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STABILITY ANALYSIS OF BRUSSELATOR MODEL USING THE JACOBIAN MATRIX METHOD

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ABSTRACT

This paper described the mathematical model of Brusselator to demonstrate the chemical oscillation using Jacobian matrix stability method. The Brusselator model is a theoretical model for a type of autocatalytic reaction. This model can also be analyzed to establish the behavior of two dimensional systems. The utility of Jacobian derives from an analysis in which only linear terms are kept in analyzing the effect of the perturbation on the study state. Marginal stability is an unusual situation that typically occurs as a parameter changes and a state goes from being stable to unstable or vice versa.

Key words: Irreversible thermodynamics, Brusselator model, Autocatalytic reaction, Jacobian Matrix.

1. Introduction

1.1 Jacobion Matrix stability

The Jacobion matrix stability involve the identification of suitable complex reaction and define the Jacobion matrix J and its determinantal equation then find the solution of determinantal equation. The sign of the trace of the Jacobion matrix tr(J) and determinant of the Jacobion matrix det (J) tells us whether the dynamical complex system is stable, asymptotically stable and the region where it oscillate periodically. The gist of this method is described below.

The Poincare Bendixson theorem states that if two dimensional system is confined to a finite region of concentration space then it must ultimately reach to a steady state or oscillate periodically. The system cannot wander through the concentration space indefinitely; the only possible asymptotic solution, other than the steady state, is oscillations. This result is extremely powerful, but it holds only for two dimensional systems. Thus if we can show that a two –dimensional system has no stable steady state and that all concentrations are bounded_ that is, the system cannot explode then we have proved that the system has stable periodic solution, whether or not we can find that solution explicitly.

To examine the issue of stability in two or more dimensions, we need to generalized the notion of the Jacobion J.

We will consider a model with two independent concentrations, α and β, whose time derivatives are represented by two functions f and g respectively;

$$\frac{d\alpha}{dt} = \mathsf{f}(\alpha, \beta) \tag{1}$$

$$\frac{d\beta}{dt} = \mathsf{f}(\alpha, \beta) \tag{2}$$

To state the stability of steady state $(\alpha_{ss,}\beta_{ss})$,we add a perturbation to each variable;

$$\alpha = \alpha_{ss} + \delta\alpha \tag{3}$$

$$\beta = \beta_{ss} + \delta\beta \tag{4}$$

Substitute the expression (3) and (4) into (1) and (2) and expand the function of f and g in the Taylor series about the steady state point $(\alpha_{ss,}\beta_{ss})$, where $\mathsf{f} = g = 0$. If the perturbation is small enough that we may neglect second and higher order terms our equation becomes

$$\frac{d\delta\alpha}{dt} = (\partial\mathsf{f}/\partial\alpha)_{ss}\,\delta\alpha + (\partial\mathsf{f}/\partial\beta)_{ss}\,\delta\beta \tag{5}$$

$$\frac{d\delta\beta}{dt} = (\partial g/\partial\alpha)_{ss}\,\delta\alpha + (\partial g/\partial\beta)_{ss}\,\delta\beta \tag{6}$$

Eqs(5)and(6)are just the differential equation in $\delta\alpha$ and $\delta\beta$. Equations of this form have solutions that are the sums of exponentials, where the exponents are found by assuming that each variable is of the form $c_i \exp(\lambda t)$.Let

$$\delta\alpha(t)=c_1e^{\lambda t},\ \ \delta\beta(t)=c_2e^{\lambda t} \tag{7}$$

where c_1 and c_2 are the vector coefficient. Now define the Jacobion matrix J as

$$J=\begin{pmatrix}\frac{\partial f}{\partial\alpha} & \frac{\partial f}{\partial\beta}\\ \frac{\partial g}{\partial\alpha} & \frac{\partial g}{\partial\beta}\end{pmatrix} \tag{8}$$

The result of substituting eqs (7) into eqs (5) and (6) and dividing by $\exp(\lambda t)$ can be written in the compact form as

$$(J-\lambda I)C=0 \tag{9}$$

where J is the Jacobion matrix difined in eq (8) and C is the vector coeficients $(c_{1,}\ c_2)$ in eq (7), I is the 2x2 identity matrix and 0 is a 2x1 vector of zeros. Eq(9) have the non trivial solution-that is the solutions other than all the coefficient c being zero- only when λ is a solution of the determinantal equation

$$\det\begin{pmatrix}\frac{\partial f}{\partial\alpha}-\lambda & \frac{\partial f}{\partial\beta}\\ \frac{\partial g}{\partial\alpha} & \frac{\partial g}{\partial b}-\lambda\end{pmatrix}_{ss}=\left(\frac{\partial f}{\partial\alpha}-\lambda\right)_{ss}\left(\frac{\partial g}{\partial b}-\lambda\right)_{ss}-\left(\frac{\partial g}{\partial\alpha}\right)_{ss}\left(\frac{\partial f}{\partial\beta}\right)=0. \tag{10}$$

Eq(10) can be expanded to give

$$\lambda^2-\lambda tr(J)+\det(J)=0 \tag{11}$$

where $tr(J)$ is the trace of the Jacobion matrix . Eq(11) is the quadratic in the exponant λ.If either eigen value λ has a positive real part,the solution will grow ;the steady state is unstable. If both λ values have negative real part,the steady state is stable.

The behavior of two-dimenssional systems based on the nature of the solution to eq(11)and are obtained by applying the quadratic formula.we will consider the several possibilities of for the sign of the trace, determinant, and discriminant $\left(tr(J)^a - 4\det(J)\right)$.

$$tr(J)^a < 0, \quad \det(J) > 0, \quad tr(J)^2 - 4\det(J) > 0 \tag{12}$$

Any perturbation to this steady state will monotonically decrease and disappear. The steady state is stable node and nearby points in the concentration are space are drawn to it.

$$tr(J)^a < 0, \quad \det(J) > 0, \quad tr(J)^2 - 4\det(J) < 0 \tag{13}$$

The perturbation will decay back to the steady state. This steady state is called as a stable focus.

$$tr(J)^a > 0, \quad \det(J) > 0, \quad tr(J)^2 - 4\det(J) < 0 \tag{14}$$

The perturbation will grow and spiral away from the steady state, which is an unstable focus.

$$tr(J)^a > 0, \quad \det(J) > 0, \quad tr(J)^2 - 4\det(J) > 0 \tag{15}$$

Any perturbation will grow exponentially away from the steady state which is an unstable node.

$$\det(J) > 0, \tag{16}$$

Trajectories approach the steady state along the eigen vector corresponding to the negative eigen value. But then move away from the steady state along the transverse direction. The steady state is called a saddle point.

$$tr(J) = 0, \quad \det(J) > 0, \tag{17}$$

This condition indicates the onset of sustained oscillations through a Hopf bifurcation.

Discussion of Brusselator model

In this paper we discussed the application of stability analysis to the Brusselator model using theJacobian matirx method .We will now analyze the Brusselator to illustrate how one might use the techniques that we have discussed to establish the behavior of two dimensional systems. The reaction scheme is as follows.

$$A \xrightarrow{k_1} E \tag{18}$$

$$B + X \xrightarrow{k_2} Y + D \tag{19}$$

$$2X + Y \xrightarrow{k_3} 3X \tag{20}$$

$$X \xrightarrow{k_4} E \tag{21}$$

Let the concentrations, like the species, be represented by capital letters, and call the time .Then the rate equation for the X and Y corresponding to the equations (18), (19), (20), (21) with the concentration of A and B held constant, are

$$\frac{dX}{dT} = k_1 A - k_2 BX + k_3 X^2 Y - k_4 X \tag{22}$$

$$\frac{dY}{dT} = k_2 BX - k_3 X^2 Y \tag{23}$$

We set eqs (22) and (23) in the simpler form as follows

$$X = \alpha x,\ Y = \beta y,\ B = \varepsilon b,\ A = \delta a,\ B = \varepsilon b \tag{24}$$

where α, β, γ, ε, δ are the scaling factors. Substitute eq(24) into eqs(22)and (23) to obtained ,after multiplying through by α/γ and α/β in eqs (25) and(26) respectively,

$$\frac{dx}{dt} = \left(k_1\delta\gamma/\alpha\right)a - \left(k_2\varepsilon\gamma\right)bx + \left(k_3\alpha\beta\gamma\right)x^2 y - \left(k_4\gamma\right)x \tag{25}$$

$$\frac{dy}{dt} = \left(k_2\varepsilon\alpha\gamma/\beta\right)bx - \left(k_3\gamma\alpha^2\right)x^2 y \tag{26}$$

Eqs(25) and(26) not only the rate constant but also the scaling factor α, β, γ, ε, and δ .now let us pick all the scaling factor in eq(25) and(26) equal to unity

$$k_1\delta\gamma/\alpha = k_2\varepsilon\gamma = k_3\alpha\beta\gamma = k_4\gamma = k_2\varepsilon\alpha\gamma/\beta = k_3\gamma\alpha^2 = 1 \tag{27}$$

Eq (27) gives the following five conditions as

$$\alpha = \beta = \left(k_4/k_3\right)^{1/2},\ \ \gamma = 1/k_4,\ \ \delta = \left(k_4/k_1\right)\left(k_4/k_3\right)^{1/2},\ \ \varepsilon = k_4 k_2 \tag{28}$$

Now substitute eq(28) into eq(25) and(26) ,we obtained much prettier version of the Brusselator in terms of unitless variable.this rescaling proccedure reduces the number of parameters before analysing the properties of a modeland we get the equations as

$$\frac{dx}{dt} = a - bx + x^2 y - x \tag{29}$$

$$\frac{dy}{dt} = bx - x^2 y \tag{30}$$

To obtain the steady state(s)of the Brusselator,we set equations (29)and (30) equal to zero and solve for x and y

$$x_{ss} = a, \qquad y_{ss} = b/a \tag{31}$$

To analyze the stability of this state,we must calculate the elements of Jacobion matrix:

$$J = \begin{pmatrix} \frac{\partial(dx/dt)}{\partial x} & \frac{\partial(dx/dt)}{\partial y} \\ \frac{\partial(dy/dt)}{\partial x} & \frac{\partial(dy/dt)}{\partial y} \end{pmatrix} \tag{32}$$

The elements of Jacobion matrix are

$$\left.\frac{\partial(dx/dt)}{\partial x}\right|_{ss} = -b + 2a(b/a) - 1 = b - 1 \tag{33}$$

$$\left.\frac{\partial(dx/dt)}{\partial y}\right|_{ss} = a^2 \tag{34}$$

$$\left.\frac{\partial(dy/dt)}{\partial x}\right|_{ss} = b - 2a(b/a) = -b \tag{35}$$

$$\left.\frac{\partial(dy/dt)}{\partial y}\right|_{ss} = -a^2 \tag{36}$$

Now obtain the eigenvalues of the matrix whose elements are given by eqns (32),(33),(34),(35) by solving the characteristic equation:

$$\lambda^2 + (a^2 + 1 - b)\lambda + a^2 = 0 \tag{37}$$

$$\det(J) = a^2 = 0 \tag{38}$$

Or equivalently

$$\lambda^2 + \left(a^2 + 1 - b\right)\lambda + a^2 = 0 \tag{39}$$

Compareing eqs (11) and (37) we observe that

$$tr\left(J\right) = -a^2 + b - 1 \qquad \left(\text{either positive or negative}\right) \tag{40}$$

$$\det\left(J\right) = a^2 \qquad \left(\text{positive}\right) \tag{41}$$

The stability of the steady state will depend on the sign of the trace .As we vary, a and b when passes through zero, the character of the steady state will change; a bifurification occurs.

$$b > a^2 + 1 \qquad \left(\text{unstable}\right) \tag{42}$$

Thus by the Poincare-Bendixson theorem, the system either oscillate or explode and confined to a finite region of the $x - y$ phase space. Equation(42)determines the boundary in the $a - b$ constraint space between the region where the system will asymptotically approach a stable steady state and the region where it oscillate periodically.

Conclusion

In this paper we have seen how to construct and analyze the mechanism for complex reaction, and introduced the notion of feedback and open system, which are key to the development of complex dynamics in chemical system and we learned how to analyze the stability of steady states.

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