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MATHEMATICAL MODELING AND THE STABILITY STUDY OF SOME CHEMICAL PHENOMENA

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Abstract: *In this paper is studied a chemical phenomenon, an example of an autocatalytic reaction. Using the stability in first approximation and the theory of bifurcations is studied the stability the autocatalytic reaction. The mathematical modelling was made using the Maple software.*

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1. INTRODUCTION

Reaction–diffusion systems are mathematical models which explain how the concentration of one or more substances distributed in space changes under the influence of two processes: local chemical reactions in which the substances are transformed into each other, and diffusion which causes the substances to spread out over a surface in space. This description implies that reaction–diffusion systems are naturally applied in chemistry. However, the system can also describe dynamical processes of non-chemical nature. Examples are found in biology, geology and physics and ecology. The nonlinear reaction-diffusion systems are the general form:

$$\begin{cases} \dfrac{\partial x}{\partial t} = a_1 x + b_1 y + f(x,y) + g_1(l) \\ \dfrac{\partial y}{\partial t} = a_2 x + b_2 y + f(x,y) - g_2(l) \end{cases} \tag{1}$$

The Brusselator is a theoretical model for a type of autocatalytic reaction. The Brusselator model was proposed by Ilya Prigogine and his collaborators at the Free University of Brussels. The Brusselator is originally a system of two ordinary differential equations as the reaction rate equations for an autocatalytic, oscillating chemical reaction, [2,3,4]. In many autocatalytic systems, complex dynamics are seen, including multiple steady states, periodic orbits, and bifurcations. The Belousov - Zhabotinsky reaction [2,3,4] is a generic chemical reaction in which the concentrations of the reactants exhibit somewhat oscillating behaviour.

To obtain the Brusselator model in systems (1) we denote by: $a_1 = -(B+1)$, $b_1 = 0$, $a_2 = B$, $b_2 = 0$, $f(x,y) = x^2 y$, $g_1(l) = A$, $g_2 = 0$ where A and B are positive constants.

In particular, the Brusselator model describes the case in which the chemical reactions follow the scheme:

$$A \to X$$
$$2X + Y \to 3X$$
$$B + X \to Y + D$$
$$X \to E$$

where *A, B, D, E, X*, and *Y* are chemical compounds. Let $x(t)$ and $y(t)$ be the concentrations of *X* and *Y*, and assume that the concentrations of the input compounds A and B are held constant during the reaction process.

2. THE DYNAMICAL SYSTEM

The dynamical system which models these processes is:

$$\begin{cases} x' = A - (B+1)x + x^2 y \\ y' = Bx - x^2 y \end{cases} \quad (2)$$

We are proposing to study the stability and the existence of limit cycles for this dynamical system making a discussion about the real, positive parameters A and B. The main aim is to evaluate what are the values that lead us to obtain an attractor solution.

For this it is a must to find the equilibrium point of the system (2), by computing the following system:

$$\begin{cases} A - (B+1)x + x^2 y = 0 \\ Bx - x^2 y = 0 \end{cases} \quad (3)$$

We'll find that the equilibrium point is: $P(x^*, y^*) \equiv P\left(A, \frac{B}{A}\right)$.

We are interesting about the behaviour of the null solution. For the stability study of the solution we have to make the translation to arrive in the origin, so: $X = x - x^*, Y = y - y^*$.

The new form of the system (2) is:

$$\begin{cases} X' = A - (B+1)(X + x^*) + (X + x^*)^2 (Y + y^*) \\ Y' = B(X + x^*) - (X + x^*)^2 (Y + y^*) \end{cases} \quad (4).$$

Because (x^*, y^*) is the solution of system (3) is obtained the following system:

$$\begin{cases} X' = (B-1)X + A^2 Y + \frac{B}{A} X^2 + 2AXY + X^2 Y \\ Y' = -BX - A^2 Y - \frac{B}{A} X^2 - 2AXY - X^2 Y \end{cases} \quad (5)$$

Which has the equilibrium point in origin $(X^*, Y^*) = (0,0)$.

The stability study is made using the method in the first approximation. So, we have:

$$J(x,y) = \begin{pmatrix} \frac{\partial f}{\partial X} & \frac{\partial f}{\partial Y} \\ \frac{\partial g}{\partial X} & \frac{\partial g}{\partial Y} \end{pmatrix} =$$

$$= \begin{pmatrix} B - 1 + 2XY + 2\frac{B}{A} X + 2AY & A^2 + X^2 + 2AX \\ -B - 2XY - 2X\frac{B}{A} - 2AY & -A^2 - 2XY - 2AY \end{pmatrix}$$

The Jacobi matrix in the equilibrium point $O(0,0)$ is

$$H = J(0,0) = \begin{pmatrix} B-1 & A^2 \\ -B & -A^2 \end{pmatrix}.$$

This is equivalent with the linear homogeneous system:

$$\begin{cases} X' = (B-1)X + A^2 Y \\ Y' = -BX - A^2 Y \end{cases} \quad (6)$$

The characteristically polynomial is:

$$P(\lambda) = \det(H - \lambda I_2) = \begin{vmatrix} B - 1 - \lambda & A^2 \\ -B & -A^2 - \lambda \end{vmatrix} =$$

$$= \lambda^2 + \lambda(A^2 - B + 1) + A^2$$

We'll study the solutions' stability taking into account the type of the characteristically polynomial's solutions. Because the product of these two roots is A^2, which is always a positive number, the study is made for the discriminant and the trace of the matrix H:

$$\Delta = \left[(A-1)^2 - B\right]\left[(A+1)^2 - B\right]$$

$$S = Tr(H) = B - 1 - A^2$$

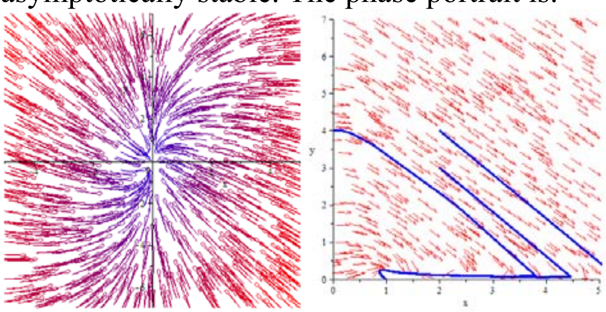
The characteristically equation roots are:

$$\lambda_{1,2} = \frac{-(A^2 - B + 1) \pm \sqrt{\left[(A-1)^2 - B\right]\left[(A+1)^2 - B\right]}}{2}$$

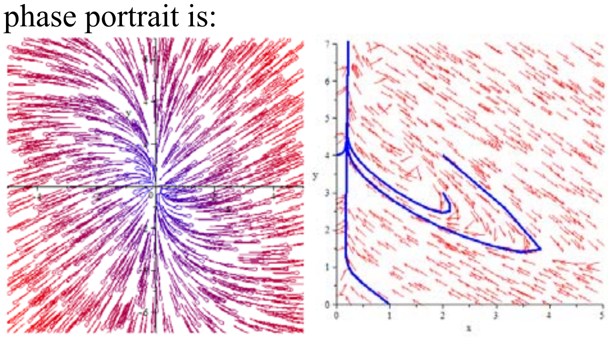
3. STABILITY ANALISYS

We consider the following cases:

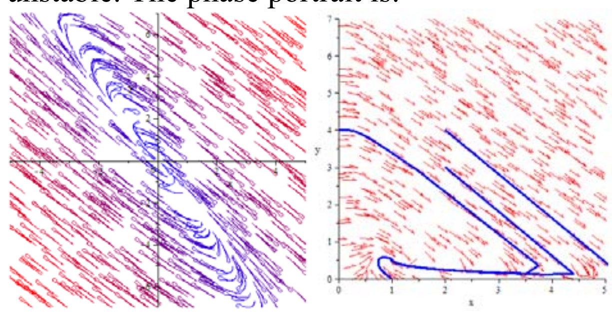
Case 1. If $0 < B < (A-1)^2$, implies that: $\begin{cases} \Delta > 0 \\ TrF_x < 0 \end{cases}$. In this case the roots are real, negative and different: $\lambda_{1,2} \in \mathbf{R}, \lambda_{1,2} < 0, \lambda_1 \neq \lambda_2$. Results that the equilibrium point $\left(A, \frac{B}{A}\right)$ is an attractive node non degenerate, the system is asymptotically stable. The phase portrait is:



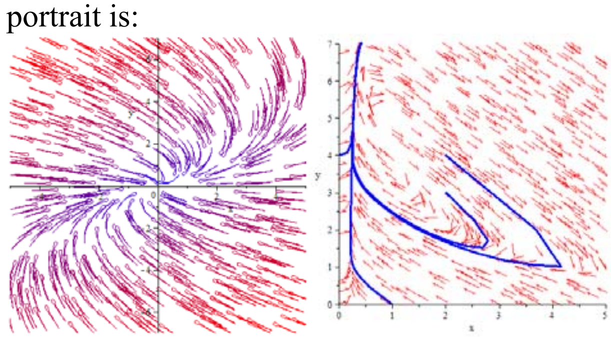
Case 2. If $B > (A+1)^2$, implies that: $\begin{cases} \Delta > 0 \\ TrF_x > 0 \end{cases}$. In this case the roots are real, positive and different: $\lambda_{1,2} \in \mathbf{R}, \lambda_{1,2} > 0, \lambda_1 \neq \lambda_2$. Results that the equilibrium point $\left(A, \frac{B}{A}\right)$ is a rejector node non degenerate, the system is unstable. The phase portrait is:



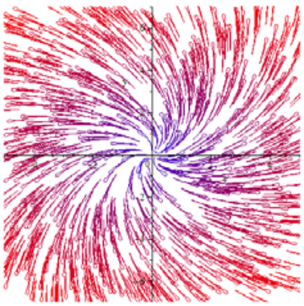
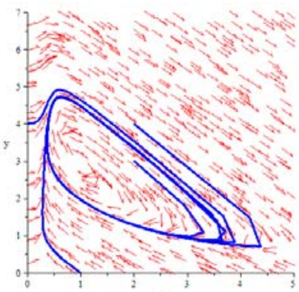
Case 3. If $B = (A+1)^2$, implies that: $\begin{cases} \Delta = 0 \\ TrF_x > 0 \end{cases}$. In this case the roots are real, positive and equal: $\lambda_{1,2} \in \mathbf{R}, \lambda_{1,2} > 0, \lambda_1 = \lambda_2$. Results that the equilibrium point $\left(A, \frac{B}{A}\right)$ is rejector node non degenerate after the line $y = Ax$, the system is unstable. The phase portrait is:



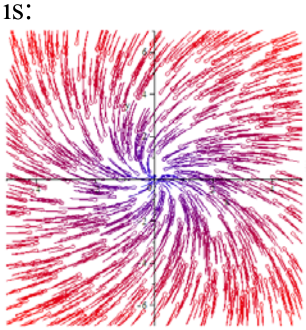
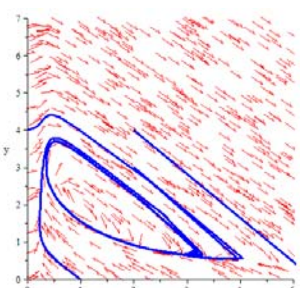
Case 4. If $B = (A-1)^2$, implies that: $\begin{cases} \Delta = 0 \\ TrF_x < 0 \end{cases}$. In this case the roots are real, negative and equal: $\lambda_{1,2} \in \mathbf{R}, \lambda_{1,2} < 0, \lambda_1 = \lambda_2$. Results that the equilibrium point $\left(A, \frac{B}{A}\right)$ is an attractor node non degenerate after the line $y = -Ax$, the system is asymptotically stable. The phase portrait is:



Case 5. If $A^2+1<B<(A+1)^2$, implies that $\begin{cases} \Delta<0 \\ TrF_x>0 \end{cases}$. In this case the roots are complex, with the imaginary part positive $\lambda_{1,2}\in \mathbf{C}\setminus\mathbf{R}$, $\mathrm{Re}(\lambda_{1,2})>0$. Results that the equilibrium point $\left(A,\frac{B}{A}\right)$ is a rejector focus. The phase portrait is:

Case 6. If $(A-1)^2<B<A^2+1$, implies that $\begin{cases} \Delta<0 \\ TrF_x<0 \end{cases}$. In this case the roots are complex, with the imaginary part negative $\lambda_{1,2}\in \mathbf{C}\setminus\mathbf{R}$, $\mathrm{Re}(\lambda_{1,2})<0$. Results that the equilibrium point $\left(A,\frac{B}{A}\right)$ is an attractive focus. The phase portrait is:

Case 7. If $B=A^2+1$, implies that $\begin{cases} \Delta<0 \\ TrF_x=0 \end{cases}$. In this case the roots are complex, with the imaginary part null $\lambda_{1,2}\in \mathbf{C}\setminus\mathbf{R}$, $\mathrm{Re}(\lambda_{1,2})=0$. We have: $\lambda_{1,2}=\mu(B)+i\omega(B)$ where $\mu(B)=0$ and $\omega(B)=A>0$ and $\frac{d\mu}{dB}=\frac{1}{2}\neq 0$. Results that the Hopf theorem's conditions [5] are fulfilled for these values of parameter B.

The new matrices form of the system (5) is:

$$\begin{pmatrix} X' \\ Y' \end{pmatrix}=\begin{pmatrix} A^2 & A^2 \\ -(A^2+1) & -A^2 \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix}+$$
$$+\begin{pmatrix} \frac{A^2+1}{A}X^2+2AXY+X^2Y \\ -\frac{A^2+1}{A}X^2-2AXY-X^2Y \end{pmatrix}$$

With $h(X,Y)=\begin{pmatrix} \frac{A^2+1}{A}X^2+2AXY+X^2Y, \\ -\frac{A^2+1}{A}X^2-2AXY-X^2Y \end{pmatrix}$

For the eigenvalue $\lambda=-iA$ we have the vector: $q=(q_1,q_2)=\left(q_1,-\frac{A-i}{A}q_1\right)$, and for the eigenvalue $\lambda=iA$ we have the vector: $p=(p_1,p_2)=\left(p_1,-\frac{A+i}{A}p_1\right)$, where q_1,p_1 are random numbers. A choice for the vector q is $q=\left(1,-\frac{A-i}{A}\right)$. Taking into account that $q\cdot\overline{p}=A^2$, from the relation: $q\cdot\overline{p}=q_1\cdot\overline{p}_1+q_2\cdot\overline{p}_2$ it is obtained $p_1=\frac{A^4}{A^2+(A-i)^2}$. The vector p has the new form:

$$p=\left(\frac{A^4}{A^2+(A-i)^2},-\frac{A+i}{A}\cdot\frac{A^4}{A^2+(A-i)^2}\right).$$

We introduce a new variable z, using the diffeomorphic transformation:

$(X,Y)=z\cdot q+\overline{z}\cdot\overline{q}$. In this case it is obtained:

$$X=z+\overline{z}$$
$$Y=-\frac{A-i}{A}z-\frac{A+i}{A}\overline{z}.$$

Compute the new function in the new variables:

$$g(z,\bar{z}) = h(X,Y)\cdot\bar{p} =$$
$$= \frac{g_{20}}{2}z^2 + g_{11}z\bar{z} + \frac{g_{02}}{2}\bar{z}^2 + \frac{g_{21}}{2}z^2\bar{z} + \frac{g_{12}}{2}z\bar{z}^2 +$$
$$+\frac{g_{30}}{2}z^3 + \frac{g_{03}}{2}\bar{z}^3 + O(|z|)^4$$

For B we evaluate the expression:

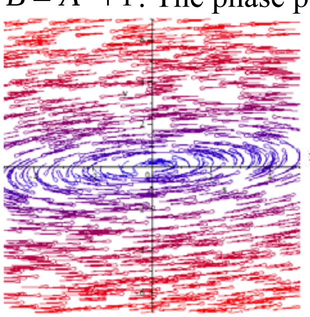
$$C_1(B) = \left(g_{20}g_{11} - 2|g_{11}|^2 - \frac{1}{3}|g_{02}|^2\right) + \frac{g_{21}}{2}$$

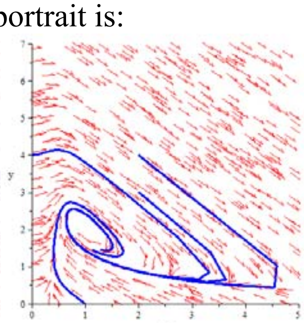
The first coefficient of Liapunov for B is a real number and it is defining by

$$L_1(\alpha_0) = \frac{\operatorname{Re} C_1(B)}{\omega}.$$

Using the affirmations above if $\operatorname{sgn} L_1(B) = \operatorname{sgn}\operatorname{Re}(ig_{20}g_{11} + \omega_0 g_{21}) < 0$ results that in the vicinity of $B = A^2 + 1$ the system admits a stable limit cycle, that means a supercritical bifurcation; $\operatorname{sgn} L_1(B) > 0$ results that in the vicinity of $B = A^2 + 1$ the system admits an unstable limit cycle, that means a subcritical bifurcation.

Because $L_1(B) = \dfrac{2(A^2+1)^2 - A^3}{4A^2}$ the system admits an unstable limit cycle in the vicinity of $B = A^2 + 1$. The phase portrait is:





The trajectory is a rotating ellipse. Next we'll determine the equation of the trajectory corresponding to the system described above. Making the ratio between X' and Y' from the linear system, we obtain the differential total exact equation:

$$[(A^2+1)X + A^2Y]dX + A^2(X+Y)dY = 0$$

By integration it is obtained the equation of trajectory:

$$A^2(X+Y)^2 + X^2 = C$$

REFERENCES

1. Neamțu M., *The study of Differential Systems using geometrical structures*, PhD Thesis, 2001
2. Vernic C., *Analytical methods for the study of biodynamical systems*, Ed. Augusta, Timisoara, 143pg, 2004 ISBN 973-695-107-3
3. Yuncheng You, *Global Dynamics Of The Brusselator Equations*, Dynamics Of Pde, Vol.4, No.2, 167-196, 2007
4. I.R. Epstein, *Complex Dynamical Behavior In Simple Chemical Systems*, J. Phys. Chemistry, 88 (1984), 187-198.
5. O. Florea, C. Ida, *Practical Applications of dynamical systems in engineering*, Ed. LuxLibris, Brasov, 2010