Physica D ▮ (▮▮▮▮) ▮▮▮–▮▮▮

Contents lists available at ScienceDirect

Physica D

journal homepage: www.elsevier.com/locate/physd

The stability and slow dynamics of spot patterns in the 2D Brusselator model: The effect of open systems and heterogeneities

J.C. Tzou *, M.J. Ward

Department of Mathematics, University of British Columbia, Vancouver, BC, Canada

HIGHLIGHTS

- We study effects of open systems and heterogeneities on localized spot patterns.
- Localized bulk feed acts to pin spots away from their usual equilibrium locations.
- Sufficiently strong localized feed pulls spots to the source location in finite time.
- Robin BC's induce a saddle–node bifurcation for the existence of quasi-equilibria.

ARTICLE INFO

Article history:
Received 15 December 2016
Received in revised form 1 February 2018
Accepted 3 February 2018
Available online xxxx
Communicated by Y. Nishiura

Keywords:
Localized spike patterns
Domain heterogeneity
Permeable boundary
Hybrid asymptotic-numerical method

ABSTRACT

Spot patterns, whereby the activator field becomes spatially localized near certain dynamically-evolving discrete spatial locations in a bounded multi-dimensional domain, is a common occurrence for two-component reaction–diffusion (RD) systems in the singular limit of a large diffusivity ratio. In previous studies of 2-D localized spot patterns for various specific well-known RD systems, the domain boundary was assumed to be impermeable to both the activator and inhibitor, and the reaction-kinetics were assumed to be spatially uniform. As an extension of this previous theory, we use formal asymptotic methods to study the existence, stability, and slow dynamics of localized spot patterns for the singularly perturbed 2-D Brusselator RD model when the domain boundary is only partially impermeable, as modeled by an inhomogeneous Robin boundary condition, or when there is an influx of inhibitor across the domain boundary. In our analysis, we will also allow for the effect of a spatially variable bulk feed term in the reaction kinetics. By applying our extended theory to the special case of one-spot patterns and ring patterns of spots inside the unit disk, we provide a detailed analysis of the effect on spot patterns of these three different sources of heterogeneity. In particular, when there is an influx of inhibitor across the boundary of the unit disk, a ring pattern of spots can become pinned to a ring-radius closer to the domain boundary. Under a Robin condition, a quasi-equilibrium ring pattern of spots is shown to exhibit a novel saddle–node bifurcation behavior in terms of either the inhibitor diffusivity, the Robin constant, or the ambient background concentration. A spatially variable bulk feed term, with a concentrated source of "fuel" inside the domain, is shown to yield a saddle–node bifurcation structure of spot equilibria, which leads to qualitatively new spot-pinning behavior. Results from our asymptotic theory are validated from full numerical simulations of the Brusselator model.

1. Introduction

Localized spot patterns, whereby a solution component becomes concentrated near certain dynamically-evolving discrete spatial locations in a bounded multi-dimensional domain, is a well-known phenomena for certain two-component reaction–diffusion (RD) systems in the singular limit of a large diffusivity ratio (cf. [1–11]). As surveyed in [12], localized spot patterns arise in many diverse physical and chemical experiments, and they represent a particular class of "far-from equilibrium" patterns [13]. Spot patterns can exhibit a rather wide variety of instabilities such as spot self-replication, spot annihilation due to overcrowding effects, and spot amplitude temporal oscillations, all of which can, typically, be triggered through dynamic bifurcations resulting from the slow spot evolution. In 2-D spatial domains, the stability and dynamics of localized spot patterns have been analyzed for many prototypical RD systems, including the Gierer–Meinhardt (GM) model [1,5,8], the Gray–Scott model [2,3,7], the Schnakenberg model

* Corresponding author.
E-mail addresses: justin.tzou@mq.edu.au (J.C. Tzou), ward@math.ubc.ca (M.J. Ward).

https://doi.org/10.1016/j.physd.2018.02.002
0167-2789/

[4,6,11], and the Brusselator model posed on the boundary of the unit sphere [9,10]. More recently, in [14], the Schnakenberg model was used to provide the first study of spot stability and dynamics in a bounded 3-D domain. A more extensive set of references for the analysis of 2-D spot patterns, and corresponding 1-D spike patterns, is given in the references of these cited articles and in the monograph [15].

The primary new focus of this paper is to provide the first systematic analysis of 2-D spot patterns for a RD system that accounts for some exchange of material between a bounded 2-D domain and the outside environment. Previous studies of spot patterns in a 2-D domain have considered only "closed" systems, modeled by homogeneous Neumann boundary conditions, where the domain boundary is impermeable. While in many cases this may be a realistic assumption, there are other modeling scenarios, such as in skeletal limb development [16], where the boundary is either a source of some chemical morphogen or is only partially impermeable. In the latter case, the boundary is modeled by an inhomogeneous Robin-type condition. We will show that such "open systems" can have rather pronounced effects on the bifurcation properties, stability, and dynamics of localized spot patterns. In our 2-D model we will also consider the effect of a spatially inhomogeneous term in the reaction kinetics, which can lead to new pinning behavior of spot patterns. For concreteness, we will analyze spot patterns for two classes of "open" systems for the classic Brusselator RD model [17] in the singular limit of a large diffusivity ratio, while allowing for a spatially inhomogeneous bulk feed term. We remark that a similar analysis can be done for other RD systems in the large diffusivity ratio limit.

The non-dimensional Brusselator RD model with small activator diffusivity $0 < \varepsilon_0^2 \ll 1$ takes the form [17]

$$U_\sigma = \varepsilon_0^2 \Delta U + \mathcal{E} - (B+1)U + VU^2 \,, \qquad V_\sigma = \mathcal{D}\Delta V + BU - VU^2 \,; \qquad \sigma > 0 \,, \quad \mathbf{x} \in \Omega \,, \tag{1.1a}$$

where the bulk feed $\mathcal{E} = \mathcal{E}(\mathbf{x}) > 0$ is allowed to be spatially dependent. In contrast to the usual analysis of closed systems in which $\partial_n U = \partial_n V = 0$ on the boundary $\partial\Omega$, we will consider two scenarios for the inhibitor V on $\partial\Omega$ that model an exchange of material with the outside environment:

$$\text{(I):} \quad \mathcal{D}\partial_n V = \mathcal{A} \,, \quad \partial_n U = 0 \,, \quad \mathbf{x} \in \partial\Omega \,; \qquad \text{(II):} \quad \mathcal{D}\partial_n V + k(V - V_{\text{out}}) = 0 \,, \quad \partial_n U = 0 \,, \quad \mathbf{x} \in \partial\Omega \,. \tag{1.1b}$$

Here, ∂_n denotes the outward normal derivative on $\partial\Omega$. When $\mathcal{A} > 0$ in (1.1b), Case I models influx of the inhibitor from the boundary, while in Case II with $k > 0$ and $V_{\text{out}} > 0$, we have influx (leakage) when $V(\mathbf{x}) < V_{\text{out}}$ ($V(\mathbf{x}) > V_{\text{out}}$) for $\mathbf{x} \in \partial\Omega$. We refer to (1.1a) with boundary conditions I and II as "open" systems in contrast to a closed system with homogeneous Neumann boundary conditions. For these open systems, our goal is to investigate new behavior regarding the existence, dynamics, and stability of spot patterns. As shown in [9,10], spot patterns occur when $\mathcal{E} = \mathcal{O}(\varepsilon_0)$. Therefore, in (1.1a) we introduce $\mathcal{E} = \varepsilon_0 \mathcal{E}_0 E(\mathbf{x})$, with $\mathcal{E}_0 > 0$, and assume that $\mathcal{A} = \mathcal{O}(\varepsilon_0)$ and $V_{\text{out}} = \mathcal{O}(\varepsilon_0)$. We then rescale $U = \mathcal{E}_0 u/\varepsilon_0$, $V = \varepsilon_0 B v/\mathcal{E}_0$, and $\sigma = t/(B+1)$, so that (1.1b) reduces to

$$u_t = \varepsilon^2 \Delta u + \varepsilon^2 E(\mathbf{x}) - u + f v u^2 \,, \qquad \tau v_t = D\Delta v + \frac{1}{\varepsilon^2}\left(u - vu^2\right) \,; \qquad t > 0 \,, \qquad \mathbf{x} \in \Omega \,, \tag{1.2a}$$

with either of the following two sets of boundary conditions (Case I and Case II):

$$\text{(I):} \quad \partial_n u = 0 \,, \quad D\partial_n v = A \,, \quad \mathbf{x} \in \partial\Omega \,; \qquad \text{(II):} \quad \partial_n u = 0 \,, \quad \partial_n v + \kappa_0 (v - v_b) = 0 \,, \quad \mathbf{x} \in \partial\Omega \,; \quad \kappa_0 \equiv \kappa/D \,. \tag{1.2b}$$

In (1.2a) and (1.2b), the positive $\mathcal{O}(1)$ parameters are

$$f \equiv \frac{B}{B+1} < 1 \,, \quad \tau \equiv \frac{(B+1)^2}{\mathcal{E}_0^2} \,, \quad D \equiv \frac{\mathcal{D}(B+1)}{\mathcal{E}_0^2} \,, \qquad \mathcal{A} = \varepsilon_0 f \mathcal{E}_0 A \,, \quad \varepsilon \equiv \frac{\varepsilon_0}{\sqrt{B+1}} \,, \quad V_{\text{out}} = \frac{\varepsilon_0 B}{\mathcal{E}_0} \,, \quad k \equiv \frac{\mathcal{D}}{D}\kappa \,. \tag{1.2c}$$

There have been relatively few studies of the effect of open systems on pattern formation in RD systems. In [16] a numerical study of an RD system comparing a variety of different boundary conditions was performed, showing that a Robin condition can lead to more predictable transitions between Turing-type patterns as the domain length increases. In [18] the effect of a Robin condition on periodic wave generation for a class of RD systems was analyzed. A boundary flux has also been used to both control and select certain spatio-temporal patterns in specific RD systems (cf. [19,20]). Boundary fluxes also arise in RD systems that couple nonlinear bulk diffusion to surface diffusion effects [21]. For spike solutions, [22] proves the existence of a new class of near-boundary steady-state spike solutions for the scalar problem $\varepsilon^2 \Delta w - w + w^2 = 0$ in a multi-dimensional domain under a Robin boundary condition. For the shadow limit of the GM model, corresponding to a large inhibitor diffusivity, the linear stability properties of this class of near-boundary spikes under a Robin condition were analyzed in [23]. For the singularly perturbed Brusselator model in a 1-D domain, the existence, linear stability, and slow dynamics of spike patterns were analyzed in [24] and [25] for Case I flux-type boundary conditions. One key finding of [24] is that steady-state spikes are located closer to the endpoints of the 1-D spatial domain whenever there is an influx of material from the boundary. The present study can be viewed as an extension of [24] and [25] to 2-D domains, imposing boundary conditions of either type I and II in (1.2b).

A further goal of this paper is to analyze spot-pinning phenomena resulting from a spatially variable bulk feed $E = E(\mathbf{x})$ in (1.2a). For the 1-D GM model, spike-pinning behavior resulting from a piecewise constant inhibitor diffusivity was analyzed in [26]. Spot-pinning behavior associated with two types of precursor gradients in the 2-D GM model was studied in [27] and [5]. In [28], spot alignment due to a spatially inhomogeneous auxin gradient was analyzed for a generalized Schnakenberg system modeling root hair profusion in plant cells. Reflection and transmission properties of pulses and spots across a step-function type barrier in a three-component Fitzhugh–Nagumo system has been studied in [29] and [30]. Pulse dynamics in a 1-D model with strongly localized spatial coefficients was studied recently in [31]. For front-type or transition-layer solutions, pinning effects due to either spatial inhomogeneities or jumps in the nonlinear kinetics were analyzed for various specific RD models in [32,33], and [34] (see also the references therein).

The outline of this paper is as follows. In Section 2 we use the method of matched asymptotic expansions to construct N-spot quasi-equilibrium patterns for (1.2a) for both types of boundary conditions in (1.2b). For the Case I flux-type condition, we will also allow for $E = E(\mathbf{x}) > 0$. In our construction, which accounts for all logarithmic terms of order $\nu \equiv -1/\log\varepsilon$ in the expansion, we will focus primarily on aspects of the analysis that differ from that in [9] for N-spot quasi-equilibria on the surface of the sphere with a constant bulk feed. The problem of constructing quasi-equilibrium spot patterns is shown to reduce to the study of a nonlinear algebraic system that is defined in terms of the local spot profile, the Neumann Green's function for the Case I flux-type boundary condition or the Robin Green's function for the Case II Robin condition, and certain integrals that incorporate the spatial heterogeneities in the system. In Section 3 we use a higher order matching procedure to derive a DAE system characterizing slow