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Turing pattern formation for reaction–convection–diffusion systems in fixed domains submitted to toroidal velocity fields

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ABSTRACT

We have studied the effect of advection on reaction–diffusion equations by using toroidal velocity fields. Turing patterns formation in diffusion–advection–reaction problems was studied specifically, considering the Schnackenberg and glycolysis reaction kinetics models. Four cases were analyzed and solved numerically using finite elements. For glycolysis models, the advective effect modified the form of Turing patterns obtained with diffusion–reaction; whereas for Schnackenberg problems, the original patterns distorted themselves slightly, making them rotate in direction of the velocity field. We have also determined that the advective effect surpassed the diffusive one for high values of velocity and instability driven by diffusion was eliminated. On the other hand the advective effect is not considerable for very low values in the velocity field, and there was no modification in the original Turing pattern.

1. Introduction

Many physical problems can be modeled by balancing of three phenomena: diffusion, advection and reaction [1]. The first is defined as the dispersion of the species involved in the process through physical dominion of the problem. Advection is related to species transport due to the presence of velocity fields. Reaction is an interaction process in which involved species are generated or consumed. The advection–diffusion–reaction equation includes these terms, as expressed in (1) for a phenomenon with one species problem [1]:

$$\frac{\partial u}{\partial t} = \nabla \cdot (\mathbf{K}\nabla u) + \mathbf{a} \cdot \nabla u + f(u), \tag{1}$$

where u is the concentration, $\mathbf{a}$ is the associated velocity of the advective phenomena, $\mathbf{K}$ is the diffusion matrix and $f(u)$ is the reaction function. This equation has been used for problems in fields as fluid dynamics [2], heat transfer [3–5], semiconductor physics [6], engineering materials [7], chemistry [8], biology [9–12], population dynamics [13–15], astrophysics [16], biomedical engineering [17–19] and financial mathematics.

A particular case, driven by reaction and diffusion phenomenon, is characterized by the presence of space stable distributions of concentration species, commonly known as patterns. Turing [20] defined the conditions in which reactive phenomena at equilibrium cannot be stabilized by the presence of a diffusive term, forming spatial heterogeneous patterns known as instabilities driven by diffusion or Turing instabilities.

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Turing [20], Madzvamuse [11,12,17,21–26] and Garzón-Alvarado [1] have proposed numerical simulations considering growing dominion conditions and particular geometries modifying distribution patterns. Their articles have a two species reaction–diffusion system in common as defined in (2b)

$$\frac{\partial u}{\partial t} = \nabla^2 u + \gamma f(u, v), \tag{2a}$$

$$\frac{\partial v}{\partial t} = d\nabla^2 v + \gamma g(u, v) \tag{2b}$$

which will present spacial instability in the concentration patterns (of species u and v) if (2b) satisfies the next inequations (3d) [20,21,27]

$$f_u g_v - f_v g_u > 0, \tag{3a}$$

$$f_u + g_v < 0, \tag{3b}$$

$$df_u + g_v < 0, \tag{3c}$$

$$(df_u + g_v)^2 > 4d(f_u g_v - f_v g_u), \tag{3d}$$

where f_i and g_i indicate the derivates of the reaction functions regarding concentration variables (for example $f_u = \frac{\partial f}{\partial u}$). In expressions (2b) and (3d), $d = \frac{D^u}{D^v}$ is the relationship between these species diffusion coefficients, while γ is a dimension coefficient associated with reactive processes f and g.

In his seminal work, Turing found pattern formation in several physical and chemical processes. The present authors have been studying another biological situations like animal skin pattern formation [10–12,28–31], bone, tissue and tumor formation [17–19,32], animal population distribution [13,14], in recent papers.

Different numerical techniques for solution of the reaction–diffusion problem have thus been implemented, like finite differences [29,30,33,34], finite elements [11,22–25,32] and spectral elements [35]. Many initial studies on Turing pattern formation have been devoted to work on fixed meshes. However, the growing nature of reaction–diffusion problems (in a biological context) have led to studies on growing meshes. For example, Madzvamuse [11] has studied the incidence of mesh growth in diffusion pattern formation. In a seminal work, Madzvamuse [11] presented an algorithm for 2D diffusion–reaction problem solution using a continuously growing Eulerian dominion. For example, [23] introduced a mesh growing finite element technique application for biological problems. In 2007, Madzvamuse [26] presented the effect of a structured growth mesh on Turing pattern formation using a Lagrangian approach analyzing two specific techniques: an implicit finite difference method and finite elements with second order semi-implicit time discretization (2-SBDF). The latter work complemented to [36] where results from the 2-SBDF technique were compared to a finite element implementation that linearized the reaction terms. It should be pointed out that in the previously mentioned references, where a mesh growth effect was included, an advective term was used within the differential equation. However, the role of this transport phenomenon is not quite clear because the Lagrangian approach eliminates this term from the differential equation.

Here, we focus on Turing pattern formation without mesh growth, including advective terms with toroidal velocity fields. A numerical solution of the reaction–advection–diffusion equation was implemented using finite elements, with Backward-Euler temporal discretization. The results showed the influence of convective terms on pattern type and the relationship between advective term magnitude and the appearance or not of diffusion instability. Five study cases are presented, three of them include Schnackenberg reaction terms while the other two were analyzed using a glucolysis reaction model. The results illustrate that glucolysis reaction models are much sensitive to advective field presence, since the resulting Turing pattern is alter for small velocity values. Schnackenberg reaction models showed that Turing pattern changes were proportional to toroidal velocity field magnitude.

2. Materials and methods

2.1. Finite element method solution of the reaction–advection–diffusion equation

Here, we will focus on the study of reaction–advection–diffusion equations in 2D (4):

$$\frac{\partial \mathbf{u}}{\partial t} + \mathbf{a} \cdot \nabla \mathbf{u} - \nabla \cdot (\mathbf{D}\nabla \mathbf{u}) - \mathbf{f}(\mathbf{u}) = \mathbf{0}, \tag{4}$$

where $\mathbf{u} = [u, v]^T$ is the species concentration vector, $\mathbf{a} = [a_x, a_y]^T$ is the velocity vector associated with transport term, while $\mathbf{f}(\mathbf{u}) = [f(u, v), g(u, v)]^T$ is the reaction vector.

Applying weighted residue method to expression (4) on the 2D-domain Ω for variable u, we can obtain (5):

$$\int_\Omega \mathbf{w}\left(\frac{\partial \mathbf{u}}{\partial t} + \mathbf{a} \cdot \nabla \mathbf{u} - \nabla \cdot (\mathbf{D}\nabla \mathbf{u}) - \mathbf{f}(\mathbf{u})\right) d\Omega = \mathbf{0}, \tag{5}$$

where $\mathbf{w}$ is the weighting function. Now, working on each term separately and integrating by parts, Eq. (6) is obtained:

$$\int_\Omega \mathbf{w}\left(\frac{\partial \mathbf{u}}{\partial t}\right) d\Omega + \int_\Omega \mathbf{w}(\mathbf{a} \cdot \nabla \mathbf{u}) d\Omega + \int_\Omega (\nabla \mathbf{w} \cdot \mathbf{D}\nabla \mathbf{u}) d\Omega - \int_\Omega \mathbf{w}(\mathbf{f}(\mathbf{u})) d\Omega - \int_\Gamma (\mathbf{w}(\mathbf{D}\nabla \mathbf{u}) \cdot \mathbf{n}) d\Gamma = \mathbf{0}, \tag{6}$$