

Article

Semi-Analytical Solutions of the Schnakenberg Model in a Circularly Symmetric Reaction–Diffusion Annulus

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Abstract

This paper investigates the semi-analytical solutions of the Schnakenberg reaction system in a circularly symmetric reaction–diffusion annulus. The Galerkin method is used to approximate spatial concentration profiles of both the autocatalyst and reactant. This method transforms governing partial differential equations into a system of ordinary differential equations, allowing a semi-analytical investigation of this special geometric domain. Singularity theory is then used to determine the regions of the parameter space where different steady states are obtained, and a degenerate Hopf bifurcation analysis is used to determine the region where the Hopf bifurcation points are located. A novel result is that the width of the annulus significantly influences both static and dynamic multiplicity; specifically, a thicker annulus expands the region of parameter space where multiple steady-state solutions and Hopf bifurcations exist. Finally, the reliability and precision of these semi-analytical results are confirmed through direct comparison with numerical solutions of the original partial differential equations.

Keywords: reaction–diffusion annulus; Schnakenberg model; singularity theory; Hopf bifurcations; semi-analytical model

MSC: 37Gxx; 35B10; 35B32; 35B35; 35K57; 35Q92; 37G15; 35B05; 62P10

1. Introduction

Chemical and biochemical reactions exhibit a remarkable diversity of nonlinear phenomena, including multiple steady states, autonomous oscillations, and deterministic chaos. These behaviors have been the subject of interdisciplinary studies for the past several decades. In particular, experimental studies of chemical reactions have investigated oscillatory behavior in great detail. The Belousov–Zhabotinsky, Briggs–Rauscher and Bray–Liebhafsky reactions are classic examples of reactions that display periodic changes in concentration with visually striking color changes [1–4]. The Schnakenberg model is an oscillatory system that describes spontaneous pattern formation and sustained oscillations linked to biochemical processes within cells [5]. Oscillatory behavior in such systems has been studied using continuous-flow well-stirred tank reactors (CSTRs) in which the concentration dynamics are modeled by ordinary differential equations (ODEs). These reactors have proven highly effective in both theoretical and experimental analyses of steady states and oscillations. Another important reactor for investigating oscillatory reactions is the reaction–diffusion cell, which is described by partial differential equations (PDEs) and allows for the characterization of a wide range of emergent phenomena.



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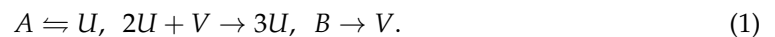
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Schnakenberg [5] proposed a simplified autocatalytic model to describe sustained oscillations. The kinetic mechanism of this model consists of the following three elementary steps:



The second step is a trimolecular autocatalytic process. In this system, U acts as a self-activating catalyst, and V is a reactant whose concentration increases significantly before being depleted. The substances A and B serve as source terms supplying the system.

The Schnakenberg model has been widely applied to model processes such as pattern formation in embryogenesis and skin dynamics [6,7]. Previous studies [8] have demonstrated the existence of steady state solutions and various bifurcation phenomena such as spatially inhomogeneous patterns and periodic instabilities. The importance of the steady-state and Hopf bifurcations in the generation of temporal oscillations has been discussed in detail. Furthermore, the authors of [9] studied the role of geometric factors in the pattern formation of biological systems such as organ primordia and embryonic structures.

Al Noufaey [10,11] studied the irreversible and reversible Schnakenberg models. These studies concentrated on singularity and stability, showing that the model has a hysteresis bifurcation pattern. You [12] studied asymptotic components of reversible Schnakenberg equations and identified the existence of a global attractor semiflow solution of the model, which is part of the Dirichlet boundary. Yang [13] investigated spatiotemporal pattern formation caused by cross-diffusion in the Schnakenberg model. The author found that linear cross-diffusion in the model can cause Turing instability and determined regions of the parameter space in which hexagon-like, stripe-like, and coexistence patterns are formed. Din and Haider [14] investigated a discrete version of the Schnakenberg model and demonstrated that discretization in time can dramatically alter the dynamics of the original continuous system. Their analysis revealed local stability conditions, flip and Neimark–Sacker bifurcations, chaotic behavior and possible chaos–control mechanisms. Their study showed that discrete Schnakenberg systems can exhibit dynamical regimes that are not apparent in the corresponding continuous-time formulation. Alfifi [15] considered a diffusive Schnakenberg model incorporating gene-expression time delays. A Galerkin approximation was employed to reduce the delayed partial differential equations to a system of delay differential equations. Steady states, stability boundaries, and Hopf bifurcation curves were then obtained analytically and numerically. The results showed that increasing the delay can shift the Hopf threshold and reduce the parameter values at which oscillatory instability occurs. Diffusion coefficients were also shown to affect the location and extent of the stability regions. Al Saadi et al. [16] studied spikes and localized solutions of a modified one-dimensional Schnakenberg system with source terms in the equations for the activator and inhibitor. Their work connected semi-strong asymptotic analysis with the theory of pattern localization near a subcritical Turing bifurcation. The results indicate that localized states can exist in a pinning region where spatially periodic and homogeneous states coexist. Xu et al. [17] considered a Schnakenberg system with main reversible reactions under homogeneous Neumann boundary conditions. They used semigroup theory to prove the existence and uniqueness of strong solutions. The reversible system can have up to four positive homogeneous equilibria as opposed to the classical irreversible model. Explicit conditions for local stability, Turing instability, steady-state bifurcation and Hopf bifurcation were obtained. The presence of several positive equilibria makes the reversible formulation particularly suitable for the investigation of multistability, hysteresis, and switching between chemical states. The model has also been analyzed for noise and uncertainty. Recently, a stochastic Schnakenberg model has been proposed to investigate the effects of environmental fluctuations on the positivity, boundedness and

asymptotic behavior of the chemical concentrations. Stochastic modeling is important because molecular fluctuations, uncertain reaction rates and external disturbances affect the experimentally observed biochemical patterns. Thus, the stochastic framework is a more realistic representation than a fully deterministic system, especially when the numbers of reacting molecules are small; see [18].

In semi-analytical solutions to reaction–diffusion systems, the original PDEs can be approximated and replaced by a set of lower-order ODEs using the Galerkin method [19,20]. Marchant [21] used this approach to obtain semi-analytical solutions of the Gray–Scott cubic autocatalytic reaction–diffusion model. This approximation yielded parameter regions corresponding to different bifurcation diagrams and a Hopf bifurcation map that aligned closely with numerical solutions. The Galerkin method has also been successfully applied to several other reaction–diffusion systems. For example, it was used to analyze a mixed quadratic–cubic autocatalytic system [22] and a reversible Selkov model with feedback delay in oscillatory glycolysis [23]. In addition, this approach has elucidated the dynamics of the Selkov model, accounting for precursor and final product effects [24]. It has also been applied to ecological and biological models such as the Lotka–Volterra predator–prey model with diffusion and time-delay variables [25–27]. In addition, the effect of time delay in gene expression was studied with the Brusselator model [28].

Reaction–diffusion systems with cylindrical and spherical geometries are commonly used to model a variety of biological phenomena, including morphogenesis of tissue during development and tumor growth [29–31]. For example, Liu and Tavener [32] used a two-dimensional reaction–diffusion annulus to model intracellular protein trafficking. This annular geometry has also proven useful for the study of rotating chemical waves. Farr and Golubitsky [33] considered the Gray–Scott model in a circular geometry and investigated the appearance of rotating wave solutions via Hopf bifurcations. Their results indicated that stable rotating waves can be found for a wide range of parameter values and that even simple models can have complicated bifurcation phenomena such as two- and three-frequency motions. Lubkin and Rand [34] determined the conditions for the formation of spiral waves and evaluated the influence of disk sizes and diffusion coefficients on wave properties in a circular domain. The authors of [35] developed semi-analytical solutions for cubic autocatalytic reactions in a circularly symmetric reaction–diffusion annulus. An important result concerned the influence of the physical width of the annulus on static and dynamic multiplicity. Specifically, the annulus can be widened to expand the parameter regions where both multiple steady states and Hopf bifurcations occur. Wakil et al. [18] considered a reaction–diffusion system with linear cross-diffusion and an activator-depleted kinetics as a main example on rectangular domains. They obtained lower and upper bounds for the domain size for the occurrence of instability and provided a parameter classification in terms of Turing, Hopf and transcritical bifurcations. The authors found that even with the reaction parameters fixed, changing the spatial scale can create or eliminate regions of instability. Cross-diffusion enlarged the domain of parameters where patterns may occur.

Contrary to our previous studies that were restricted to one-dimensional reaction–diffusion systems or alternative reaction mechanisms, we derive in this study a semi-analytical Galerkin formulation that is specifically designed for the Schnakenberg reaction–diffusion model (2) in a circularly symmetric annulus. Thus, the novel highlights of the present work are the development of the Galerkin approximation for annular geometry, the study of the effect of annulus thickness on steady-state multiplicity and Hopf bifurcations, the derivation of parameter maps for hysteresis and Hopf bifurcations in annular domains, and a rigorous comparison with full numerical PDE solutions to prove the reliability of the reduced model.

The rest of this paper is organized as follows: Section 2 introduces the governing PDEs of the annular Schnakenberg model and details the methodology for applying the Galerkin method to the PDEs and their associated boundary conditions to derive the system of ODEs that comprise the semi-analytical model. Section 3 presents the profiles of both steady-state concentrations and a comprehensive analysis of the steady-state concentration multiplicity alongside the corresponding steady-state concentration patterns. In Section 4, singularity theory is used to locate the positions of the hysteresis bifurcation points. The positions are plotted, and the parameter space is divided into regions for which two different steady-states are obtained. Section 5 presents a local stability analysis of the semi-analytical model. This reveals degenerate Hopf points, allowing us to map out the parameter boundaries where Hopf bifurcation arises. Section 6 considers the influence of altering the width of the annulus on the stability of the model.

2. The Semi-Analytical Model

2.1. Governing Equations of the Schnakenberg Model

Consider the Schnakenberg scheme represented by (1) in a circularly symmetric annulus, shown in Figure 1. The non-dimensional form of the governing PDEs is expressed as

$$u_t = \alpha - \delta u + u^2 v + \frac{1}{r} u_r + d_1 u_{rr}, \quad v_t = \beta - u^2 v + \frac{1}{r} v_r + d_2 v_{rr}, \quad (2)$$

$$u = v = 0, \text{ at } r = r_1, r_1 \leq r \leq 1 \quad u = v = 0, \text{ at } r = 1 \text{ and } t = 0. \quad (3)$$

In (2), u and v represent the dimensionless concentrations of the chemical autocatalyst U and reactant V , respectively. This reactor operates as an open system; the annulus features permeable boundaries at $r = 1$ and $r = r_1$, each interfacing with reservoirs where the concentrations of u and v are maintained at zero. This geometric configuration allows the reactant to flow at the outer boundary and the autocatalyst at the inner boundary. An important feature of this geometry is that the inner radius of the annulus can be changed ($r_1 \in (0, 1)$). As r_1 approaches zero, the geometry becomes a solid disk, and the internal reservoir is removed, eliminating the source for the autocatalyst u . On the other hand, when r_1 approaches one, the annulus becomes infinitesimally thin. The positive, non-dimensional parameters α , δ , β , d_1 , and d_2 are defined in (2) and represent the following physical properties: α and δ are the rate constants for the forward and reverse reactions of the first step described in (1). The parameter β is the rate at which component B is transformed into the reactant V . The diffusion coefficients for the autocatalyst concentration u and the reactant concentration v are represented by the parameters d_1 and d_2 , respectively. r_1 is the radius of the inner boundary of the annulus, which is depicted in Figure 1.

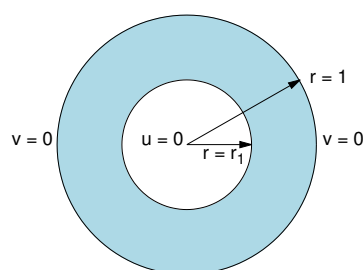


Figure 1. The geometry of the circularly symmetric reaction–diffusion annulus, where u is the autocatalyst concentration, v is the reactant concentration, and r_1 is the radius of the inner boundary of the annulus.

To compute the numerical solution to Equation (2), an explicit finite-difference scheme accurate to $O(\Delta t, \Delta x^2)$ [36,37] is employed, while the system of ODEs is solved using a fourth-order Runge–Kutta (RK4) method [38].

2.2. The Galerkin Method

The Galerkin method transforms the governing PDEs (2) and boundary conditions (3) to a system of ODEs by prescribing the spatial structure of the concentration profiles. The method is based on approximating the concentrations by a series of orthogonal basis functions. The following function expansion is used:

$$\begin{aligned} u(r, t) &= u_1(t) \sin(\theta) + u_2(t) \sin(2\theta), \\ v(r, t) &= v_1(t) \sin(\theta) + v_2(t) \sin(2\theta), \end{aligned} \quad (4)$$

where $\theta = \pi \frac{r-r_1}{1-r_1}$. This is known as the two-term method. Although the function expansion (4) complies with the boundary conditions in (3), it does not satisfy the governing PDEs (2) exactly. The unknown parameters in (4) are determined by averaging the governing PDEs and weighting with the corresponding basis functions. This is done by inserting expansion (4) into the governing PDE equations (2), multiplying the results by the basis functions $\sin(\theta)$ and $\sin(2\theta)$, and integrating numerically, using the composite midpoint rule [39], over the interval $[r_1, 1]$. Thus, this approach provides a set of ODEs for any given value of r_1 . The ODE model is fairly simple to analyze for a fixed r_1 . However, the reactor geometry is not static, so changing r_1 alters the integration boundaries, and the coefficients must be numerically recomputed for each value. As a result, the effect on the system must be assessed by solving a separate ODE model for each value of r_1 . The following ODE model represents the case $r_1 = 0.2$:

$$\begin{aligned} \frac{d}{dt} u_1 &= 0.75u_1^2v_1 + u_1u_2v_2 + 0.5u_1^2v_1 - \delta u_1 - 13.710d_1u_1 - 4.914d_1u_2 + 1.274\alpha \\ \frac{d}{dt} v_1 &= -0.75u_1^2v_1 - 0.5u_2^2v_1 - u_1u_2v_2 + 1.274\beta - 13.710d_2v_1 - 4.914d_2v_2 \\ \frac{d}{dt} u_2 &= +6.754d_1u_1 - 59.539d_1u_2 + 0.5u_1^2v_2 + u_1u_2v_1 + 0.75u_2^2v_2 - \delta u_2 \\ \frac{d}{dt} v_2 &= -0.5u_1^2v_2 + 6.754d_2v_1 - 59.539d_2v_2 - u_1u_2v_1 - 0.75u_2^2v_2. \end{aligned} \quad (5)$$

This set of ODEs (5) is derived by truncating series (4) after two terms. The two-term approximation yields accurate results without unnecessarily complicating the mathematical expressions. The one-term approximation is also calculated by setting $u_2 = v_2 = 0$.

Although both the Schnakenberg and cubic autocatalytic reaction–diffusion systems can be reduced using the Galerkin method, the resulting reduced-order models exhibit distinct nonlinear coupling structures. The Schnakenberg model contains the reaction term u^2v , whereas the cubic autocatalytic model [21,35] is governed by the term uv^2 . After Galerkin projection, the quadratic dependence on the activator variable u generates stronger self-interaction and additional cross-mode coupling terms among the modal amplitudes.

3. Steady-State Profiles and Bifurcation Diagrams

In this section, we describe the steady-state solution of the ODEs (5). All time-dependent derivative terms are neglected, and the system is reduced to a set of four simultaneous equations, which is numerically solved with Maple. This system simplifies to two simultaneous equations for the simplified one-term approximation in which $u_2 = v_2 = 0$.

Figure 2a,b display the steady-state concentration profiles of the autocatalyst u and the reactant v versus r , respectively. The basic system parameters are chosen as $r_1 = 0.2$, $\alpha = 2$, $\beta = 6$, $\delta = 8$, and $d_1 = d_2 = 0.1$. These curves illustrate the results of both the one- and two-term approximation models alongside those from the direct numerical simulation of the governing PDEs, (2) and (3). Inside the annular reactor, the concentration profiles assume a rounded peak geometry. The peak concentrations are located at the center of the annulus ($r_c = \frac{1+r_1}{2}$), and the following solution pairs (u, v) are obtained from the three approaches: $(u, v) = (0.313, 5.289)$ for the one-term, $(u, v) = (0.311, 5.097)$ for the two-term models, and $(u, v) = (0.270, 4.80)$ for the numerical solution. The relative error rates are less than 16% for u and 7% for v . The reduced Schnakenberg system is more strongly nonlinear and more sensitive to mode truncation, particularly in the approximation of u . In contrast, the nonlinear interactions in the cubic autocatalytic model are distributed differently, leading to a comparatively weaker coupling of the activator variable and typically smaller truncation errors. This structural difference could be a reasonable explanation for the relatively larger error found for u in this figure.

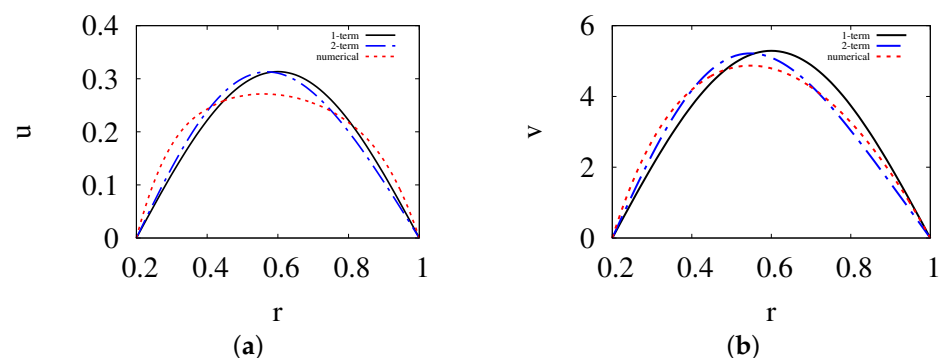


Figure 2. Steady-state profiles of (a) autocatalyst concentration u and (b) reactant concentration v versus r . The system parameters are established at $r_1 = 0.2$, $\alpha = 2$, $\beta = 6$, $\delta = 8$, and $d_1 = d_2 = 0.1$.

The steady-state concentrations u and v at the centre of the annulus r_c are mapped against the bifurcation parameter δ to construct the bifurcation diagrams. Figure 3a,b show the corresponding bifurcation diagrams for the two concentrations, u and v , with the bifurcation parameter δ . The calculations are carried out with the parameter set $r_1 = 0.2$, $\alpha = 0.3$, $\beta = 1.5$, and $D_1 = D_2 = 0.05$. The results obtained with the one- and two-term truncated models are plotted together with the numerical solutions of the governing PDEs. In this case, it can be seen that the bifurcation curves have a unique steady-state branch, which means that there is only one steady-state solution in the considered concentration range. It can also be seen that u decreases and v increases as δ increases. In contrast, Figure 4a,b exhibit the bifurcation pattern of the breaking-wave type for the same parameter values as those of Figure 3a,b except for $\alpha = 0.1$ and $\beta = 2.5$. In this case, the steady-state branch folds back on itself in the interval $\delta \in (0.58, 1.09)$, giving rise to two turning points. Between these points, the system admits multiple steady-state solutions with a steep decline in the autocatalyst concentration u . The concentration of the reactant v increases sharply near the bifurcation point $\delta = 1.088$. The two-term semi-analytical approximation model is found to be accurate across the unique and breaking-wave steady-state patterns, with solutions in close agreement with numerical solutions of the governing PDE.

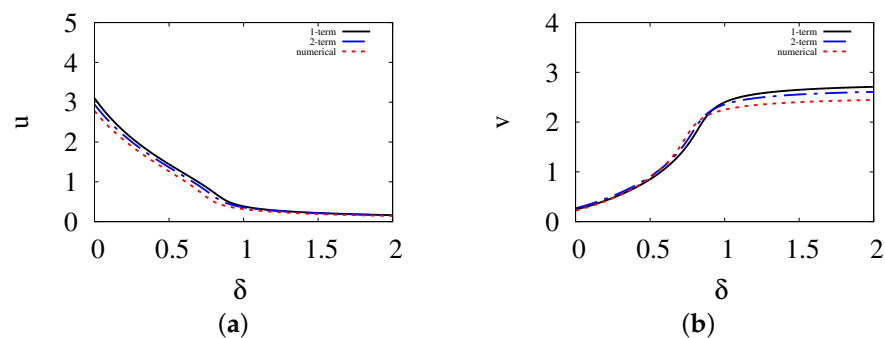


Figure 3. Bifurcation diagrams for (a) autocatalyst concentration u and (b) reactant concentration v versus δ at the centre of the annulus r_c . A unique steady-state pattern is exhibited. The parameter values used are $r_1 = 0.2$, $\alpha = 0.3$, $\beta = 1.5$, and $D_1 = D_2 = 0.05$.

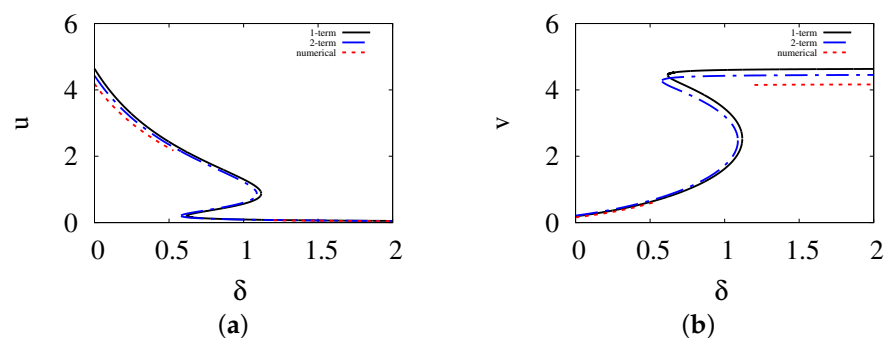


Figure 4. Bifurcation diagrams for (a) autocatalyst concentration u and (b) reactant concentration v versus δ at the centre of the annulus r_c . A breaking-wave pattern is exhibited. The parameter values are the same as in Figure 3, except $\alpha = 0.1$ and $\beta = 2.5$.

4. Singularity Theory

Singularity theory provides a systematic tool to find the complete set of steady-state solutions of ODE systems, as shown in [40]. This approach was used in [41] to describe bifurcation phenomena in chemical reactions, specifically isolas and hysteresis. Several benchmarks including first-order, non-isothermal CSTR models were used to demonstrate the usefulness of the method.

This section uses singularity theory to investigate the semi-analytical approximation model (2). This allows the construction of a map of the parameter space showing the regions yielding the primary bifurcation behaviors, namely unique steady-state and breaking-wave patterns. For the steady-state scenario, the two-term semi-analytical approximation model is expressed by the following general formula:

$$f_i(u_j, v_j, \alpha, \delta, \beta, d_j) = 0, i = 1, \dots, 4, j = 1, 2. \quad (6)$$

Consequently, δ is chosen as bifurcation parameter. The unique and breaking-wave steady-state behaviors discussed in Section 3 are directly related to the emergence of a hysteresis bifurcation curve, which is obtained by imposing the conditions below:

$$\frac{d\delta}{du_1} = 0, \frac{d^2\delta}{du_1^2} = 0. \quad (7)$$

The first condition indicates that the steady-state branch has a turning (fold) point. The second condition implies that this fold is degenerate, where two fold points merge to form a cusp. Therefore, the system shifts from a unique steady state to a region of multiple steady states with hysteresis behavior. Since (6) defines an implicit relation in the model

with respect to δ , the criteria in (7) have to be implemented using implicit differentiation. Thus, the first total derivative of (6) with respect to u_1 , under constraints (7), is

$$\frac{df_i}{du_1}(u_j, v_j) = f_{i u_1} + f_{i u_2} \frac{du_2}{du_1} + f_{i v_1} \frac{dv_1}{du_1} + f_{i v_2} \frac{dv_2}{du_1} = 0, i = 1, \dots, 4, j = 1, 2, \quad (8)$$

where f_i are defined as functions of u_1, u_2, v_1 , and v_2 . This implies that the functions f_i vary with u_1 explicitly and implicitly through the other variables. Note that the remaining parameters are held constant. The second total derivative of (6) under condition (7) becomes

$$\frac{d^2 f_i}{du_1^2}(u_1, v_1, u_2, v_2) = 0, i = 1, \dots, 4. \quad (9)$$

The hysteresis bifurcation points for the two-term approximation model are obtained by evaluating (6), (8) and (9) via Maple. Under the one-term approximation, these hysteresis conditions reduce to

$$f = f_{u_1} = f_{u_1 u_1}. \quad (10)$$

Figure 5 illustrates how the α - β parameter space is divided into two regions that dictate the various bifurcation states. Here, the hysteresis curves for the one- and two-term semi-analytical approximations are mapped with $r_1 = 0.2$ and $d_1 = d_2 = 0.05$. The parameter space to the left of the hysteresis curve generates a breaking-wave pattern with multiple steady-state solutions, whereas the domain to the right corresponds to a bifurcation pattern with a unique steady-state solution. Generally speaking, both hysteresis curves follow a linear upward trend as δ increases. These curves are governed approximately by the linear equations $\beta = 0.1445\delta + 0.099$ (one-term) and $\beta = 0.1576\delta + 0.0717$ (two-term). For context, the system configuration from Figure 3 ($\alpha = 0.3$ and $\beta = 1.5$) falls in the right of the curves in Figure 5, resulting in a unique steady-state pattern. On the other hand, the case shown in Figure 4 ($\alpha = 0.1$ and $\beta = 2.5$) is located on the left of the curve and demonstrates a breaking-wave pattern.

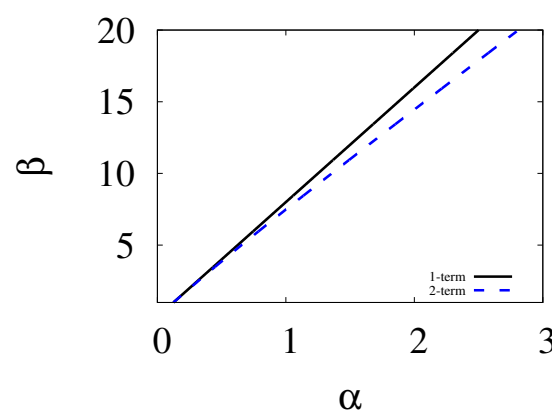


Figure 5. Partition of the α - β plane into regions corresponding to the different bifurcation diagrams. The parameters are $r_1 = 0.2$ and $d_1 = d_2 = 0.05$.

5. Local Stability and Oscillatory Solutions

Oscillations and Hopf bifurcations are basic phenomena that occur frequently in many biological and chemical systems. The theory of Hopf bifurcations is well developed in the literature on dynamical systems and bifurcations (see, for instance, Guckenheimer and Holmes [42] or Golubitsky and Schaeffer [43]). In particular, these bifurcations have been described within the context of a one-dimensional Schnakenberg reaction–diffusion cell by Al Noufaey [10,11], who used the Jacobian matrix of a lower-order ODE system to analyze

stability. The method successfully identified a region in the parameter space where Hopf bifurcations occur. In this section, the stability of the semi-analytical model (2) is studied and analyzed. By computing degenerate Hopf points, we construct a semi-analytical map to predict the emergence of Hopf bifurcations and limit cycles. The theoretical predictions are compared with numerical simulations to validate the method.

We first investigate the stability of the system of ODEs (5) describing the two-term semi-analytical approximation model. In this case, the Jacobian matrix J_m is

$$J_m = \begin{bmatrix} \frac{\partial f_1}{\partial u_1} - \kappa & \frac{\partial f_1}{\partial v_1} & \frac{\partial f_1}{\partial u_2} & \frac{\partial f_1}{\partial v_2} \\ \frac{\partial f_2}{\partial u_1} & \frac{\partial f_2}{\partial v_1} - \kappa & \frac{\partial f_2}{\partial u_2} & \frac{\partial f_2}{\partial v_2} \\ \frac{\partial f_3}{\partial u_1} & \frac{\partial f_3}{\partial v_1} & \frac{\partial f_3}{\partial u_2} - \kappa & \frac{\partial f_3}{\partial v_2} \\ \frac{\partial f_4}{\partial u_1} & \frac{\partial f_4}{\partial v_1} & \frac{\partial f_4}{\partial u_2} & \frac{\partial f_4}{\partial v_2} - \kappa \end{bmatrix}.$$

The entries of J_m are the first-order partial derivatives of the nonlinear ODE functions f_i , evaluated at the equilibrium state (u_1, v_1, u_2, v_2) . Consequently, the Jacobian provides a linear approximation of the nonlinear dynamics in a neighbourhood of the steady state and describes how small perturbations evolve over time. Assuming perturbations of the exponential form,

$$\chi(t) = ce^{\kappa t},$$

where c is a constant vector and κ is the growth rate, substitution into the linearized system gives

$$(J_m - \kappa I)c = 0.$$

Nontrivial solutions exist only if

$$\det(J_m - \kappa I) = 0,$$

which is the characteristic equation of the Jacobian matrix. Since the reduced semi-analytical model contains four state variables, the characteristic polynomial is of the fourth degree,

$$\kappa^4 + \omega_1\kappa^3 + \omega_2\kappa^2 + \omega_3\kappa + \omega_4 = 0, \quad (11)$$

where

$$\omega_1 = 73.25d_1 + 73.25d_2 + 1.25u_1^2 + 1.25u_2^2 + 2\delta - 2.5u_1v_1 - 2.5u_2v_2.$$

$$\begin{aligned} \omega_2 = & 1.25u_1v_1u_2v_2 + 40.05u_2^2d_2 + 51.51u_1^2d_2 - 0.19u_1^2u_2^2 - u_1^2v_2^2 - u_2^2v_1^2 \\ & + 1.5u_1^2v_1^2 + 1.5u_2^2v_2^2 + 73.25\delta d_1 - 1.5u_1^3v_1 - 1.5u_2^3v_2 + 2.5\delta u_1^2 + 2.5\delta u_2^2 \\ & + 146.5\delta d_2 + 91.56d_1u_1^2 + 91.56d_1u_2^2 + 5365.38d_1d_2 + \delta^2 + 849.48d_1^2 \\ & + 0.38u_2^4 + 0.38u_1^4 - 2.5\delta u_2v_2 - 80.11d_1u_2v_2 - 2.5\delta u_1v_1 - 103.02d_1u_1v_1 \\ & - 1.84d_1u_1v_2 - 1.84d_1u_2v_1 + 1.84d_2u_1u_2 + 0.38u_1v_1u_2^2 - 183.12d_2u_2v_2 \\ & - 183.12d_2u_1v_1 + 0.38u_1^2u_2v_2 + 849.48d_2^2, \end{aligned} \quad (12)$$

while the coefficients ω_3 and ω_4 are too long to be presented here.

The Hopf bifurcations occur precisely when a single pair of eigenvalues κ is purely imaginary, which implies

$$q = \omega_4\omega_1^2 + \omega_3^2 - \omega_1\omega_2\omega_3 = 0. \quad (13)$$

Thus, the degenerate Hopf points are determined by solving the following conditions:

$$f_i = q = \frac{dq}{d\delta} = \frac{df_i}{d\delta} = 0, \quad i = 1, \dots, 4. \quad (14)$$

Figure 6 shows the degenerate Hopf curve mapped across the α - β parameter plane. The figure compares the numerical solution of (2) with the two-term semi-analytical approximate solutions derived from (5) for fixed parameters $r_1 = 0.2$ and $d_1 = d_2 = 0.05$. By solving the conditions in (14), the degenerate Hopf curve is obtained. This curve divides the parameter space into two regions, with the part below the curve containing only stable solutions without Hopf bifurcation points and the part above the curve containing Hopf bifurcations. We can see that the two-term semi-analytical approximation aligns closely with the numerical simulation of the PDE system. For example, at $\delta = 6.01$, the numerical values are $(\alpha, \beta) = (2.20, 6.14)$. At the same position, the two-term semi-analytical approximation yields values of $(\alpha, \beta) = (2.198, 6.31)$. The errors in these estimates are less than 3%.

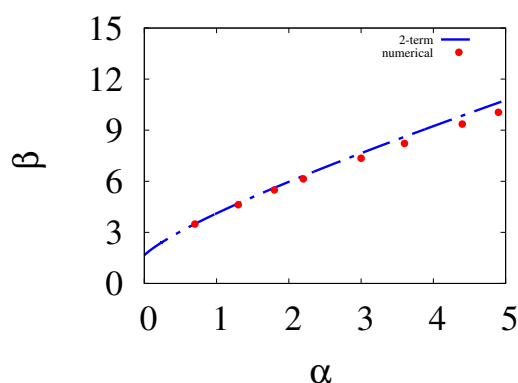


Figure 6. Degenerate Hopf bifurcation curve in the α - β parameter space. The other fixed parameters are $r_1 = 0.2$ and $d_1 = d_2 = 0.05$.

The dynamic behavior of the system in Figure 7a approaches a limit cycle in the u - v phase plane. Complementing this, Figure 7b,c show the temporal evolutions of the concentrations u and v , respectively, demonstrating how the system approaches steady oscillatory dynamics. The chosen parameter values are $r_1 = 0.2$, $\delta = 4.56$, $\alpha = 1.5$, $\beta = 5.7$, and $d_1 = d_2 = 0.05$. Figure 7 illustrates the trajectories obtained from the two-term semi-analytical approximation with the numerical solution. Because these parameters are in the region above the Hopf bifurcation curve shown in Figure 6, the obtained limit cycle matches the theoretical predictions of the underlying ODE model (5). From these figures, the period and the amplitude of the oscillations can be deduced. The value of the period obtained from the numerical solution is 3, which is close to the two-term semi-analytical value of 2.89. Moreover, the two-term semi-analytical model predicts oscillation amplitudes of 1.548 for the autocatalyst and 3.481 for the reactant, which are in close agreement with the numerical amplitudes of 1.637 and 3.432 for u and v , respectively.

To investigate another dynamical regime, a second set of parameters are evaluated: $r_1 = 0.2$, $\delta = 4.56$, $\alpha = 1.5$, $\beta = 4.8$, and $d_1 = d_2 = 0.05$. This configuration is also below the Hopf bifurcation curve shown in Figure 6, but it produces a non-oscillatory response. The corresponding time series of the autocatalyst and reactant concentrations are shown in

Figure 8a,b. For $t > 50$, the system converges to a steady state. In particular, the steady-state concentrations converge to $(u, v) \simeq (0.917, 4.533)$ for the two-term approximation model and $(u, v) \simeq (0.854, 4.455)$ for the numerical solution of the governing PDEs (2). The comparative data in Figures 7 and 8 demonstrate the robustness and precision of the two-term semi-analytical approximation model results with respect to the numerical solutions.

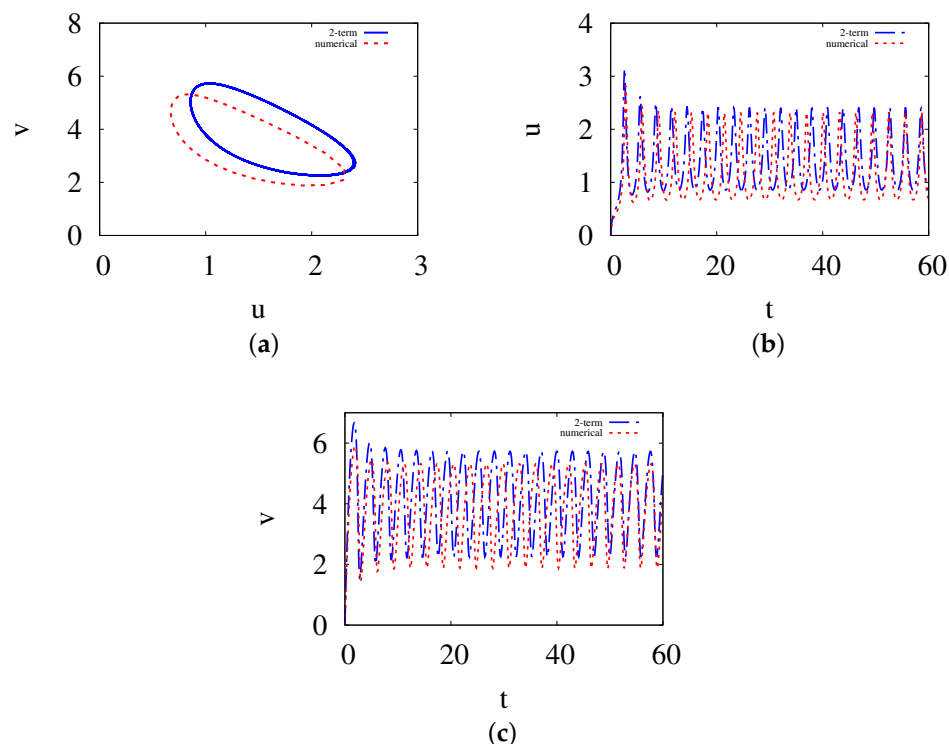


Figure 7. Plots of (a) the limit cycle in the u - v phase plane and the time evolution of (b) u and (c) v against t . The parameter values are $r_1 = 0.2$, $\delta = 4.56$, $\alpha = 1.5$, $\beta = 5.7$, and $d_1 = d_2 = 0.05$.

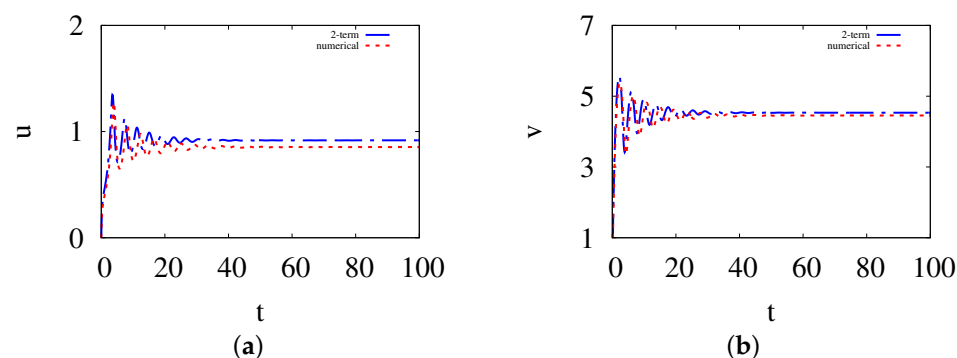


Figure 8. Evolution of the concentrations (a) u and (b) v with time t . The parameters are $r_1 = 0.2$, $\delta = 4.56$, $\alpha = 1.5$, $\beta = 4.8$, and $d_1 = d_2 = 0.05$.

6. The Effect of Altering the Thickness of the Annulus

This section examines the effect of altering the inner edge radius of the annulus $r_1 \in (0, 1)$. The semi-analytical model can be used to determine the transitions in the bifurcation diagrams and changes to the parameter regions where Hopf bifurcations occur as the value of r_1 is varied. However, this presents significant computational challenges due to the change in the model of the ODEs as r_1 changes. In biological systems, varying the thickness of an annular domain directly influences the effective diffusion path and the spatial constraints under which morphogens interact. Our results demonstrate that altering this geometric parameter dictates whether the Schnakenberg system exhibits steady-state

multiplicity, underlying localized pattern selection, or undergoes Hopf bifurcations, leading to sustained spatio-temporal oscillations. Biologically, this means that tissue geometry and domain growth can act as primary mechanical triggers that control either the static zoning of cell fates or the onset of periodic, dynamic signaling waves without requiring a change in the underlying biochemical reaction kinetics, see [44–47].

Figure 9 illustrates the partition of the α – β parameter space, contrasting the various bifurcation diagrams corresponding to different values of annulus thickness, namely $r_1 = 0.1$, $r_1 = 0.3$, and $r_1 = 0.7$. The parameters are $d_1 = d_2 = 0.05$. Altering the thickness of the reactor, defined by $1 - r_1$, induces substantial shifts in the bifurcation diagrams. Specifically, increasing the inner radius of the annulus r_1 shifts the hysteresis curve to the left, which expands the parameter space in which unique steady-state patterns can occur and shrink the breaking-wave region. Figure 10 shows bifurcation diagrams of the concentrations u and v for two different annuli. The inner radius is $r_1 = 0.1$ in Figure 10a,b, whereas it is $r_1 = 0.4$ in Figure 10c,d. The parameters used to create these are $d_1 = d_2 = 0.05$, $\alpha = 0.1$, and $\beta = 2.5$. The system displays the breaking-wave pattern at $r_1 = 0.1$ and then transitions to the unique steady-state pattern when the inner radius is increased to $r_1 = 0.4$. Hence, reducing the thickness of annulus suppresses the emergence of multiple steady-state solutions.

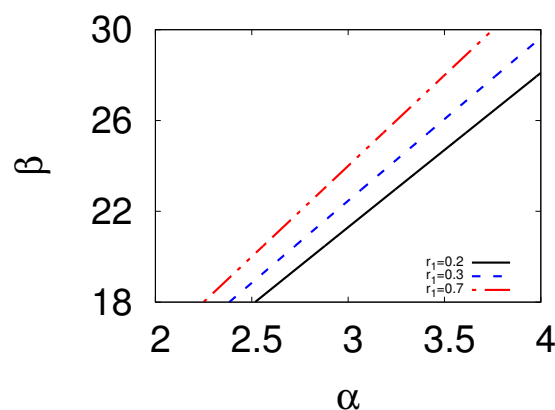


Figure 9. Partition of the α – β plane into regions corresponding to the different bifurcation diagrams for different values of annulus thickness: $r_1 = 0.1$, $r_1 = 0.3$, and $r_1 = 0.7$. The parameters are $d_1 = d_2 = 0.05$.

Figure 11 displays the Hopf curves across the α – β and d_1 – d_2 parameter planes for three different values of r_1 : 0.2, 0.5, and 0.7. The parameters are $d_1 = d_2 = 0.05$ in Figure 11a, shown as the one- and two-term semi-analytical solutions, whereas in Figure 11b, they are $\alpha = 2$ and $\beta = 6$, shown as the two-term semi-analytical model and numerical solutions of PDE. It can be clearly seen that with increasing r_1 , the degenerate Hopf curve moves upwards in Figure 11a and downwards in Figure 11b. This also expands the overall parameter space, and so the region where stable solutions can occur is enlarged. Consequently, the region where oscillatory behaviors can occur shrinks. For $r_1 = 0.5$ and $d_1 = 0.03$, the two-term semi-analytical solution yields $d_2 = 0.018$, which is in close agreement with the numerical value of $d_2 = 0.017$, with relative error less than 6%. Generally, a thin annulus, which corresponds to a large value of r_1 , leads to a reduction in the likelihood of Hopf bifurcations and oscillatory solutions.

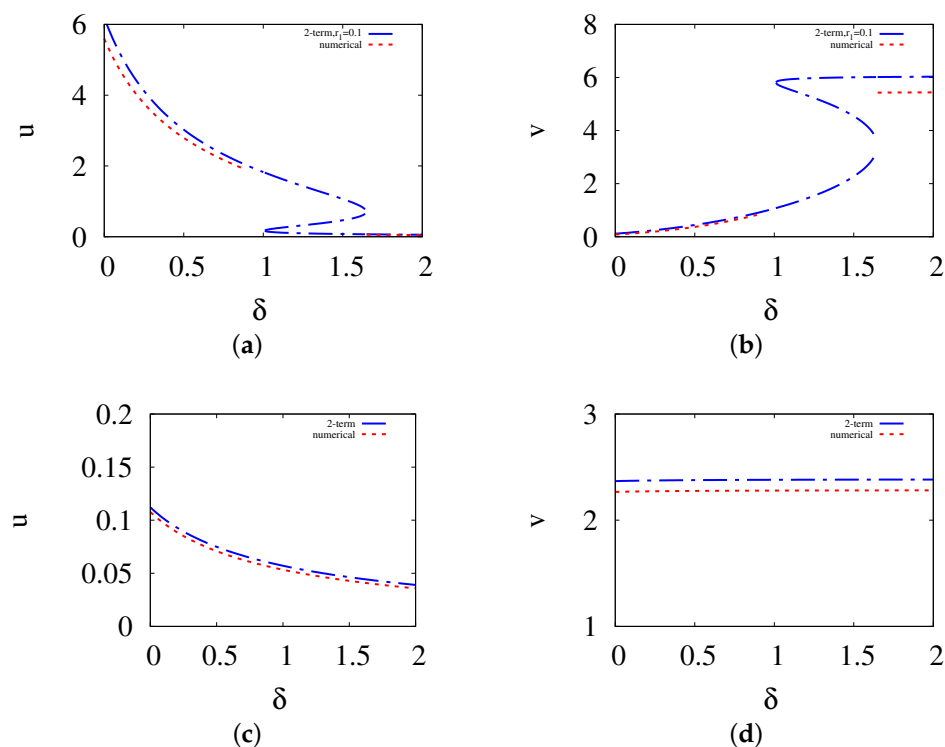


Figure 10. Steady-state autocatalyst u and reactant v concentration bifurcation diagrams versus δ for $r_1 = 0.1$ (showing the breaking-wave pattern in (a,b)) and $r_1 = 0.4$ (showing the unique steady-state pattern in (c,d)). The two-term semi-analytical solutions and the numerical solution are shown. The parameters used are $d_1 = d_2 = 0.05$, $\alpha = 0.1$, and $\beta = 2.5$.

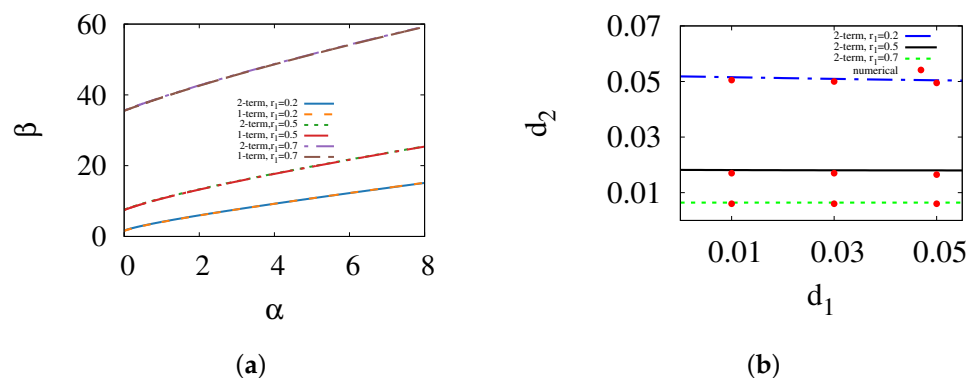


Figure 11. Hopf curves across the (a) α - β and (b) d_1 - d_2 parameter planes for three different values of r_1 : 0.2, 0.5, and 0.7. The other parameters used are $d_1 = d_2 = 0.05$ in (a) and $\alpha = 2$ and $\beta = 6$ in (b).

7. Conclusions

In this paper, semi-analytical solutions have been constructed to investigate the Schnakenberg model within a reaction–diffusion annulus. Both the singularity behavior and stability of the model have been considered. The influence of the annular thickness on the system has been studied, and it has been shown that the behavior of the model is very complex, especially with respect to the bifurcation patterns and Hopf bifurcation points. A thicker annulus usually expands the region of the parameter space in which multiple steady-state and Hopf bifurcations occur. Comparing these results with numerical solutions indicated that the two-term semi-analytical approach yields a high accuracy.

Future work may include the study of symmetry-breaking Hopf bifurcations and the existence and stability of rotating waves in annular reactors. Furthermore, the annular

reaction–diffusion framework developed here could be extended to chemically realistic models with experimental relevance, such as the Brusselator, Selkov, or Belousov–Zhabotinsky reaction schemes.

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Abbreviations

The following abbreviations are used in this manuscript:

ODEs	Ordinary differential equations
PDEs	Partial differential equations
CSTRs	Continuous-flow well-stirred tank reactors

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