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Instabilities In A Reaction Diffusion Model: Spatially Homogeneous And Distributed Systems*

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Abstract

The theory of instability in a detailed Lotka-Volterra model has been investigated for the spatially homogeneous and inhomogeneous cases. In the spatially homogeneous case, we show that the occurrence of oscillation (instability) is due to the partial neglect of the initiation step and/or constant reactant approximation– a violation of the detailed chemistry. In the spatially distributed case, the existence of a finite blow-up time (t_b) is found to be due to a combination of diffusion coefficient and the reaction rates. The intervals of existence of t_b are obtained.

1 Introduction

In the strict sense of the term, reaction-diffusion systems are systems involving constituents locally transformed into each other by chemical reactions and transported in space by diffusion. The word reaction has been used in a very broad sense, much broader than the one used in physical chemistry to mean "chemical reaction". Although they arise quite naturally in chemistry and chemical engineering, they also serve as a reference for the study of a wide range of phenomena encountered beyond the strict realm of chemical science such as environmental and life sciences [1–11, 13–16]. For example, the reaction-diffusion equation has served as a means of explaining competitions between birth and death rates, relation between people and disease, activator and inhibitor system, prey and predator model, see e.g. [1, 2].

The mathematical theory of reaction-diffusion systems in a closed vessel in the absence of external forces evolve eventually to a state of equilibrium, whereby the constituents involved are distributed uniformly in space and each elementary reactive step is counteracted by its inverse. Thus, there is a spontaneous transfer from the zones of high concentrations of the constituents to those of lower concentration. In this case, diffusion provides the transport of the constituents, the coupling between species reaction and also create organizations in space [10].

In the past, the sustained oscillations in the Lotka scheme has been shown to be due to an effective source term arising from the neglect of fuel consumption [3], while [4]

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further stressed the need to be careful when making approximations as the inclusion of a small parameter could alter the stability of a system. The reaction step in which the reactant species decomposes to produce the intermediates (radical or chain carrier), which propagates reactions is known as the initiation step and is often neglected. This neglect, which is largely due to its transient nature serves as a safe simplification for easy mathematical handling [6]. However, since emphasis is laid on satisfying basic physical principles and on preserving chemical reasonableness as simple as possible, the initiation step is sometimes included [11, 15]. In the spatially distributed system, diffusion was known to be a stabilizing quantity [10]. However, it has been shown that for a given parameter regime and realistic approximations, diffusion could be a destabilizing quantity [8.16]. A frequently used approximation is the constant reactant or chemical pool approximation. In this case, intermediates are supposed to be much more reactive than the relatively stable reactant F, so that their concentrations will always be relatively low compared with the initial concentration of the reactant F [3–7].

In view of the above, we study the behaviour of solutions in a detailed or modified Lotka-Volterra model, which is formulated by incorporating the hitherto neglected initiation step into the Lotka-Volterra model [3].

2 Problem Formulation

We consider a complete reaction kinetics consisting of the following elementary steps: (1)-initiation, (2)-branching, (3)-propagation and (4)-termination steps

$$F \xrightarrow{k_i'} A, \qquad w_i = k_i' F, \tag{1}$$

$$F + A \xrightarrow{k_1'} 2A, \qquad w_1 = k_1' F A, \tag{2}$$

$$A + B \xrightarrow{k_2'} 2B, \qquad w_2 = k_2' A B, \tag{3}$$

$$F + B \xrightarrow{k_3'} P, \qquad w_3 = k_3' F B, \tag{4}$$

where F represents reactant concentration and P is the inert product; A and B represent the two intermediates (radicals) formed autocatalytically; w_i, w_1, w_2 and w_3 represent the local reaction rates and k_i', k_1', k_2' and k_3' are the rate constants. The above example involves the irreversible conversion of a reactant F to a final product P through two intermediates A and B. The initiation step kick starts the reaction and also lead to the production of radicals; the propagation step leads to the production of radicals of the same proportion; the branching step is a form of propagation usually leading to the production of additional radicals of same or different types; while the termination reaction leads to the consumption or termination of the radicals.

In view of the reaction (1)-(4), the one-dimensional governing equations for the reactive system taking place within an interval Ω are,

$$\frac{\partial F}{\partial t} = D_1 \frac{\partial^2 F}{\partial x^2} + W_F, \tag{5}$$

$$\frac{\partial A}{\partial t} = D_2 \frac{\partial^2 A}{\partial x^2} + W_A, \tag{6}$$

$$\frac{\partial B}{\partial t} = D_3 \frac{\partial^2 B}{\partial x^2} + W_B, \tag{7}$$

where $D_i (i = 1, 2, 3)$, denote the diffusion species; W_F, W_A and W_B represent the global reaction rates. The relations between the global and local reaction rates are

$$\begin{array}{ll} W_F & = -w_i - w_1 - w_3 = -k_i' F - k_1' FA - k_3' FB, \\ W_A & = w_i + w_1 - w_2 = k_i' F + k_1' FA - k_2' AB, \\ W_B & = w_2 - w_3 = k_2' AB - k_3' FB. \end{array} \tag{8}$$

Assuming that the reactant F diffuses into the system from the outside, where its value is assumed constant at F_0, then, (5)-(8) become

$$\frac{\partial F}{\partial t} = D_1 \frac{\partial^2 F}{\partial x^2} - k_i'(F - F_0) - k_1' FA - k_3' FB, \tag{9}$$

$$\frac{\partial A}{\partial t} = D_2 \frac{\partial^2 A}{\partial x^2} + k_i'(F - F_0) + k_1' FA - k_2' AB, \tag{10}$$

$$\frac{\partial B}{\partial t} = D_3 \frac{\partial^2 B}{\partial x^2} + k_2' AB - k_3' FB. \tag{11}$$

The relevant initial and boundary conditions for the system are

$$\begin{array}{l} F(x,0) = F_0(x) \geq 0, \ A(x,0) = A_0(x) \geq 0, \quad B(x,0) = B_0(x) \geq 0, \quad x \in \Omega, \\ F(x,t) = A(x,t) = B(x,t) = 0, \quad t > 0, \quad x \in \partial\Omega. \end{array} \tag{12}$$

It is convenient to use the dimensionless variables

$$f = \frac{F}{F_0}, u = \frac{A}{F_0}, v = \frac{B}{F_0}, \ \tau = k_2 t, \text{ and } x' = \frac{x}{L}, \tag{13}$$

where L is a characteristic length. After dropping primes, equations (9)-(12) become

$$\frac{\partial f}{\partial \tau} = d_1 \frac{\partial^2 f}{\partial x^2} + k_i(1 - f) - k_1 F_0 fu - k_3 F_0 fv, \tag{14}$$

$$\frac{\partial u}{\partial \tau} = d_2 \frac{\partial^2 u}{\partial x^2} - \eta k_i(1 - f) + k_1 F_0 fu - F_0 uv, \tag{15}$$

$$\frac{\partial v}{\partial \tau} = d_3 \frac{\partial^2 v}{\partial x^2} + F_0 uv - k_3 F_0 fv, \tag{16}$$

where

$$k_i = \frac{k_i'}{k_2}, \ k_j = \frac{k_j'}{k_2}, d_j = \frac{D_j}{k_2 L^2}, \quad \text{where } (j = 1, 2, 3),$$

and η is introduced for case study;

$$\eta = \begin{cases} 0, \text{ Lotka-Volterra model} \\ 1, \text{ modified Lotka-Volterra model.} \end{cases} \tag{17}$$

The dimensionless initial and boundary conditions are

$$f(x,0) = f_0(x), \quad u(x,0) = u_0(x), \quad v(x,0) = v_0(x), \quad x \in \Omega \tag{18}$$

and

$$f(x,\tau) = 0, \quad u(x,\tau) = 0, \quad v(x,\tau) = 0, \quad x \in \partial\Omega \tag{19}$$

where $u_0 = \frac{A_0}{F_0}$, $v_0 = \frac{B_0}{F_0}$. Investigations and analysis of most practical applications require detailed information of the physics of the problem. Often times, studies are based on simplifying mathematical approximations in order to allow for easy mathematical handling and interpretations.

3 Spatially Homogeneous System

The reduced spatially homogeneous forms of (14)-(16) are

$$\frac{df}{d\tau} = k_i(1-f) - k_1 F_0 f u - k_3 F_0 f v, \tag{20}$$

$$\frac{du}{d\tau} = -\eta k_i(1-f) + k_1 F_0 f u - F_0 u v, \tag{21}$$

$$\frac{dv}{d\tau} = F_0 u v - k_3 F_0 f v. \tag{22}$$

The steady-state, or time-independent solutions of the above systems are obtained by setting $\frac{df}{d\tau} = \frac{du}{d\tau} = \frac{dv}{d\tau} = 0$. It may be desirable to study these equilibrium solutions and their stability for the 3-dimensional space for some special cases. The Jacobian matrix of a 3-dimensional system has 3 eigenvalues; one which must be real and the other two can be either both real or complex conjugate. The nature of these stationary points depend on the signs of these eigenvalues.

3.1 Modified Lotka-Volterra Model ($\eta = 1$, $k_i \neq 0$)

This case represents the detailed reaction scheme incorporating initiation with rate constant k_i and fuel consumption.

$$\frac{df}{d\tau} = k_i(1-f) - k_1 F_0 f u - k_3 F_0 f v, \tag{23}$$

$$\frac{du}{d\tau} = -k_i(1-f) + k_1 F_0 f u - F_0 u v, \tag{24}$$

$$\frac{dv}{d\tau} = F_0 u v - k_3 F_0 f v. \tag{25}$$

The above system has a non-trivial singularity at the point $f = u = \frac{1}{4}\left(-k_i + \sqrt{k_i^2 + 8k_i}\right)$, $v = 0$. The characteristic equation obtained from the Jacobian matrix shows that the eigenvalues are given by $(\lambda_1, \lambda_2, \lambda_3) = (0, 0, -k_i)$. There is no indication of any oscillation and the system will decay to equilibrium. The field and parametric plots are shown in Figures 2 and 3 respectively.

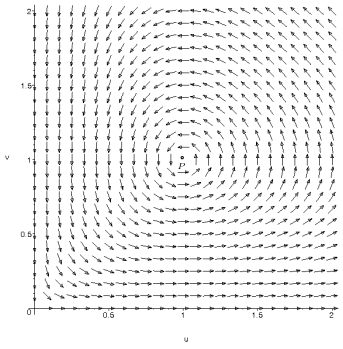

Figure 1: Field plot $v(t)$ and $u(t)$ k_i=k_1=k_3=1, η=0.

3.2 Modified Lotka-Volterra Model ($\eta = 0$)

This case corresponds to partial initiation process and the system of equations (20)-(22) reduce to the Lotka-Volterra scheme.

$$\frac{df}{d\tau} = k_i(1-f) - k_1 F_0 f u - k_3 F_0 f v, \tag{26}$$

$$\frac{du}{d\tau} = k_1 F_0 f u - F_0 u v, \tag{27}$$

$$\frac{dv}{d\tau} = F_0 u v - k_3 F_0 f v. \tag{28}$$

It is evident that the system possesses singularities at points $P_1\,(f = 1, u = v = 0)$ and $P_2\left(f = u = v = \frac{1}{4}\left(-k_i + \sqrt{k_i^2 + 8k_i}\right)\right)$. The steady state P_1 which corresponds to the initial data is saddle in nature, which is unstable. This is because there is at least one positive eigenvalue. Similarly, at point P_2, computation shows that the eigenvalues have one real and a pair of complex conjugate eigenvalues with positive real part, which is an unstable focus. This is consistent with the oscillatory behaviour obtained numerically [3, 4]. The field and parametric plots are shown in Figures 1 and 4 respectively.

3.3 Neglect of Initiation ($k_i = 0$)

In the absence of initiation process, equations (20)-(22) reduce to

$$\frac{df}{d\tau} = -k_1 F_0 f u - k_3 F_0 f v, \tag{29}$$

$$\frac{du}{d\tau} = k_1 F_0 f u - F_0 u v, \tag{30}$$

$$\frac{dv}{d\tau} = F_0 u v - k_3 F_0 f v. \tag{31}$$

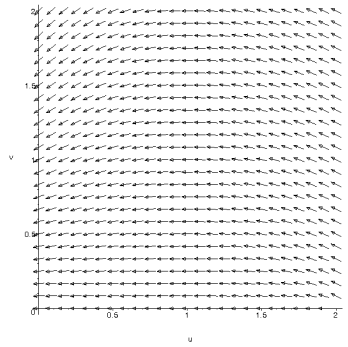

Figure 2: Field plot $v(t)$ and $u(t)$ k_i=k_1=k_3=η=1.

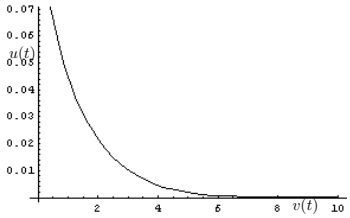

Figure 3: Parametric plots $u(t)$ and $v(t)$, $u(0)$=$v(0)$=0.1, $f(0)$=1.

There is no realistic non-trivial steady state solution satisfying the system. However, since the system can be obtained by fixing $k_i = 0$ in section 3.2, the trivial steady state solution depicts stability as there is no indication of any oscillation. The non-oscillatory character is shown in Figure 5, which confirms [3].

3.4 Neglect of Reactant ($F = F_0$)

In this case, assuming that the reactant is constant($f = F_0 = 1$), then equations (20)-(22) reduce to a two-dimensional system

$$\frac{du}{d\tau} = k_1 F_0 f u - F_0 u v, \tag{32}$$

$$\frac{dv}{d\tau} = F_0 u v - k_3 F_0 f v. \tag{33}$$

The singularity of equations (32) and (33) occur at (u, v)=$(0, 0)$ and (u, v)=(k_3, k_1). The corresponding eigenvalues for the trivial(initial data) steady state is $\lambda_1 = k_1$ and $\lambda_2 = -k_3$ (saddle), while it is $\lambda_{1,2} = \pm i\sqrt{k_1 k_3}$(spiral) for the non-trivial case. Further analysis shows that oscillation is in the non-trivial critical point [3, 4].

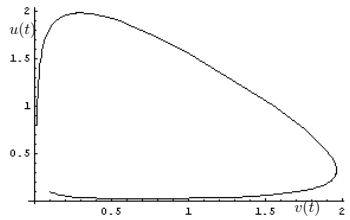

Figure 4: Parametric plots $u(t)$ and $v(t)$, $u(0)$=$v(0)$=0.1, $f(0)$=1.

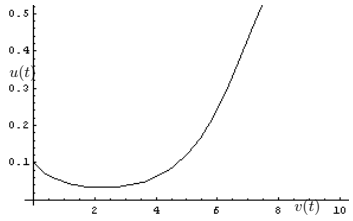

Figure 5: Parametric plots $u(t)$ and $v(t)$, $u(0)$=$v(0)$=0.1, $f(0)$=1.

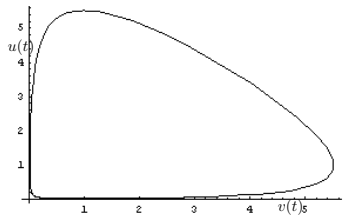

Figure 6: Parametric plots $u(t)$ and $v(t)$, $u(0)$=$v(0)$=0.1.

4 Spatially Distributed System

Assume that the reactant (F) is constant ($f = 1$), the system of equations reduce to

$$\frac{\partial u}{\partial \tau} = d_2 \frac{\partial^2 u}{\partial x^2} + k_1 u - uv, \tag{34}$$

$$\frac{\partial v}{\partial \tau} = d_3 \frac{\partial^2 v}{\partial x^2} + uv - k_3 v, \tag{35}$$

subject to

$$u(x,0) = u_0(x), \quad v(x,0) = v_0(x). \tag{36}$$

A solution of the above system of partial differential equation is a signal that is propagated into a space-time domain from the boundary of that domain. Thus, using these initial conditions, we apply ansatz to equations (33) and (34) in the forms [8, 16],

$$u(x,\tau) \;=\; \theta(\tau)\left(\psi(\tau) + x^2\right) \quad \text{and} \quad v(x,\tau) = \phi(\tau)\exp(-x^2\mu(\tau)). \tag{37}$$

For a one dimensional system with concentrations $u(x,t)$ and $v(x,\tau)$, the system can be maintained at

$$u(0,t) = 1 \;\text{ and }\; v(0,t) = \frac{1}{\sqrt{2\pi}}, \tag{38}$$

$$u(x,0) = x^2 \qquad \text{and} \qquad v(x,0) = \frac{1}{\sqrt{2\pi}} \exp\left(\frac{-x^2}{2}\right). \tag{39}$$

It is obvious from (39) that

$$\theta(0) = 1, \psi(0) = 0, \phi(0) = \frac{1}{\sqrt{2\pi}}, \mu(0) = \frac{1}{2}. \tag{40}$$

After putting equations (37) into (34)-(35) and collecting terms (in x^0 and x^2), we obtain the ordinary differential equations,

$$x^0: \quad \theta\psi' + \theta'\psi = 2d_2\theta + k_1\theta\psi, \tag{41}$$

$$x^2: \quad \theta' = k_1\theta, \tag{42}$$

$$x^0: \quad \phi' = -2d_3\mu\phi + \phi\theta\psi - k_3\phi, \tag{43}$$

$$x^2: \quad -\mu' = 4d_3\mu^2 + \theta. \tag{44}$$

By direct integration of (41)–(42) subject to initial conditions (40)

$$\psi(\tau) = 2d_2\tau \text{ and } \theta(\tau) = \exp(k_1\tau). \tag{45}$$

After inserting the expression for $\theta(\tau)$ in (45) into (44), the Riccati equation (44) gives [12, 14]

$$\mu(\tau) = \sqrt{\frac{\exp(k_1\tau)}{4d_3}} \left(\frac{Y_1\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) - C_1 J_1\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)}{-Y_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) + C_1 J_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)} \right), \tag{46}$$

where $C_1 = \frac{\sqrt{d_3}Y_0\left(\frac{4\sqrt{d_3}}{k_1}\right)+Y_1\left(\frac{4\sqrt{d_3}}{k_1}\right)}{\sqrt{d_3}J_0\left(\frac{4\sqrt{d_3}}{k_1}\right)+J_1\left(\frac{4\sqrt{d_3}}{k_1}\right)}$. Substituting (45) and (46) into (43), we have a separable first order differential equation

$$\frac{d\phi}{\phi} = \left[-\sqrt{d_3\exp(k_1\tau)}\frac{Y_1\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) - C_1J_1\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)}{-Y_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) + C_1J_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)} + U\right]d\tau, \quad (47)$$

where $U = U(\tau) = 2d_2\tau\exp(k_1\tau) - k_3$. Taking integration of (47) and using the fact that $\frac{d}{dx}J_0(x) = -J_1(x)$, $\frac{d}{dx}Y_0(x) = -Y_1(x)$,

$$\phi = C_2\frac{\exp\left[V(\tau)\right]}{\sqrt{-Y_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) + C_1J_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)}}, \quad (48)$$

where

$$V(\tau) = \frac{2d_2}{k_1}\left(\tau - \frac{1}{k_1}\right)\exp(k_1\tau) - k_3\tau, \quad (49)$$

and C_2 can be determined using $\phi(0) = \frac{1}{\sqrt{2\pi}}$. The closed-form solutions are

$$u(x,\tau) \;=\; \exp(k_1\tau)\left[2d_2\tau + x^2\right], \quad (50)$$

$$v(x,\tau) = \frac{C_2\exp\left(V(\tau) - x^2\mu(\tau)\right)}{\sqrt{-Y_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right) + C_1J_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)}}. \quad (51)$$

It is observed from (51) that $v(x,\tau)$ exhibits finite time blow-up, which occurs when

$$\begin{aligned} &J_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)\left(\sqrt{d_3}Y_0\left(\frac{4\sqrt{d_3}}{k_1}\right) + Y_1\left(\frac{4\sqrt{d_3}}{k_1}\right)\right) \\ &-Y_0\left(\frac{4\sqrt{d_3\exp(k_1\tau)}}{k_1}\right)\left(\sqrt{d_3}J_0\left(\frac{4\sqrt{d_3}}{k_1}\right) + J_1\left(\frac{4\sqrt{d_3}}{k_1}\right)\right) = 0, \end{aligned} \quad (52)$$

provided

$$k_1 > 0, \text{and} \;\; d_3 > 0. \quad (53)$$

Analysis of (52) in an interactive manner shows that as $k_1 \to \infty$ for d_3 fixed, the blow-up time satisfies the condition

$$1 < \tau_b \leq 1.5. \quad (54)$$

Similarly, for fixed k_1 ($k_1 = 1$) shows that d_3 is bounded in the interval $0 < d_3 \leq 1$, while the blow-up time satisfies the condition

$$1 < \tau_b < \infty. \quad (55)$$

5 Conclusion

The behaviour of the modified Lotka-Volterra model for the spatially homogeneous and distributed cases have been examined. In the spatially homogeneous case, using stability analysis, the destabilizing effect of approximations on the system is observed and confirms previous works in the literature. In the spatially distributed case, it has been suggested that not only is the diffusion coefficient responsible for finite time blow-up, the rate constant(s) are also significant. Finally, it is necessary to state that the conjectures raised in this paper may provoke mathematical questions in other areas other than kinetic theory.

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