

Non-linear Chemical Reactions*

A Comparison Between an Experiment and a Theoretical Model

Abiya Rajans, Neelima Gupte, P C Deshmukh

In this article, we discuss the Belousov–Zhabotinsky (BZ) reaction and its relation with the Oregonator model of chemical reactions. The Oregonator model has a limit cycle, and the BZ reaction shows chemical oscillations. We compare the time series obtained from the Oregonator model, with the time series obtained from an experimental study of the BZ reaction and show that the qualitative behaviour is similar. We also construct the limit cycle from the experimental data using the Takens' embedding theorem and compare it with the limit cycle from the Oregonator model. We conclude with a demonstration of the spatio-temporal patterns which can be seen in the two-dimensional version of this system.

1. Introduction

Chemical reactions are important processes in which the components of the reactants of the process combine to give rise to products which are distinct from the reactants. Such reactions are essential in the laboratory, in industry, as well as in nature and biological processes. Most chemical reactions familiar to us from school days can be modelled by linear equations, and result in a smooth decrease of reactants and a corresponding increase of resultants. However, more complex reactions which occur in a variety of contexts need to be modelled by non-linear equations and result in complex phenomena such as chemical oscillations and spatio-temporal patterns. We study the Belousov–Zhabotinsky model and the chemical oscillations occurring in the experiment with a theoretical model, which is known as the Oregonator. We



Abiya Rajans is a BS-MS student at IISER Tirupati. She is interested in dynamical systems, divisibility graphs, network theory.



Neelima Gupte was earlier on the faculty of the University of Pune, and is now at IIT Madras where she presently holds the Girija Vaidyanathan Chair Professorship in the Department of Physics. She specialises in Nonlinear Dynamics, Chaos and Statistical Mechanics.



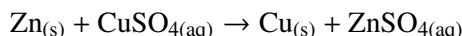
P C Deshmukh served the IIT Madras for more than three decades and has now moved to the IIT Tirupati. He also holds an adjunct position at the IISER Tirupati. He specializes in quantum collision physics.

*Vol.25, No.3, DOI: <https://doi.org/10.1007/s12045-020-0952-8>



also demonstrate the spatio-temporal patterns, which are spiral waves visible in the reaction in a two-dimensional context.

Consider a chemical reaction studied in high school chemistry like,



Keywords

BZ reaction, Oregonator model, limit cycle, chemical oscillations, spatio-temporal patterns.

In the case of non-linear chemical reactions, the reactants form intermediate species before forming the products, and the concentration of these intermediate species changes in a non-linear fashion which causes the oscillations in colour. These oscillations stop when the final product is formed, and the reactants are depleted.

When zinc (Zn) is added to copper sulphate solution (CuSO_4), zinc displaces copper (Cu) from copper sulphate and forms zinc sulphate (ZnSO_4). There is a colour change of the solution from blue to colourless indicating the product formation. Copper sulphate is blue while zinc sulphate is colourless, and the copper formed is deposited as reddish-brown residue. One may remember from elementary chemistry that zinc has higher reactivity than copper in the reactivity series, hence the reverse reaction is not possible. In this case, as the reaction proceeds, the concentration of copper sulphate decreases while at the same time, the concentration of zinc sulphate increases. In other words, the solution changes colour from blue to colourless. However, there are some non-linear chemical reactions in which the solution seems to be oscillating periodically between two colours. In the case of non-linear chemical reactions, the reactants form intermediate species before forming the products, and the concentration of these intermediate species changes in a non-linear fashion which causes the oscillations in colour. These oscillations stop when the final product is formed, and the reactants are depleted.

Usually in chemical reactions, during product formation the concentrations fall smoothly to an equilibrium value. However, in non-linear chemical reactions, the concentrations can oscillate before reaching equilibrium or the way the concentrations change before reaching equilibrium can be sensitive to the initial value of the concentrations. In such non-linear chemical reactions, there is a myriad of patterns that have been found under different experimental conditions. These are about changes in the concentration with time and, hence this is non-linearity in time or temporal non-linearity. There is also non-linearity in space, called spa-



tial non-linearity. In this article, we will focus only on one type of temporal non-linearity manifested through oscillations of the concentrations of intermediate chemicals with time.

In 1951, a Russian biochemist Boris Belousov was trying to study the Krebs cycle. He mixed citric acid, bromate ions and sulfuric acid in the presence of a cerium catalyst. He found that the colour of the solution oscillated between yellow and colourless. This oscillation continued for some time before the solution finally settled down to equilibrium. Such reactions are known as oscillating chemical reactions. They were known before 1921. However, many scientists doubted their existence since it was believed that all reactants linearly go to equilibrium. In 1968, Zhabotinsky confirmed Belousov's results and also proposed a possible mechanism for this non-linear behaviour. He also observed beautiful patterns of concentric rings or spirals of propagating waves in the thin unstirred layers of the reaction, with ferroin as a catalyst. Such spiral waves are similar to excitation waves observed in neural or cardiac tissues. Hence such oscillating reactions are not only an eccentricity of interest, but they also have applications in biology.

We discuss this complex chemical reaction, which was named as the Belousov–Zhabotinsky (BZ) reaction after those pioneers of non-linear reaction studies. The mechanism of BZ reaction is complex containing more than eighteen elementary reactions. The dynamics are modelled by a system of three non-linear ordinary differential equations (ODEs) [1]. We briefly discuss the mechanism of BZ reactions and the ODEs modelling the reactions. Then we solve these ODEs computationally to plot its phase portrait. Then we experimentally obtain the time series (values of concentration at different times) of one of the three variables and reconstruct the phase portrait from it. Finally, we compare the time series and phase portrait from the experiment vs the model.

Russian biochemist Boris Belousov, studying the Krebs cycle, mixed citric acid, bromate ions and sulfuric acid in the presence of a cerium catalyst. He found that the colour of the solution oscillated between yellow and colourless. This oscillation continued for some time before the solution finally settled down to equilibrium.



2. Mechanism and Modelling – A Brief Discussion

2.1 The Belousov–Zhabotinsky (BZ) Reaction Mechanism

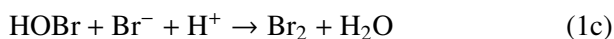
In this section, we discuss how to arrive at the equations modelling the dynamics of the BZ reaction and simplify it in a way suitable for computational analysis.

BZ reaction is a family of reactions, characterized by the reaction between an organic acid substrate that can be easily brominated and oxidized, in the presence of a strong acid, a bromate ion and a transition metal catalyst.

BZ reaction is a family of reactions, characterized by the reaction between an organic acid substrate that can be easily brominated and oxidized, in the presence of a strong acid, a bromate ion and a transition metal catalyst [2]. To be specific, we choose the commonly used reactants – malonic acid ($\text{CH}_2(\text{COOH})_2$), sulfuric acid (H_2SO_4), sodium bromate (NaBrO_3) with traces of sodium bromide (NaBr), and ceric ammonium nitrate ($(\text{NH}_4)_2\text{Ce}(\text{NO}_3)_6$).

We briefly discuss the mechanism of BZ reaction to understand how non-linearity arises in the system. The following mechanism is called the FKN mechanism named after Field, Koros and Noyes who proposed it in 1972 [3].

In the first step (1), the bromate ion (BrO_3^-) reacts with bromide (Br^-) in the presence of acid (H^+) to produce bromine (Br_2) and water (H_2O). Reaction (1) takes place through three elementary reactions (1a), (1b) and (1c). The elementary reactions (1a), (1b) and (1c) give the mechanism of (1) as $(1) = (1a) + (1b) + 3(1c)$.



The Br_2 formed in (1) combines with malonic acid to form bromomalonic acid (reaction (g) given in *Table 1*). The mechanism proceeds through enolization followed by bromination. The slowest of the two steps controls the rate of the overall reaction. Bromomalonic acid undergoes further bromination to form dibromo-



malonic acid, again through a two-step process. Dibromomalonic acid being unstable in acidic medium decarboxylates to form dibromoacetic acid, which again brominates to form tribromoacetic acid. Thus, many brominated organic compounds keep forming. Ce(IV) and malonic acid oxidize these compounds to produce Br^- and CO_2 . Thus this sequence of reactions produce Br^- , while the reaction (1) consumes Br^- (reaction (i) in *Table 1*).

Ce(IV) is reduced to Ce(III) during oxidation of brominated organic compounds (reactions (h), (i) in *Table 1*). This Ce(III) reduces BrO_3^- through a sequence of intermediate steps and is oxidized back to Ce(IV) (reaction (f) in *Table 1*). The important reactions of the FKN mechanism are listed in *Table 1*.

In the BZ system, several reactions proceed simultaneously. rate of change of chemical concentrations in these reactions is given by first-order ODEs. When we write down the rate equations for the intermediate species, we have a system of first-order coupled non-linear ODEs which contain non-linear terms. Next, we shall discuss how the FKN mechanism is simplified with some assumptions to obtain these ODEs, also called the Oregonator model. We use the methods of non-linear dynamics to analyze these non-linear ODEs.

In the BZ system, several reactions proceed simultaneously. The rate of change of chemical concentrations in these reactions is given by first-order ODEs.

2.2 The Oregonator Model

In our discussion about the mechanism of BZ reaction, we did not assume any transfer of matter between the system and the surrounding. The system is also stirred to keep it homogeneous. Hence, it is a closed stirred system (CSS). The Oregonator [4] model is a kinetic model of FKN mechanism proposed by Field and Noyes in 1974. Different models have been proposed since then. However, this model is good for our purpose of visualizing the oscillations and obtaining a phase portrait.

Reactions (c), (b), (e), (f), (d) and (i) from *Table 1* are the major steps in the BZ mechanism. We rewrite the important reactions by substituting $\text{A} = \text{BrO}_3^-$, $\text{P} = \text{HOBr}$, $\text{X} = \text{HBrO}_2$, $\text{Y} = \text{Br}^-$, $\text{Z} = \text{Ce}^{4+}$, $\text{B} = \text{MA}$ to get (2), (3), (5).



Table 1. The FKN mechanism of the BZ reaction [1, 3].

	Reaction	Rate Law / Rate Constants
o)	$\text{BrO}_3^- + 3\text{CH}_2(\text{COOH})_2 + 2\text{H}^+ \rightarrow 2\text{BrCH}(\text{COOH})_2 + 3\text{CO}_2 + 4\text{H}_2\text{O}$	Overall reaction
a)	$\text{HOBr} + \text{Br}^- + \text{H}^+ \rightleftharpoons \text{Br}_2 + \text{H}_2\text{O}$	$k_a = 8 \times 10^9 \text{ M}^{-2}\text{s}^{-1}$, $k_{-a} = 110 \text{ s}^{-1}$
b)	$\text{HBrO}_2 + \text{Br}^- + \text{H}^+ \rightarrow 2\text{HOBr}$	$k_b = 2 \times 10^9 \text{ M}^{-2}\text{s}^{-1}$
c)	$\text{BrO}_3^- + \text{Br}^- + 2\text{H}^+ \rightarrow \text{HBrO}_2 + \text{HOBr}$	$k_c = 2.1 \text{ M}^{-3}\text{s}^{-1}$
d)	$2\text{HBrO}_2 \rightarrow \text{BrO}_3^- + \text{HOBr} + \text{H}^+$	$k_d = 4 \times 10^7 \text{ M}^{-1}\text{s}^{-1}$
e)	$\text{BrO}_3^- + \text{HBrO}_2 + \text{H}^+ \rightleftharpoons 2\text{BrO}_2 + \text{H}_2\text{O}$	$k_e = 1 \times 10^4 \text{ M}^{-2}\text{s}^{-1}$, $k_{-e} = 2 \times 10^7 \text{ M}^{-1}\text{s}^{-1}$
f)	$\text{BrO}_2 + \text{Ce}^{3+} + \text{H}^+ \rightleftharpoons \text{HBrO}_2 + \text{Ce}^{4+}$	(fast)
g)	$\text{Br}_2 + \text{CH}_2(\text{COOH})_2 \rightarrow \text{BrCH}(\text{COOH})_2 + \text{Br}^- + \text{H}^+$	$r_g = 1.3 \times 10^{-2} \text{ M}^{-1}\text{s}^{-1} [\text{H}^+][\text{MA}]$
h)	$6\text{Ce}^{4+} + \text{CH}_2(\text{COOH})_2 + 2\text{H}_2\text{O} \rightarrow 6\text{Ce}^{3+} + \text{HCOOH} + 2\text{CO}_2 + 6\text{H}^+$	$r_h = \frac{8.8 \times 10^{-2} \text{ s}^{-1} [\text{Ce}^{4+}][\text{MA}]}{0.53\text{M} + [\text{MA}]}$
i)	$4\text{Ce}^{4+} + \text{BrCH}(\text{COOH})_2 + 2\text{H}_2\text{O} \rightarrow 4\text{Ce}^{3+} + \text{Br}^- + \text{HCOOH} + 2\text{CO}_2 + 5\text{H}^+$	$r_i = \frac{1.7 \times 10^{-2} \text{ s}^{-1} [\text{Ce}^{4+}][\text{BrMA}]}{0.2\text{M} + [\text{BrMA}]}$
j)	$\text{Br}_2 + \text{HCOOH} \rightarrow 2\text{Br}^- + \text{CO}_2 + 2\text{H}^+$	$r_j = \frac{7.5 \times 10^{-3} \text{ s}^{-1} [\text{Br}_2][\text{HCOOH}]}{[\text{H}^+]}$



(4) has the stoichiometry of (C) and the kinetics of (e). (6) gives the production of Br^- from MA and Ce^{4+} . Finally, h is a stoichiometric parameter whose value is adjusted as given in the literature [5].

Assuming the depletion of A to be negligible over a timescale of minutes and all the reactions to be irreversible, the rate of change of the concentrations of X (denoted by [X] or simply X), Y, Z are given by three coupled non-linear ODEs [1], [5]:

$$\frac{dX}{dt} = k_1AY - k_2XY + k_3AX - 2k_4X^2 \quad (7)$$

$$\frac{dY}{dt} = -k_1AY - k_2XY + hk_5Z \quad (8)$$

$$\frac{dZ}{dt} = 2k_3AX - k_5Z, \quad (9)$$

where

$$\begin{aligned} k_1 &= k_c[\text{H}^+]^2 = 2.1 \text{ M}^{-3}\text{s}^{-1}[\text{H}^+]^2, \\ k_2 &= k_b[\text{H}^+] = 2 \times 10^9 \text{ M}^{-2}\text{s}^{-1}[\text{H}^+], \\ k_3 &= k_e[\text{H}^+] = 1 \times 10^4 \text{ M}^{-2}\text{s}^{-1}[\text{H}^+], \\ k_4 &= k_d = 4 \times 10^7 \text{ M}^{-1}\text{s}^{-1}, \\ k_5 &= \frac{4r_i}{[\text{Ce}^{4+}]} \approx 0.34[\text{BrMA}] \text{ M}^{-1}\text{s}^{-1}. \end{aligned}$$

According to [1], we assume $[\text{BrMA}] \ll 0.2 \text{ M}$ and $h \approx 0.75$.

To write the equations (7), (8), and (9) in dimensionless form, substitute

$$x = \frac{k_2X}{k_1A}, \quad y = \frac{k_2Y}{k_3A}, \quad z = \frac{k_2k_5Z}{2k_1k_3A^2}, \quad \tau = k_1At,$$

$$a = \frac{k_1}{k_3}, \quad b = \frac{k_1A}{k_5}, \quad c = \frac{2k_1k_4}{k_2k_3}$$

to get

$$\frac{dx}{d\tau} = \frac{x + y - cx^2 - xy}{a} \quad (10)$$



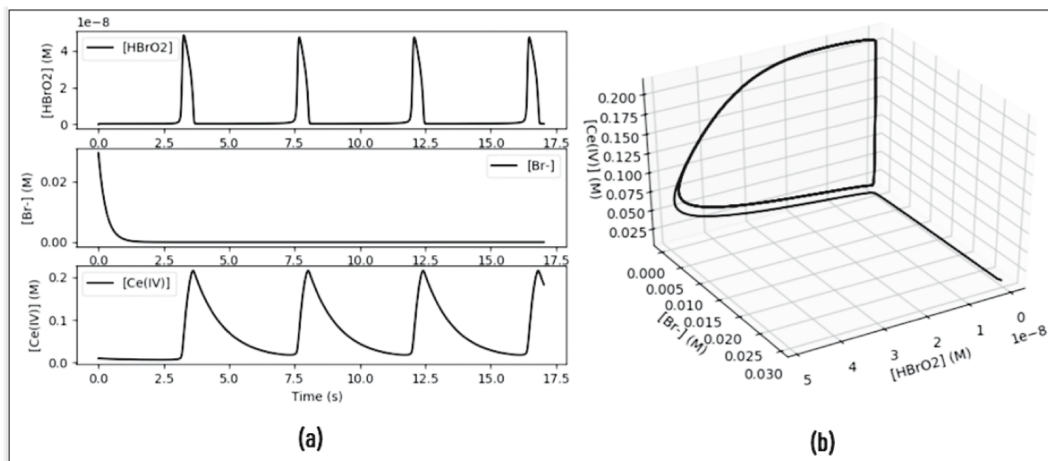


Figure 1. The Oregonator model based on Field-Körös-Noyes (FKN) mechanism for the BZ reaction in a closed stirred system with initial concentrations of $[BrO_3^-] = 0.115\text{ M}$, $[MA] = 0.155\text{ M}$, $[Ce(IV)] = 0.0095\text{ M}$, $[H^+] = 2.7\text{ M}$, $[Br^-] = 0.0295\text{ M}$, $stepsize = 0.01$, $time = 17.5$, the value for adjustable parameter, h was chosen to be the same as the one used in [1] $h = 0.75$. (a) The temporal oscillations of X,Y,Z which are the concentrations of $[HBrO_2]$, $[Br^-]$, $[Ce(IV)]$ in CSS. (b) The phase portrait corresponding to the data plotted in (a).

$$\frac{dy}{d\tau} = -y - xy + 2hz \tag{11}$$

$$\frac{dz}{d\tau} = \frac{x - z}{b} \tag{12}$$

(10), (11), (12) are the non-linear ODEs modelling the BZ reaction. They are the Oregonator equations in dimensionless form suitable for computational analysis.

3. Computationally Solving the Oregonator Model

Equations [10],[11],[12] are known as the Oregonator equations. By setting the RHS to zero in these three equations and solving the resulting expressions, we can get the equilibrium values of x, y, z . What we are interested in is the patterns in the values of x, y, z before reaching equilibrium. It involves some complicated arguments and background knowledge to understand why the values of x, y, z must oscillate due to these equations. Reference [1] discusses the proof for the existence of at least one periodic solution to this system of differential equations.

However, we approach this system of ODEs computationally to observe the oscillations in the values of x, y, z with time. Equations (10) , (11) , (12) are stiff ODEs, called so because they cannot be solved using ordinary Runge–Kutta like methods with a



Range (s)	No. of oscillations, N (per 500 s)	No. of oscillations, $n = N/500$ (per s)	Time period, $T = 1/n$ (s)
590–2090	4	0.008	125
2090–5090	3	0.006	166.67
5090–5590	4	0.008	125
5590–9090	3	0.006	166.67
9090–9590	2	0.004	250
9590–10090	3	0.006	166.67
10090–10590	2	0.004	250
10590–11590	3	0.006	166.67
11590–17590	2	0.004	250

fixed step size [6]. Hence, these equations need to be solved using a method with variable step-size. After solving these equations computationally, we obtain the values of the x , y , z with time. Writing x , y , z back in terms of X , Y , Z we get the concentrations of HBrO_2 , Br^- , Ce(IV) at different times.

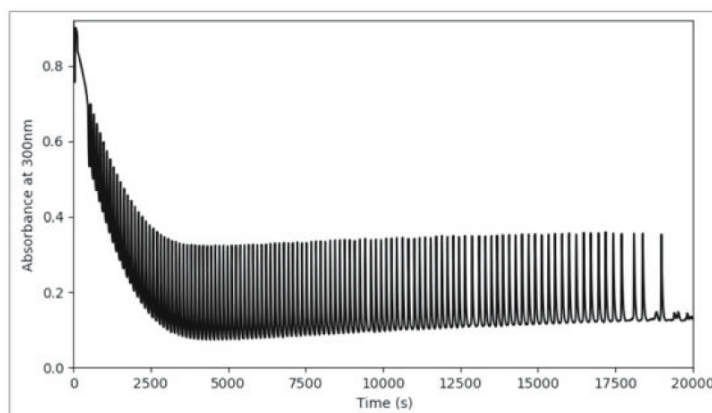
From the plots of X vs time, Y vs time and Z vs time given in *Figure 1a*, the concentrations exhibit oscillations in time. Next, we plot the phase portrait. It is the set of points towards which the triplet (X, Y, Z) approach after a long period. The three-dimensional plot of (X, Y, Z) given in *Figure 1b* shows the phase portrait for this system.

Observe that ignoring the transients, the phase portrait is a closed-loop. Therefore, after a sufficiently long time, the variables (X, Y, Z) cycle between the values on this loop only. This closed-loop structure is called a limit cycle. Hence, we have computationally shown that for this values of parameters and initial conditions, this system of ODEs modelling the BZ reaction reaches a limit cycle.

Table 2. Table showing time period of oscillations increasing with time. Time period was calculated by counting the frequency of oscillations for every 500 seconds in *Figure 2*.



Figure 2. Time series from experiment. The BZ reaction in a closed stirred system with initial concentrations $[\text{BrO}_3^-] = 0.115 \text{ M}$, $[\text{MA}] = 0.155 \text{ M}$, $[\text{Ce(IV)}] = 0.0095 \text{ M}$, $[\text{H}^+] = 2.7 \text{ M}$, $[\text{Br}^-] = 0.0295 \text{ M}$. Stirring was started 90 seconds after the measurement began.



4. Experiment

We perform the BZ reaction in the laboratory in order to observe the concentrations oscillating with time and compare them to *Figure 1*. We carry out the BZ reaction in a 10 mm × 10 mm × 45 mm cuvette, continuously stirred at nearly 660 rpm, in order to keep the system homogeneous. The reaction mixture consisted of NaBrO_3 (0.115M), MA (0.155M), $\text{Ce}(\text{NO}_3)_6(\text{NH}_4)_2$ (0.0095M), NaBr^- (0.0295M) and H_2SO_4 (2.7M).

The Beer–Lambert law states that the absorbance of a solution is proportional to the concentration of the absorbing chemical in the solution.

The Beer–Lambert law [7] states that the absorbance of a solution is proportional to the concentration of the absorbing chemical in the solution. Thus, a UV-visible spectrophotometer can be used to determine the concentration of the absorbing chemical in a solution. We use a UV-visible spectrophotometer to measure the concentrations.

The concentrations we have taken are small enough to avoid high absorbance values which cannot be read by the machine. The oscillations are not visible to eyes but are detected by the sensitive UV-visible spectrophotometer. The pale yellow coloured solution had a maximum absorbance at a wavelength of 300 nm. The time series was obtained at a wavelength of 300 nm with the machine taking readings at an interval of 5 seconds. The UV-visible spectrophotometer was equipped with a stirrer in order to maintain the homogeneity of the solution. Stirring was started 90 seconds after



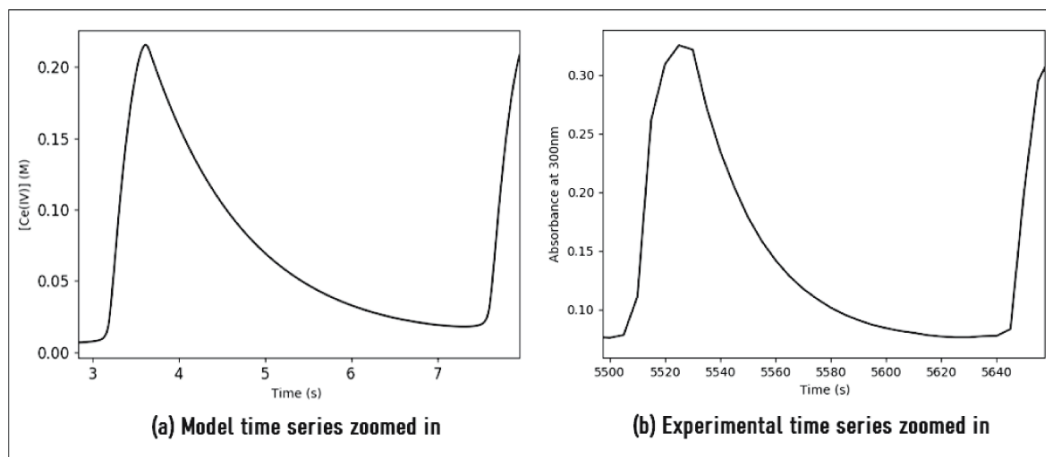


Figure 3. (a) Zoomed in view of *Figure 1a* $[\text{Ce(IV)}] = 0.0095 \text{ M}$. (b) Zoomed in view of *Figure 2*.

the spectrometer started taking readings.

It is difficult to infer from the figure the period of oscillations since the oscillations went on for nearly 20000 seconds (which is about five hours). So, the average frequency and period, counted for every 500 seconds are tabulated in *Table 2*. If one carefully sees the column entitled Range, it is clear from the table that the period increases with increasing time. In other words, the frequency of oscillations is high during the beginning of the reaction. Rows 3, 5 and 7 can be ignored since the error is most likely due to more than half of one cycle lying in different bins. Looking back at *Figure 2*, we again see that the oscillations are less crowded towards the right and abruptly stop after 17600 when the equilibrium is reached.

5. Comparison of Experiment With Model

Figure 3 shows a qualitative comparison between the oscillations observed in the experiment with the oscillations from the model. Thus we have observed the oscillations in this chemical reaction both experimentally and from the Oregonator model.

Due to experimental limitations, we could only obtain one of the



Box 1. Phase Portrait and Method of Phase Portrait Reconstruction

The phase space is an abstract mathematical space spanned by the dynamical variables X , Y , Z of the system. A point in the phase portrait represents the state of the system at an instant of time. Our system has three variables. Hence the state at a given time t is represented by a point $(X(t), Y(t), Z(t))$ in the three-dimensional Euclidean space R^3 . As the values of $(X(t), Y(t), Z(t))$ change with time, these form a trajectory or the path of the point in the phase portrait. Usually, the initial transient points are ignored, and only the values of $(X(t), Y(t), Z(t))$ for large t are plotted.

Takens' embedding theorem states that if a time series y is one of the components of an attractor that can be represented by a smooth d -dimensional manifold (like the limit cycle in our case), then the topological properties of the attractor are equivalent to the topological properties of the embedding formed by the m -dimensional phase-space vectors,

$$X_i = (y(i\Delta t), y(i\Delta t + \tau), y(i\Delta t + 2\tau), \dots, y(i\Delta t + (m - 1)\tau)),$$

whenever $m \geq 2d + 1$ [8]. τ is called the delay time, and m is called the embedding dimension. Since our system is three-dimensional, the embedding dimension, m is 3. There are different methods to choose an optimal time delay, but our system is simple, so we are good with finding τ by trial and error. This reconstructed attractor can be used to compute the Lyapunov exponents of the experimental system for comparison with the model. However, in this article, we are content with pointing out the visual similarity between the experimental and model limit cycles.

three variables X , Y , Z . So, we use the method of phase portrait reconstruction (see *Box1*) to reconstruct the phase portrait using the time series given in *Figure 2*.

Figure 4 gives a comparison between the model phase portrait and the experimental phase portrait. The reconstructed experimental phase portrait looks like a limit cycle and is qualitatively very similar to the model phase portrait.

The BZ reaction can also show complex spatial patterns when studied in a two-dimensional context. Images in *Box 2* show the complex spatial pattern in the form of concentric circular rings of propagating waves seen in a petri dish containing a thin layer of unstirred BZ solution. The waves are seen due to the propagation of reduced ferroin in a wave pattern. Breaking these patterns will result in spiral waves which can also be theoretically modelled. It



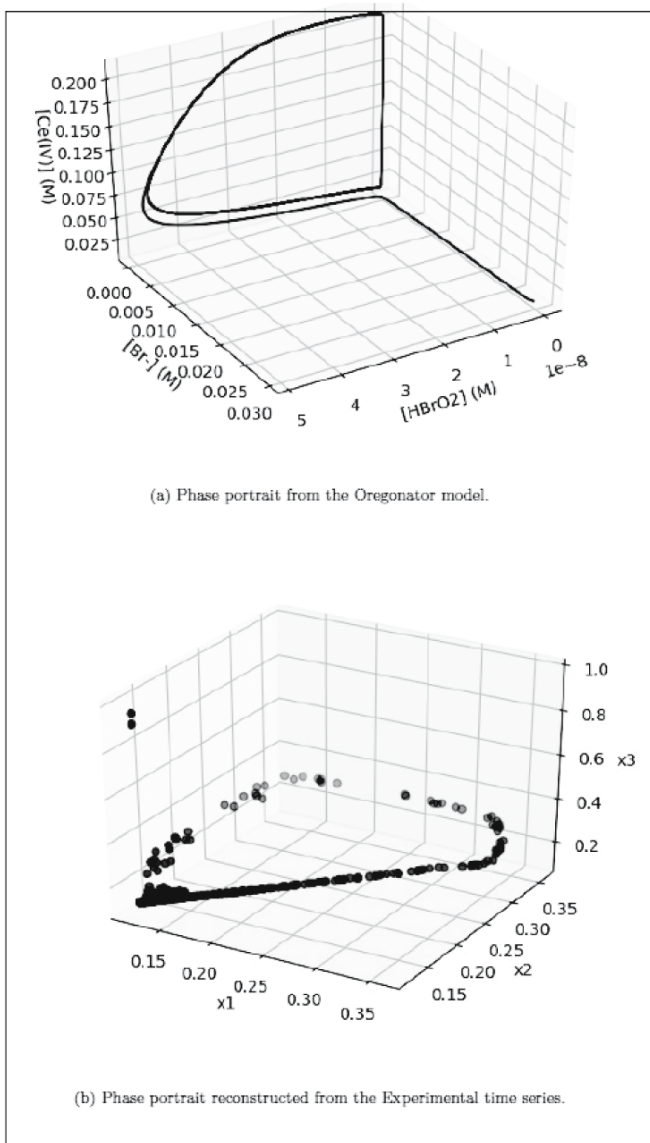


Figure 4. (a) Phase portrait from the Oregonator model. (b) Reconstructed phase-space from experimental [Ce] time series in *Figure 2*, with delay, $\tau = 2$ and embedding dimension, $m = 3$, after removing transients.

is, however, a challenging problem due to the spatially extended nature of the system.



Box 2. Temporal Oscillations and Spatial Pattern Formation

The first two images in *Figure A* show the temporal oscillations in the BZ reaction with malonic acid as a substrate and ferroin as a catalyst carried out in a beaker placed on a setup for stirring. The solution is oscillating (periodically changing) between blue and maroon due to the oscillations in the concentrations of oxidized ferroin (blue) and reduced ferroin (red). In the absence of ferroin, if only cerium ions are used as a catalyst, then the solution will oscillate between yellow and colourlessness.

The third image in *Figure A* shows the spatial pattern formation of concentric circular rings of propagating waves formed in a thin layer of unstirred BZ solution in a petri dish, due to the propagation of oxidized/reduced ferroin as waves in space. Breaking these ring patterns will result in propagating spiral waves. This experiment shows an example of the spatial non-linearity in the BZ reaction.

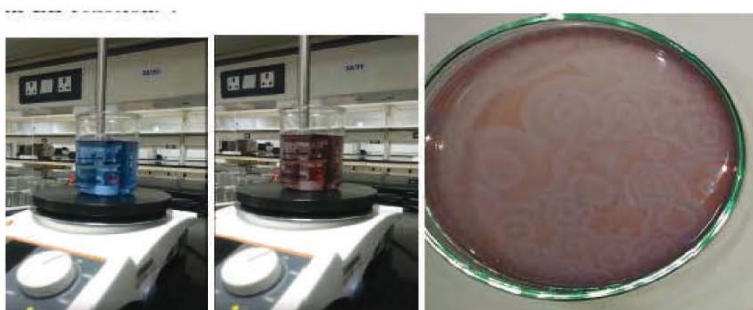


Figure A. The first two images shows the BZ solution in blue color at some time, which turns to maroon colour after some time. The solution keeps oscillating between blue and maroon for hours until the final products are formed. The last image shows the concentric circular rings formed in a thin layer of unstirred BZ solution in a petri dish.

6. Conclusion

We have carried out a study of the Belousov–Zhabotinsky reaction with its theoretical model the Oregonator. The comparison is carried out by comparing the temporal oscillation of the concentrations in the two, as well as by constructing a phase portrait of the underlying limit cycle via the methods of non-linear dynamics, and a good match is obtained. We have also observed the spatial pattern in the form of concentric rings which are formed in a thin layer of the BZ solution in a petri dish. We hope to analyze these theoretically in future.



Acknowledgements

Abiya Rajans is thankful to Anupama Roy from Dynamical Systems Lab IITM for fruitful discussions. Experiments requiring UV-visible spectrophotometer with stirring facilities were carried out in Prof. A K Mishra's laboratory, IITM under his guidance, with the help of Dr Saugata Sahu. Many thanks for their valuable support and advice.

Suggested Reading

- [1] John J Tyson, *The Belousov-Zhabotinskii Reaction*, Springer, 1976.
- [2] Anatol M. Zhabotinsky, Belousov–zhabotinsky reaction, *Scholarpedia*, Vol.2, No.9, 1435, 2007.
- [3] Richard J. Field, Endre Koros, and Richard M. Noyes, Oscillations in chemical systems. ii. Thorough analysis of temporal oscillation in the bromate-cerium-malonic acid system, *J. Am. Chem. Soc.*, Vol.94, No.25, pp.8649–8664, 1972.
- [4] Richard J. Field and Richard M. Noyes, Oscillations in chemical systems. v. Quantitative explanation of band migration in the Belousov–Zhabotinskii reaction, *J. Am. Chem. Soc.*, Vol.96, No.7, pp.2001–2006, 1974.
- [5] Richard J. Field, Oregonator, *Scholarpedia*, Vol.2, No.5, 1386, 2007.
- [6] Irving R. Epstein and John A. Pojman, *An Introduction to Non-linear Chemical Dynamics*, Oxford University Press, 1998.
- [7] D. F. Swinehart, The Beer–Lambert law, *J. Chem. Educ.*, Vol.39, No.7, 333, 1962.
- [8] Nigel Lovell Bruce Henry and Fernando Camacho, *Non-linear Biomedical Signal Processing, Volume 2 Dynamic Analysis and Modelling Chapter 1, Non-linear Dynamics Time Series Analysis*, John Wiley & Sons, 2000.

Address for Correspondence

Abiya Rajans
Department of Physics
Indian Institute of Science
Education and Research
Tirupati 517 607.

Email:

abiya.r@students.iiser
tirupati.ac.in

Neelima Gupte
Department of Physics
Indian Institute of Technology
Madras

Chennai 600 036

Email: gupte@iitm.ac.in
P C Deshmukh

Department of Physics
Indian Institute of Technology
Tirupati

Tirupati 517 506.

Email: pcd@iittp.ac.in

