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Transport System Effects On Cross Diffusion

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Abstract

Cross diffusion is a phenomena in which a gradient in the concentration of one species induces a flux of another chemical species which was generally been neglected in the study of reaction-diffusion systems. We study the Turing bifurcation of two species reaction transport systems, where particle dispersal is governed by diffusion and cross diffusion. we performed linear stability analysis to find the conditions for the Turing instability and compare results with the standard Turing conditions and we applied our results to one model system, the Schnakenberg reaction Kinetics to see it effects on cross diffusion.

Keywords: Bifurcation, Transport, dispersal, cross diffusion, stability analysis, Turing instability conditions.

1. Introduction

Turing showed in one of his seminal work [1] that the interaction of diffusion and kinetics can destabilize the uniform steady state of reaction diffusion systems and generate stable, stationary concentration patterns. The Turing instability theory has been studied extensively in the literature and typically reaction diffusion systems with two species are considered. We know that Turing instability is diffusion driven, but how different dispersal processes will affect bifurcation. Numerous studies have addressed aspects of this problem. For example, the conditions for Turing instability have been derived for systems of self and cross diffusion [4].

Our concerned here is that how molecules, organisms or animal dispersed in space can interact with each other. Actually, the dispersal is diffusive and the evolution of our system can be modelled by a standard reaction diffusion equation of the form.

$$\nabla w_c = D_c \Delta w_c + H_{c(w)}\,, \qquad c = 1,2,\ldots,M. \qquad (1)$$

Here $w_c = w_c(r,t)$ is the density of the species c at point r at time t. The vector $\boldsymbol{w}$ consists of the densities w_i, i=1,2,…M species. The first term on the right hand side of equation (1) describes the spatial dispersal, representing simple diffusive motion with diffusion constant D_c, the second term represent diffusive motion while the third term is the reaction term representing the interaction among the species. One of the species effects are subdiffusive and the other diffusive are investigated in [3] Most of the reaction diffusion models for pattern formation assumed particle dispersal to simple diffusion, where diffusive flux of the given species is driven by only the gradient of that species. But in our own case we studied the Turing bifurcation in the presence of cross diffusion, where the diffusive flux of the given species is also affected by derivatives of the other species. One of the easiest example of cross diffusion is chemotaxis [5 and 6] in which cells and other organism direct their movements by sensing the presence of certain chemicals in their environment, the tumbling motion in E-coli bacteria is one of the examples of chemotaxis, the bacteria make a straight line excursion called run and if they sense some nutrients or poison they respond by changing their direction called tumbling and followed again by the next straight line excursion.

In chemical systems, cross diffusion arises from interaction between the species and occurs in strong electrolytes and microemulsions[11]. Cross diffusion can be large compared to main or diagonal diffusion coefficients which are expected to play an important role in the formation of pattern mechanism in oil microemulsion[12].

Our cross diffusion terms are not negligible these are described as follows;

$$\nabla w_c = D_{cc}\Delta w_c + \sum_{i\neq c} D_{ci}\Delta w_i + H_{c(\boldsymbol{w})}, \qquad (2)$$

With c = 1,2,…, M. If the cross diffusion term Is positive, that is $D_{ci} > 0$, then the flux of the species c is directed downwards values of the concentration of species i, and if it is negative then the flux is directed upward values of the concentration of the species i. The cross diffusion term goes to zero as c goes to zero, that is

$$D_{ci}(\boldsymbol{w}) \to 0 \; as \; w_c \to 0, \qquad (3)$$

Which implies that there can be no flux of species c if w_c = 0. All eigenvalues of the diffusion matrix D = D_{ci} must be real and positive and the trace(D_{ci}) > 0 , Determinant(D_{ci}) > 0 [12]. If $w_c(r,0) > 0$ for all c, the concentration $w_k(r,t)$ are not guarantee to remain positive for all t > 0. Some researchers have recently analyzed the Turing instability of a two variable model where the cross diffusion coefficients behave as;

$$D_{ci}(\boldsymbol{w}) = D_{ci}\, {}^{w_i}/_{\alpha_i} + w_i \,, \qquad (4)$$

Where α_i is very small, and considered the region where $w_i \gg \alpha_i$ and performed a stability analysis of (2) with constant D_{ci} .

We carried out the stability analysis of the uniform steady state of (2) for the general concentration dependent cross diffusion terms, the cross diffusion coefficients become constant, their values are determined by the homogeneous steady state of the system.

2. Scope of Work

We performed the linear stability analysis in section **3** which provides the conditions for Turing Instability, we give some remarks on our results in section **4**, we then applied our results to Schnakenberg model which was analyzed to see the effects on cross diffusion on the stability of the uniform steady state in the activator- inhibitor in section **5,** Finally we discussed and concluded in section **6.**

3. Linear Stability Analysis

We considered a two species reaction diffusion system, W and X, where the dispersal of each species depends on the gradient of its own density. Let w = w(r,t) and x = x(r,t) be the local densities of the two species as follows;

$$\frac{\partial w}{\partial t} = D_w \frac{\partial^2 w}{\partial r^2} + E_w \frac{\partial^2 x}{\partial r^2} + f(w,x) \quad (5)$$

$$\frac{\partial x}{\partial t} = D_x \frac{\partial^2 x}{\partial r^2} + E_x \frac{\partial^2 w}{\partial r^2} + g(w,x) \quad (6)$$

Where D_w and D_x are the primary diagonal diffusion constants for the two species, on our own assumption is the density independent, and the cross diffusion on the secondary diagonal are E_w and E_x which is a measure for the strength of the cross diffusive effects depending on the sign which will give rise to attraction or repulsion. That is if both of them are positive, both species will move away from each other but if they are both negative they attract each other. Their interactions are described by the kinetic terms $(w,x) and\ g(w,x)$. In equations (5 and 6) is to model chemical system, then all the eigenvalues of the diffusion matrix are positive, which leads to the following three conditions for 2 variable systems [7];

$$\text{Tr D} = D_w + D_x > 0, \quad (7)$$

$$\text{Det D} = D_w D_x - E_w E_x > 0, \quad (8)$$

$$(D_w + D_x)^2 - 4E_w E_x > 0, \quad (9)$$

If the diffusion coefficients in the primary diagonal is positive then condition (7) is satisfied.

Now, performing the linear analysis of our model (5 and 6) to obtain the condition for Turing instability[7]

Let (w_0, x_0) be the steady state of the spatially homogeneous system,

$$\frac{dw}{dt} = f(w,x) \quad (10)$$

$$\frac{dx}{dt} = g(w,x) \quad (11)$$

And at the steady state

$$f(w_0,x_0) = g(w_0,x_0) = 0, \quad (12)$$

Let J be the Jacobian matrix at the steady state with its elements J_{ij},

$$J_{11} = f_w\ ,\ J_{12} = f_x,\ J_{21} = g_w\ and\ J_{22} = g_x, \quad (13)$$

Which was evaluated at the steady state (w_0, x_0) , by conventional stability analysis[9],

$$tr(J) = f_w + g_x < 0, \quad (14)$$

$$\det(J) = f_w g_x - f_x g_w > 0, \quad (15)$$

In order to find conditions for instability, let the perturbations depend on both time and space that is;

$$w(r,t) = w_0 + \delta w(r,t), \quad (16)$$

$$x(r,t) = x_0 + \delta w(r,t), \quad (17)$$

On linearizing our model around the steady state and neglecting the higher terms in δw we realized the following,

$$\partial_t \delta \boldsymbol{w} = \left(D_w \partial_r{}^2 + E_w \partial_r{}^2 + J_{11} + J_{12}\right)\delta w, \quad (18)$$

$$\partial_t \delta \boldsymbol{w} = \left(D_x \partial_r{}^2 + E_x \partial_r{}^2 + J_{21} + J_{22}\right)\delta w, \quad (19)$$

by rewriting our linearized equations in the form;

$$\partial_t \delta \boldsymbol{w} = D\partial_r{}^2 \delta \boldsymbol{w} + E\partial_r{}^2 \delta \boldsymbol{w} + J(\delta \boldsymbol{w}) \quad (20)$$

Where $D = \begin{pmatrix} D_w & 0 \\ 0 & D_x \end{pmatrix}$, $E = \begin{pmatrix} 0 & E_w \\ E_x & 0 \end{pmatrix}$, $J(\delta w) = \begin{pmatrix} J_{11} & J_{12} \\ J_{21} & J_{22} \end{pmatrix} = \begin{pmatrix} f_w & f_x \\ g_w & g_x \end{pmatrix}$ evaluated at the steady state (w_0, x_0).

To solve equation (20) we need a solution both in time and space which was resolved by separation of variables using $\partial_r{}^2 \delta \boldsymbol{w}$ and $\partial_t \delta \boldsymbol{w}$, and we assumed no flux Neumann boundary conditions at r = 0, and r = L we found the perturbation as

$$\delta w(r,t) = Ce^{\lambda t} \sin\left(\frac{n\pi}{L} r\right) \quad (21)$$

The eigenvalue k = $\frac{n\pi}{L}$ is called the wave number[7], we substituted (21) into (20), we have the following;

$$\begin{pmatrix} f_w - D_w k^2 - \lambda & f_x - E_w k^2 \\ g_w - E_x k^2 & g_x - D_x k^2 - \lambda \end{pmatrix} \begin{pmatrix} \delta w \\ \delta w \end{pmatrix} = 0 \quad (22)$$

The eigenvalue λ is the root of the following quadratic equations:

$$\lambda^2 - G(k^2)\lambda + H(k^2) = 0 \quad (23)$$

Where we defined

$$G(k^2) = f_w + g_x - (d_w + d_x)k^2 \quad (24)$$

$$H(k^2) = Det - \left(D_x f_w + D_w g_x - (E_x f_x + E_w g_w)\right)k^2 + \left(D_w D_x - (E_x E_w)\right)k^4 \quad (25)$$

The uniform steady state is stable against inhomogeneous perturbations, $k \neq 0, if\ G(k^2) < 0\ and\ H(k^2) > 0$

Then $G(k^2) < 0$ is always satisfied, because the main diffusion constants are positive and $f_w + g_x < 0$

according to equation (14). The only way for the uniform steady state to be unstable to inhomogeneous perturbations requires that $H(k^2) < 0$ for some values of k[7-9], that is

$$\left(D_w D_x - (E_x E_w)\right)k^4 - \left(D_x f_w + D_w g_x - (E_x f_x + E_w g_w)\right)k^2 + f_w g_x - f_x g_w < 0 \quad (26)$$

But we noticed from equation (25) that the following conditions must be satisfied, since (25) need to be negative, we have;

$$D_x f_w + D_w g_x - (E_x f_x + E_w g_w) > 0 \quad (27)$$

Which is necessary but not sufficient condition for a Turing instability. By convention in reaction diffusion systems(1), condition(27) would have been,

$$D_x f_w + D_w g_x > 0 \quad (28)$$

This implies that a Turing bifurcation can occur only if the coefficients of f_w *and* g_x do not have the same sign and the diffusion coefficients are not equal. If we have two variable systems, Turing instabilities require activator and inhibitor kinetics, where $f_w > 0$ and $g_x < 0$ and equation (14) requires that $|g_x| > f_w$ and equation (15) requires $f_x g_w < 0$. If $f_w > 0, g_x < 0, f_x < 0, g_w > 0$ then systems (5) and (6) would be pure activator-inhibitor system and on the other hand the systems would be cross activator-inhibitor if $f_x g_w < 0$. If $f_w > 0, g_x < 0, f_x > 0, g_w < 0$.

Defining $D = \frac{D_x}{D_w}$, we obtained from (28) that $D = \frac{D_x}{D_w} > \frac{-g_x}{f_w} > 1$

That is in the absence of cross diffusion, the inhibitor X must diffuse faster than the activator W, but in the presence of cross diffusion renders the necessary condition less restrictive.

The values of k in equation (25) can be determined by the zeros of $H(k^2)$, which imply that we would have real and positive values of k if the following conditions are satisfied;

$$\left(D_x f_w + D_w g_x - (E_x f_x + E_w g_w)\right)^2 - 4Det(D_w D_x - E_w E_x) > 0 \quad (29)$$

If we defined $D_{w,x} = \frac{D_x}{D_w}$, where the subscript on D indicate that W and X are subject to cross diffusion and by expanding (29) we have

$$f_w{}^2 D_{w,x}{}^2 - R D_{w,x} + S > 0 \quad (30)$$

Where $R = 2f_w g_x - 2\rho_w f_w g_w - 2\rho_x f_w f_x - 4Det$ (31)

$$S = g_x{}^2 + \rho_w{}^2 g_w{}^2 + \rho_x{}^2 f_x{}^2 + 2\rho_w \rho_x g_w f_x - 2\rho_w g_x g_w - 2\rho_x g_x f_x + 4\rho_w \rho_x Det \quad (32)$$

Where $\rho_w = \frac{E_w}{D_w}$ *and* $\rho_x = \frac{E_x}{D_w}$ (33)

Which implies that the root of the (30) is

$$D_{w,x} = \frac{R \pm \sqrt{R^2 - 4f_w{}^2 S}}{2f_w{}^2} \quad (34)$$

But D must be greater than zero which is the appropriate root and which is the condition for Turing instability therefore,

$$D_{w,x} = \frac{R + \sqrt{R^2 - 4f_w{}^2 S}}{2f_w{}^2} \quad (35)$$

$$D_{w,x} = \frac{(Det - f_x g_w + f_w(\rho_w g_w + \rho_x f_x)) + 2\sqrt{Det(\rho_w f_w - f_x)(g_w - \rho_x f_w)}}{f_w{}^2} \quad (36)$$

Equation (36) corresponds to Turing threshold condition only if conditions (8),(9) and (27) are satisfied; by dividing conditions (8) and (9) by $D_w{}^2$ and condition (27) by D_w, we have [7]

$$D_{w,x} - \rho_w \rho_x > 0, \quad (37)$$

$$\left(D_{w,x}-1\right)^2 + 4\,\rho_w\rho_x > 0 \tag{38}$$

$$g_x + D_{w,x}f_w - \rho_w g_w - \rho_x f_x > 0 \tag{39}$$

Which implies that $D_{w,x}$ is a real number and $R^2 - 4{f_w}^2S$ = Det$(\rho_w f_w - f_x)(g_w - \rho_x f_w)$ must be positive, since we know that Det is always positive by (15), we have

$$(\rho_w f_w - f_x)(g_w - \rho_x f_w) > 0, \tag{40}$$

Which implies that

$(\rho_w f_w - f_x)$ *and* $(g_w - \rho_x f_w)$ have the same sign, which gives us the coefficients of the cross diffusion as

$$T_1 = \{(\rho_w,\rho_x)|\rho_w f_w - f_x \geq 0,\; g_w - \rho_x f_w \geq 0\} \tag{41}$$

$$T_2 = \{(\rho_w,\rho_x)|\rho_w f_w - f_x \leq 0,\quad g_w - \rho_x f_w \leq 0\} \tag{42}$$

From equation (26) we found the critical wave number for the Turing bifurcation [10], as

$$k_c{}^2 = \sqrt{\frac{Det}{D_wD_x - E_wE_x}} \tag{43}$$

If both cross diffusion terms have the same sign at the steady state then the critical wave number would be larger which implies that the wave length of the Turing patterns would be smaller than the standard Turing pattern. But if on the other hand the cross diffusion terms have opposite signs then the critical wave number would be smaller and the wave length of the Turing Pattern would be larger than the standard Turing pattern.

4. Remarks

Two cases of the general results were considered;

(1) That's both species w and x are not affected by cross diffusion. In this case $E_w = E_x = 0$(or $\rho_w = \rho_x = 0$) which implies that condition(36) yields the standard Turing Condition as;

$$D_{0,0} = \left(\frac{(\sqrt{Det} + \sqrt{-f_xg_w})}{f_w}\right)^2 \tag{44}$$

Which is a real number for $-f_xg_w > 0$, this shows that condition (40) represents the extension of the activator inhibitor requirement for standard reaction diffusion systems to cross diffusion.

(2) Only one species displays cross diffusion and if one of the cross diffusion vanishes that is $\rho_w = 0$ *or* $\rho_x = 0$, then conditions (37) and (38) are trivially satisfied.

(3) The dispersal of W depends on the gradient of x but X is not affected by the gradient of w that is $\rho_x = 0$ and we have;

$$D_{w,0} = \frac{(Det - f_x g_w + \rho_w f_w g_w) + 2\sqrt{Det g_w\,(\rho_w f_w - f_x)}}{{f_w}^2} \tag{45}$$

(4) The dispersal of X depends on the gradient of w but W is not affected by the gradient of x that is $\rho_w = 0$ and we have;

$$D_{0,x} = \frac{(Det - f_x g_w + \rho_x f_w f_x) + 2\sqrt{Det f_x\,(\rho_x f_w - g_w)}}{{f_w}^2} \tag{46}$$

5. Model Systems

We now apply our results to Schnakenberg model.

Schnakenberg Model

This is one of the simplest reaction diffusion models. It is derived from a series of hypothetical tri-molecular autocatalytic reactions that was proposed in 1979 by Schnakenberg. The non-dimensionalised kinetic terms are given by

$$f(w,x) = a - w + w^2 x \tag{47}$$

$$g(w,x) = b - w^2 x \tag{48}$$

Where $a \; and \; b$ are positive constants with uniform steady state as

$$(w_0, x_0) = \left(a + b, \frac{b}{(a+b)^2}\right), \tag{49}$$

with the jacobian matrix; $$J = \begin{pmatrix} \frac{b-a}{b+a} & (b+a)^2 \\ \frac{-2b}{b+a} & -(b+a)^2 \end{pmatrix} \tag{50}$$

The Schnakenberg belongs to the class of cross activator –inhibitor systems. The stability conditions
(14) and (15) read

$$tr(J) = \frac{(b-a)-(b+a)^3}{b+a} < 0 \tag{51}$$

$$det(J) = (b+a)^2 > 0 \tag{52}$$

The later is always fulfilled. The steady state (49) is stable if $(b+a)^3 > (b-a)$ and the Turing instability occurs as

$$D_{w,x} = \left(\frac{b+a}{b-a}\right)^2 \left[\frac{(b+a)(3b+a) + \left(\frac{b-a}{b+a}\right)\left(\frac{\rho_x (b+a)^3 - 2b\rho_w}{b+a}\right) +}{2\sqrt{[(b^2-a^2)\,\rho_w + (b+a)^3][2b + \rho_x (b-a)]}}\right] \tag{53}$$

Provided that conditions (37)- (40) are satisfied at the threshold. We considered the cases where $\rho_w \; or \; \rho_x = 0$
Just to gain the effects of cross diffusion on the Turing instability in the Schnakenberg. Because $f_x > 0 \; and \; g_w < 0$ this imply that it is the set T_2 that contains the standard Schnakenberg reaction diffusion system,

$$T_2 = \{(\rho_w, \rho_x) | \rho_w \leq \frac{(b+a)^3}{(b-a)}, \;\; \rho_x \geq \frac{-2b}{b-a} \} \tag{54}$$

The condition (39) is given by

$$2\left(\frac{(b+a)^3}{b-a}\right) + \frac{\rho_x (b+a)^3 - 2b\rho_w}{b+a}$$

$$+2\left(\frac{b+a}{b-a}\right)\sqrt{\rho_w(b^2 - a^2) + (b+a)^3\big(2b + \rho_x(b-a)\big)} > 0 \tag{55}$$

Which is positive for $(\rho_w, \rho_x) \in T_2$

For $\rho_x = 0$, the threshold condition reduces to

$$D_{w,0} = \left(\frac{b+a}{b-a}\right)^2 \left[\Big((b+a)(3b+a) - \frac{2b\rho_w}{(b+a)^2}(b-a) + 2\sqrt{2b[(b+a)^3 - \rho_w(b-a)]}\right] \tag{56}$$

The derivative of $D_{w,0}$ with respect to ρ_w and evaluated at $\rho_w = 0$, which correspond to the standard Turing condition is given by

$$\frac{\partial D}{\partial \rho_w} \Big|_{\rho_w = 0} = \frac{-2b}{b-a} \tag{57}$$

This shows that the derivative is negative and it implies that Turing instability in the Schnakenberg becomes favourable and the threshold value $D_{w,0}$ decreases as ρ_w becomes positive that is the activator and inhibitor repel each other. Conversely, the conditions for Turing instability become less favourable that is the threshold value $D_{w,0}$ increases as ρ_w becomes negative that is the activator and inhibitor attract each other.

We illustrated our results for specific values of the parameters a *and* b. We chose $a = 0.1$ *and* $b = 0.9$ [2], for these values,

$$T_2 = \{(\rho_w, \rho_x) | \rho_w \leq 1.25, \;\; \rho_x \geq -2.25 \} \tag{58}$$

In figure 1 we plot the dependence of the Turing threshold value $D_{w,0}$ on the strength of the cross diffusion coefficient ρ_w.

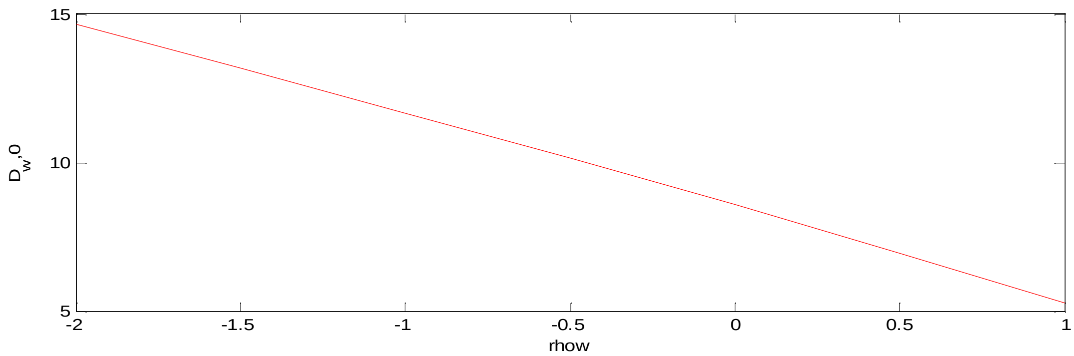

Fig 1. $D_{w,0}$ vs rhow(ρ_w) for the Schnakenberg with a = 0.1 and b = 0.9

For $\rho_w = 0$, the threshold condition reduces to

$$D_{0,x} = \left(\frac{b+a}{b-a}\right)^2 \left[(b+a)\big(3b+a+\rho_x(b-a)\big) + 2\sqrt{(b+a)^3(\rho_x(b-a)+2b)}\right] \quad (59)$$

And the derivative of $D_{0,x}$ with respect to ρ_x are evaluated at $\rho_x = 0$ that is, the point corresponding to standard Turing condition is given by,

$$\frac{\partial D}{\partial \rho_x}\Big|_{\rho_{x=0}} = (b+a)^2 \quad (60)$$

Which is clearly positive. This implies that conditions for the Turing instability in the Schnakenberg become less favourable and the threshold value D increases as ρ_x becomes positive. The activator and inhibitor rebel each other. Conversely, Turing instability become more favourable and the threshold value $D_{0,x}$ decreases as the ρ_x becomes negative. The activator and inhibitor attract each other.

In figure 2 we plot the dependence of the Turing threshold value $D_{0,x}$ on the strength of the cross diffusion coefficient ρ_x.

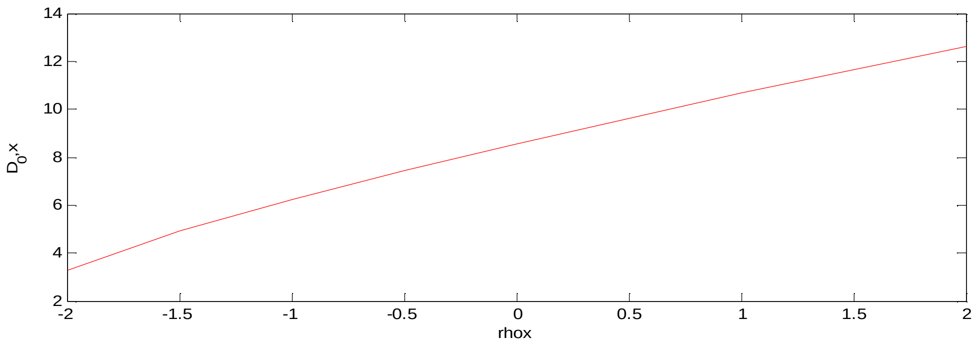

Fig 2. $D_{0,x}$ vs rhox(ρ_x) for the Schnakenberg with a = 0.1 and b = 0.9

But the minimum value of the Turing threshold attained at the boundaries of T_2, is $D_{min} = 1.5625$, that is the ratio of diffusion coefficients at $D = \frac{D_x}{D_w}$ which is greater than 1. Recall that a Turing instability can occur in standard reaction diffusion systems only if D > 1, that is if the inhibitor diffuses faster than the activator, which is known as the principle of short-range activation and long-range inhibition. This implies that the parameter values chosen, the inhibitor in the Schnakenberg diffuses faster than the activator which makes it possible for the Turing instability to occur.

6. Discussion and Conclusion

After studying the stability analysis of a uniform steady state of the reaction diffusion systems, our results shows that cross diffusion affects the conditions for the Turing instability and cause them less limited than those that apply in standard reaction diffusions with a nondiagonal diffusion matrix. In the Schnakenberg reaction kinetics, a cross activator-inhibitor system reveals that the effects of the cross-diffusion depend on the cross-kinetic behaviour of the system. Consider, for example, the case that the activator is affected by the gradient of the inhibitor while the latter has a vanishing cross-diffusion coefficient. Then attraction between the activator and the inhibitor facilitates the Turing instability in the pure activator-inhibitor model, while it prevents it in the cross activator-inhibitor model. Conversely, repulsion between the activator and the inhibitor facilitates the Turing instability in the cross activator-inhibitor model.

Finally, the inhibitor in the Schnakenberg diffuses faster than the activator which makes it possible for the Turing instability to take place.

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