Modeling the oscillating Belousov – Zhabotinsky chemical reaction

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Abstract: In this communication, the kinetics of the well-known Belousov-Zhabotinsky oscillating reaction is studied. The choice of this particular reaction came from its similitude with circadian rhythms and the molecular clocks involved in the human response to microgravity conditions and the presence of electro-magnetic fields. In the present communication, the chemical kinetics is modeled as a system on nonlinear differential equations following the scheme NKF. Critical points and conditions of stability are obtained, as well as the conditions leading to an oscillatory behavior. Since the study is limited to the kinetics only, convection effects were neglected cause the influence of the magnetic field on the reaction could not be addressed. Even though a system of partial differential equations will include such effect, in this communication, a possible explanation for the Magnetic Field Effect (MFE) is advanced which is in qualitative agreement with experiments performed by another research team from the School of STEM at St. Thomas University.

Keywords: *Belousov-Zhabotinsky, chemical reaction, magnetic field, circadian rhythms, dynamical systems, NKF scheme, chemical kinetics.*

Introduction

Many phenomena in Nature display periodic patterns. Chemical oscillating reactions are involved in biochemical processes, neurological responses, and circadian rhythms [1,2]. One of the conditions that might compromise the life of future astronauts venturing into long term space travels (for example to Mars) is the disruption of circadian rhythms due to outer space electromagnetic fields. Since most of the rhythms are controlled by the central nervous system, and the later operates on neurons, the use of a more simple system to study the expected changes will be desired. In this end, the Belousov-Zhabotinsky (BZ) reaction has emerged as one of the simplest dynamical models capable to address this problem. It is a non-linear oscillatory reaction that involves the production of molecular bromine from bromate and bromide ions in the presence of malonic acid. A realistic and a simple way of studying it would be using the same mathematical model of the Oregonator, created by Richard Field and Richard M. Noyes at the University of Oregon [1].

According to [3], the mechanisms of a magnetic field effect (MFE) on chemical reactions are classified into: (1) Radical pair mechanism, (2) Lorenz force, and (3) Magnetic force, proportional to the product of the magnetic susceptibility gradient of solutes and the square of magnetic flux density. Such a problem is important when addressing long-term space-travel physiology, in particular, the effect of magnetic fields on internal clocks of future astronauts. In this communication, the time evolution of the oscillating BZ chemical reaction is modeled and possible effects of magnetic field are addressed.

Model and Results

This communication is aimed at explaining the changes observed during the experiments performed at the chemistry laboratories in St. Thomas university school of STEM. The set up consists of two Helmholtz coils separated at a distance d, and generating a magnetic field distribution in between. At the middle point between the two coils, a petri dish with the chemical reagents is located such that the BZ reaction can be recorded in both conditions, in absence and presence of magnetic field.

The magnetic field distribution between the two coils was computed in [4] and is given by:

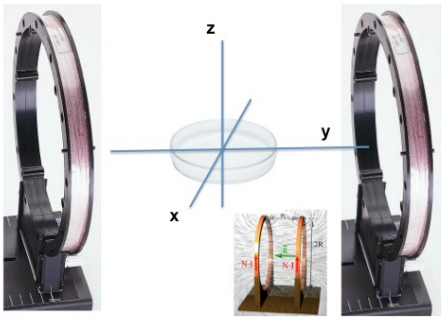

Fig. 1: Experimental setup to study the influence of the magnetic field on the BZ reaction.

$$B_r(r,y) = \frac{\mu_0 I}{2\pi}\frac{y}{r\sqrt{(r+a)^2+y^2}}\left[\frac{a^2+r^2+y^2}{(a-r)^2+y^2}E(k)-K(k)\right]$$
$$B_y(r,y) = \frac{\mu_0 I}{2\pi}\frac{y}{r\sqrt{(r+a)^2+y^2}}\left[\frac{a^2-r^2-y^2}{(a-r)^2+y^2}E(k)-K(k)\right]$$

where $k^2 = \frac{4ar}{(a+r)^2+y^2}$ and E(k) and K(k) are the elliptical integrals of first and second type respectively.

The kinetics of the BZ along with the fluid dynamics is considered as a reaction – diffusion problem. The kinetics follows the scheme FKN modified into the Oregonator model [1], which considers the chemical species X = $HBrO_2$, Y = Br^-, and Z = M_{ox}=Ferroin/Ferritin. The dynamical system in dimensionless form and following the quasi-static approximation (slow variation of Y) can be cast into:

$$\varepsilon\frac{dx}{d\tau} = x(1-x)-\frac{(x-q)}{(x+q)}f_0 z = f(x,z)$$
$$\frac{dz}{d\tau} = x-z = g(x,z)$$

where f_0 is the stoichiometric factor, q is a constant including several rate constants. The value of ε is small.

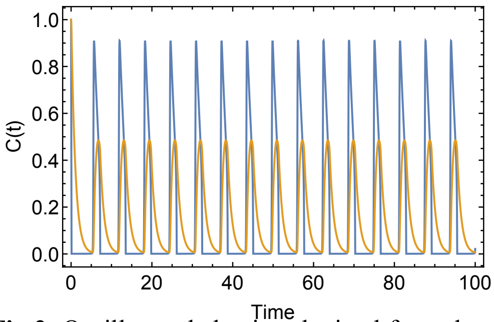

Fig 2: Oscillatory behavior obtained from the Oregonator model of the BZ reaction.

The condition for an oscillatory behavior (center) is equivalent to the requirement of Trace A = 0, while the Det A ≠ 0 (Hopf bifurcation), where A is the Jacobian of the above system.

In order to address the effect of the magnetic force, we will focus on the Ferroin/Ferritin ion. Hence the equation for z must be complemented with the Euler equation:

$$\frac{\partial\vec{v}}{\partial\tau}+(\vec{v}\cdot\vec{\nabla})\vec{v} = \frac{1}{\rho}\vec{\nabla}\left(\frac{B^2}{8\pi}\right)+\frac{(\vec{B}\cdot\vec{\nabla})\vec{B}}{4\pi\rho}$$

The term with B^2 conrresponds to the magnetic pressure and based on the spatial effects observed it does not seem responsible for their inner working. On the other hand, the last term is related with the tension along the magnetic lines, and it seems to be the source of the observed patterns [3]. Further modeling is going on in order to verify this hypothesis.

Conclusions

The Oregonator model is capable to reproduce the oscillatory behavior observed in experiments. The values of the parameter f_0 are critical to the stability of the system. Wave-trains, spirals and other two dimensional patterns require the inclusion of a diffusion term, transforming the Oregonator into a reaction-diffusion system. Magnetic field effects could be accounted by including an advection term, and it is part of an ongoing effort.

Conflicts of Interest

The authors declare no conflict of interest.

Acknowledgments

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References and Notes

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