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AN ANALYSIS OF MORPHOGENESIS IN REACTION-DIFFUSION SYSTEMS WITH A CATALYST

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Abstract : A Two-species, one-dimensional, reaction-diffusion system with a catalyst is considered. The catalytic action enhances the diffusion coeficients of the reactants and the catalyst itself is subject to a reaction-diffusion kinetics (with decaying reaction part) which is fast compared with that of the other two species. Global existence is analyzed and is applied to the particular case of a Schnackenberg kinetics.

1. Problem setting and first approximations

Many processes involve complex interactions of several species (chemical, biological, etc.) In some instances some of them are ctalysts, enhancing reactions between the other species and following a kinetic depending on its own concentration. Here we concentrate on the study of a three-species model, where one catalyzes the interaction between the other two. A dimensionless model for such a problem can be written down giving the following reaction-diffusion system [Murray, 1988]

$$\frac{\partial X_1}{\partial t} = \gamma f_1(X_1, X_2) + div(D_1 grad X_1) \tag{1}$$

$$\frac{\partial X_2}{\partial t} = \gamma f_2(X_1, X_2) + div(D_2 grad X_2) \tag{2}$$

$$\frac{\partial X_3}{\partial t} = \gamma f_3(X_3) + div(D_3 grad X_3) \tag{3}$$

plus appropriate supplementary conditions.

In many interesting cases the spatial extent is one-dimensional, so the diffusion terms become $\frac{\partial}{\partial x}\left(D_i \frac{\partial X_i}{\partial x}\right)$. This will be the framework of our study.

Key words : Reaction-diffusion, Morphogenesis, Global existence, Schnackenberg kinetics, spatial patterns.

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One the other hand, the catalytic action usually acts by enhancing diffusion of the reactants, whereas the catalyst has a constant diffusion rate. Some loss of catalyst must be accounted for (poisoning or similar problems), and the above system becomes

$$\frac{\partial X_1}{\partial t} = \gamma f_1(X_1, X_2) + \frac{\partial}{\partial x}\left(D_1(X_3)\frac{\partial X_1}{\partial x}\right) \tag{4}$$

$$\frac{\partial X_2}{\partial t} = \gamma f_2(X_1, X_2) + \frac{\partial}{\partial x}\left(D_2(X_3)\frac{\partial X_2}{\partial x}\right) \tag{5}$$

$$\frac{\partial X_3}{\partial t} = -dX_3 + k\frac{\partial^2 X_3}{\partial x^2} \tag{6}$$

where D_1 and D_2 depend on the concentration X_3. The spatio-temporal domain of definition is $[0,1]\times[0,\infty)$ and the supplementary conditions are zero-flux conditions at both ends of $[0,1]$ for the species X_1 and X_2, while we impose a zero-flux condition on X_3 at $x = 0$ and a constant value at $x = 1$, i.e. $X_3(1, t) = c$. These conditions are natural if the hypothesis is assumed that there is some external supply of the catalyst to maintain it constant at $x = 1$.

A plausible hypothesis is that concentration X_3 must attain quickly a certain level for the reaction between species 1 and 2 to take place. Therefore, equation (6) represents a fast evolution as compared with (4)-(5) and (6) can be replaced by the equilibrium solution of $\frac{\partial X_3}{\partial t} = 0$. A direct solution of the boundary problem for X_3 yields.

$$X_3(x) = c\frac{Ch\left(x\sqrt{\frac{d}{k}}\right)}{Ch\left(\sqrt{\frac{d}{k}}\right)} \tag{7}$$

This equation suggests that the conflict between decay and diffusion of the catalyst, represented by the quotient $\frac{d}{k}$, will play an important role. As a matter of fact, it will be shown later that this is a bifurcation parameter.

Now our model reads :

$$\frac{\partial X_1}{\partial t} = \gamma f_1(X_1, X_2) + \frac{\partial}{\partial x}\left(D_1(X_3(x))\frac{\partial X_1}{\partial x}\right) \tag{8}$$

$$\frac{\partial X_2}{\partial t} = \gamma f_2(X_1, X_2) + \frac{\partial}{\partial x}\left(D_2(X_3(x))\frac{\partial X_2}{\partial x}\right) \tag{9}$$

According to the standard Turing theory, systems of this type can develop spatial patterns if the diffusion coefficients are different [Turing, 1952]. Here we assume a relationship $D_2 = mD_1$, $m > o$, and $D_1(X_3)$ is taken as some affine function of X_3, i.e.

$$D_1(X_3)=\alpha X_3+\beta \quad (\alpha<0,\beta>0)$$

where α, β are chosen to keep $D_1>0$ on the interval [0, 1]. Summing up, we have

$$D_1=D_1(X_3(x))=\alpha X_3(x)+\beta=\alpha c\frac{Ch\left(x\sqrt{\frac{d}{k}}\right)}{Ch\left(\sqrt{\frac{d}{k}}\right)}+\beta=D_1(x)$$

$$D_2=mD_1(x)$$

2. Linear analysis and morphogenesis

Morphogenesis appears when durable spatial patterns can be observed. These patterns are wavelike structures and they can be stationary or else have some wandering features [Panfilov and Keener (1995)]. Some analysis have been carried on by the authors elsewhere [García Cortí and Pacheco (1993); García Cortí, Fernandez and Pacheco (1994)]. Duration implies some type of global existence results, a problem analyzed in the next part of this paper. We apply in a straightforward way the general linear theory. Let $f_i(X_1,X_2)(i=1,2)$ satisfy conditions for the diffusionless system to have a compatible singular point, i.e. (X_{10},X_{20}) with $X_{10}>0,X_{20}>0$ and let

$$J=\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

be the jacobian at (X_{10},X_{20}). We look for patterns as solutions of the global systems bifurcating from (X_{10},X_{20}):

$$X_1=X_{10}+e^{\lambda t}Y_1(x), \qquad X_2=X_{20}+e^{\lambda t}Y_2(x)$$

where λ are eigenvalues and $Y_i=(x)\,(i=1,2)$ are the shape coefficients. Now we plug these expresions in the system together with that for $D_i=(x_3)$ and obtain the following *ODE* system :

$$(\alpha X_3+\beta)Y_1''+\alpha X_3'Y_1'+(a_{11}-\lambda)Y_1+a_{12}Y_2=0$$

$$m(\alpha X_3+\beta)Y_2''+m\alpha X_3'Y_2'+a_{21}Y_1+(a_{22}-\lambda)Y_2=0$$

In fact this is a single *ODE* for the new variable Y_1+AY_2 if A is properly chosen. The first equation puls $\frac{A}{m}$ times the second yields

$$(\alpha X_3+\beta)(Y_1''+AX_2'')+\alpha X_3'(x)(Y_1'+AY_2')+$$

$$+\left((a_{11}-\lambda)+\frac{a_{21}A}{m}\right)\left(Y_1+\frac{a_{12}+(a_{22}-\lambda)\frac{A}{m}}{a_{11}-\lambda+\frac{a_{21}A}{m}}Y_2\right)=0 \tag{10}$$

Therefore we must choose $A = \dfrac{a_{12} + (a_{22} - \lambda)\frac{A}{m}}{a_{11} - \lambda + \frac{a_{21}A}{m}}$, a quadratic euation whose roots we represent as A_1 and A_2. Writing $Z_j = Y_1 + A_j Y_2 (j = 1,2)$, we have two *ODE's* for the spatial perturbations Z :

$$(\alpha X_3 + \beta) Z_j'' + \alpha X_3'(x) Z_j' + \left((a_{11} - \lambda) + \frac{a_{21} A_j}{m} \right) Z_j = 0 \quad (j = 1,2) \tag{11}$$

whose general solutions are $Z_j(x) = c_{1j} e^{x(H_1 - H_{2j})} + c_{2j} e^{x(H_1 + H_{2j})}$

where $H_1 = \dfrac{-\alpha c \sqrt{\frac{d}{k}} Sh\left(x\sqrt{\frac{d}{k}}\right)}{2\left(\beta Ch\left(\sqrt{\frac{d}{k}}\right) + \alpha c Ch\left(x\sqrt{\frac{d}{k}}\right)\right)}$

$$H_{2j} = \frac{\sqrt{-4\beta p_j Ch^2\left(\sqrt{\frac{d}{k}}\right) - 4\beta p_j c Ch\left(\sqrt{\frac{d}{k}}\right) Ch\left(x\sqrt{\frac{d}{k}}\right) + a^2 c^2 \frac{d}{k} Sh^2\left(x\sqrt{\frac{d}{k}}\right)}}{2\left(\beta Ch\left(\sqrt{\frac{d}{k}}\right) + \alpha c Ch\left(x\sqrt{\frac{d}{k}}\right)\right)}$$

with $p_j = (a_{11} - \lambda) + \dfrac{a_{21} A_j}{m}$

The zero-flux conditions at $x = 0$ imply $c_{1j} = c_{2j}$, and the following system appears :

$$Z_1(x) = Y_1 + A_1 Y_2 = c_{11}\left(e^{x(H_1 - H_{21})} + e^{x(H_1 + H_{21})} \right)$$

$$Z_2(x) = Y_1 + A_2 Y_2 = c_{12}\left(e^{x(H_1 - H_{22})} + e^{x(H_1 + H_{22})} \right)$$

Now, Y_1 and Y_2 are expressed as :

$$Y_1 = 2\frac{e^{xH_1}}{A_2 - A_1}\left(c_{11} A_2 Ch(xH_{21}) - c_{12} A_1 Ch(xH_{22})\right)$$

$$Y_2 = 2\frac{e^{xH_1}}{A_2 - A_1}\left(c_{12} Ch(xH_{22}) - c_{11} Ch(xH_{21})\right)$$

Combining these expressions with $e^{\lambda t} Y_j(x) = X_j - X_{j0} (j = 1,2)$, we obtain $Y_j(0) = X_j(0,0) - X_{j0}$, and the constants c_{11} and c_{12} are given by

$$c_{11} = \frac{Y_1(0) + A_1 Y_2(0)}{2}; \qquad c_{12} = \frac{Y_1(0) + A_1 Y_2(0)}{2}$$

Equation (11) deserves a more detailed analysis. Its charactreistic equation is

$$r^2+\frac{\alpha X_3'}{\alpha X_3+\beta}r+\frac{(a_{11}-\lambda)+\frac{a_{21}A_j}{m}}{\alpha X_3+\beta}=0 \tag{12}$$

where $\frac{\alpha X_3'}{\alpha X_3+\beta}<0$. Therefore $H_1=-\frac{1}{2}\frac{\alpha X_3'}{\alpha X_3+\beta}>0$, so the real part of the (possibly complex) roots is positive. For complex roots to appear, the relationships

$$\left(\frac{\alpha X_3'}{\alpha X_3+\beta}\right)^2-4\frac{(a_{11}-\lambda)+\frac{a_{21}A_j}{m}}{\alpha X_3+\beta}<0 \tag{13}$$

must hold, which is equivalent to H_{2j} being a pure imaginary, i.e. $H_{2j}=iK_{2j}$ for some real K_{2j}. Summing up, the following expression for Y_1, Y_2 are obtained :

$$Y_1=\frac{e^{xH_1}}{A_2-A_1}(Y_1(0)+A_1Y_2(0))A_2\cos(xK_{12})-(Y_1(0)+A_2Y_2(0))A_1\cos(xK_{22})$$

$$Y_2=\frac{e^{xH_1}}{A_2-A_1}(Y_1(0)+A_2Y_2(0))\cos(xK_{22})-(Y_1(0)+A_1Y_2(0))\cos(xK_{21})$$

thus showing their oscillatory nature, a distinguished feature for morphogenesis. Relationship (13) can be interpreted as two dispersion relationships $F_j(x,\lambda)$, and (13) becomes simply $F_j(x,\lambda)<0$. Figures 3 and 4 show the functions $z_1=F_1(x,\lambda), z_2=F_2(x,\lambda)$ with the bifurcation parameter $\sqrt{\frac{d}{k}}$ set to 1.

3. Existence theory and numerical experiments

The model equations can be written in abstract form as

$$\frac{\partial X}{\partial t}+GX=f(X) \tag{14}$$

where $X=(X_1,X_2)^{\mathrm{T}}$, $f(X)=(f_1,f_2)^{\mathrm{T}}$ and $G=-\begin{pmatrix}\frac{\partial}{\partial x}\left(D_1\frac{\partial}{\partial x}\right) & 0\\ 0 & \frac{\partial}{\partial x}\left(D_2\frac{\partial}{\partial x}\right)\end{pmatrix}$

Boundary conditions are zero-flux ones at $\{0,1\}$ and an initial condition $X(x,0)=X_0(x)$ is also given. In this language we face an initial value problem for the operator "G+Boundary conditions" [Holland (1992)] in some Banach space E. This can be solved formally through the variation of constants formula

$$X(t)=e^{-Gt}X_0+\int_0^t e^{-G(t-s)}f(X(s))ds \tag{15}$$

where e^{-Gt} is the analytic semigroup whose infinitesimal generator is G. The formula can be justified because G is a sectorial operator and therefore generates an analytic semigroup [Henry, 1981]. the emergence of stable spatial patterns needs the existence of the solutions for all $t > 0$. Geometrically, this is equivalent to avoiding blow-up of solutions and can be adrieved through an application of Gronwall's lemma, if an estimate

$$\|f(x)\|_E < cte(1 + \|X\|_\delta) \tag{16}$$

holds, where $\|X\|_\delta$ is the norm in the space $E_\delta = Dom(G + aI)^\delta$ and δ is some fractional power characterizing the Banach space where initial conditions X_0 ensure existence and uniquenes. The norm is defined as

$$\|X\|_\delta = \left\|(G + aI)^\delta X\right\|_2 \quad a \in IR \tag{17}$$

In practice $\| \ \|_\delta$ is not computed directly, the norm of the adequate Sobolev space $H_k[0,1]$ such that $E_\delta \subseteq H_k[0,1]$ for $\delta > \frac{k}{2}$ is employed. Moreover, the Sobolev embedding theorem guarantees that for $n = 1$ the elements of E_δ can be considered as continuous functions, and the same holds for solutions of our problem. See, e.g. [Grindrod (1991)]. The so-called Schnackenberg kinetics is described by the reaction term

$$f(X) = \begin{pmatrix} f_1(X) \\ f_2(X) \end{pmatrix} = \begin{pmatrix} w_1 - X_1 + X_1^2 X_2 \\ w_2 - X_1^2 X_2 \end{pmatrix}$$

where $\mathbf{f} \in L_2(\Omega)$ whenever $f_1, f_2 \in L_2(\Omega)$. This happens only if $X_1, X_2 \in L_{2p}(\Omega)$, where $\Omega = [0,1]$ and $p = 3$. Now we apply the Nirenberg-Gagliardo inequality

$$\|X_i\|_{L_{2p}} \leq cte\|X_i\|^\theta{}_{H_q} \quad \|X_i\|_{L_r}^{1-\theta}$$

if $0 \leq \theta \leq 1, p \geq q, p \geq r$, and $-\frac{n}{p} \leq \theta\left(q - \frac{n}{2}\right) - (1-\theta)\frac{n}{r}$. The inequality is strict for $r = 1$.

Putting $\theta = 1$ we have $\|X_i\|_{L_{2p}} \leq \|X_i\|_{H_q}$, where one of $\frac{-n}{p} \leq \left(q - \frac{n}{2}\right)$ or $q \geq \dfrac{n(p-1)}{2p}$ must hold. This is true if $2q \geq n$. Therefore we take the initial condition in $H_1(\Omega)(q = 1)$, and because $n = 1(\text{i.e.}\,\Omega \subset IR)$, there is no restriction on p. Therefore f_1 and f_2 map H_1 on $L_2(\Omega)$. To see taht $\mathbf{f}$ is lipschitz we write, for f_1:

$$\|f_1(X) - f_1(Y)\|_{L_2} = \left\|-X_1 + X_1^2 X_2 + Y_1 - Y_1^2 Y_2\right\|_{L_2} \leq$$

$$\leq \|X_1 - Y_1\|_{L_2} + \left\|X_1^2 X_2 - X_1^2 Y_2 + X_1^2 Y_2 - Y_1^2 Y_2\right\|_{L_2} \leq$$

$$\leq \|X_1 - Y_1\|_{L_2} + \left\|X_1^2 (X_2 - Y_2)\right\|_{L_2} + \left\|(X_1 - Y_1)(X_1 + Y_1) Y_2\right\|_{L_2}$$

and the Hölder inequality yields that this last expression is bounded by:

$$cte\|X_1 - Y_1\|_{H_1} + cte\left\|X_1^2\right\|_{H_1} \|X_2 - Y_2\|_{H_1} + cte\left\|(X_1 + Y_1) Y_2\right\|_{H_1} \|X_1 - Y_1\|_{H_1} =$$

$$\left(cte+cte\left\|(X_1+Y_1)Y_2\right\|_{H_1}\right)\left\|X_1-Y_1\right\|_{H_1}+cte\left\|X_1^2\right\|_{H_1}\left\|X_2-Y_2\right\|_{H_1}$$

An analogous result holds for f_2 and, summing up, existence of solutions is guaranted. Numerical experiments have been carried on for $\alpha=-1$, $\beta=20$, $\lambda=1000$, $c=15$, $m=10$, $w_1=0\cdot 1$, $w_2=0\cdot 9$ y $\sqrt{\frac{d}{k}}=1$ (figures 5*a* and 5*b*), and $\sqrt{\frac{d}{k}}=2$ in figures 6*a* y 6*b*, showing the stable wavelike patterns appearing in the reaction-diffusion equations.

4. Figures

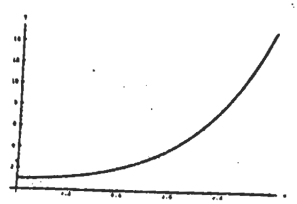

Figure 1

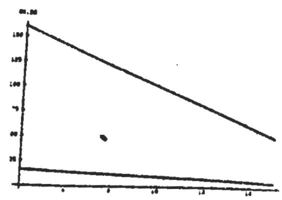

Figure 2

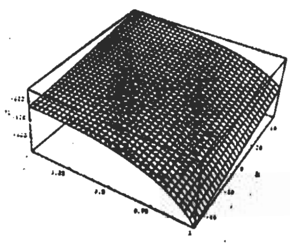

Figure 3

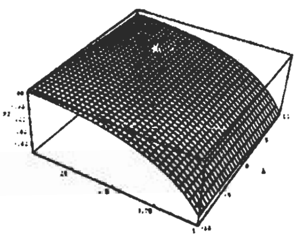

Figure 4

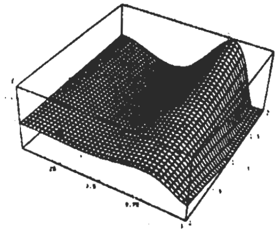

Figure 5a

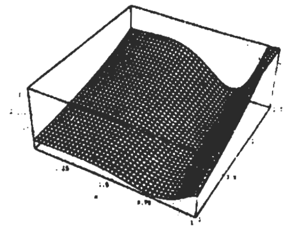

Figure 5b

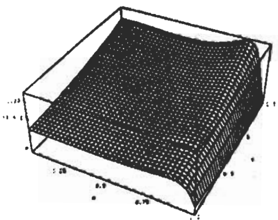

Figure 6a

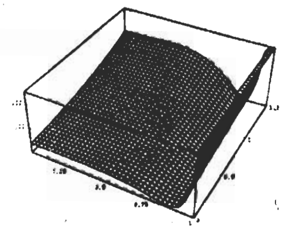

Figure 6b

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