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Classification of parameter spaces for a reaction-diffusion model on stationary domains

Wakil Sarfaraz*, Anotida Madzvamuse*

University of Sussex, School of Mathematical and Physical Sciences, Department of Mathematics, Pevensey 3, Brighton, BN1 9QH, UK

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ABSTRACT

This paper explores the classification of parameter spaces for reaction-diffusion systems of two chemical species on stationary rectangular domains. The dynamics of the system are explored both in the absence and presence of diffusion. The parameter space is fully classified in terms of the types and stability of the uniform steady state. In the absence of diffusion the results on the classification of parameter space are supported by simulations of the corresponding vector-field and some trajectories of the phase-plane around the uniform steady state. In the presence of diffusion, the main findings are the quantitative analysis relating the domain-size with the reaction and diffusion rates and their corresponding influence on the dynamics of the reaction-diffusion system when perturbed in the neighbourhood of the uniform steady state. Theoretical predictions are supported by numerical simulations both in the presence as well as in the absence of diffusion. Conditions on the domain size with respect to the diffusion and reaction rates are related to the types of diffusion-driven instabilities namely Turing, Hopf and Transcritical types of bifurcations. The first condition is a lower bound on the area of a rectangular domain in terms of the diffusion and reaction rates, which is necessary for Hopf and Transcritical bifurcation to occur. The second condition is an upper bound on the area of domain in terms of reaction-diffusion rates that restricts the diffusion-driven instability to Turing type behaviour, whilst forbidding the existence of Hopf and Transcritical bifurcation. Theoretical findings are verified by the finite element solution of the coupled system on a two dimensional rectangular domain.

1. Introduction and model equations

1.1. Introduction

Reaction-diffusion systems (RDSs) attract a significant degree of attention from researchers in applied mathematics [1–9], mathematical and computational biology [10–14], chemical engineering [15–17] and so forth. Alan Turing was one of the first scientists to realise the significance of RDSs as a self-governing dynamical system [18], and showed that RDSs can be responsible for the emergence of spatial patterns in nature. A large number of scientists [1,2,8,11,19–21], since the publication of Turing [18], have contributed to investigating RDSs, with various types of reaction kinetics. The most popular models of reaction kinetics explored in the literature are the *activator-depleted* model (also known as the Schnakenberg reaction kinetics) [2,20,22–24], Meinhardt [12,13] and Thomas [25] reaction kinetic models. From a research perspective the study of RDSs is conducted through different types of approaches, one of which focuses on the local behaviour of the dynamics of the RDS near a uniform steady state, which in turn relates to the subject of stability analysis [6,8,12,20,26,27] of RDSs using the stability matrix. Linear stability analysis offers a great deal of insight regarding the behaviour of RDSs in the neighbourhood of a uniform steady state of a particular system. The other usual approach is numerical computation of the actual solution of RDSs using finite element, finite difference and other numerical methods [1,2,4,5,7,9,28–30]. Numerical solution of RDSs helps to visualise the evolution of the dynamics in time. Numerical computations of RDSs with non-linear reaction kinetics with a particular choice of parameters partially encapsulates the possible types of dynamics that a certain RDS can exhibit. In order to better understand the behaviour of RDSs, it is necessary to have prior knowledge on the classification of the parameter values. Madzvamuse et al., in [20,27] found regions of parameter space, corresponding to diffusion-driven instability with and without cross-diffusion respectively using the well-known *activator-depleted* reaction kinetics. Their approach to finding unstable regions in the parameter

* Corresponding authors. Tel.: +447832903102.
E-mail addresses: wakilsarfaraz@gmail.com, ws49@sussex.ac.uk (W. Sarfaraz), A.Madzvamuse@sussex.ac.uk (A. Madzvamuse).

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space is restricted to Turing instability only. One of the few complementary contributions from the present work is the application of a numerical method (exclusive to this paper) in order to obtain the full classification of parameter space. The numerical method is also employed to solve the equations for the implicit curves forming the partitioning of the classification within the parameter space. Iron et al., present a detailed study in [28] on the stability analysis of Turing patterns generated by *activator-depleted* reaction kinetics in one spatial dimension. Despite the presentation of rigorous and well-demonstrated proofs in [28], their results are restricted to spatial patterns with focus on the emergence of the number of spatial peaks relative to the eigenvalues of the one-dimensional diffusion operator. Xu and Wei investigated *activator-depleted* reaction-diffusion model in [31] with restriction to one spatial dimension focusing mainly on Hopf bifurcation. The approach in [31] is not aimed to produce any results that relate the domain size (length) to the reaction-diffusion rates. Yi *et al.* studied bifurcation analysis and spatiotemporal patterns of a diffusive predator-prey system in one space dimension [32]. The results obtained in [32] are mainly theoretical with limited numerical demonstration and in comparison with the current work, no attention is given to analyse whether domain size have any role in the bifurcation behaviour of the system in [32]. Reaction-diffusion system with *activator-depleted* reaction kinetics is investigated in [33] with time delay in one-dimensional space and it is theoretically proven with limited numerical verifications that Hopf bifurcation can occur with given constraints on the parameter values of the system. Liu *et al.*, in [34] attempted to find constraints on the parameters of RDSs with *activator-depleted* reaction kinetics that causes the system to exhibit Hopf and transcritical bifurcations. The proofs in [34] are focused on the existence of bifurcation points for some theoretical constraints of parameterised variables of the actual parameters, with no relation between the domain size and reaction-diffusion rates. Comparing their work to the present study, our results are robust in the sense that we explicitly relate domain size to the reaction-diffusion rates. Using this relationship, the parameter space is classified for different types of bifurcations. Moreover, in the present work the parameter constraints are a consequence of the relationship between the domain size and the reaction-diffusion rates. An additional drawback in the analysis of Liu et al. [34] is that their results are produced on parameterised variables of the model and not on the actual parameters of the equations, which makes their results applicable to non-realistic possibilities (negative values) of the actual parameters of the model. This drawback is effectively resolved in the current work as the analysis is conducted on the actual two-dimensional positive real parameter space, which in addition to confirming the existence of different bifurcation regions, it offers concrete quantitative classification of the parameter space that guarantees the dynamics of RDSs to exhibit these bifurcations.

The majority of RDSs in the literature [2,3,9,19,21,35] that exhibit spatial or temporal pattern, contain nonlinear terms in their reaction kinetics, which makes the mathematical and numerical analysis of such systems extremely challenging. With no closed analytical solutions, studies of the local behaviour of the systems are generally conducted by use of linear stability theory close to bifurcation points. Here, the behaviour of a system can be theoretically predicted in the neighbourhood of the uniform steady states. Linear stability analysis can help derive certain conditions on the reaction kinetics, which lead to causing instability in the dynamics of RDSs in the presence of diffusion. Numerous papers [6,8,20,24,27] exist in literature that routinely apply linear stability analysis to RDSs. A routinely used approach related to stability analysis of RDSs [6,24,27,31,32] focuses on deriving linear stability conditions in terms of the characteristics of the stability matrix for diffusion-driven instability, lacking to explore what the numerical application of these conditions induce on the admissible choice of the parameter space for a certain RDS. Spatio-temporal pattern formation occurs when an RDS undergoes diffusion-driven instability [18,23,36]. This occurs when a uniform steady state which is stable in the absence of diffusion becomes unstable upon adding diffusion to the system. Diffusion-driven instability crucially depends on the values of diffusion and reaction rates of each reactant, however, more importantly it depends on the parameter choice of the reaction kinetics. In the current work the existing knowledge on the conditions for diffusion-driven instability in the literature is extended using a series of analytical and numerical techniques, to obtain new insights on the combined effects of diffusion and reaction rates, and in turn relating these to domain size of the evolution of the pattern. The detailed and quantitative analysis on the relationship between the domain size and diffusion-reaction rates in light of the parameter classification is an aspect that has not been studied in the literature. The usual approach in selecting parameters for numerical computations of RDSs [14,36] is based on the behaviour of RDSs in the absence of diffusion by use of trial and error or is based on previously published work, to observe instability caused by diffusion [1,2,6,9,19]. The absence of a robust method to fully classify the parameter space for an RDS, creates an arguable platform for the importance of this work. Efficient analytical as well as computational methods are used to demonstrate the quantitative relationship between the domain size and diffusion rate for an *activator-depleted* RDS. The main findings of the present work, which relate the domain size to the diffusion and reaction rates, are presented in the form of theorems with rigorous mathematical proofs and these theoretical results are supported computationally by finite element numerical solutions corresponding to the *activator-depleted* RDS on fixed rectangular domains. For each numerical demonstration the relative error plots of the solutions for each successive time-step are presented to visualise the convergence of the numerical approximate solutions.

This article is therefore structured as follows. In Section 1.2 we state model equations with the corresponding initial and boundary conditions. Section 2 presents a detailed theoretical linear stability analysis of the system (1) in the absence of diffusion. Linear stability analysis is conducted by computing the stability matrix through which, the non-dimensional parameter space is derived and classified. Section 2.3 presents the methodology to compute the solutions of the partitioning curves for the classification on the parameter space. A combination of analytical and numerical methods using polynomials are applied. In Section 3, the linear stability analysis of the system is conducted in the presence of diffusion and the parameter space is explored to understand the consequences of including diffusion in the analysis. The parameter space is further explored to find the change in regions of the parameter space through varying the non-dimensional diffusion coefficient. Section 4 contains the finite element solution of system (1), where the theoretical predictions proposed by the linear stability theory subject to conditions on the domain size and parameter spaces are numerically verified. Section 5 presents conclusions, future directions and possible extensions of the current work.

1.2. Model equations

The dynamics of two chemical species u and v in a coupled system of nonlinear parabolic equations is considered. Both species diffuse with independent rates and satisfy the well-known *activator-depleted* reaction-diffusion system in a closed two-dimensional rectangular domain denoted by $\Omega \subset \mathbb{R}^2$ with area $L_x \times L_y$, where L_x and L_y are the corresponding side lengths in the direction of x and y axes respectively. The reaction-diffusion system satisfying the *activator-depleted* model for u and v in its non-dimensional form with Neumann boundary conditions and positive