

Activator-Inhibitor Model of a Dynamical System: Application to an Oscillating Chemical Reaction System

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Abstract

In this paper we have first studied the role of activator-inhibitor technique in modelling a general dynamical system and then as application investigated the criteria of oscillation of a non-linear chemical reaction system.

Keywords: Activator-Inhibitor Model, Informational Network, Dynamical System, Chemical Reaction System, Criteria of Oscillation.

1. Introduction

A complex system is composed of many parts, elements or components which are connected in a more or less complicated fashion[1,2,3]. In dealing with complex systems we are confronted with the challenge of finding unifying principles covering all systems irrespective of the branches of science they belong to. In order to describe a complex system at microscopic level, we need an enormous amount of data or information[4]. A macroscopic description allows an enormous compression

of information which are concerned not with the individuals microscopic data but rather with the global properties of the system establishing various relations among the various macroscopic quantities. Non-equilibrium thermodynamics is the appropriate branch of science dealing with such relations of a complex system[5]. The method is analogous to Rosen's mathematical representation of a complex system[2]. It is based on Higgins activation and inhibition model of oscillating chemical reaction[6]. In the present paper we have first discussed the mathematical techniques of activation-inhibition in the modelling of a general dynamical system. We have then investigated the role of activation-inhibition technique in the modelling of an oscillating chemical reaction system.

2. Activation and Inhibition in Dynamical System

Let us consider a general dynamical system described by the system of differential equations

$$\frac{dx_i}{dt} = f_i(x_1, x_2, \dots, x_n), (i = 1, 2, \dots, n) \quad (2.1)$$

The functions f_i are assumed to be continuous and to have continuous partial derivatives in some open set $\Omega = \{x_i, x_i \geq 0\}$. Following Higgin's activation and inhibition model of dynamical system we consider the following observational quantities[2]

$$a_{ij}(x_1, x_2, \dots, x_n) = \frac{\partial}{\partial x_j} \left(\frac{dx_i}{dt} \right) = \frac{\partial}{\partial x_j} V_{x_i}, (i, j = 1, 2, \dots, n) \quad (2.2)$$

where V_{x_i} is the net rate at which the substance (or reactant) is being produced as a result of interaction occurring in the system. The quantities a_{ij} , ($i, j = 1, 2, \dots, n$) as Higgin noted have informational correlation. For instance, the quantities a_{ij} defined above have three possibilities[1]

$$(a) a_{ij} > 0, (b) a_{ij} < 0, (c) a_{ij} = 0 \quad (2.3)$$

If (a) holds, then the increase (or decrease) in the instantaneous value of x_j will cause the rate of production of

$x_i \left(i.e. \frac{dx_i}{dt} = V_{x_i} \right)$ to be increased (or

decreased). In this case we shall call x_j to be an activator of x_i . If $x_j = x_i$, then x_i is a self-activator.

If (b) holds, the reverse is true, an increase (or decrease) in the instantaneous value of x_j will cause the rate of production of x_i to be decreased (or increased). In that case x_j

is said to be an inhibitor of x_i . For $x_j = x_i$, x_i is then a self-inhibitor.

if (c) holds, the rate of production of x_i is independent of alterations in the instantaneous values of x_j .

The quantity a_{ii} is the interaction of x_i with its flux V_{x_i} is known as the self-coupling and the quantities $a_{ij} (i \neq j)$, which is the interaction of x_i with the flux of x_j (i.e. V_{x_j}) is known as the cross-coupling.

An important problem about the quantities a_{ij} is to find out the ranges of validity of the activator and inhibitor a_{ij} which are defined relative to some initial state (a stationary point or a critical point). Since by hypothesis all the partials of the production rates are continuous, it follows that if x_j is an activator for x_i relative to some initial state, it is an activator for x_i in some entire

neighbourhood of that state ; likewise if x_j is an inhibitor for x_i relative to some initial state, we can thus, decompose the state space Ω of the system into a set of subregions, such that, in any sub-region, the sign of all first partial derivatives $\frac{\partial V_{x_i}}{\partial x_j}$ is

the same for all points in the subregion[1]. On the basis of activator- inhibitor any dynamical system (biochemical, morphogenetic, ecological or neutral etc) can be converted into an informational network of activator and inhibitor which seems more natural than the dynamical one[2]. The quantities a_{ijk} defined by[2]

$$a_{ijk} = \frac{\partial}{\partial x_k} a_{ij} = \frac{\partial}{\partial x_k} \left[\frac{\partial}{\partial x_j} \left(\frac{dx_i}{dt} \right) \right] \quad (2.4)$$

$i, j, k = 1, 2, \dots, n$

also have the characters of informational correlations. It is easy to show that if $a_{ijk} > 0$ in a state, it means that x_k enhances or potentiates the effect of x_j on x_i . Under these considerations we call x_k an agonist of x_j . Likewise if $a_{ijk} < 0$ in a state, x_k attenuates the effect of x_j on x_i and hence we call x_k antagonist of x_i . We can continue the iterating process in this way to get successive networks a_{ij}, a_{ijk}, \dots to give an informational

description of the dynamical system (2.1). The system of networks $\{a_{ij}\}$ play significant role in the study of stability, instability and periodicity of the dynamical system. In the next section we shall study the role of the network $\{a_{ij}\}$ in finding out the criteria of stability, instability and periodicity of a chemical reaction system

3. Activation and Inhibition in Chemical Reaction System

Let us consider a system of two chemical species described by the kinetic equations[7]

$$\begin{aligned} \frac{dx_1}{dt} &= a - bx_2 + \frac{x_1^2}{x_2} = f_1(x_1, x_2) \\ \frac{dx_2}{dt} &= x_1^2 - x_2 = f_2(x_1, x_2) \end{aligned} \quad (3.1)$$

where x_1 and x_2 are the concentrations of two reactants depending on time, a and b are externally given fixed in time. Let us assume that the system is homogeneous such that the chemical species are distributed uniformly throughout its entire whole space. The steady state (or stationary point) of the system is

$$x^0 = (x_1^0, x_2^0) = \left\{ \sqrt{\left(\frac{1+a}{b} \right)}, \left(\frac{1+a}{b} \right) \right\} \quad (3.2)$$

such that

$$f_i(x^0) = f_i(x_1^0, x_2^0) = 0, \quad (i = 1, 2)$$

(3.3)
 Expanding the functions

$f_i(x_1, x_2)$, ($i = 1, 2$) about the stationary point (x_1^0, x_2^0) we have the system of equations

$$\frac{dx_i}{dt} = f_i(x_1^0, x_2^0) + \sum_{j=1}^2 \left(\frac{\partial f_i}{\partial x_j} \right)_{(x^0)} (x_j - x_j^0) + \frac{1}{2} \sum_{j=1}^2 \sum_{k=1}^2 \left(\frac{\partial^2 f_i}{\partial x_k \partial x_j} \right)_{(x^0)} (x_j - x_j^0)(x_k - x_k^0) + \dots$$

(3.4)

neglecting higher order terms of δx_j , we have the system of linear equations,

$$\frac{dx_i}{dt} = \sum_{j=1}^2 a_{ij}(x_1^0, x_2^0) \delta x_j = \sum_{j=1}^2 a_{ij}(x^0) \delta x_j, \quad (i = 1, 2)$$

(3.5)

where

$$a_{ij}(x^0) = \left(\frac{\partial f_i}{\partial x_j} \right)_{(x^0)} = \left[\frac{\partial}{\partial x_j} \left[\frac{dx_i}{dt} \right] \right]_{(x^0)}$$

(3.6)

is the value of the informational correlation function at the stationary point $x^0 = (x_1^0, x_2^0)$. $a_{ij}(x^0)$ are the elements of the Jacobian matrix J at the stationary state.

$$J = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}_{(x^0)} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}_{(x^0)}$$

$$= \begin{pmatrix} 2\sqrt{\frac{b}{1+a}} & -b\left(\frac{a+2}{a+1}\right) \\ 2\sqrt{\frac{a+1}{b}} & -1 \end{pmatrix}$$

(3.7)

The term $a_{11} = \frac{\partial}{\partial x_1} V_{x_1} = 2\sqrt{\frac{b}{1+a}} > 0$

implies that x_1 is self-activator of x_1 .

$$a_{12} = \frac{\partial}{\partial x_2} V_{x_1} = -b\left(\frac{a+2}{a+1}\right) < 0$$

implies that x_2 is an inhibitor of x_1 .

$$a_{21} = \frac{\partial}{\partial x_1} V_{x_2} = 2\sqrt{\frac{a+1}{b}} > 0$$

implies

that x_1 is an activator of x_2 .

$$a_{22} = \frac{\partial}{\partial x_2} V_{x_2} = -1 < 0$$

implies that x_2

is a self-inhibitor of x_2 .

The system (3.1) whose Jacobian matrix has the sign matrix of the form

$$Sign(J) = \begin{pmatrix} + & - \\ + & - \end{pmatrix}$$

(3.8)

is an activator-inhibitor system[8].

Let us now turn to the stability analysis of the system (3.1) on the basis of the system

of linear equations (3.5). The eigenvalue equation is

$$\begin{pmatrix} a_{11} - \lambda & a_{12} \\ a_{21} & a_{22} - \lambda \end{pmatrix} = 0$$

or

$$\lambda^2 - \beta\lambda + \gamma = 0 \tag{3.9}$$

with eigenvalues

$$\gamma_{1,2} = \frac{\beta \pm \sqrt{\beta^2 - 4\gamma}}{2} \tag{3.10}$$

where

$$\beta = \text{Trace}(J) = 2\sqrt{\frac{b}{a+1}} - 1 \tag{3.11}$$

$$\gamma = \det(J) = 2\sqrt{b(a+1)} > 0 \tag{3.12}$$

We keep the concentration a fixed and change the concentration b . $\beta = 0$ if

$$b = b_c = \frac{1+a}{4}. \text{ If } b_c = \frac{1+a}{4} < b \text{ then}$$

$\beta > 0$ implying that stationary point (3.2)

is unstable focus. Again if $b_c = \frac{1+a}{4} > b$,

then $\beta < 0$ implying that the stationary point is a stable focus. If

$\beta = 0$ i.e. $b = b_c = \frac{1+a}{4}$, we have a

bifurcation point at $\beta = 0$ or

$$b = b_c = \frac{1+a}{4}. \text{ This situation}$$

corresponds to the transition of the system from the stable focus ($\beta < 0$) to the unstable focus crossing through the

bifurcation point $\beta = 0$ or $b = \frac{1+a}{4}$.

Hopf-bifurcation theorem then predicts the existence of a stable limit cycle provided $\gamma > 0$ [8].

Let C be a closed orbit enclosing the stationary point as the only singular point. In order that the closed orbit be the limit cycle it is necessary that

$$\gamma > 0$$

or

$$a_{11}a_{22} - a_{12}a_{21} > 0$$

or

$$\frac{\partial V_{x_1}}{\partial x_1} \frac{\partial V_{x_2}}{\partial x_2} - \frac{\partial V_{x_1}}{\partial x_2} \frac{\partial V_{x_2}}{\partial x_1} > 0 \tag{3.13}$$

The partials in the above l.h.s. expression are evaluated at the stationary point. In view of the continuity of the partials we have seen that, if these partials have a definite character at the stationary point, this character must be retained throughout the entire neighbourhood of the stationary point,

and thus the inequality (3.13) must hold throughout this entire region[1]. We now suppose that the closed curve C lies entirely within this region of constant character. So also the reaction

$$a_{11} + a_{22} = \frac{\partial V_{x_1}}{\partial x_1} + \frac{\partial V_{x_2}}{\partial x_2} = 0 \quad (3.14)$$

valid for the stationary point is valid throughout the entire region in the neighbourhood of the stationary point. We have thus see that the self-couplings $\frac{\partial V_{x_1}}{\partial x_1}$

and $\frac{\partial V_{x_2}}{\partial x_2}$ must be of opposite sign. From

this and (3.13) it follows that

$$\frac{\partial V_{x_2}}{\partial x_1} + \frac{\partial V_{x_1}}{\partial x_2} = 0 \quad (3.15)$$

implying that the cross coupling terms

$\frac{\partial V_{x_2}}{\partial x_1}$ and $\frac{\partial V_{x_1}}{\partial x_2}$ are of opposite sign.

From the above analysis of self-coupling and cross-coupling we see that

$$a_{11}a_{22} < 0 \Rightarrow \frac{\partial V_{x_1}}{\partial x_1} \frac{\partial V_{x_2}}{\partial x_2} < 0 \quad (3.16)$$

and

$$a_{12}a_{21} < 0 \Rightarrow \frac{\partial V_{x_1}}{\partial x_2} \frac{\partial V_{x_2}}{\partial x_1} < 0 \quad (3.17)$$

where the elements $a_{ij}, (i, j = 1, 2)$ are defined in the neighbourhood of the stationary point. The signed matrix corresponding to the Jacobian matrix (3.7) is given by

$$Sign(J) = \begin{pmatrix} + & - \\ + & - \end{pmatrix} \quad (3.18)$$

which characterises an activator inhibitor system[8].

4. Conclusion

In the present paper we have studied two problems. We have first studied the role of the technique of activator-inhibitor in the modelling of a general dynamical system. As application of the activator-inhibitor technique we have studied a non-linear chemical reaction system and determined the conditions or criteria of oscillating behaviour of the system. The activator-inhibitor network a_{ij} play a significant role in the study of stability, instability and the periodicity of the chemical reaction system.

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