)
\]
where $|A|<a, |B|<b$. We do the calculations in general and later we specialize for the kinetics (2.3). Substituting Eq. (2.4) into Eqs. (2.1) and (2.2) we obtain, after linearizing,

$$\frac{\partial A}{\partial t} = \delta \frac{\partial^2 A}{\partial x^2} - \phi \frac{\partial A}{\partial x} + a_{11}A + a_{12}B, \quad (2.5)$$

$$\frac{\partial B}{\partial t} = \delta \frac{\partial^2 B}{\partial x^2} - r \frac{\partial B}{\partial x} + a_{21}A + a_{22}B, \quad (2.6)$$

where $a_{11} = \partial f/\partial a, a_{12} = \partial f/\partial b, a_{21} = \partial g/\partial a$, and $a_{22} = \partial g/\partial b$ are evaluated at $S$.

The conditions for spatiotemporal instability are satisfied when the spectrum of the linearized operator for the system (2.5), (2.6) enters the right-hand plane. Using the exponential solution ansatz $A,B \sim \exp[\omega + i k(\omega)]$, where $\omega$ is the eigenvalue and $k$ is the wave number of the perturbation, and substituting into Eqs. (2.5) and (2.6) gives the dispersion relation

$$D(\omega,k) = \omega^2 + [(1 + \delta)k^2 - Tr + i \phi(r + 1)] + \omega \delta k^2$$

$$+ i \phi \delta^3(1 + r \delta) - k^2 \delta a_{11} + \delta a_{22} - r \delta a_{22}^2$$

$$- i k \phi(r a_{11} + a_{22}) + \Delta, \quad (2.7)$$

where $Tr = a_{11} + a_{22} < 0, \Delta = a_{11}a_{22} - a_{12}a_{21} > 0. \quad (2.8)$

Equation (2.8) implies that $\min(a_{11},a_{22}) < 0$. Without restricting the generality we shall henceforth assume that $a_{11} < 0$. Clearly there are two main cases of instability possible through a primary bifurcation, namely, when $\omega = 0$, corresponding to a steady or FDS bifurcation (the Turing case is included), or when $\Re(\omega) = 0, \Im(\omega) \neq 0$, corresponding to a periodic solution (Hopf or DIFI bifurcation).

**A. FDS instabilities**

The FDS situation has been analyzed for some special cases before [1,3]. For the general case the critical FDS flow is given by

$$\phi_{FDS}^2 = \frac{(1 + r^2 \delta^2) a_{12}a_{21} + r(a_{11} - \delta a_{22})^2 + 2 \delta a_{12}a_{21} r}{(1 + r \delta)(a_{11}r + a_{22})}, \quad (2.9)$$

for $r \neq 0$ and $ra_{11} + a_{22} \neq 0$. Generically, Eq. (2.9) has a strictly positive minimum $\phi_{FDS}^c$, and the FDS instability is predicted for all $\phi > \max(0,\phi_{FDS}^c)$. This is similar to the Turing case which occurs in the domain $\delta > \delta_T > 1$ where $\delta_T$ is the critical Turing ratio of the diffusivities [3]. Space-periodic FDS waves have purely imaginary wave numbers $k_{FDS} = iz_{FDS}, \ z_{FDS} > 0$ given by

$$z_{FDS} = \sqrt{\frac{a_{11}r + a_{22}}{1 + r \delta}}. \quad (2.10)$$

These exist only when $r < a_{22}/a_{11}$. A more detailed analysis of the neutral curve (2.9) shows that $a_{22} > 0$ and $a_{12}a_{21} < 0$. Figures 1(a) and 1(b) show typical plots of the neutral curve (2.9) for kinetics (2.3). Another feature of the model is the relative insensitivity of the critical FDS value $\phi_{FDS}^c$ to variations in $\delta$ as shown in Fig. 1(a).

**B. Differential-flow instability**

The case Re(\omega) = 0 in Eq. (2.7) leads to a Hopf bifurcation giving rise to space- and time-periodic traveling DIFI waves. The neutral curve $\phi_{DIFI}(k,d)\text{ }\delta, f, g$ that corresponds to bifurcation to spatiotemporal traveling DIFI solutions is

$$\phi_{DIFI}^2(k, d, f, g) = \frac{[\delta k^4 - (a_{11} + \delta a_{22})k^2 + \Delta][(1 + \delta)k^2 - Tr]^2}{(r - 1)^2(a_{22} - k^2)(\delta k^2 - a_{11})k^2} \quad (2.11)$$

for $r \neq 1, a_{22} - k^2 \neq 0, a_{11} - \delta k^2 \neq 0$. From Eq. (2.11) we recover the previously published results for the cases when $\delta = 0, r = 1$, and for the ionic model [11].

A detailed analysis of the neutral curve (2.11) shows that the differential-flow instability occurs for any $r \neq 1$ as follows. In the FDS regime $0 < \delta < \delta_T$, necessary conditions for instability are that $a_{11}a_{22} < 0$ and $a_{12}a_{21} < 0$. Let $\phi_{DIFI}^c > 0$ be the minimum of the neutral function (2.11) [see Fig. 1(c)]. In this case we require that $\phi = \phi_{DIFI}^c$, and for instability we require that $\phi > \phi_{DIFI}^c$. In our case traveling waves are predicted even if differential diffusion is not present in the system, i.e., for $\delta = 1$, which is an unusual property for models of differential-flow instability. Figure 1(c) shows a typical neutral DIFI curve for the model (2.1), (2.3) for the case $\delta = 1, r = 0.05, \mu = 3.0$ giving $\phi_{DIFI}^c = 21.65$.

**C. The relation between FDS and DIFI instabilities**

Our analysis shows that FDS and DIFI instabilities can occur simultaneously for $0 < r < -a_{22}/a_{11}, \phi > \max(0,\phi_{FDS}^c, \phi_{DIFI}^c)$. Then the FDS critical wave number (2.10) is in the range $0 < k_{FDS} < a_{22}$. Since the FDS condition Re(\omega) = 0 is guaranteed at the neutral FDS boundary $\omega = 0$ we find from Eqs. (2.9) and (2.11) that

$$\phi_{FDS}^2 = \phi_{DIFI}^2(k_{FDS}^2) \geq \min_{0 < k_{FDS}^2 < a_{22}} \phi_{DIFI}^2 = (\phi_{DIFI}^2)^2. \quad (2.12)$$

Hence the two neutral curves are always tangent at $k_{FDS}$. In particular, the DIFI instability is always generated first as the flow rate $\phi$ is increased from 0 to large values. We have explored these predictions numerically for the system (2.3). The result is given in Fig. 1(d). $\delta = 1.0, \mu = 3.0$ gives $-a_{22}/a_{11} = 0.11$. For $0 < r < 0.11$, as established above, $\phi_{FDS}^c = \phi_{DIFI}^c$. In the range $0.04 < r < 0.055$ the critical flow values for FDS and DIFI are relatively close and the two critical wave numbers have similar magnitudes. As seen below [Fig. 2(c)] the stationary FDS waves dominate the behavior in this range. Outside this traveling and stationary
waves may coexist. Figure 1(d) also predicts that for values of \( r \) near a certain vicinity of zero or for \( r \) in a certain vicinity of 0.11 only traveling waves are expected (for such \( r \)’s the difference \( F_{DS} - D_{IFI} \) is very large). Finally note that for \( r > 0.11 \) only DIFI waves are predicted with \( F_{DIFI} \rightarrow \infty \) as \( r \rightarrow 1^- \).

**III. NUMERICAL SIMULATIONS**

In order to illustrate our results we have explored numerically the spatiotemporal behavior of the model (2.3), using Fig. 1(d) as a guide to choosing parameters. The coupled parabolic system (2.1), (2.2) with reaction terms (2.3) was...
integrated using an implicit Crank-Nicolson code with vari-
able time stepping [3,11]. At the inflow \( x=0 \) we used a
Dirichlet boundary condition in the form of a constant devia-
tion from the uniform steady state \( S \). At the outflow \( x=L \) we
used the free boundary condition \( \partial^2 a/\partial x^2 = \partial^2 b/\partial x^2 = 0 \).
The system was left to evolve for a sufficient long time for a
permanent structure to be established in the full computa-
tional domain.

For the reaction kinetics (2.3) we have \( \delta_T = (3 + 2\sqrt{2})\mu^2 \)
(see [1,11]). Typical results for the case \( 0 < \delta \leq \delta_T \) are shown
in Figs. 2(a)–2(d) for representative parameter values. Con-
istent with our analytical predictions [Fig. 1(a)] the critical
flow \( \phi_{FDS} \) is not sensitive to variations in \( \delta \). For simulations
it was fixed to \( \delta = 1 \). On the other hand, \( \phi_{FDS} \) depends sen-
sitively on \( r \), the differential-flow rate, as expected from the
above analysis. For Figs. 2(a)–2(d) we fixed \( \mu = 3.0 \) and \( \phi = 30.0 \Rightarrow \phi_{FDS} \approx 22.0 \) [see also Fig. 1(d)]. Figure 2(a) shows
a contour plot of the autocatalyst density profile for \( r = 0.01 \).
Following the initial sequential propagation of the perturbation in the domain, periodic upstream traveling DIFI
waves establish themselves. However, at about \( t\sim 600 \) an
extinct state with zero autocatalyst \( (b \sim 0) \) begins to invade
the whole domain at the outflow boundary. This picture is
valid for all \( r \) sufficiently small and \( 0 < \delta < \delta_T \). These waves
moving against the flow are interesting especially when com-
pared with previous studies [11] which showed that a DIFI
bifurcation is associated with a convective instability at least
when the uniform stationary state is stable as is the present
case. As \( r \) is increased further, the traveling waves become
increasingly unstable and split into two parts. The region
close to the inflow boundary develops into stationary FDS
waves [Fig. 2(b)]. Between approximatively \( r = 0.04 \) and
0.055 only stable stationary waves are formed [Fig. 2(c)].
For \( 0.095 \approx r > 0.6 \) there is again a structure composed of two
sections, illustrated by Fig. 2(d), with the front part forming
downstream propagating high amplitude DIFI waves and the
rear section settling into stationary, low amplitude FDS
waves as \( t \to \infty \). Finally, for \( r > a_{11} \approx 0.11 \), only down-
stream propagating DIFI waves survive, forming a transient
structure in the domain due to the convective instability of
the uniform steady state (not shown). The overall picture is
much the same in the Turing domain where \( \delta > \delta_T = (3 + 2\sqrt{2})\mu^2 \).

Further study shows that the above wave behavior is a
robust and generic feature among a wide class of autocata-
lytic coupled systems of RDA that are widely employed in
biological and chemical modeling. In all cases we found that
similar waves arise in systems with the Belousov-
Zhabotinskii (BZ) Oregonator [12], FitzHugh-Nagumo [13],
and CIMA [14] kinetics. In the BZ-Oregonator case we
found traveling waves that accelerate and decelerate (jump).
These results will be given elsewhere [15].

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