NONLINEAR DYNAMICS OF REACTION DIFFUSION SYSTEMS: TURING'S ANALYSIS

Abstract

The target of this chapter is to give a brief outline about Nonlinear Dynamics of reaction diffusion systems. When diffusion is coupled with chemical kinetics some interesting spatio temporal structures arise such as stationary patterns, spatially-varying concentrations of chemical species, spirals, traveling waves, solitons, targets etc. In view of Alan Turings phenomenological theory on Morphogenesis the pattern formation of reaction diffusion systems can be understood. The theoretical prediction of spatio-temporal instability and its experimental demonstration is illustrated in this chapter.

Keywords: Stability, Nonlinear dynamics, diffusion, bifurcation, instability.

Author

Shrabani Sen
Department of Chemistry
Rammohan College
102/1, Raja Rammhan Sarani
Kolkata, West Bengal, India.

I. INTRODUCTION

The study of Non linear dynamics is an important tool for understanding various bio physical and chemical phenomena such as glycolytic oscillations, Ca^{+2} oscillations, circadian cycles, cell cycles and so on[1-4]. In one of the previous book chapters the emergence of oscillation from Nonlinear dynamical point of view had already been discussed [5]. When reaction kinetics is accompanied with diffusion, dynamical evolution of the system becomes more significant resulting in stationary patterns, spatially inhomogeneous concentration of chemical species, spirals, traveling waves, solitons, targets, wave propagations etc. These spatial and spatio-temporal structures can be realized by coupling the reaction part with diffusion at discrete spatial points [6,7]. The dynamics of these systems are governed by reaction-diffusion equations. Alan Turing, in one of his seminal papers on the theory of Morphogenesis [8], had revealed the mystery behind the structural evolution of patterns in biological systems, such as, coat patterns of animals like tigers, zebras, pigmentation patterns of fish, spots, stripes and spiral patterns of various biological species. Turing's analysis illustrates that the necessary and sufficient condition for generation of pattern is the disparity in diffusivities of the reacting species. Thermodynamically open system took a long time to understand its consequences. As a result Turing pattern could not be understood for a long time even after its theoretical explanation With gradual development of suitable experimental techniques unambiguous experimental evidences on Turing pattern were clearly explained in the last decade of twentieth century[9,10]. Thus the theoretical prediction of spatio-temporal instability and its experimental demonstration have now opened up a new horizon in the field of reaction-diffusion systems. In this present chapter we will focus on some of the primary features of the spatio temporal structures.

II. TURING'S ANALYSIS

Let us think A and B are two reactants.. Without diffusion they react with each other to reach the equilibrium state following chemical kineics. Now the parameter domain of the system determines the stability of the steady state. It can be stable or unstable. Or it can lead to oscillation resulting in limit cycle in phase space. Now comes the question whether reaction is coupled with diffusion then what happens.Turing raised the fact that when a chemical reaction is coupled with diffusion then kinetically stable steady state becomes unstable. Turing concluded that instability is possible when the diffusion coefficients of the species differs with each other significantly among themselves. Diffusion although is a stabilizing phenomena leading to homogeneity but coupling reaction with diffusion contradicts the thought. We will proceed the analytical understandings but now it is better to elaborate the intrinsic theory first. Let us consider an auto-catalytic reaction which involves an 'activator' and an 'inhibitor'. Activator diffuses much slowly than inhibitor. Let us consider that a small region of space feels a sudden increase in concentration of the activator. This subsequently enhances the autocatalytic reaction rate and as a result concentrations of both the species A and B increases. Now the diffusion coefficient of inhibitor is higher than activator resulting in faster diffusion than activator. Consequently the activator concentration increases in a particular space but the surrounding domain becomes inhibitor rich. Thus a very small perturbation of any reactants evolves with time and results differential distribution of the concentration of the species which ultimately leads to inhomogeneity. Following is the analytical explanation of the Turings's analysis.

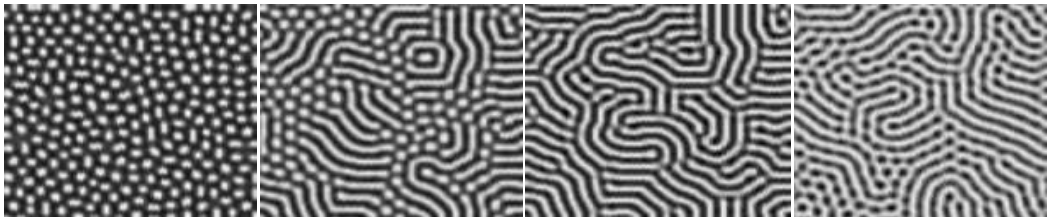

Figure 1: Different types of coat patterns generated in animals fish. This is predicted theoretically [10]

Let us consider a kinetic model of two chemical species $u(x,t)$ and $v(x,t)$ in one dimension. Here one is acting as an activator $u(x,t)$ and other one is an inhibitor $v(x,t)$. The corresponding reaction-diffusion equations are given by

$$u_t = \gamma f(u,v) + \nabla^2 u$$

$$v_t = g(u,v) + d\nabla^2 v \qquad (1).$$

Where $d = Dv/Du.$, Du and Dv are the respective diffusion coefficients and d representing the ratio. The parameter space of the system has to be chosen in such a way that without diffusion both u and v tend to steady state linearly stable in nature and spatially homogeneous. That means the concentration of the chemical species remains constant throughout the space. In presence of diffusion with variable diffusion coefficients the spatially inhomogeneous patterns may develop which are stationary in time under certain conditions by diffusion-driven instability. Diffusion is usually considered as a stabilizing process. Diffusion makes homogeneity out of inhomogenous nature. But in this case diffusion is the cause of instability. We are in search for the necessary and sufficient conditions for diffusion-driven instability of the homogeneous steady state and the generation of stationary pattern. As per Turing's analysis the boundary conditions are chosen to be zero flux. For the homogeneous kinetic steady state (u_0, v_0) the following condition holds

$$f(u_0, v_0) = 0$$
$$g(u_0, v_0) = 0 \qquad (2).$$

Now in absence of diffusion u and v the dynamical equations become

$$u_t = \gamma f(u,v)$$
$$v_t = g(u,v) \qquad (3).$$

The equations are linearised around the steady state (u_0, v_0). (u,v) is changed to $u_0 + \delta u$ and $v_0 + \delta v$. where δu and δv are the small amount of perturbations applied. Now the time evolution of the perturbations are given by

$$y_t = \gamma A y, \quad A = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \qquad (4).$$

Where A the stability matrix . f and g are the partial derivatives of the corresponding kinetic part. This forms matrix A. The partial derivatives are needed to be evaluated at the steady state (u_0, v_0) . y has the form

$$y = \begin{pmatrix} \delta u \\ \delta v \end{pmatrix} \tag{5}.$$

The solutions of the above dynamical equations Eq 4 must be of the exponential form $y \sim e^{\lambda t}$ where λ is the eigen value. The steady state will be linearly stable only when the real part of the eigen value is negative as a consequence perturbation matrix $y \rightarrow 0$ as t tends to infinity. As a result the steady state becomes stable. We proceed in the same way and obtain the following algebraic equation for the eigenvalues

$$\lambda^2 - \gamma(f_u + g_v)\lambda + \gamma^2(f_u g_v - g_u f_v) = 0 \tag{6}.$$

From the above equation Eq (6) λ will be negative that means the steady state will be linearly stable if $f_u + g_v < 0$ and $f_u g_v - g_u f_v > 0$. The inequality implies the steady state to be homgeneosly stable in the aforementioned parameter domain . We now proceed for the analysis of entire reaction diffusion system and apply the same linearization technique. Thus we get

$$y_t = \gamma A y + D\nabla^2 y, \quad D = \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix} \tag{7}.$$

Here the small perturbations in the variables u and v are allowed to grow both in space and time around steady state as $du \sim e^{\lambda t} \cos kx$ and dv accordingly. Here k is the wavenumber. The significant inclusion of both spatial and temporal part in the trial wave function is notable. The boundary condition to be applied is no flux. Result is $k = \frac{n\pi}{a}$. n is an integer and a is the parameter by which the domain size can be determined in single dimension. Putting the trial solution in Eq (7) ultimately the following equation is obtained

$$\lambda^2 + [k^2(1+d) - \gamma(f_u + g_v)]\lambda + h(k^2) = 0 \tag{8}.$$

$$h(k^2) = dk^4 - \gamma(d f_u + g_v)k^2 + \gamma^2|A|.$$

Where

Note that as a function of k^2 h is quadratic that opens upward, that is it has minimum. Since |A| >0, we know that h cannot be less than zero or equal to zero for any positive value of k^2 unless

$$d f_u + g_v > 0 \tag{9}.$$

Because if Eq (9) does not hold, all the terms in Eq (8) would be positive for any k^2>0. This Eq (9) is a necessary condition for Turing instability.

Eq (9) provides an important physical insight. We know from the stability analysis that the sum of the Jacobain elements that is $f_u + g_v < 0$. If both the terms are individually negative and on the above condition will not held. Therefore both the condition to hold true i.e. $f_u + g_v < 0$ and $df_u + g_v > 0$ one must be negative and one positive element. That is one species enhances the rate of its own production and the other decreases the rate production as its production grows. If one species is called the activator, other is inhibitor and the model is called activtator-inhibitor model. This type of model plays an important role in investigating Turing pattern.

Inorder o hold $f_u + g_v < 0$ $|f_u| < |g_v|$. Eq (9) provides an important restriction on the diffusion coefficients of the activator and inhibitor in any system that permits Turing pattern formation. The inhibitor must diffuse more rapidly that the activator. This condition is referred to as 'local activation and lateral inhibition'.

Thus we can conclude if the requisite conditions hold then the initial infinitesimal perturbation will ultimately evolve to a stable spatially inhomogeneous structure, the Turing pattern.

Extension of the analytic treatment upto two dimension will elaborate further experimental findings of Turing pattern formations. Application of external effects such as electric field, magnetic field, effect of deterministic and stochastic time delay will further reveal the control of the pattern generations. Depending on the nature of nonlinearity one may observe various types of patterns ranging from stripes to spots for the systems obeying the conditions discussed above.

III. SOME REACTION DIFFUSION SYSTEMS EXHIBITING TURING'S PATTERN

1. **The Pigmentation Fish Model:** *It* is a two variable reaction diffusion sytem. Bario et al first proposed this model where pattern in fish arises due to physical interaction between cells with external surrounding leading to cell aggregation and differentiation. The equations are as follows

$$\frac{\partial u}{\partial t} = \alpha u(1 - r_1 v^2) + v(1 - r_2 u) + \delta d\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right)$$

$$\frac{\partial v}{\partial t} = \beta v(1 + \alpha r_1 uv/\beta) + u(\gamma + r_2 v) + \delta\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right)$$

Where α, β, γ, r_1, r_2 are the given parameters of the dynamics. d is the length scale. When the diffusion not present v = -(α + γ)u/(1 + β) is the another steady state. apart from the steady state (0,0) can be ensured as the only uniform steady state by setting the parameter $\alpha = -\gamma$.

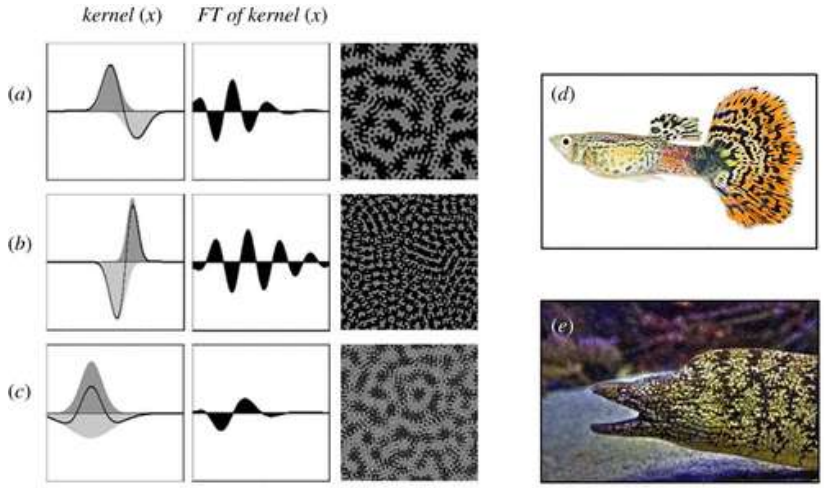

Figure 2: Generation of patterns in Fish as a result of different activator inhibitor concentrations [9]

IV. GIERER MEINHERDT MODEL

To take into consideration the two central features of pattern forming phenomena, viz. the local self-enhancement and the long range inhibition, Gierer and Meinhardt introduced the two species (A and B are the concentrations of the two reacting species) model.

$$\frac{\partial A}{\partial t} = D_A \Delta^2 A + \rho_A \frac{A^2}{1+K_A^2}\frac{1}{B} - \mu_A A + \sigma_A$$
$$\frac{\partial B}{\partial t} = D_B \Delta^2 B + \rho_B A^2 - \mu_B B + \sigma_B$$

In this model the species B is an antagonist and consequently *DB >> DA* which is the condition for formation of spatial instabilities. The coefficients μ_A and μ_B are the removal rates. The basic production terms are given by σ_A and σ_B, the cross reaction coefficients are given by ρ_A and ρ_B. The constant *KA* is called the saturation constant and is believed not that necessary for pattern forming instability to develop, rather it determines the shape of the pattern.

There are some experimental systems which have been studied to illustrate the instabilities but we will elaborate those in some other reviews rather we will focus on some different tyes of instabilities eg spirals.

V. SPIRALS

Spirals are fascinating spatio-temporal patterns in reaction diffusion system where circular symmetry is disrupted. A wave created from a point due the infinitesimal perturbation of any one of the reactants can form circles having unique centre. It is due to fact that waves can propagate uniformly in all directions. It can form spots, stripes, labyrinth patterns and so on. But local disruption of concentric waves lead to curl and results spirals.

Spirals are one of the most commonly featured phenomena in several areas in involving living systems as well as complex systems. Spirals have been detected in aggregating slime molds , carbon monoxide oxidation on single crystals of platinum, developing frog eggs, heart muscle, ferrocin-catalyzed BZ reaction, Gierer-Meinhardt model and other related systems [13,14]. However, the most studied of all these systems is Beluosov-Zhabotinskii reaction.

Figure 3: Theoretical prediction of spiral patterns generated in CDIMA system which has quite relevance with experimental observations [13].

Before going to review some of the mathematical techniques that are in frequent use it is necessary, however, to make it clear what precisely we mean by the term spiral. In the case of BZ reaction, it is a rotating, time-periodic, spatial structure of reactant concentrations as noted by Murray[6,11]. If one stands at the center of a spiral he would see a periodic wave train is passing by him since every time the spiral turns a wave front moves past him. A simple rotating spiral is described by a periodic function of the phase φ with

$$\varphi = \psi\,(t) + m\,(\theta) \pm \psi\,(r)$$

Where ψ is the frequency, m is the number of arms on the spiral and ψ (r) is a function which describes the type of spiral. The ± in the m (θ) term determines the sense of rotation. Numerous authors have investigated spiral wave trains of general reaction diffusion mode. These involved analyses usually make use of asymptotic methods. The λ-w system has been very extensively used as a model system because of the relative algebraic simplicity of the analysis. In this section we present some representative solutions for the λ -w system for illustration, following Murray, keeping in mind the direct relevance to real reaction-diffusion mechanism. The λ -w reaction diffusion mechanism for two reactants is

$$\begin{pmatrix} u \\ v \end{pmatrix}_t = \begin{pmatrix} \lambda(A) & -\omega(A) \\ \omega(A) & \lambda(A) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix}$$

Where $w(A)$ and $\lambda\,(A)$ are real functions of A.

If we consider w as a complex function of A and re do the analysis we will get the following dynamical equations as a solution of u and v.

$$\begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} r^m \cos[\Omega t + m\theta + \psi(0)] \\ r^m \sin[\Omega t + m\theta + \psi(0)] \end{pmatrix}$$

Another way to deal with the problem of spiraling is to arrive at a linear amplitude equation from the solvability criterion applied at first order in a perturbation expansion of the model involved using multiple scales. It can then be shown that a general solution of a spiral exists for the amplitude equation in a region of phase space where a homogeneous oscillatory state is stable. Targets and stars are some special cases.

VI. CONCLUSIONS

So far we have discussed the generation of different patterns in animal, fish etc. It is an analytical support to morphogenesis. Non linear dynamical studies have utmost strength to describe the pattern generations. Now to differentiate between spots, stripes and spirals we have to study the effect of different nodes on the reaction diffusion system. We can also study the effect of external noise, electric field, magnetic field , stochasticity on the systems. Worthmentioned will be to tune the pattern generations above any critical threshold through any of the external applications. In an upcoming issue it is planned to elaborate the effects on reaction diffusion systems.

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