BELOUSOV-ZHABOTINSKII REACTION

Manish Baral

14 May 2019

1 Abstract

Oscillation chemical reaction. Modeling the Belousov–Zhabotinskii reaction. The mathematical modeling of the Belousov–Zhabotinskii reaction was pioneered by Field, Koros and Noyes who proposed what is now known as the FNK mechanism. We use the adaptation to the ferroin catalyzed variant of the reaction proposed by Rovinsky and Zhabotinskii with simplification and in the notation of , which leads to the following:

2 Introduction

A Belousov–Zhabotinsky reaction, or BZ reaction, is one of a class of reactions that serve as a classical example of non-equilibrium thermodynamics, resulting in the establishment of a nonlinear chemical oscillator. The only common element in these oscillators is the inclusion of bromine and an acid. The reactions are important to theoretical chemistry in that they show that chemical reactions do not have to be dominated by equilibrium thermodynamic behavior. These reactions are far from equilibrium and remain so for a significant length of time and evolve chaotically. In this sense, they provide an interesting chemical model of nonequilibrium biological[clarification needed] phenomena; as such, mathematical models and simulations of the BZ reactions themselves are of theoretical interest, showing phenomenon as noise-induced order.

The discovery of the phenomenon is credited to Boris Belousov. In 1951, while trying to find the non-organic analog to the Krebs cycle, he noted that in a mix of potassium bromate, cerium(IV) sulfate, malonic acid, and citric acid in dilute sulfuric acid, the ratio of concentration of the cerium(IV) and cerium(III) ions oscillated, causing the colour of the solution to oscillate between a yellow solution and a colorless solution. This is due to the cerium(IV) ions being reduced by malonic acid to cerium(III) ions, which are then oxidized back to cerium(IV) ions by bromate(V) ions.

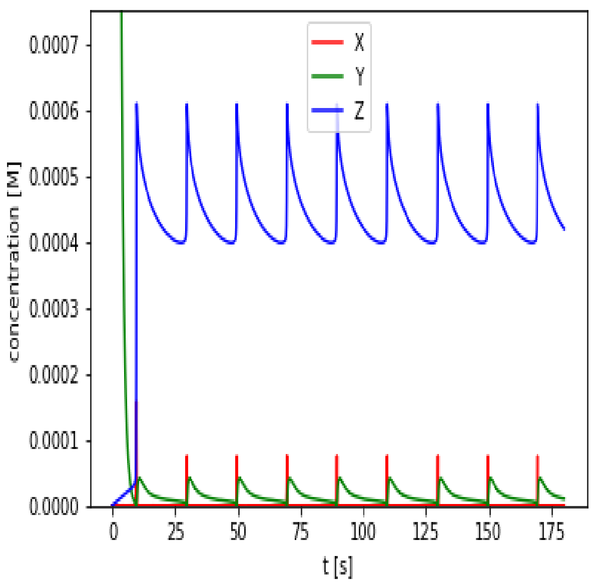
3 Methods

a. calculate the corresponding value of A,B,C H constant using table 3-4: A = 0.39 ,B=0.097, C=0.0006, H=0.39 (using molar formula)

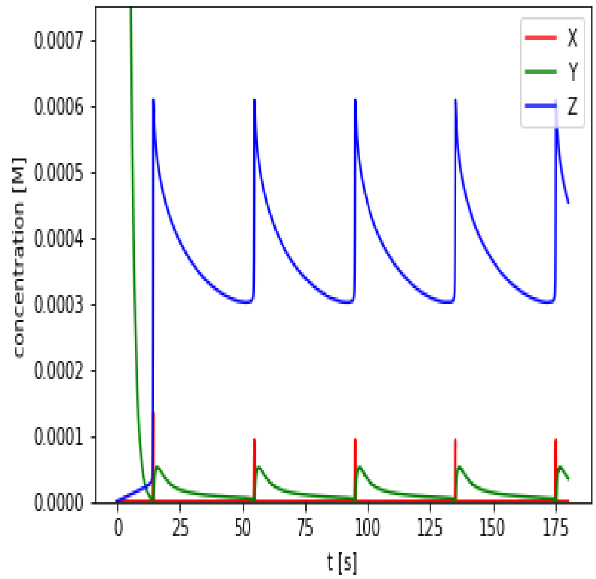
4 Results

b. solve system of differential eqns , measure period of oscillations and obtain graph.

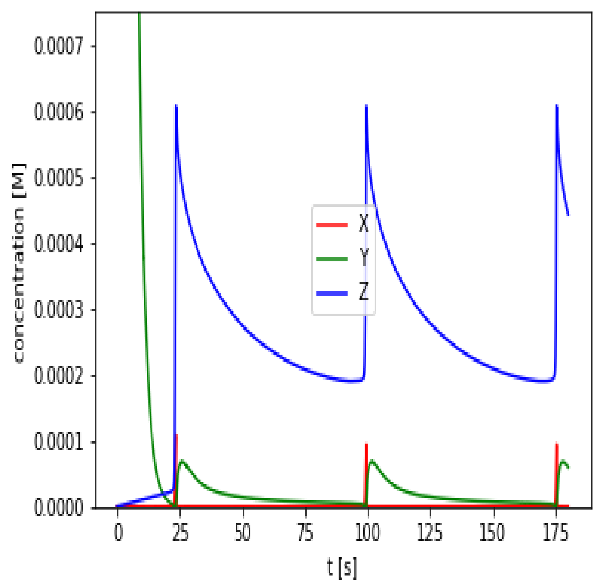
4.1 SOLUTION 1 (VARYING)



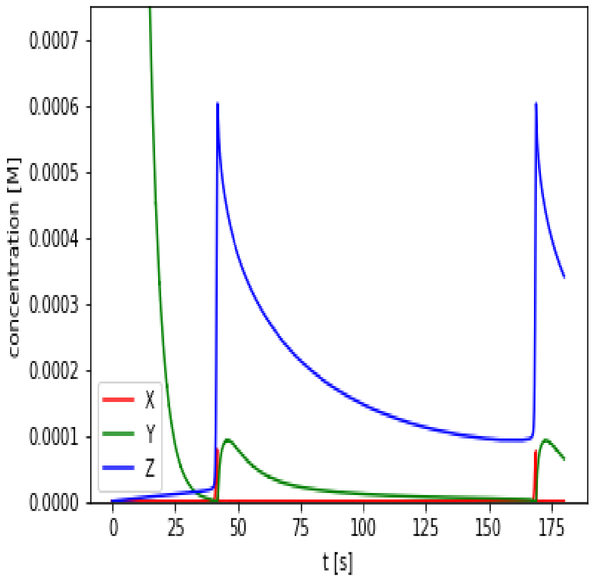
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 800 l of Solution 1, 0.5 M H2SO4+ 0.5 M N aBr were used. The period of oscillation is approximately 20 s. The experimental value was 6.6 s.



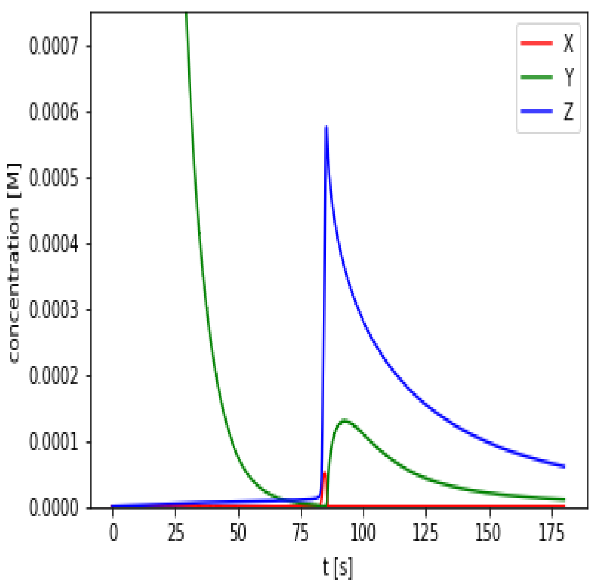
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 700 l of Solution 1, 0.5 M H2SO4+ 0.5 M N aBr were used. The period of oscillation is approximately 40 s. The experimental value was 21.1 s.



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 600 l of Solution 1, 0.5 M H2SO4+ 0.5 M N aBr were used. The period of oscillation is approximately 75 s. The experimental value was 76.6 s.



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 500 l of Solution 1, 0.5 M H2SO4+ 0.5 M N aBr were used. The period of oscillation is approximately 130 s. The experimental value was 137.1 s.

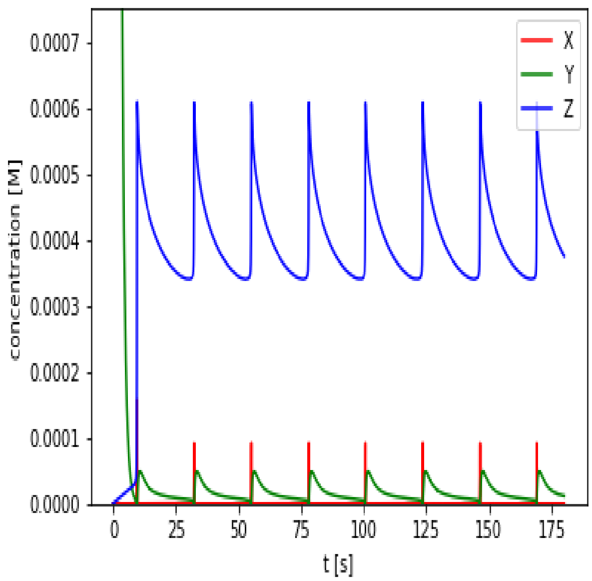


- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 400 l of Solution 1, 0.5 M H2SO4+ 0.5 M N aBr were used. The period of oscillation is approximately 180 s. The experimental value was 182.8 s.

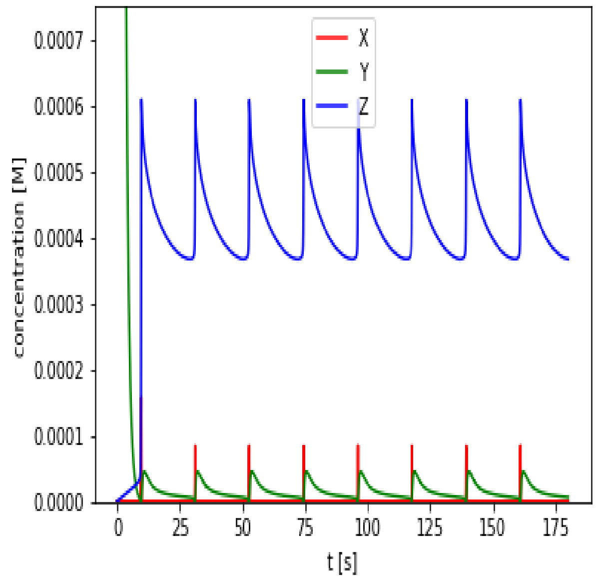
4.2 REASONS FOR NUMERICAL RESULT DON'T AGREE EXPERIMENTAL RESULT, IN SOME PLACES

1. RZ84 quote values of H between 2 M and 2.5 M
2. Numerical result is a simplified model.

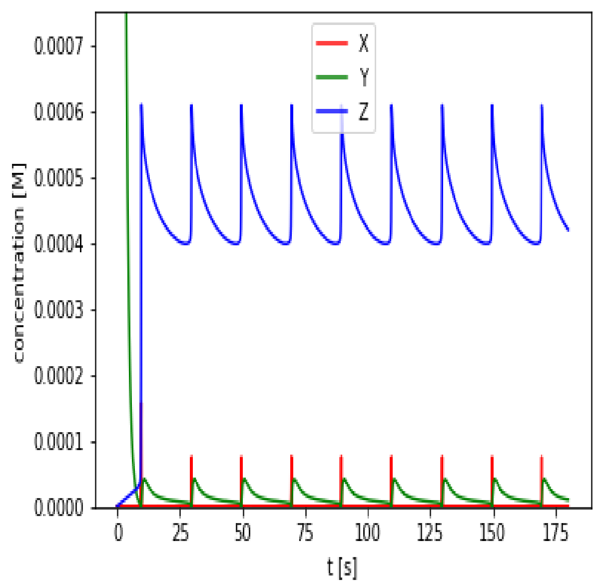
4.3 SOLUTION 2(VARYING)



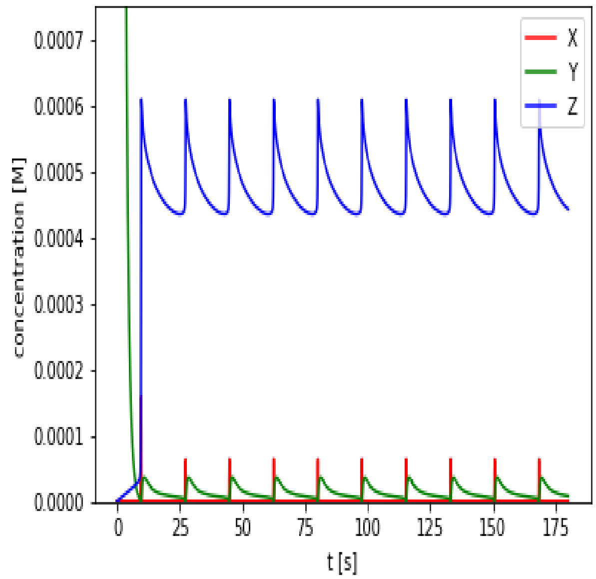
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 150 l of Solution 2, 0.5 M Malonic acid was used. The period of oscillation is approximately 22 s. The experimental value was 12.9s



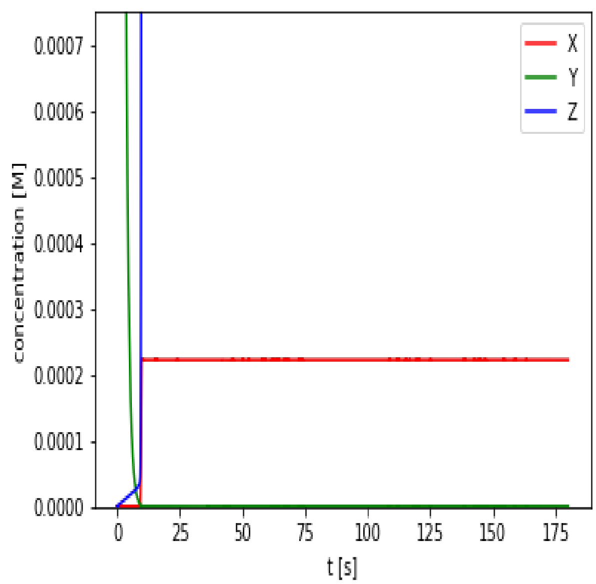
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 125 l of Solution 2, 0.5 M Malonic acid was used. The period of oscillation is approximately 21 s. The experimental value was 8.8s



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 100 l of Solution 2, 0.5 M Malonic acid was used. The period of oscillation is approximately 19 s. The experimental value was 8.8s

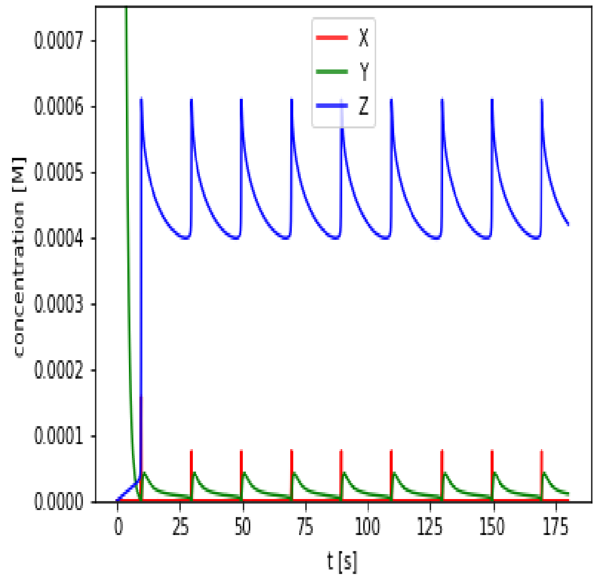


- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 75 l of Solution 2, 0.5 M Malonic acid was used. The period of oscillation is approximately 17 s. The experimental value was 6.6s

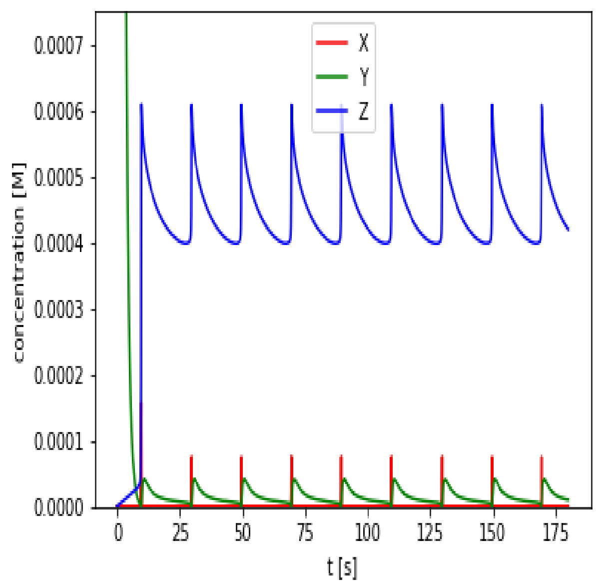


- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 50 l of Solution 2, 0.5 M Malonic acid was used. The system fails to oscillate. The experimental value was 31 s.

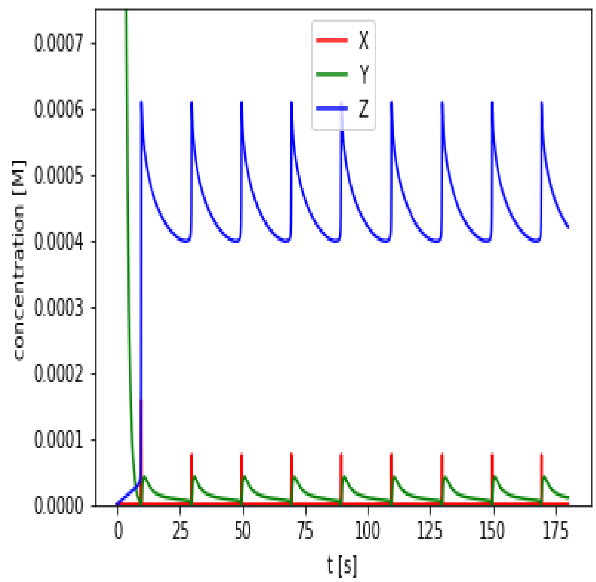
4.4 SOLUTION 3(VARYING)



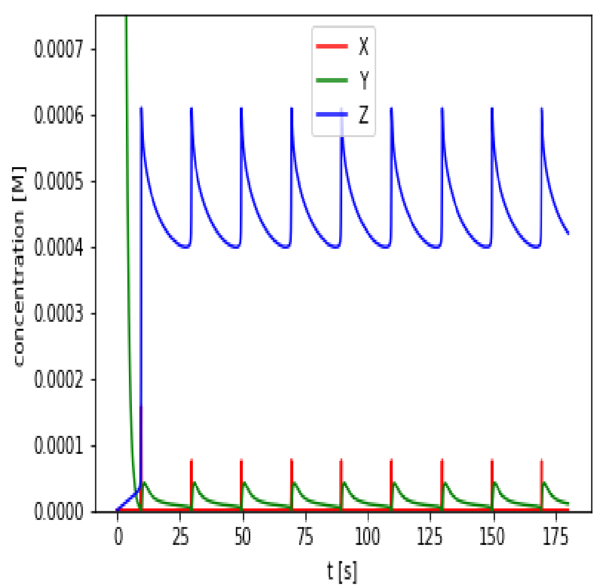
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 100 l of Solution 3, 1 M N aBr was used. The period of oscillation is approximately 20 s. The experimental value was 76.4 s



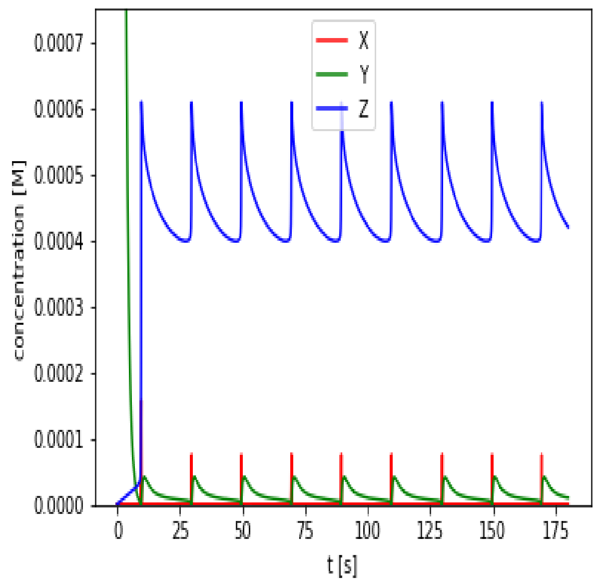
- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 80 l of Solution 3, 1 M N aBr was used. The period of oscillation is approximately 20 s. The experimental value was 38.5 s.



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 60 l of Solution 3, 1 M N aBr was used. The period of oscillation is approximately 20 s. The experimental value was 7.9 s.



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 40 l of Solution 3, 1 M N aBr was used. The period of oscillation is approximately 20 s. The experimental value was 5.8 s.



- Molar concentration of X = [HBrO3], Y = [Br] and Z = [F e3+] over time of 200 seconds. 20 l of Solution 3, 1 M N aBr was used. The period of oscillation is approximately 20 s. The experimental value was 19.8 s.

5 References

[1] A. F. Taylor, V. Gaspar, B. R. Johnson, and S. K. Scott, Analysis of reactiondiffusion waves in the ferroin-catalysed Belousov–Zhabotinsky reaction, Phys. Chem. Chem. Phys., 1 (1999), pp. 4595–4599.

[2] R. J. Field, E. Kor os, and R. M. Noyes , Oscillations in chemical systems. II. Thorough analysis of temporal oscillation in the bromate-cerium-malonic acid system, J. Am. Chem. Soc., 94 (1972), pp. 8649–8664.

[3] C. R. Gray, An analysis of the Belousov–Zhabotinskii reaction, Rose-Hulman Undergrad. Math J., 3 (2002), pp. 1–15.

[4] E. Mori, I. Schreiber, and J. Ross, Profiles of chemical waves in the ferroincatalyzed Belousov–Zhabotinskii reaction, J. Phys. Chem., 95 (1991), pp. 9359–9366.

[5] A. Rovinsky and A. Zhabotinsky, Mechanism and mathematical model of the oscillating bromate-ferroin-bromomalonic acid reaction, J. Phys. Chem., 88 (1984), pp. 6081– 6084.

[6] Partial help from Avinash Niraula for code section