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A BRUSSELATOR TYPE POPULATION MODEL BASED ON OSCILLATING CHEMICAL REACTIONS

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ABSTRACT

In this paper we study a two-gender population model similar to the Brusselator equations which is based on oscillating chemical reactions. This is a two-gender population model where the rate of growth of the population is proportional to the square of the members. We examine and study the stability of the system by observing phase plane analysis and nature of Eigen values at equilibrium points.

Keywords: Autocatalytic model, Dynamical behavior, Phase plane analysis, Stability of equilibrium points.

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1. INTRODUCTION

During autocatalysis, the concentrations of reactants, intermediates form as well as products with periodicity. Chemical oscillation is analogous to electrical oscillation, where autocatalysis replaces positive feedback. Oscillating reactions are known to occur in several places [1]. Generally, the reactions proceed smoothly with varying rates, till they reach a state of equilibrium. These reactions give rise to observable oscillations of the concentrations. Some examples of oscillating reactions are Belousov-Zhabotinskii reaction (B-Z reaction) and The Bray-Liebhafsky reaction

The reaction consists of the breakup of hydrogen peroxide in oxygen and water with $IO_3^{\,-}$. The phenomenon can be described by the following equations [2].

$$IO_3^- + 2H_2O_2 + H^+ = HOI + 2O_2 + 2H_2O$$

$$HOI + CH_2\left(CO_2H\right)_2 = ICH\left(CO_2H\right)_2 + H_2O$$

Oscillating reactions, their dynamics and chemistry has been studied from the past 50 years. This work was started by the work of B. Belousov [3].

In 1961, A.M. Zhabotinskii [4] reproduced Belousov's work. The oscillations in the system were observed by the changes in electrical potential and optical density of the reacting solutions.

This is known as the Belousov-Zhabotinskii or B-Z reaction. Many people have studied this reaction. There are now a large number of mathematical models of this kind. Some important examples of such reactions are Brusselator, Lotka Volterra, Oregonator and Bubbelator.

Here we explained briefly about these reaction mechanisms.

2. THE B-Z REACTION MECHANISM:

The complete mechanism of the B-Z reaction was studied by Noyes et.al.,[5]. There are some 18 reactions and 21 chemicals [6]. The mechanism is

$$Br^- + BrO_3^- + 2H^+ \rightarrow HBrO_2 + HOBr$$

$$Br^- + HOBr + H^+ \rightarrow Br_2 + H_2O$$ Catalytic production of $HBrO_2$

$$BrO_3^- + HBrO_2 + H^+ \rightarrow 2BrO_2 + H_2O$$

$$BrO_2 + Ce^{3+} + H^+ \rightarrow HBrO_2 + Ce^{4+}$$

The final reaction is a combination of above two reactions. $HBrO_2$ Catalyses the reaction and the reaction rate is proportional to it [7].

3. IDEALIZED B-Z REACTION

3.1. Lotka Volterra Mechanism for oscillating reactions:

This is one of the simplest mechanisms which has served as the model for many other mechanisms. It has been studied in great mathematical detail, and it has been used in several other branches of science, especially in ecology. This mechanism is known as the Lotka-Volterra mechanism named after two scientists, Lotka (the physical chemist) and the mathematician Volterra. Volterra had described it independently in 1925.

In 1920, A. J. Lotka suggested that a chemical system might undergo oscillations which would be sustained [8]. The Lotka-Volterra mechanism is given by the following set of equations:

$$a) A + X \rightarrow 2X \qquad \frac{d[A]}{dt} = -k_a\left[A\right][X]$$

$$b) X + Y \rightarrow 2 \qquad \frac{d[X]}{dt} = -k_b\left[X\right][Y]$$

$$c) Y \rightarrow B \qquad \frac{d[B]}{dt} = k_c[Y]$$

The system of equations for Lotka-Voltera model is

$$\frac{dA}{dt} = -k_a AX$$

$$\frac{dX}{dt} = -k_b XY$$

$$\frac{dB}{dt} = k_c Y$$

Figure 1 Reaction

Where A, B and X are the concentrations of the reactants. Lotka was modeling a chemical system but there are numerous examples of this kind in ecology. The Lotka-Volterra equations can be numerically solved using various techniques and the results can be shown in two ways. The first way is to plot both X and Y with respect to time. The same information can be displayed more concisely by plotting X versus Y that is one concentration versus the other. In 2005 Zhang et al. [9] study the dynamical behavior of Lotka-Volterra predator prey model concerning with pest manangement. L.Nie et.al. [10] study the existence and stability of periodic solutions with state dependent impulsive effects.

Some oscillating reactions approach a closed trajectory whatever their starting conditions. The closed trajectory is called a 'limit cycle' [11].

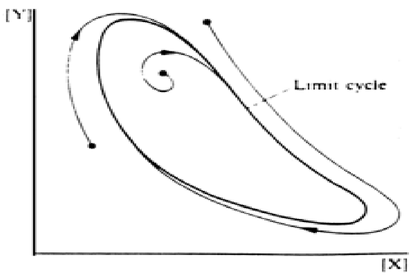

Figure 2 Limit cycle

3.2. The Oregonator Model

The Oreganaotor model was studied by Noyes et al. in [12] demonstrates the B-Z reaction. It has three independent composition variables and five steps which are irreversible. The underlying dynamics of the Oregonator is an inhibitor system containing an autocatalytic step as well as a negative feedback loop with a delay. In 2018 Yuting Cai et al. [13] study the Hopf-zero bifurcation of oreganator oscillator with time delay. Here we briefly discuss the dynamical equations involved in oreganator model.

$$A + Y \rightarrow X + P$$

$$X + Y \rightarrow 2P$$

$$A + X \rightarrow 2X + 2Z$$

$$X + X \rightarrow A + P$$

$$B + Z \rightarrow \frac{1}{2} f$$

Where $X = HBrO_2, Y = Br^- = Ce(IV)$

$A = Bro_3^-, B = CH_2\left(COOH\right)_2, P = HOBr$ or $BrCH\left(COOH\right)_2$.

The differential equations for the Oregonator are

$$\frac{dX}{dt} = K_1AY - K_2XY + K_3AX - 2K_4X^2$$

$$\frac{dY}{dt} = -K_1AY - K_2XY + \frac{1}{2}K_c fBZ$$

$$\frac{dZ}{dt} = 2K_3AX - K_cBZ$$

For giving some particular values to the parameters the limit cycle for Oreganator exist.

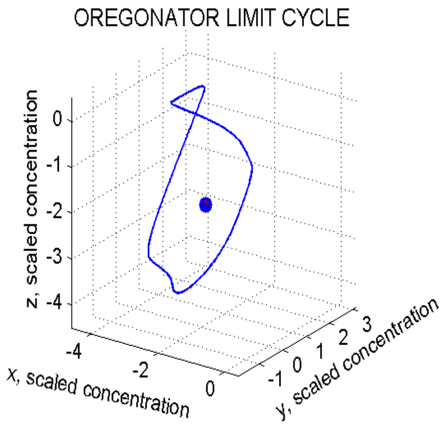

Figure 3 The limit cycle in the Oregonator

3.3. The Brusselator Model

Brusselator is an autocatalytic model which is based on oscillating chemical reactions. The mechanism for the Brusselator is given by [14]

$$A \rightarrow X$$

$$2X + Y \rightarrow 3X$$

$$B + X \rightarrow Y + C$$

$$X \rightarrow D$$

The ordinary differential equations for brusselator model are

$$\dot{X} = 1 - \left(b + 1\right)X + aX^2Y$$

$$\dot{Y} = bX - aX^2Y$$

4. REVIEW OF BRUSSELATOR MODEL

Changzhao et.al [15] study the stochastic stability and bifurcation of brusselator system with multiplicative white noise. Wenjie Zuo et.al. [16] study the diffusive Brusselator model with delayed feedback control subject to dirchlet boundary conditions and the equilibrium point changes its stability and became unstable for some critical values. They also studied about direction and stability of Hopf bifurcation. B.Kostet et.al [17] study the Brusselator reaction diffusion model and formation of localized structures. They established pitchfork bifurcation for showing the emergence of localized spots and using delayed feedback control a motion of localized and dissipative structures occurs.

Ram Jiwari et.al [18] proposed a modified cubic B-spline differential quadrature method for two-dimensional reaction-difussion brusselator system. They solved these nonlinear differential equations using Runge-Kutta 4th order method and they tested the stabililty of the equilibrium point. A.K.M. Nazimuddin et.al. [19] proposed a nonlinear reaction-diffusion Brusselator model and they established a parameter plane to investigate the existence of periodic waves and stability of the model using continuation method. The existence of hopf bifurcation for ordinary and partial differenntial equations in general models of brusselator subject to homogeneous Neumann boundary conditions was studied by Yan li [20]. He also studies the stability of bifurcating periodic solutions using center manifold theory. Manjun ma et.al [21] study the structure of non-negative steady state solutions of a Brusselator model. They also studied about existence and boundedness of steady state solutions using global bifurcation theory.

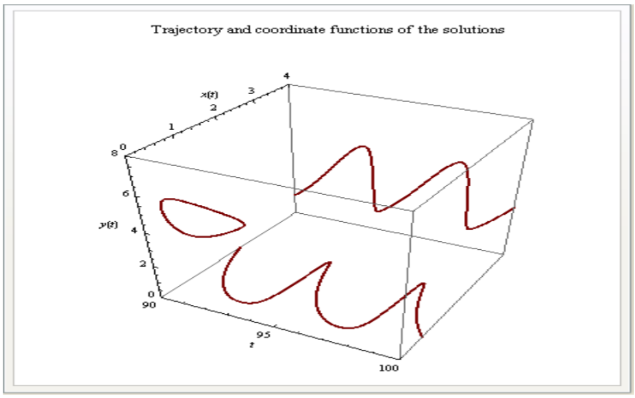

Figure 4 Hopf Bifurcation in the Brusselator reaction

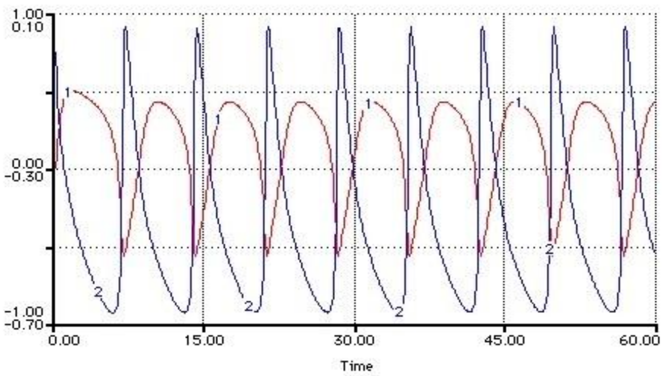

Figure 5 Oscillating reactions for Brusselator

In this paper we will be studying a Brusselator type model. The Brusselator is an auto catalytic oscillating reaction. We will investigate the system's dynamics by observing behavior in the phase plane, proving the existence of stable cyclic orbits.

4.1. Brusselator type model

The dynamics of the population Model can be described by a system of two ordinary differential equations. They are

$$X' = 1 - (b+1)X + aX^2 Y$$

$$Y' = bX - aXY^2$$

where a and b are constants and positive and X, Y *are* population of females and the males. In this proposed model there an X^2 and Y^2 term, It is known that in a two gender population the rate of growth of the population is proportional to the square of the members [22]. The model could be interpreted to be a predator-prey model in a two gender population. Mathematical models have been developed to prevent the extinction of the species due to several reasons. Nishant Juneja et.al [23], proposed a prey-predator model and it has been shown that the dynamics of the prey-predator is largely affected by getting alternative food for predator population. They also studied existence and uniform stability of equilibrium points. Qamar Din et.al. [24] study the qualitative behavior of a modified Prey-Predator model with local asymptotic stability of equilibria and in the case of discrete time prey-predator model, it attains period-doubling and Neimark-sacker bifurcation at its positive steady state.

4.2. Equilibrium Points

We obtain the equilibrium points of this system by solving

$$1 - (b+1)X + aX^2 Y = 0$$

$$bX - aXY^2 = 0$$

The four equilibrium points are

$$E_1 = \left(\frac{1+b+\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, \frac{\sqrt{b}}{\sqrt{a}}\right)$$

$$E_2 = \left(\frac{1+b-\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, \frac{\sqrt{b}}{\sqrt{a}}\right)$$

$$E_3 = \left(\frac{-1-b+\sqrt{4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, -\frac{\sqrt{b}}{\sqrt{a}}\right)$$

$$E_4 = \left(\frac{-1-b-\sqrt{4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, -\frac{\sqrt{b}}{\sqrt{a}}\right)$$

4.3. Nullclines

We next find the nullclines of the given system by equating X' and Y' to zero

$$1-(b+1)X + aX^2Y = 0 \text{ and } bX - aXY^2 = 0$$

The first equation gives the X-nullcline and the second gives the Y-nullcline. We plot the nullclines for different values of a and b. We choose the values of a from 0 to 1 and b from 0 to 3.

The nullclines are shown in the graph as follows

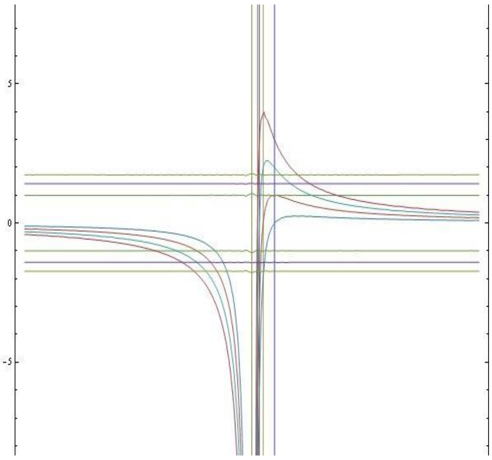

Figure 6 Nullclines

The x-nullclines are parallel to x and y-axes and y-nullclines are hyperbolic.

4.4. Phase plane Analysis

We next analyze the system by studying the direction of the level lines by plotting the force field directions. For that we choose the values for a=1 and b=3.

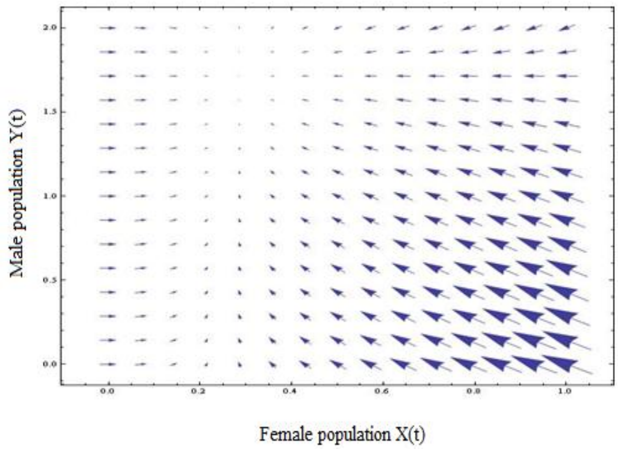

Figure 7 Equilibrium point

From this figure It can be seen that the direction field points towards an equilibrium point. We next make a plot of the system in the phase plane.

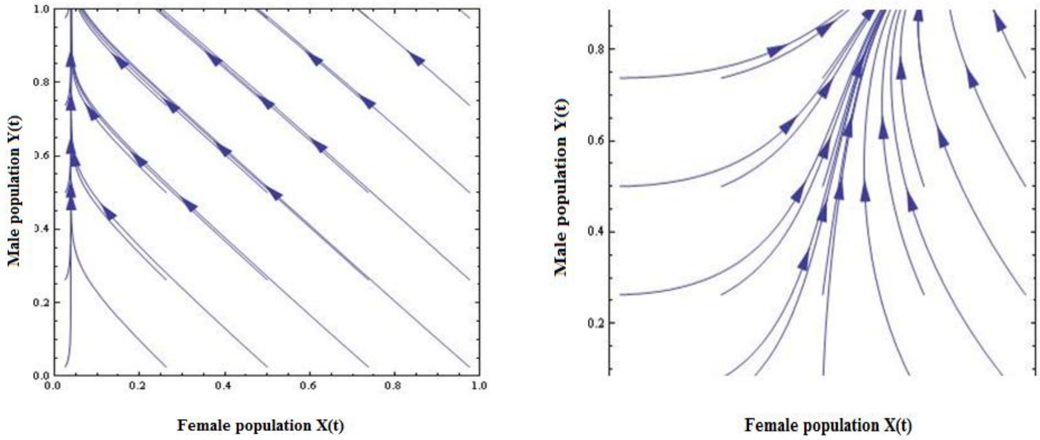

Figure 8 Phase Curves with different values for a and b

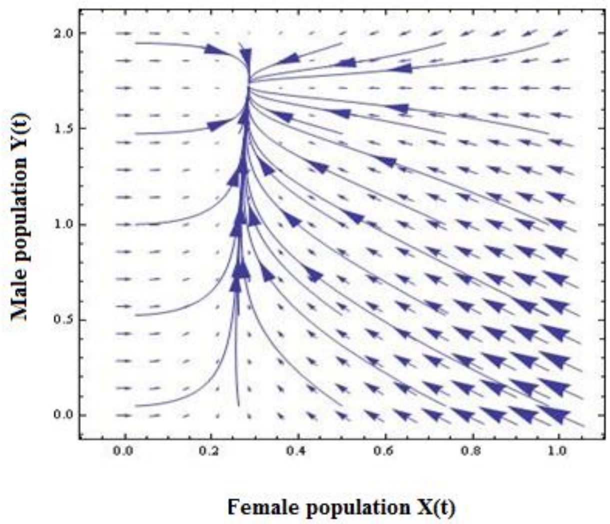

Figure 9 Phase plane

From this phase plane we can observe that the phase lines are moving towards an equilibrium point and it indicates that the equilibrium point is stable.

4.5. Mathematical Analysis of the system

We next linearize the system about its equilibrium points.

The linearized Jacobian matrix is

$$\begin{pmatrix} -1-b+2axy & ax^2 \\ b-ay^2 & -2axy \end{pmatrix}$$

At the first equilibrium point

$$E_1 = \left(\frac{1+b+\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, \frac{\sqrt{b}}{\sqrt{a}}\right)$$

The Eigen values of the Jacobian matrix are

$$-\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}, 1+b\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}$$

At the second equilibrium point $E_2 = (\frac{1+b-\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, \frac{\sqrt{b}}{\sqrt{a}})$

The Eigen values of the jacobian matrix are

$-\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}, -1-b+\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}$ At the third equilibrium point

$$E_3 = (\frac{-1-b+\sqrt{4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, -\frac{\sqrt{b}}{\sqrt{a}})$$

The Eigen values are

$$\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}, \sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}$$

We now evaluate the Jacobian for the equilibrium point

$$E_4 = (\frac{-1-b-\sqrt{4\sqrt{a}\sqrt{b}+(1+b)^2}}{2\sqrt{a}\sqrt{b}}, -\frac{\sqrt{b}}{\sqrt{a}})$$

The Eigen values at this equilibrium point are

$$-\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}, -b+\sqrt{-4\sqrt{a}\sqrt{b}+(1+b)^2}$$

It can be observed that for some values of a and b the Eigen values for the equilibrium points E_2 and E_4 are negative which indicates that these equilibrium points are asymptotically stable for certain values of a and b.

5. CONCLUSION

We formulated a mathematical model similar to brusselator system which is based on autocatalytic oscillating chemical reactions. We hypothesized that these could also represent a population with two genders. Initially we performed a phase plane analysis from which we observed that the equilibrium points are moving towards equilibrium point and it indicates that the equilibrium point is stable. Further we verified the stability of equilibrium point by mathematical analysis using Eigen values and at two equilibrium points E_2 and E_4 the Eigen values are negative, it illustrate that the system of equations are having stable equilibrium points.

6. FUTURE SCOPE

This model involves more complicated dynamics including limit cycles and bifurcations. As this is a vast field to explore from the dynamical systems point of view. Using this model also furtherly frame the mathematical models based on autocatalytic reactions.

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