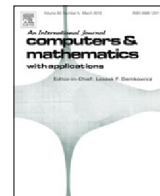




Contents lists available at ScienceDirect

## Computers and Mathematics with Applications

journal homepage: [www.elsevier.com/locate/camwa](http://www.elsevier.com/locate/camwa)

## Validation of numerical solution of diffusive part in a reaction–diffusion model

E.C. Herrera-Hernández<sup>a,\*</sup>, M. Núñez-López<sup>b</sup>, J.A. González-Calderón<sup>a</sup><sup>a</sup> CONACYT-Centro de Ingeniería y Desarrollo Industrial, Av. Playa pie de la cuesta 702, Desarrollo Sn. Pablo, 76125, Querétaro, Qro., Mexico<sup>b</sup> Departamento de Matemáticas Aplicadas y Sistemas, DMAS, Universidad Autónoma Metropolitana-Cuajimalpa, Av. Vasco de Quiroga, 4871, Sta. Fe Cuajimalpa, Cuajimalpa de Morelos, 05300, Mexico, Mexico

## ARTICLE INFO

## Article history:

Available online xxx

## Keywords:

Numerical validation

Mass conservation

Reaction–diffusion system

Finite differences method

Mean square displacement

## ABSTRACT

In this work, we present a methodological procedure to validate the numerical solution of the diffusive part in a reaction–diffusion model. Uniform explicit finite differences method is used to generate the solution in a confined circular domain with boundary condition of zero flux. For the validation of the numerical solution, we consider three different criteria applied to normal diffusion and sub-diffusive cases: (i) the moments of concentration, (ii) decay of the concentration at the origin and (iii) the mass conservation. The numerical solution fulfills the validation criteria of moments and concentration decay at the origin only in the long-term. The mass conservation criterion is fulfilled when the initial condition is imposed close to the border, whereas when it is set near to the origin a dependence on the diffusion rate appears. Pattern formation is presented after validating the numerical solution for normal diffusive case. Good agreement of stationary spatial pattern against reported results is observed.

© 2017 Elsevier Ltd. All rights reserved.

### 1. Introduction

The application of mathematical modeling to biology problems has led to the formulation of a variety of models that describe phenomena like pattern formation in spatial–temporal regimes. In reaction–diffusion models, chemical interactions generate patterns complex in space and/or time due to diffusive processes and synthesis and degradation that depends on how all species/chemicals present in the domain of analysis interact between them, and the properties of the medium. Reaction–diffusion systems describe the process by which two or more species or substances are spatially distributed as a result of diffusion process, and their interactions.

The reaction–diffusion models have been extensively studied in developmental biology as they explain several natural phenomena like tissues formation [1], predator–prey interactions [2], tumor growth [3], spread of epidemics and organs specialization like the hard wings of certain species of beetles [4]. Further, they allow to quantify the evolution of different variables involved in the morphogenesis process, and help in the understanding of tissues and organs formation in spatio-temporal regime.

Turing [5] proposed the first model of morphogenesis which assumes the existence of certain number of chemicals, called morphogens, that diffuse and interact with cells of the same kind. He showed that a reaction–diffusion system with these characteristics, defined in a closed spatial domain and under appropriate condition (defined by model parameters),

\* Corresponding author.

E-mail address: [erik.herrera@cidesi.edu.mx](mailto:erik.herrera@cidesi.edu.mx) (E.C. Herrera-Hernández).

<http://dx.doi.org/10.1016/j.camwa.2017.01.013>

0898-1221/© 2017 Elsevier Ltd. All rights reserved.

evolves in a heterogeneous spatial pattern due to the diffusive process. In this sense, the diffusion process adopts new role, contrary to the classical conception of stability, where the homogeneous steady state becomes spatially unstable. Further, they allow to quantify the evolution of different variables involved in the morphogenesis process, and allow the understanding of tissues and organs formation in spatio-temporal regime. It has been observed that the steady state holds for certain level of perturbation only if the diffusion process is not relevant, but it becomes unstable when diffusion is important. This is known as diffusion-driven instability. In this context, the diffusion process must be conservative regardless the method of solution employed, so that before solving the coupled reaction–diffusion system, it is necessary to validate the numerical solution only for diffusion process. It have been proposed explicit schemes of finite differences to validate numerical solutions of reaction–diffusion models [6,7]. Such numerical schemes reduce the anisotropy effects associated to the mesh refinement, but assume constant and dimensionless values of the discretization parameters. On the other hand, implicit–explicit methods have been explored to solve and validate reaction–diffusion models [8,9]. In such works, authors concluded that full implicit and Crank–Nicolson schemes are not well-suited for numerical solution in reaction–diffusion problems because of the severe time step restriction and the growth rate of wavenumbers in pattern formation process. Instead of using those methods, they modified them by increasing the resolution in the integration stage and showed an improvement in the numerical solutions.

In this work, a methodological procedure to validate the numerical solutions of a diffusion process in a reaction–diffusion model is presented. Explicit finite difference method is implemented to generate the numerical solution and different criteria like mass conservation, concentration decay at the origin, and moments of species concentration are used to verify the performance of the numerical solution against analytical one. After validating the diffusion process, stationary spatial patterns for different model parameters were generated.

The paper is outlined as follows: in Section 2, we present the mathematical model along with initial and boundary conditions. In Section 3 we present details of the numerical solution. Validation methodologies are presented in Section 4. Results and discussions are developed in Section 5. Finally, concluding remarks are summarized in Section 6.

### 1.1. Reaction–diffusion equations

Diffusion process describes the average movement of individuals in a specific confined environment due to local concentration gradients. Individuals can be as small as fundamental physical particles, molecules, cells and bacteria, or even more complex organisms like animals, plants or people. In this context, diffusion phenomenon is present not only at the micro-scale but also at the macro or even at mega-scale. Events like spread of epidemics or fluid flow inside oil and geothermal reservoirs, are governed by diffusion but at different length scales. Individuals concentration is limited to a region  $S$  of space that defines a volume  $V$  where their motion takes place. In the case of a single species in a  $n$ -dimensional domain,  $\mathbf{u}(\mathbf{x}, t)$  is the population density distributed in the spatial domain  $\mathbf{x}$  at time  $t$ . To know how the population varies within the space domain  $\mathbf{x}$  for a evolution time  $t$ , it is necessary to establish a relationship between local spatial gradients and diffusion rates through constitutive law which defines the flux density. It relates the population flow from zones with high concentration to those with low concentration [10]. This principle is known as Fick's law whose mathematical representation is

$$\mathbf{J}(\mathbf{x}, t) = -\mathbf{D}\nabla\mathbf{u}(\mathbf{x}, t) \quad (1)$$

where  $\mathbf{J}(\mathbf{x}, t)$  is the flux vector of  $\mathbf{u}(\mathbf{x}, t)$  and  $\mathbf{D}$  is the diffusion tensor.

The population can be modified by internal processes such as birth, death, or chemical reactions establishing an additional source/sink term in population density denoted by  $f(\mathbf{x}, t, \mathbf{u})$ . According to the conservation principle the rate of change of the quantity of matter contained in  $V$  should be equal to the net flow of matter through the surface  $S$  plus the transform amount of matter inside  $V$  due to source term, it is

$$\int_V \frac{\partial}{\partial t} \mathbf{u}(\mathbf{x}, t) dV = - \int_S (\mathbf{J} \cdot \bar{\mathbf{n}}) ds + \int_V f dV \quad (2)$$

where  $\bar{\mathbf{n}}$  is the unit normal vector pointing out of  $S$ . Using the divergence theorem in the diffusive term and combining Eqs. (1) and (2) we obtain

$$\int_V \frac{\partial}{\partial t} \mathbf{u}(\mathbf{x}, t) dV = \int_V \nabla \cdot (\mathbf{D}\nabla\mathbf{u}(\mathbf{x}, t)) dV + \int_V f dV \quad (3)$$

this equation corresponds to a differential equation in the domain  $\Omega = V$  with appropriate boundary conditions defined on  $\Gamma = S$ . Eq. (3) in its differential form is given as

$$\frac{\partial \mathbf{u}}{\partial t} = \nabla \cdot (\mathbf{D}\nabla\mathbf{u}) + f \quad (4)$$

which is known as reaction–diffusion equation and together with initial and boundary conditions predicts the evolution of  $\mathbf{u}(\mathbf{x}, t)$  within  $V$ .

Download English Version:

<https://daneshyari.com/en/article/4958431>

Download Persian Version:

<https://daneshyari.com/article/4958431>

[Daneshyari.com](https://daneshyari.com)