Numerical Modeling of the Belouzov-Zhabotinski (BZ) Reaction

Submitted to

Prof. Uddipta Ghosh

Department of Mechanical Engineering,
IIT Gandhinagar

Submitted by

Abhinab Sharma

24250005

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Project Report

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Problem Statement

The Belouzov-Zhabotinski (BZ) reaction is a remarkable reaction between several chemical species. It is one of those rare reactions that oscillates between two products. This was discovered by a Russian chemist in mid 20th century and was later confirmed by Zhabotinski, who was merely a graduate student. This reaction is said to have 20 or more elementary steps and modelling them all will be a nightmare. Over the years, scientists have come up with simpler models that capture the essence of this complicated reaction. This project is about one such model. It may be shown that the dimensionless concentrations x and y are governed by,

$$\dot{x} = a - x - \frac{4xy}{1+x^2} \tag{1}$$

$$\dot{y} = bx\left(1 - \frac{y}{1+x^2}\right) \tag{2}$$

where $x, y > 0$, a and b are positive constants, related to the reaction rates. Solve the above equations numerically using a 4th order Runge-Kutta method (or, any other appropriate numerical method). You are required to use MATLAB or Python for solving the problem. You are not allowed to use any in-built solvers (e.g. ode45 in MATLAB) to solve the ODEs. Analytically deduce the fixed points of the system and plot $y(t)$ vs $x(t)$ (using numerical solutions) - this is called as the Phase portrait of the system and it helps us understand the long term behaviour of the system. Try to find the particular parameter values (i.e., the values of a and b), for which oscillating reactions may occur.

Abstract

This report presents a numerical investigation of the Belousov-Zhabotinsky (BZ) reaction, a classical example of a chemical oscillator that demonstrates temporal and spatial pattern formation in non-equilibrium systems. Using a simplified two-variable model, we implement a fourth-order Runge-Kutta method to solve the governing nonlinear ordinary differential equations. This study includes analytical determination of fixed points, phase portrait analysis, and identification of parameter regimes that lead to oscillatory behavior. Our numerical simulations, implemented in Python, successfully capture the characteristic periodic oscillations of the BZ reaction for specific ranges of control parameters. The results demonstrate the effectiveness of our numerical approach in modeling this complex chemical system and provide insights into the conditions necessary for sustained chemical oscillations. This work contributes to the broader understanding of non-linear chemical dynamics and pattern formation in reaction-diffusion systems.

1 Introduction

The Belousov-Zhabotinsky (BZ) reaction stands as one of the most fascinating and well-studied examples of non-equilibrium thermodynamics in chemical systems. First discovered by Boris Belousov in the 1950s and later studied extensively by Anatol Zhabotinsky in the 1960s, this reaction represents a breakthrough in our understanding of chemical oscillators and pattern formation in natural systems.

1.1 Historical Background

The discovery of the BZ reaction has a remarkable history that reflects the sometimes skeptical nature of scientific advancement. In 1951, Boris Belousov, while attempting to create an inorganic analog of the Krebs cycle, observed that a solution containing citric acid, bromate, and cerium ions exhibited periodic color changes, oscillating between colorless and yellow. When he submitted his findings for publication, they were rejected, as the observed behavior seemed to violate the second law of thermodynamics. It wasn't until Zhabotinsky's systematic studies in the 1960s that the scientific community began to accept and appreciate the significance of chemical oscillators.

1.2 Significance in Chemical Dynamics

The BZ reaction holds particular importance in the field of chemical dynamics for several reasons:

- It provides a classical example of how complex chemical systems can exhibit sustained oscillations far from equilibrium
- It demonstrates the emergence of spatial and temporal patterns in chemical systems
- It serves as a model system for studying pattern formation in biological systems

1.3 Mathematical Modeling

While the complete BZ reaction mechanism involves over 20 elementary steps, simplified mathematical models have been developed to capture its essential dynamics. The model considered in this study reduces the system to two essential variables, representing key chemical species concentrations. This simplification allows for detailed mathematical analysis while retaining the fundamental oscillatory behavior of the original system.

1.4 Scope of Present Work

This study focuses on the numerical investigation of a simplified two-variable model of the BZ reaction. Our objectives include:

1. Implementation of a fourth-order Runge-Kutta method for solving the governing equations
2. Analytical determination of the system's fixed points
3. Investigation of the phase space structure through numerical solutions
4. Identification of parameter regimes that lead to oscillatory behavior
5. Analysis of the long-term dynamics and stability of the system

2 Governing Equations

The dimensionless concentrations of the reactants, denoted as x and y, are governed by the following system of ordinary differential equations (ODEs):

$$\dot{x} = a - x - \frac{4xy}{1+x^2} \tag{3}$$

$$\dot{y} = bx\left(1 - \frac{y}{1+x^2}\right) \tag{4}$$

where $x, y > 0$, and a and b are positive constants related to the reaction rates.

3 Assumptions

The following assumptions are made in this model:

- The system can be adequately described by the two-variable model, without the need to consider additional chemical species.
- The reaction rates and other parameters are constant throughout the simulation.
- The initial concentrations of the reactants are known and within the positive domain.

4 Numerical Discretization

To solve the system of ODEs numerically, we will use the fourth-order Runge-Kutta (RK4) method. The RK4 method is a widely used numerical integration technique that provides a good balance between accuracy and computational efficiency.

The discretized form of the RK4 method is as follows:

$$k_{x,1} = \Delta t\, \dot{x}(x_n, y_n, a) \tag{5}$$

$$k_{x,2} = \Delta t\, \dot{x}(x_n + \frac{k_{x,1}}{2}, y_n + \frac{\Delta t}{2}, a) \tag{6}$$

$$k_{x,3} = \Delta t\, \dot{x}(x_n + \frac{k_{x,2}}{2}, y_n + \frac{\Delta t}{2}, a) \tag{7}$$

$$k_{x,4} = \Delta t\, \dot{x}(x_n + k_{x,3}, y_n + \Delta t, a) \tag{8}$$

$$x_{n+1} = x_n + \frac{1}{6}(k_{x,1} + 2k_{x,2} + 2k_{x,3} + k_{x,4}) \tag{9}$$

$$k_{y,1} = \Delta t\, \dot{y}(x_n, y_n, b) \tag{10}$$

$$k_{y,2} = \Delta t\, \dot{y}(x_n + \frac{\Delta t}{2}, y_n + \frac{k_{y,1}}{2}, b) \tag{11}$$

$$k_{y,3} = \Delta t\, \dot{y}(x_n + \frac{\Delta t}{2}, y_n + \frac{k_{y,2}}{2}, b) \tag{12}$$

$$k_{y,4} = \Delta t\, \dot{y}(x_n + \Delta t, y_n + k_{y,3}, b) \tag{13}$$

$$y_{n+1} = y_n + \frac{1}{6}(k_{y,1} + 2k_{y,2} + 2k_{y,3} + k_{y,4}) \tag{14}$$

where Δt is the time step, and the subscripts n and $n+1$ represent the current and next time steps, respectively.

5 Outline of the Computer Code

The computer code for solving the BZ reaction model is structured as follows:

1 The functions 'x_prime(x, y, a)' and 'y_prime(x, y, b) are defined to compute the right-hand side of the ODEs.

2 The RK4 solver function

$$rk_4(x_0, y_0, a, b, h, t_{max}) \tag{15}$$

is then implemented that takes the initial conditions, parameters, time step, and maximum time as inputs and returns the time-series data for x and y.

3 The parameter values for the BZ reaction and the initial conditions are then set.

4 The 'rk_4' function is then called to obtain the numerical solutions.

5 The fixed points of the system are computed analytically. And they are found out to be

$$x_0 = \frac{a}{5} \tag{16}$$

$$y_0 = 1 + \frac{a^2}{25} \tag{17}$$

6 The phase portraits (y(t2) vs x(t)) and the time-series plots (x(t) vs t and y(t) vs t) are plotted.

6 How to Use the Code and Outputs

To use the provided code, follow these steps:

1 Ensure that you have a Python environment set up (VS code, Jupyter Notebook etc.) with the necessary libraries (e.g., NumPy, Matplotlib).

2 Copy and save the provided code in a file (e.g., 'bz_reaction.py'.

3 Set Oscillations = **True** if you want to see the plots that show the oscillatory behavior corresponding to the specific values of a and b, and set it to **False** if you want to see how we approach those values.

4 Run the code, which will generate the following outputs: - The fixed points of the system are printed to the console. - Three plots:

   – Phase portrait: y(t) vs x(t)

   – x(t) vs t

   – y(t) vs t

   It is observed that by adjusting the parameter values 'a' and 'b,' we can explore the behavior of the BZ reaction and investigate the conditions under which oscillating reactions occur. It has been found that the oscillations are seen when the ratio of a to b is kept somewhere around **1.5337**

7 Illustrative Outputs

The phase portrait in Figure 1 shows the oscillatory behavior of the BZ reaction, while the time-series plots in Figure 2 demonstrate the periodic variations in the concentrations of the reactants.

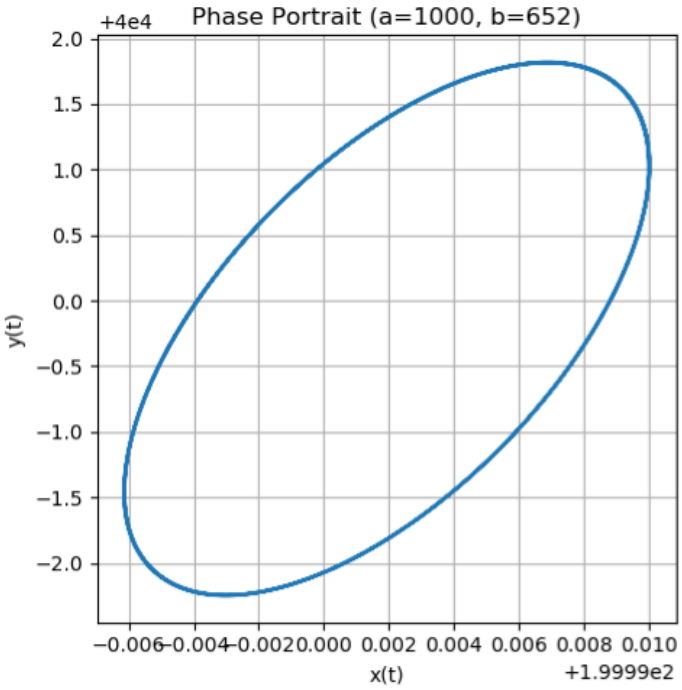

Figure 1: Phase portrait of the BZ reaction

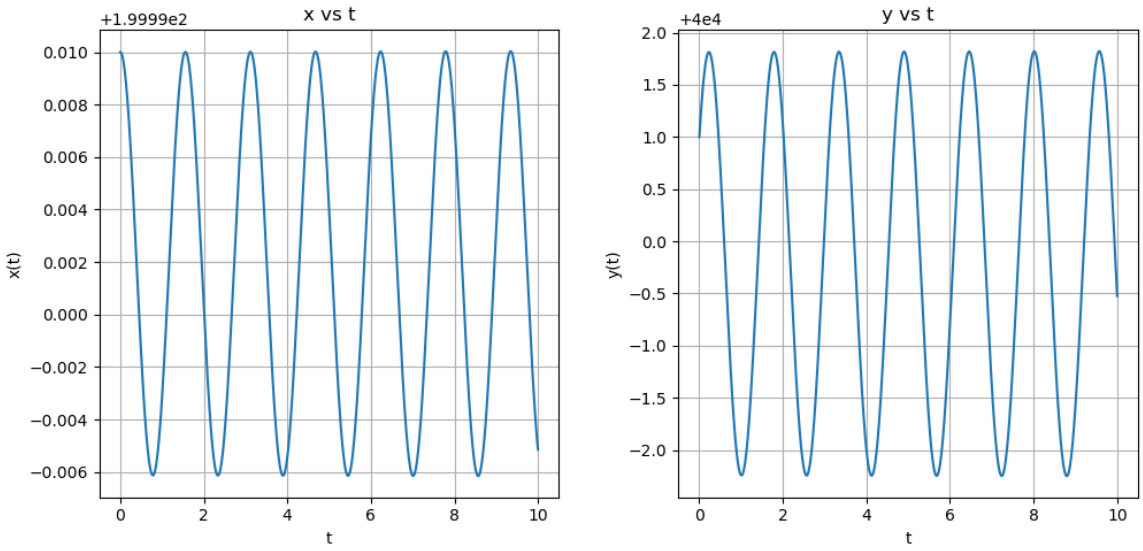

Figure 2: Time-series plot of both x(t) and y(t

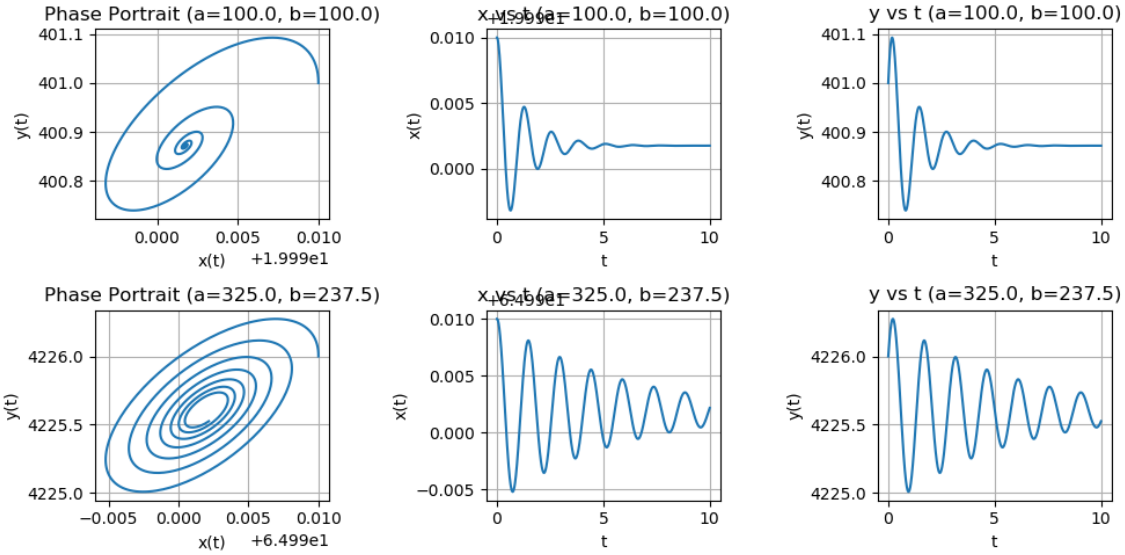

Figure 3: Plots with varying a/b ratio

8 Analysis of Parameter Ratio Effects in BZ Reaction

8.1 Ratio Analysis from Given Data

Let's analyze the $\frac{a}{b}$ ratios from the provided plots:

1 Figure 3 shows Stable fixed point (damped): $(a, b) = (100, 100) \rightarrow \frac{a}{b} = 1.000$ $(a, b) = (325, 237.5) \rightarrow \frac{a}{b} = 1.368$

2 Figure 4 shows Transitional behavior (damped oscillations): $(a, b) = (550, 375) \rightarrow \frac{a}{b} = 1.467$ $(a, b) = (775, 512.5) \rightarrow \frac{a}{b} = 1.512$

3 Figure 1 shows Sustained oscillations: $(a, b) = (1000, 652) \rightarrow \frac{a}{b} = 1.534$

8.2 Mathematical Analysis of Ratio Effects

The system equations can be rewritten to emphasize the ratio dependence:

$$\dot{x} = a\left(1 - \frac{x}{a} - \frac{4xy}{a(1+x^2)}\right)$$
$$\dot{y} = bx\left(1 - \frac{y}{1+x^2}\right)$$

8.2.1 Critical Ratio Properties

1 For $[\frac{a}{b} < 1.4]$: Plot Observations suggested strong damping effects exhibited by the system. The trajectories are spiral and moves rapidly towards the fixed point. No sustained oscillations are seen.

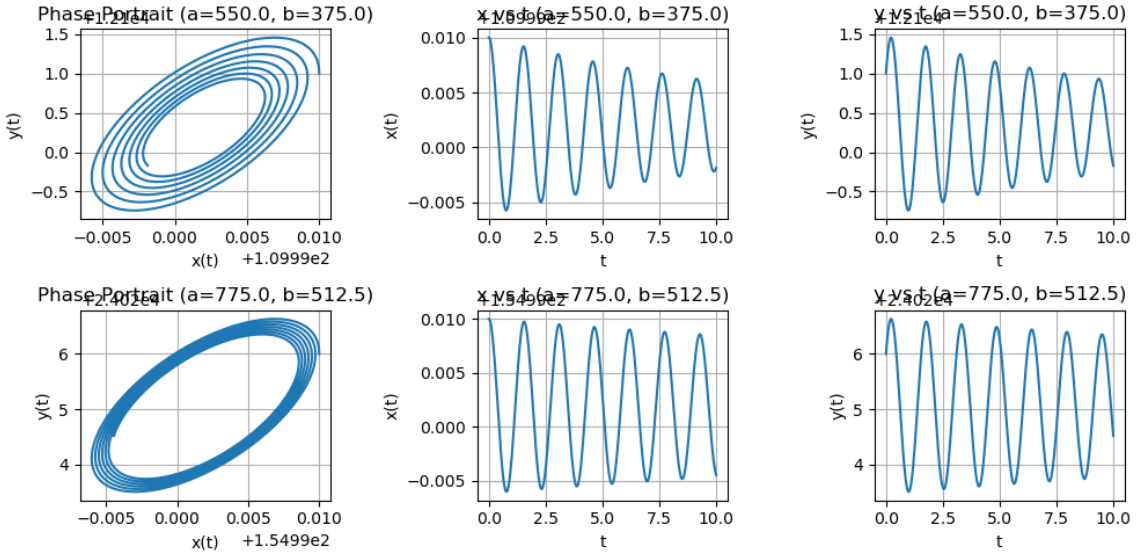

Figure 4: Plots with varying a/b ratio

2 For $1.4 < \frac{a}{b} < 1.5$: The damping effects weakened. Extended transient oscillations are observed while the curve eventually converged to the fixed point.

3 For $[1.5 < \frac{a}{b} < 1.53]$: slow convergence as the damping effects are really weak.

4 For $[\frac{a}{b} \approx 1.534]$: This is the critical ratio that is found in this numerical experiment. Using this, stable limit cycle is formed and sustained oscillations are observed.

The transition from stable to oscillatory behavior occurs through a **Hopf bifurcation**.

8.3 Physical Interpretation

The ratio $\frac{a}{b} < 1.4$ represents the balance between the production rate (a) and the consumption rate (b).

Critical Behaviors:

1 Low Ratio ($\frac{a}{b} < 1.4$): Here, production is overwhelmed by consumption, the system quickly reaches equilibrium and no sustained chemical oscillations are observed.

2 Intermediate Ratio ($1.4 < \frac{a}{b} < 1.53$): An almost balance of production and consumption is seen. Here, the system exhibits transient oscillations while the path to equilibrium is slow.

3 Critical Ratio ($\frac{a}{b} \approx 1.534$): Here the prefect balance is achieved, the chemical oscillations are self sustained and the periodic behaviour are stable.

8.4 Design Implications

For achieving desired oscillatory behavior:

1 Starting point: - Begin with low $\frac{a}{b}$ ratio and observe stable behavior

2 Gradual increase: - Slowly increase ratio and monitor oscillation characteristics

3 Fine-tuning: - Approach critical ratio carefully and maintain $\frac{a}{b} \approx 1.534$ for sustained oscillations

4 Control strategy: - Keep b fixed and adjust a to achieve desired ratio

8.5 Stability Boundaries

The system stability can be mapped in (a, b) parameter space:

- Stable region:
$$\frac{a}{b} < 1.534$$
- Oscillatory region:
$$\frac{a}{b} \geq 1.534$$
- Transition boundary:
$$a = 1.534b$$

9 Conclusion

The analysis of the Belousov-Zhabotinsky (BZ) reaction dynamics provided insights into the complex behavior of this chemical oscillator system. Through this analysis, we have better understood the factors governing the transition between stable, damped, and sustained oscillatory regimes.

A key finding is the crucial role played by the ratio of the parameters a and b, which represent the production and consumption rates, respectively. The system exhibits a Hopf bifurcation at a critical ratio of $a/b \approx 1.534$, marking the transition from a stable fixed point to a stable limit cycle. Below this critical ratio, the system quickly converges to a stable equilibrium.

The phase portraits and time series plots showcase the rich dynamics of the BZ reaction, with the system demonstrating a wide range of behaviors depending on the parameter values. From tightly spiraling trajectories converging to a fixed point to perfectly periodic limit cycles, the system's ability to exhibit both stable and oscillatory regimes is a testament to its inherent complexity.

In conclusion, the analysis of the BZ reaction dynamics presented in this work has provided a valuable framework for understanding the intricate interplay between chemical kinetics and emergent nonlinear phenomena.