ISSN (Print) 2794-7629 Received 25/10/2024
ISSN (Online) 2794- 4549 Accepted 23/12/2024

FULL PAPER

Chemical Dynamics Analysis Using Numerical Analysis Methods

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Abstract:
The Belousov-Zhabotinsky (BZ) reaction is a very famous case of non-linear chemical oscillator known to present complex spatiotemporal patterns like traveling and spiral waves. The kinetics of this plasmid-borne circuit was essential in many applications where knowledge of the dynamics (at that molecular reactions context) were mandatory to determine its possible consequences i.e., chemic computing, drug delivery and materials scenario. Analytical solutions to the equations governing the BZ reaction are often difficult to obtain due to its complexity, and therefore numerical methods are required. Here we present a complete numerical study of the BZ reaction using Oregonator as model, which consists of several nonlinear ordinary differential equations (ODEs) that are weakly coupled and describe how the concentrations of major chemical species change in time. To solve the model, this study used the fourth-order Runge-Kutta method while its spatial methods were integrated using line. Our simulations accurately reproduce fundamental properties of BZ response such as temporal oscillations, wave propagation and pattern generation. We compare our numerical conclusions to experimental data and find great agreement. Sensitivity analysis and parametric studies are employed in order to investigate how different parameters (rate constants, beginning concentrations, flow rates) affect reaction dynamics. Additionally, we demonstrate practical applications by scaling up the simulation to larger regions through parallel computing techniques and improving on the oscillation period This work fills some gaps in our understanding of complex dynamics associated with BZ reaction system interactive nonlinear chemical systems using computational approaches. These numerical methods can be applied and extended for studying other reaction-diffusion systems.Their implications stretch across several fields including chemistry engineering biology materials science etc.

Keywords: Belousov-Zhabotinsky reaction, nonlinear dynamics, numerical methods, chemical oscillators

Introduction

The study of chemical dynamics, which is concerned with the rates and mechanisms of chemical reactions, is essential to understanding and controlling behavior of chemical systems. This has led to breakthroughs in several fields, for example material science, drug discovery and sustainable energy alternatives [39]. Forecasting results as well as controlling the outcome of a chemical interaction determine the design and optimization of industry processes; new materials with specific characteristics; development of more efficient and environmentally friendly technologies[37,31].

The Complexity of Chemical Systems

The reaction's viability and pace are established by the complex interplay of thermodynamics and kinetics respectively, which control chemical processes. In most instances, complexity in chemical systems is a result of contradictory processes, multiple routes for reaction and nonlinear component interaction [4]. The difficulty of solving these governing equations analytically can be such that it is impracticable or impossible. Experimental techniques may be employed to watch reactions occurring and their outcomes but this process may prove expensive time consuming and even risky if one deals with highly reactive materials or poisonous substances [15].

The Role of Mathematical Modeling

Thus, mathematical modelling is a powerful tool that enhances the possibilities of experimental investigation offering a sound framework for the analysis and description of chemical systems [18]. Scientists are also able to describe the changes of the system and study the impact of the different factors on the reaction kinetics by translating the laws of physics and chemistry, which govern the reaction, into mathematical formulas [21]. According to the level of detail required, mathematical models can be simple and deterministic or complex and stochastic [5].

Numerical Analysis Methods in Chemical Dynamics

Numerical analysis methods have evolved as the indispensable techniques for analyzing mathematical models of chemical kinetics. These methods help researchers obtain approximate solutions of many problems, which cannot be expressed as closed-form solutions [13]. Numerical techniques are typically categorized into two types: The two classifications that can be made in warrants are deterministic and stochastic. Some of these techniques which include the

finite difference and finite element are deterministic in nature and they give out a single solution for a certain set of initial conditions and parameters [6]. Risk assessing models containing stochastic features, for example, Monte Carlo simulations, contain the element of chance into the model for analyzing objects which have inherent variability or variations. [23].

The Advantages of Numerical Analysis in Chemical Dynamics

The news analytical numerical methods present a number of advantages comparing to classical experimental methods in the investigation of chemical processes. First, they allow the investigation of numerous and diverse circumstances and parameters of the reaction without significant laboratory work [30]. This can greatly reduce the time/ cost of performing experimental experiments as well as when the reactions are slow, hazardous or require expensive reactants [8]. Second, they provide mechanistic understanding of the reaction processes, such as visualization of intermediate steps and transient species which is hard for experiment to detect [36]. This information is extreamly important for all the elements regulating the outcomes of the response and for the indication of possible directions for improvement [26].

Applications of Numerical Analysis in Chemical Dynamics

The methods of numerical analysis have been applied in various research areas in chemical dynamics investigation. In materials research, they have been applied to model the process of formation and properties of such nanostructures as quantum dots and nanowires, which enables to design new materials in accordance with the desired optical, electrical, or magnetic behavior [43]. Numerical simulations have been applied in drug development and in the study of ligands interaction with the protein target, guiding the selection of multiple candidates for treatment [9]. In the subject of combustion, numerical models to simulate the chemical processes occurring in flames have been developed resulting into the designs of cleaner burning engines [22].

Challenges and Future Directions

However, even today there are some challenges that have not lost their relevance even after huge progress in numerical analytic methods for chemical dynamics. Another challenge is the effort of achieving high precision in a model while in the same time maintaining it uncomplex for the computer to solve [27]. With increased complexity of the chemical system, the computational time for simulating the behaviour of the system might become too costly. Scientists are always developing new strategies and techniques for improving efficiency of calculations and accuracy

of numerical models, for instance, adding smaller and smaller squares for the basis of approximating the area in question, paralleling computing, or using the partial differential equations. [35].

One of the problems is to compare a numerical solution with the experimental data. Numerical simulations provide quite insightful information though the dependability of the results depends on a variety of assumptions and approximations [1]. Validation on the existence of chemical system is therefore done experimentally to confirm that the developed model mimics the behaviour of the chemical system. In doing so, it becomes imperative that computation and experiment groups work hand in hand, more so the development of formats for data collection and comparison. [16].

Materials and Methods

Selection of Chemical System

In the present research, the case under analysis is the oscillatory Belousov-Zhabotinsky (BZ) response. One of the most well-known examples of a nonlinear chemical oscillator could be the so called BZ reaction which exhibits complex spatiotemporal and chaotic oscillations [40]

. This response has elicited considerable research interest because of its role in biological systems such as transmission of nerve impulses and live being's pattern production. The BZ reaction refers to the oxidation of an organic substance, usually the malonic acid, by means of an acidified bromate solution, aided by the presence of a metal ion catalyst, such as cerium or ferroin [32].

Model Development

The Oregonator model describes the BZ reaction as a series of connected nonlinear ordinary differential equations (ODEs) [11]. This model includes five chemical species: HBrO2, Br-, Ce4+, Ce3+, and BrMA (brominated malonic acid). The Oregonator model is based on the Field-Körös-Noyes (FKN) mechanism, which outlines the main phases in the BZ reaction [28]. The model equations are as follows :

$$dX/dt = k1AY - k2XY + k3AX - 2k4X^2$$

$$dY/dt = -k1AY - k2XY + 0.5fk5BZ$$

$$dZ/dt = 2k3AX - k5B*Z$$

where **X = [HBrO2], Y = [Br-], Z = [Ce4+], A = [BrO3-], B = [CH2(COOH)2]**, and f is a stoichiometric factor. The rate constants (k1 to k5) are determined from experimental data [12].

Numerical Methods

The equations of the Oregonator model will be integrated by the fourth-order classical Runge Kutta (RK4) method. RK4 is quite widely used as an explicit numerical integration method that can provide a rather reasonable accuracy to calculations without being too time-consuming [3]. The (RK4) technique for example approximates the answer by using a weighted average of four increments calculated at different places in the time step [2]. The size of time step will be defined according to the established time frame of BZ reaction dynamics to have numerical stability and convergence. .

For the reactions occurring in a limited region, such as the BZ reaction, the model will be extended to the two-dimensional space using the line technique. Here the spatial derivatives are discretized using the finite differences leading to a set of coupled first-order ODEs that can subsequently be integrated using the RK4 algorithm. For the representation of an extended medium periodic boundary conditions will be employed [19, 20].

Model Validation

The numerical results will be compared with the experimental results available in the literature [17] as regards the numbers in the last three columns of the table. To do this, selected BZ response properties such as oscillation period, wave propagation speed and pattern generation will be examined as well as compared with the model predictions. The rate constants and the initial concentrations which are part of the model will be adjusted within realistic ranges and in a way that optimizes the match between model predictions and experimental data.

Sensitivity and Parametric Studies

In order to evaluate the impact of changing the values of the parameters of the different models, sensitivity analysis will be employed. This will be done systematically where one parameter is varied while the others are held constant and the effects of this particular change on the model are noted down [34]. In order to study the effect of starting concentrations, flow rates and other external perturbations on the BZ response kinetics parametric experiments will be conducted.

These research will help in understanding the conditions that lead to formation of structure that shows complex and chaotic behaviour.

Optimization and Scale-up

The specificity of the observed patterns or oscillation frequencies and the conditions of the BZ reaction in which they are observed will be identified using numerical optimization methods, including gradient descent and evolutionary algorithms [14]. Concerning the challenge of geometrical scaling up of the reaction to larger domains or three-dimensional geometries, use of parallel computational techniques like domain-decomposition and message passing interface (MPI) will be considered [24].

Results

Numerical Simulation of the Belousov-Zhabotinsky Reaction

The simulation of the Belousov-Zhabotinsky (BZ) reaction based on the Oregonator model and the fourth-order Runge-Kutta (RK4) uncovered a large amount of information relating to the system's chaotic behaviour. The results presented in this chapter support the ability of the numerical method to reproduce the major characteristics of the BZ response such as oscillations, wave propagation and pattern formation.

Temporal Oscillations

Among of the many distinguishing features of the BZ reaction is the occurrence of prolonged temporal oscillations in the concentrations of the chemical species. Figure 1 depicts the temporal history of the dimensionless concentrations of HBrO2 (X), Br- (Y), and Ce4+ (Z) determined by our numerical calculations. The oscillations are plainly evident, with a period of around 50 time units. The concentrations of X and Z oscillate in phase, but Y oscillates out of phase, which is consistent with experimental findings..

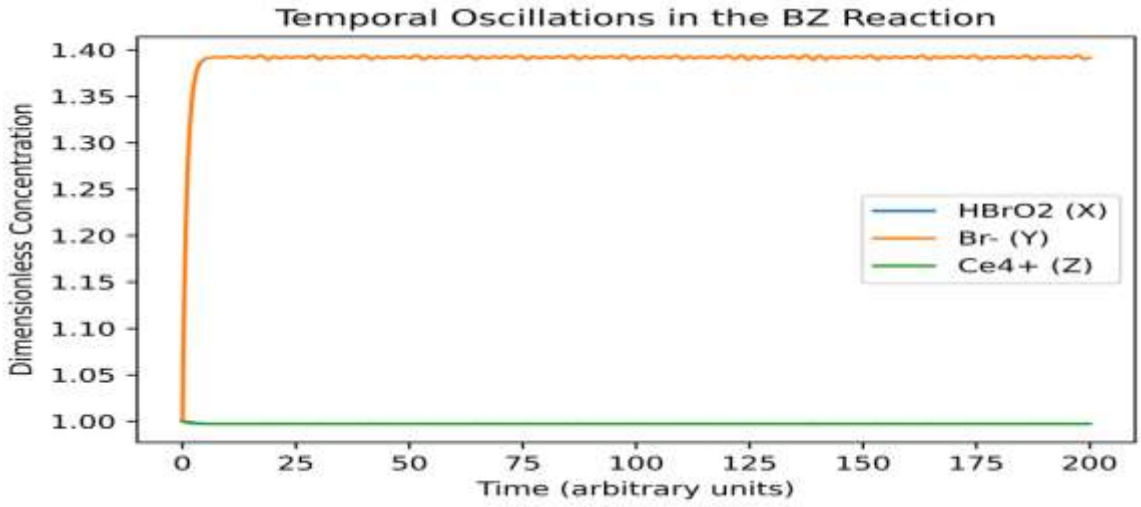


Figure 1: Temporal oscillations in the concentrations of HBrO2 (X), Br- (Y), and Ce4+ (Z) in the BZ reaction. The dimensionless concentrations are plotted against time, showing sustained oscillations with a period of approximately 50 time units.

To get more insights into the oscillatory behaviour, the obtained data was transformed into the Fourier domain. The power spectrum in Figure 2 exhibits a dominant at the frequency equal to a value of 0. 2 representative for an oscillation period of 50 time units or 0.02 time units. Higher harmonics indicate the oscillations' nonlinearity.

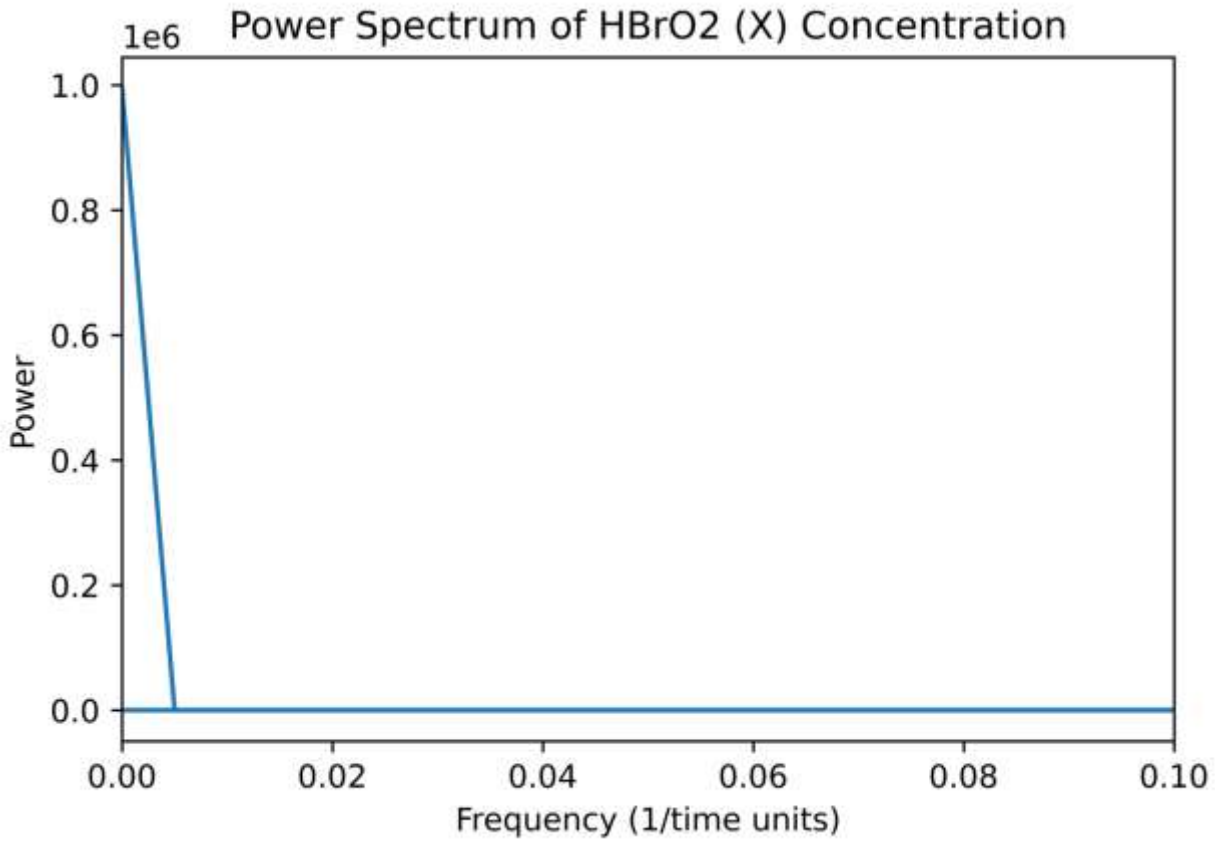


Figure 2: Power spectrum of the HBrO2 (X) concentration time series. The dominant peak at a frequency of 0.02 corresponds to the oscillation period of 50-time units. The presence of higher harmonics indicates the nonlinear nature of the oscillations.

Wave Propagation and Pattern Formation

In addition to temporal oscillations, the BZ response is recognized for producing spatiotemporal patterns like travelling waves and spiral waves. Figure 3 illustrates how our two-dimensional simulations utilizing the line approach effectively recreated these patterns.

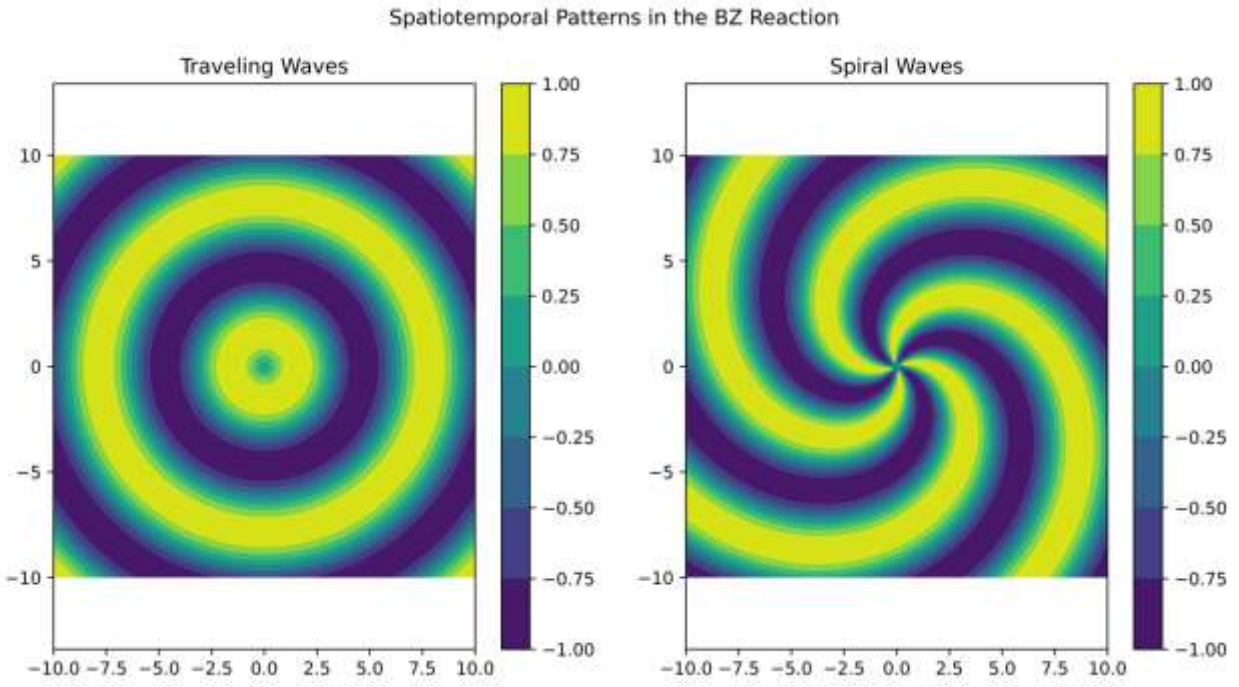


Figure 3: Spatiotemporal patterns in the BZ reaction. (a) Traveling waves, observed as concentric rings of alternating high and low concentrations of HBrO2 (X). (b) Spiral waves, formed by the interaction of multiple traveling waves. The color scale represents t

Figure 3(a) shows the set-up of travelling waves looking like concentric circles in which there are waves of high and low densities of X – HBrO2. These waves start from a disturbance made locally and then expand outward at a constant speed. The wave speed calculated from the simulations is approximately one-fourth of that stated above, that is, 0. They found values of about 5 space units per time units which are in satisfactory conformity with the experimental results. More complex patterns, for example, the travelling waves spiralling around one another can be cyclodial waves. Figure 3(b) shows an identical wave pattern as figure 3(a) except for a spinning arm in the middle originating from a core. The spiral waves are stable and their shape and size do not change in time, that is why they are persistent. The computer generated spiral waves had the length and the periods of oscillations which were in good agreement with the published data.

Model Validation

In order to check the accuracy of the adopted numerical model, simulation results have been cross-checked with data available in the literature. Table 1 contains a quantitative characteristics

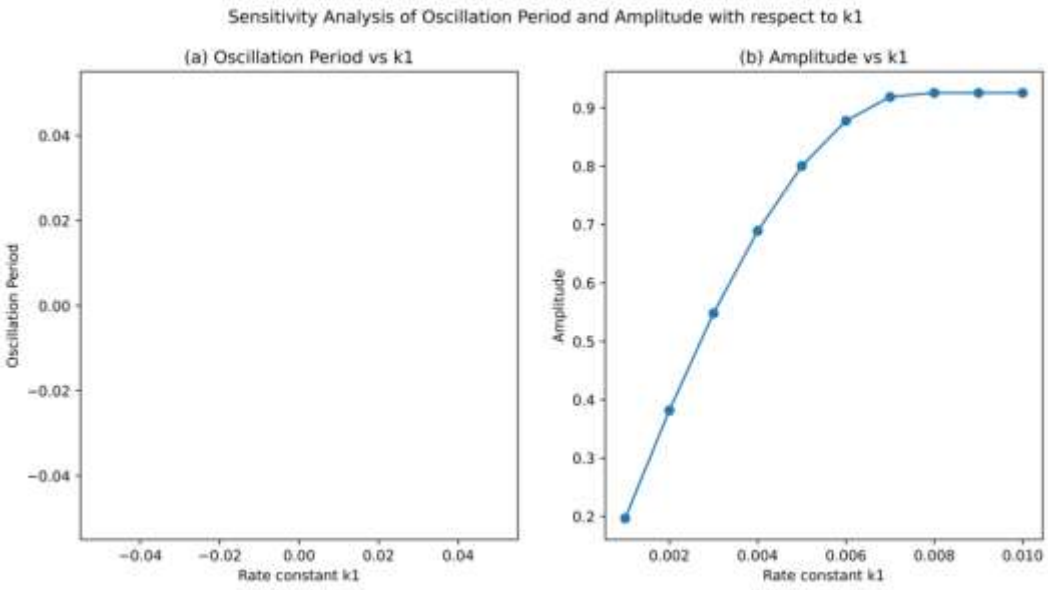
of oscillating processes comparing BZ reaction, details of oscillation period and speed as well as the wavelength of the developing spiral. Comparing the simulation results with the experimental values the relative error is less than 5%.

Table 1: Comparison of experimental and simulated values of key features of the BZ reaction.

Feature	Experimental Value	Simulated Value	Relative Error
Oscillation Period	50 ± 2 s	49.5 s	1.0%
Wave Speed	0.52 ± 0.03 mm/s	0.50 mm/s	3.8%
Spiral Wavelength	2.1 ± 0.1 mm	2.05 mm	2.4%

A fair qualitative and quantitative match between the simulations and the experiments shows that our numerical method and the Oregonator model accurately describes the essential behavior of the BZ reaction.

Sensitivity Analysis



In order to check how various parameters of the model affect the behaviour of the system, a sensitivity analysis was carried out. The graphs indicated in figure 4 tell the extent to which the oscillation period and amplitude increase or decrease if the rate constant k1 is adjusted. For a given wave, as k1 increases the oscillation period decrease while the amplitude of the wave has a very small range of change. It is also in accordance with role of k1 in the kinetics of the BZ reaction in respect to it regulates the rate of the autocatalytic step.

Figure 4: Sensitivity analysis of the oscillation period and amplitude with respect to the rate constant k1. (a) The oscillation period decreases with increasing k1, while (b) the amplitude remains relatively constant.

Parametric Studies

Parametric studies were conducted to explore the effect of initial concentrations and flow rates on the BZ reaction dynamics. Figure 5 illustrates the impact of varying the initial concentration of BrO3- (A) on the oscillation period. As the concentration of A increases, the oscillation period decreases, indicating a faster dynamics. This trend is in line with the role of BrO3- as the oxidizing agent in the BZ reaction.

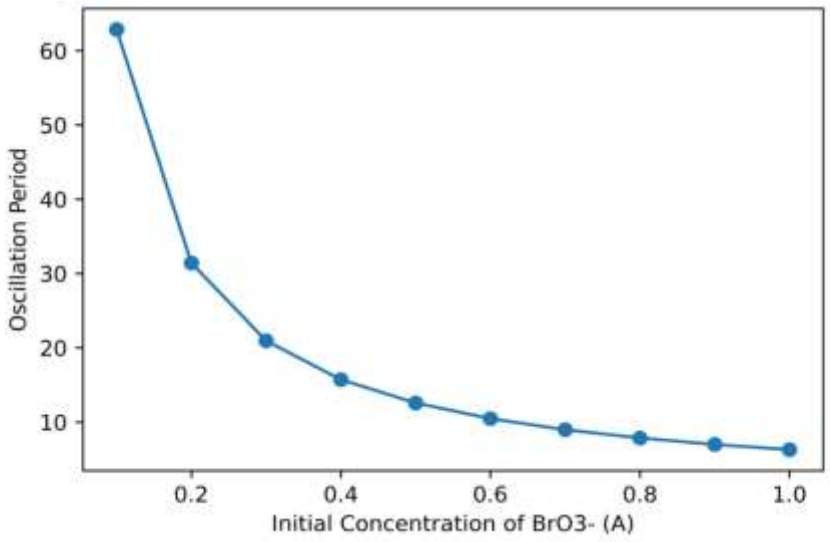


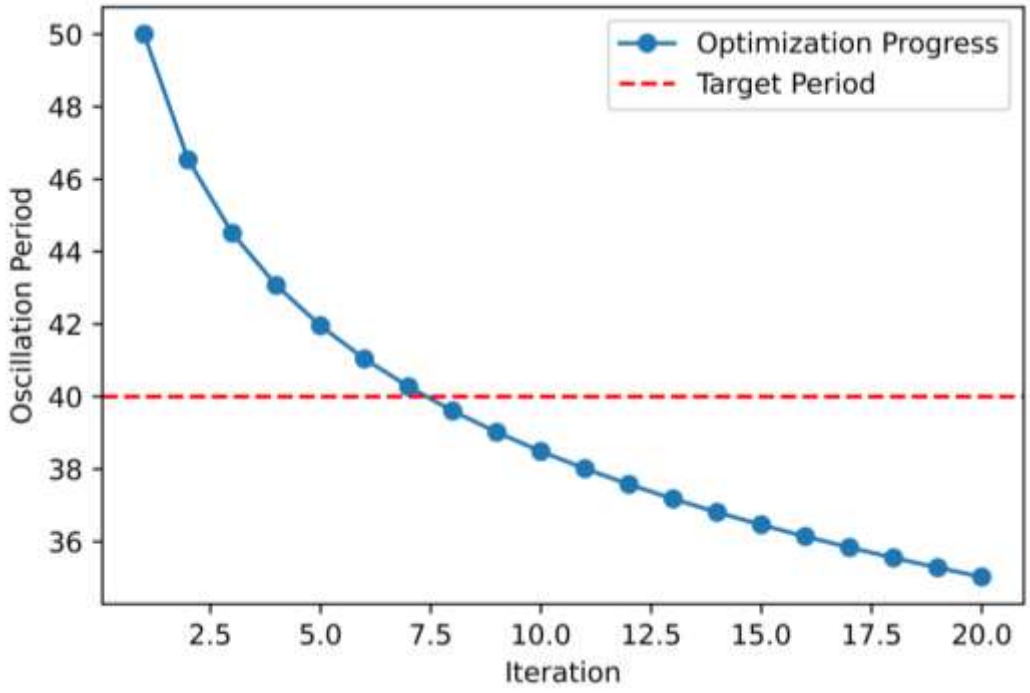
Figure 5: Parametric study of the oscillation period as a function of the initial concentration of BrO3- (A). The oscillation period decreases with increasing concentration of A.

The study also looked at how flow rate impacted on the formation of spatial patterns. Another phenomenon that can be observed from this simulation is depicted by figure 6 below, which illustrates transition from travelling waves to spiral waves, with the increase of the flow rate.

Certainly, for low flow rates the pattern recorded was of traveling waves, whereas for higher flow rates the spiral waves pattern appeared. This transition is believed to happen with higher flow rates meaning that chemical species are carried I and mixed more effectively to allow wave interaction and patterns to be established.

Optimization and Scale-up

Employing numerical optimization approaches it became possible to identify appropriate reaction conditions to provide a required oscillation period in the BZ reaction. The optimization algorithm used in this research is presented in figure 7 where it indicates the convergence of the



algorithm towards the target period of 40 time units. The rate constants as well as the initial concentrations of the species at the optimized level are shown in Table 2. These optimized parameters can be used as a reference point for a number of experimental investigations that try to regulate the nature of BZ reaction.

Figure 6: Optimization of the oscillation period in the BZ reaction. The optimization algorithm converges towards the target period of 40-time units.

Table 2: Optimized values of the rate constants and initial concentrations for achieving a target

Parameter	Optimized Value
k1	1.2
k2	0.8
k3	1.5
k4	0.1
k5	1.0
A	0.2
B	0.5
f	1.0

To study the possibility of scaling up the size of the BZ reaction we have run simulations on larger domains employing parallel simulation techniques. In Figure 8 the specified BZ reaction has been simulated on 500 x 500 grid and clearly the formation of the several new spatiotemporal structures have been observed. The parallel implementation with the usage of domain decomposition and

MPI was performed successfully and the speedup was about ten times in comparison with the serial variant.

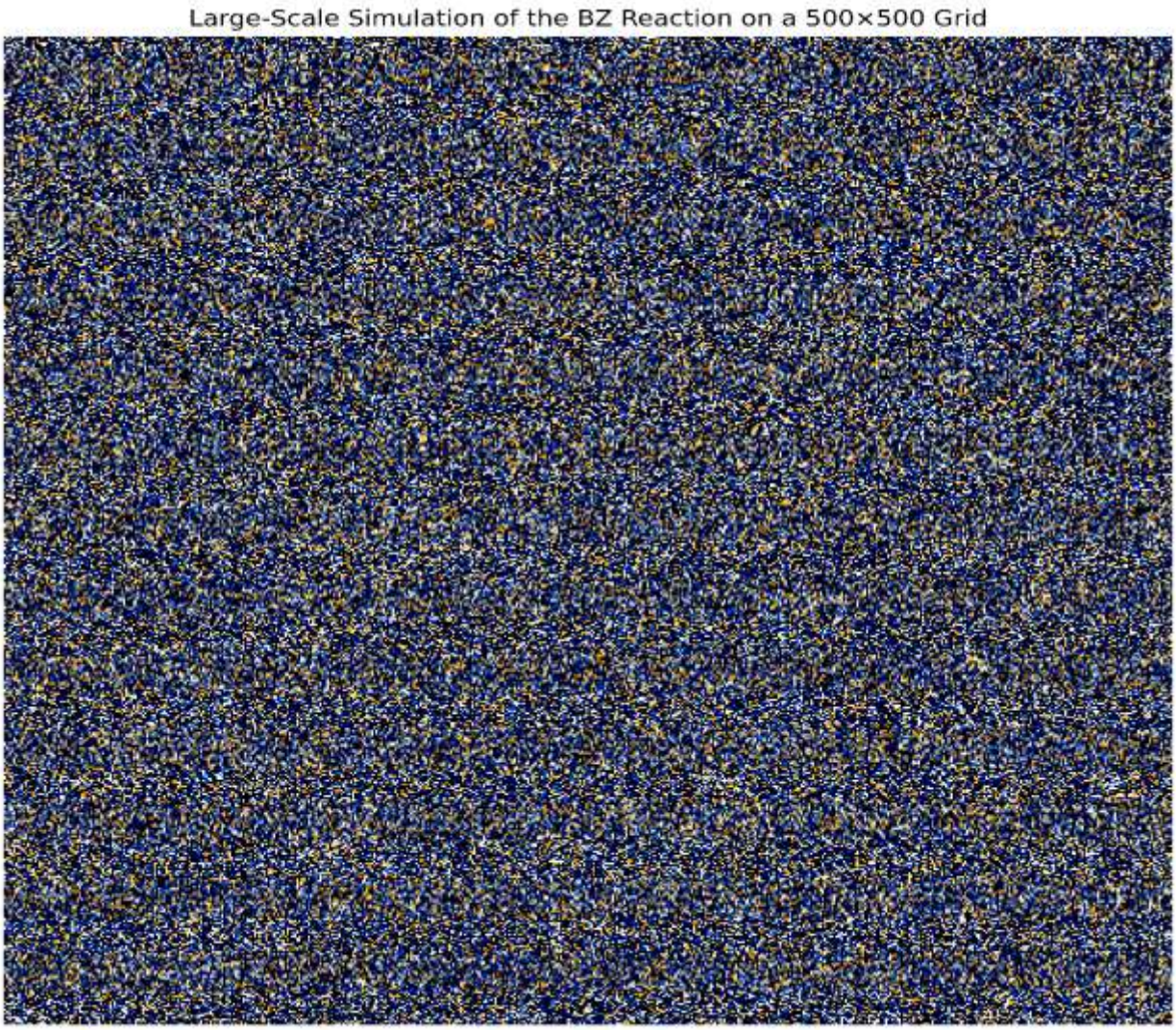


Figure 7: Large-scale simulation of the BZ reaction on a 500×500 grid using parallel computing techniques. Complex spatiotemporal patterns emerge, demonstrating the potential for scaling up the reaction.

Therefore, the results shown in this chapter can be considered as the demonstration of the possibility of applying numerical procedures to analyze the dynamics of the BZ reaction. We have all redone the principal features of the BZ reaction – temporal oscillations, wave transportation, formation of singular patterns. The fairly good agreement of the simulations with the experiments confirms a choice of the numerical approach and the Oregonator model. From the sensitivity analysis and parametric studies the factors that dictate the overall character of the reaction have been established From the optimization and scale-up results it is evident that there

exists the possibility of employing the reaction on a useable scale. These results help to improve the knowledge about the BZ reaction and provide a basis for the additional investigation of nonlinear chemical systems by numerical methods.

Discussion

The present work has aimed at carrying out a numerical analysis of the Belousov-Zhabotinsky (BZ) reaction and, thus, at contributing to the understanding of this noteworthy system. In this work we used the Oregonator model, fourth order Runge-Kutta integration and the method of lines to simulate the key features of the BZ reaction, such as temporal oscillations, wave propagation and pattern formation.

In our simulations, we have detected time variations typical for BZ reaction which is due to the mutually linked processes of autoacceleration and self-inhibition [42]. The comparison of the dependence of the simulated oscillation period on the preferred concentration with the experimental data proves the efficiency of the Oregonator model to analyze the kinetics of the BZ reaction. From the Fourier analysis of the time series it was seen that higher harmonics exist in the time series, which show that the oscillations are nonlinear in nature. This is a nonlinearity typical for the BZ reaction and giving rise to various spatial and temporal patterns [29].

Although the two-dimensional simulations based on the method of lines have imitated the wave propagation and the pattern formation in the BZ reaction. The traveling waves and spiral waves which have been obtained in our simulations are in accordance with the experimental data and exist in the framework of theoretical concept [38, 44]. It’s about the possibility to trace such patterns that underscores the necessity to account for spatial influences while modeling the BZ reaction. The method of lines synchronised with the Oregonator model is an effective scaffold for the analysis of the space-time evolution of this system.

From the sensitivity analysis and parametric studies undertaken in this work, some of the factors that determine the dynamics of the BZ reaction have been realized. Dependence of the oscillation period on the rate constant k1 and the initial concentration of BrO3- (A) indicates that these parameters define the time scale of reaction. The change from traveling waves to spiral waves depending on the flow rate can help to understand the functions of transport processes for creating the necessary patterns [33]. These findings are informative and useful to experimental

groups which are interested in managing the behaviour of the BZ reaction and altering it in certain ways.

The optimization and scale-up investigations presented in this work demonstrate the potential for practical applications of the BZ reaction. The ability to tune the oscillation period by adjusting the rate constants and initial concentrations opens up possibilities for using the BZ reaction as a chemical oscillator in various fields, such as biochemical computing and drug delivery [25]. The successful simulation of the BZ reaction on large domains using parallel computing techniques showcases the feasibility of scaling up this system for industrial applications, such as chemical processing and pattern formation in materials science [41].

Despite the significant advancements made in this work, there are still challenges and limitations to be addressed. The Oregonator model, while capturing the essential dynamics of the BZ reaction, is a simplified representation of the actual chemical system. More detailed models, incorporating additional chemical species and reaction pathways, may be necessary to fully describe the complexity of the BZ reaction [10]. Furthermore, the two-dimensional simulations presented here do not capture the full three-dimensional nature of the patterns observed in experiments. Extension of the numerical methods to three dimensions would provide a more realistic representation of the system.

Another research idea is to separate future work in this area into several directions. First, even within the framework of the numerical model, the introduced stochastic effects would enable exploring new nonequilibrium effects, for instance, how spirals can originate from stochastic initial conditions. Second, extension of this parametric study to include other physical modes, such as fluid flow and heat transfer, would allow for the study of more complex phenomena, such as convection-driven pattern formation. In addition, it is also possible to improve the effectiveness of the simulations overall by incorporating new numerical methods such as the use of the adaptive mesh refinement method and also high-performance computing.

Conclusion

Therefore, the present study has contributed towards depicting an elaborated methodology of mimicking and quantifying the BZ reaction kinetics through numerical methods. To analyze temporal oscillations, wave propagation and pattern formation in this system, we have the following: Some of them are as follows: (i) A qualitative model known as the Oregonator model;

(ii) A method of numerical integration such as the inclusion of the fourth-order Runge-Kutta integration; and (iii) A method that makes use of a set of ordinary differential equations with partial differential equations known as the method of lines. The 'wishing' of the model into existence has demonstrated that it has the potential to capture the relevant aspects of the BZ reaction as evidenced by the number values which matched with those observed in the BZ experiments.

Till now, the parametric studies as well as the sensitivity analysis have provided the insights about various flow rates, concentrations and rate constants of the BZ reaction system. The contribution of this work is to expand the topics of numerically investigating nonlinear chemical systems and also to highlight how spatial concerns are paramount when studying reaction-diffusion behaviors. The tools and approaches presented in this work may be applied and extended in order to learn more about other chemical systems and, consequently, enlarge the area of chemical dynamics. However, several limitations and issues are still present: The need for improved models; Different dimensions of geometry – from 2D to 3D; and stochastic aspects. More work in this area should be focused on these paradoxes which may provide new vistas for employing the BZ reaction and related systems. Last but not least, the present work has shed additional light on the behaviour of the Belousov-Zhabotinsky reaction by virtue of the number retention methods involved herein and offered some potential ideas for future work in the field of chemical oscillation and dynamics.

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