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ON STABILIZATION OF SOLUTIONS OF THE SYSTEM OF PARABOLIC DIFFERENTIAL EQUATIONS DESCRIBING THE KINETICS OF AN AUTO-CATALYTIC REVERSIBLE CHEMICAL REACTION

BY

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Abstract. A system of quasilinear parabolic equations arising in the theory of autocatalytic reactions is studied. A global existence result is established. Furthermore, the large time behaviour of the solution is investigated.

1. Introduction. Systems of reaction-diffusion equations enter a wide number of phenomena in ecology, biology, biochemistry, chemistry and physics. The important problems about these systems is the time evolution of the "active masses" and their relations to the steady states.

The present paper discusses a simple prototype scheme of chemical feedback (autocatalysis) occuring in simple conditions. To be precise, let us consider a region (which may be the liquid in a test tube or a living cell) in which takes place a processus in that the product of a region feeds back on its own formation. This may be represented in the "mass action" style by:

$$(1.1) \qquad U + mV \underset{\epsilon}{\overset{1}{\rightleftarrows}} (m+1)V.$$

Normally this behaviour will arise from a subscheme of elementary steps. It is assumed that (1.1) occurs under constant temperature and constant pressure.

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If u and v represent the active masses of substances U and V, then the forward and backward rates for the two equations are [cf.1, 2, 3]:

$$R_+ = uv^m \qquad \text{and} \qquad R_- = -\epsilon v^{m+1}$$

where ϵ is a positive constant.

Using second Fick's law and the law of mass action, one can write down the equations governing the reaction (1.1):

$$\text{(1.2)} \qquad u_t - a\Delta u = -uv^m + \epsilon v^{m+1}$$

$$\text{(I)}_\epsilon$$

$$\text{(1.3)} \qquad v_t - b\Delta v = uv^m - \epsilon v^{m+1}$$

for $(x,t) \in \Omega \times (0,\infty)$ (x is position, t is time and $\Omega \subset R^n$, $n = 1,2,3$ in practice, the region).

The quantities $a\Delta u$ and $b\Delta v$ are the diffusion terms while $u_t + uv^m - \epsilon v^{m+1}$ and $v_t - uv^m + \epsilon v^{m+1}$ are the reaction terms.

If we assume that reactants and products are confined in a closed system (so an equilibrium is established in which all are present in a certain proportion) then equations (1.2)–(1.3) are supplemented by boundary conditions of Neumann type:

$$\text{(1.4)} \qquad \nabla u \cdot n = \nabla v \cdot n = 0 \qquad \text{on } \partial\Omega \times (0, +\infty)$$

where n is the outward normal to $\partial\Omega$ the boundary of Ω which is assumed to be regular.

It is also assumed that initially u and v are present:

$$\text{(1.5)} \qquad u(x,0) = \phi(x) \geq 0 \quad \text{and} \quad v(x,0) = \psi(x) \geq 0 \text{ for } x \in \Omega.$$

When the effect of diffusion is not considered, namely $a = b = 0$, system (1.2)–(1.5) becomes an ordinary differential system which is simple to integrate.

In this work, we analyse the behaviour of solutions of system (1.2)–(1.5).

2. Notations and preliminaries. In order to study system (1.2)–(1.5), we introduce the Banach space $X = C(\Omega, R^2)$ (of functions $\zeta = (u,v)^{tr}$ which are continuous in Ω) endowed with the norm:

$$||\zeta|| = |u(t)|_\infty + |v(t)|_\infty$$

where $|f|_\infty = \sup|f(x)|$ for $x \in \Omega$.

Let A be defined as the unbounded linear operator

$$D\Delta = \text{diag}(a, b)\Delta$$

with domain:

$$D(A) = (\zeta \in X / D\Delta\zeta \in X \text{ and } \overrightarrow{\nabla u} \cdot \vec{n} = \overrightarrow{\nabla v} \cdot \vec{n} = 0)$$

and let F denote the nonlinear operator:

$$\zeta \in X \to F(\zeta) = (-uv^m + \epsilon v^{m+1}, uv^m - \epsilon v^{m+1}) \in X.$$

With the above notations in mind, system (1.2)-(1.5) can be written in the abstract form:

$$\frac{d}{dt}(\zeta(t)) = A\zeta + F(\zeta(t)) \tag{2.1}$$

$$\zeta(0) = (\phi, \psi) \in X_+, \tag{2.2}$$

where X_+ denotes the subset of X consisting of nonnegative valued functions in X.

It is standard to show that a unique local classical solution of problem (2.1)–(2.2) exists; by this we mean that:

$$\zeta \in C^1([0,T), X) \cap C([0,T), D(A))$$

and satisfies system (1.2)–(1.5). This can be proved by using general results concerning the semigroup theory as $D\Delta$ generates an analytic semigroup on X. Moreover we have the alternative:

either $\quad T = \infty$

or $\quad T < \infty$ and $\lim \|\zeta\| = \infty$ as t goes to T.

3. Global existence and large time behaviour. Concerning global existence we have:

Theorem 1. *The unique solution $(u(x,t), v(x,t))$ is global and bounded for all $(x,t) \in \Omega \times (0,\infty)$. That is if the positive constants K_1 and K_2 are defined by:*

$$\text{Max}(|\phi|_\infty,\ \epsilon|\psi|_\infty) \le K_1$$

$$\text{Max}(\epsilon^{-1}|\phi|_\infty,\ |\psi|_\infty) \le K_2$$

then the solution $(u(x,t), v(x,t))$ satisfies:

$$0 < u(x,t) < K_1 \quad \textit{and} \quad 0 < v(x,t) < K_2 \tag{3.1}$$

for $(x,t) \in \Omega \times (0,\infty)$.

In other words, $]0, K_1[\times]0, K_2[$ is an invariant rectangle.

Proof. It is worth noting that $0 < u(x,t)$ and $0 < v(x,t)$ whenever $0 < \phi(x)$ and $0 < \psi(x)$. Now, assume that (3.1) does not hold for all $(x,t) \in \Omega \times (0,\infty)$. Define the sets B and C as:

$$B := \{(u,v) : 0 < u < K_1, 0 < v < K_2\}$$

$$C := \{t > 0 : (u(x,t), v(x,t)) \in B \text{ for all } (x,t) \in \Omega \times (0,t)\}.$$

Let t_* be the least upper bound for the set C. Then there must be an $x_* \in \Omega$ such that $(u(x_*, t_*), v(x_*, t_*)) \in \partial B$. Since the solution (u,v) is stricktly positive when either $\phi(x) = 0$ or $\psi(x) = 0$, at least one of the following equalities holds:

$$\begin{aligned} u(x_*, t_*) &= K_1 \\ v(x_*, t_*) &= K_2 \end{aligned} \tag{3.2}$$

suppose $u(x_*, t_*) = K_1$, then $u(x_*, t_*)$ must be the maximum of $u(x, t_*)$ for all $x \in \Omega$ by the definition of t_*. Suppose $x_* \in \Omega$; then $a\Delta u(x_*, t_*) < 0$ and $-uv^m + \epsilon v^{m+1} < 0$ at (x_*, t_*) since $-K_1 v^m + \epsilon v^{m+1} < 0$ for $v > 0$; consequently equation (1.2) implies that $u_t < 0$ at (x_*, t_*) and hence $u(x_*, t) > K_1$ for $t < t_*$; this contradicts the definition of t_*. Suppose now $x_* \in \partial\Omega$; we can claim that $a\Delta u(x_*, t_*) \leq 0$. Otherwise $\Delta u(x, t_*) > 0$ for x in a domain with x_* as a boundary point and $u(x_*, t_*)$ as maximum; by Theorem 7 of [6] it will then imply that $\nabla u(x_*, t_*) \cdot n > 0$ which will contradict the boundary condition on u. Once again we have $-uv^m + \epsilon v^{m+1} < 0$ at (x_*, t_*) and as before equation (1.2) will lead to $u(x_*, t_*) > K_1$ for some $t < t_*$ contradicting the definition of t_*. Consequently the set C is unbounded and hence the solution (u,v) remains bounded for all $t > 0$.

To investigate the asymptotic behaviour of the system, we shall make use of its free energy defined by: for $t > 0$

$$G(u,v)(t) = \int_\Omega (u \ln(u/\bar{u}) - u + \bar{u} + v \ln(v/\bar{v}) - v + \bar{v}) dx$$

where $(\bar{u},\bar{v})=(\epsilon c_0,c_0)$, $c_0\in R^+$, are the marginally locally stable stationary solutions. The other steady states are $(c,0), c\in R^+$. Calculating the rate of change of G along the trajectories:

$$\frac{d}{dt}(G)=\int_\Omega(u_t\ln(u/\bar{u})+v_t\ln(v/\bar{v}))dx$$

$$=\int_\Omega((a\Delta u-uv^m+\epsilon v^{m+1})\ln(u/\bar{u})+(b\Delta v+uv^m-\epsilon v^{m+1})\ln(v/\bar{v}))dx$$

$$=-4a\epsilon\int_\Omega|\nabla u^{1/2}|^2-4b\int_\Omega|\nabla v^{1/2}|^2-$$

$$\int_\Omega(uv^m-\epsilon v^{m+1})(\ln(uv^m)-\ln(\epsilon v^{m+1}))$$

as $(a-b)(\ln(a)-\ln(b))>0$ when $a>0$ and $b>0$, we have:

$$\frac{d}{dt}(G)<0, \tag{3.3}$$

as $G>0$ and (3.3) holds, G is a Liapounov functional and hence:

Lemma 2. *It hold $\frac{d}{dt}(G)<0$ and $\frac{d}{dt}(G)=0$ if and only if $u=\bar{u}$ and $v=\bar{v}$ for all $x\in\Omega$. Then $G_\infty=\lim G(u(t),v(t))$ as t goes to ∞ exists.*

As an immediate consequence of (3.3) we have:

Corollary. *System (1.2)–(1.5) does not have t-periodic or (x,t)-periodic, nonnegative and nonconstant solutions.*

At this point, we can state our main theorem.

Theorem 3. *There exists a constant $M<\infty$ such that for all ϕ and ψ continuous and positive, the solution (u,v) satisfies:*

$$\|u(\cdot,t)\|_1\le M \quad \textit{and} \quad \|v(\cdot,t)\|_1\le M \quad \textit{for } t\ge 1. \tag{3.4}$$

Moreover $\lim|u(\cdot,t)-\bar{u}|_\infty=0$ *and* $\lim|v(\cdot,t)-\bar{v}|_\infty=0$ *as t goes to ∞. Where $\|\ \ \|_1$ denotes the norm of $C^1(\Omega)$ and*

$$C_0(1+\epsilon)=(1/meas(\Omega))\int_\Omega(\phi(x)+\psi(x))dx. \tag{3.5}$$

Proof. With $\omega=u$ or $v,\alpha=a$ or b, each equation of the system may be written in the form:

$$\omega_t-(\alpha\Delta-\eta)\omega=\Gamma(x,t) \tag{3.6}$$

where $\Gamma(x,t) = \eta\omega(x,t) \pm (uv^m - \epsilon v^{m+1})$, and $\omega(x,0) = \phi(x)$ or $\psi(x)$. It is clear that we may consider $\omega \in C^2$, for otherwise the initial value problem starting at $t = 1/2$ may be considered. From boundedness of the solution we infer the existence of a constant N such that $|\Gamma|_\infty \leq N$ for all $t > 0$.

By [5, p.88], for some η, under homogeneous Neumann boundary conditions $\Delta - \eta I$ generates an analytic semigroup in $L^p(\Omega)$ (norm $|\cdot|_p$) for $p > 1$ and with $-\Sigma$ the associated operator, there is a $\rho > 0$ such that $Re\,\sigma(\Sigma) > \rho$ (where $\sigma(S)$ denotes the spectrum of Σ). Equation (3.6) may then be written as:

$$\omega_t + \Sigma\omega = \Gamma,$$

with integral solution

$$\omega(t) = e^{-\Sigma t}\omega_0 + \int_o^t e^{-\Sigma(t-s)}\Gamma(s)ds. \tag{3.7}$$

From [5, p.26], for $\sigma > 0$,

$$|\Sigma^\sigma e^{-\Sigma t}|_p < C(\sigma)t^{-\sigma}e^{-\rho t}, \tag{3.8}$$

where $|\cdot|_p$ is also used to denote the operator norm. Taking some $0 < \sigma < 1$, applying Σ^σ to (3.7), and taking norms, we obtain:

$$|\Sigma^\sigma\omega(t)|_p \leq C(\sigma)\Big(t^{-\sigma}e^{-\rho t}|\omega_0|_p + \max_{0\leq s\leq t}|\Gamma|_p \int_0^t (t-s)^{-\sigma}e^{-\rho(t-s)}ds\Big)$$

by (3.7), we infer:

$$|\Sigma^\sigma\omega(t)|_p \leq N_0 \quad \text{for } t \geq 1. \tag{3.9}$$

From the definition of the fractional space $L = (L^p(\Omega))^\sigma$ [5, p.29], and a standard imbedding theorem [5, p.39], respectively,

$$|\Sigma^\sigma\omega(t)|_p = |\omega(t)|_L, \tag{3.10}$$

$$|\omega(t)|_\theta \leq C|\omega(t)|_L \quad \text{for } 0 \leq \theta \leq 2\sigma - n/p \tag{3.11}$$

where C is a constant independent of ω. Taking $\sigma = 3/4$, $p = 2n$ and $\theta = 1$, we obtain the result of combining (3.9), (3.10), (3.11).

Now, to prove the global attractivity of (u,v), we make use of the positive ω-limit set ω^+:

$$\omega^+ = ((u,v) \in X : \exists t_n \to \infty \text{ such that } (u(t_n), v(t_n)) \to (u,v) \text{ in } X)$$

it is well known that:

- The limit set ω^+ is nonvoid, compact and connect.
- The trajectory approches its own limit set in the X-norm.
- The limit set ω^+ is invariant: new trajectories starting from any point in ω^+ remain in ω^+ for all future time.

Now, it is clear that it suffices to show that the ω-limit set consists only of the stationary solution $(\bar{u}, \bar{v})$. But this can be done using the well known La Salle's invariance principle [4], which is here reproduced just for convenience. Let $(U(x), V(x)) \in \omega^+$; it is clear that $U(x)$ and $V(x)$ are bounded. Let, now, the trajectory $(U(x,t), V(x,t))$ starts at $(U(x), V(x))$. By our results, $U(x,t)$ and $V(x,t)$ are bounded. So by the continuity of G we have: $G(U(\cdot,t), V(\cdot, \ )) = G_\infty$ for all $t > 0$, hence G is constant along this trajectory, so $U(x,t) = \bar{u}$ and $V(x,t) = \bar{v}$ for all $(x,t) \in \Omega \times (0,\infty)$; hence $U(x) = \bar{u}$ and $V(x) = \bar{v}$.

Moreover, adding (1.2) and (1.3) and integrating over $\Omega \times (0,t)$ yields:

$$\int_\Omega (u(x,t) + v(x,t))dx = \int_\Omega (\phi(x) + \psi(x))dx \tag{3.12}$$

combining (3.12) with $\lim |u(\cdot,t) - \bar{u}|_\infty = 0$ and $\lim |v(\cdot,t) - \bar{v}|_\infty = 0$ as t goes to infinity yields (3.5).

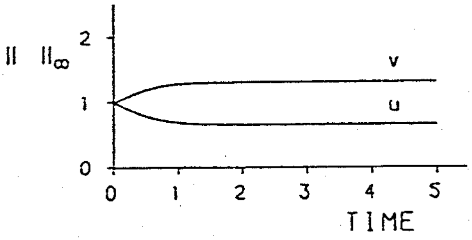
In studying $(I)_\epsilon$, we wished to get a global solution to $(I)_0$ using the uniform estimates (3.4) and passing to the limit as ϵ goes to 0 in contrast with the work of Masuda [7] where a judicious functional (not natural) of Liapounov was used. Unfortunatly we have not succeeded in doing so but we continue to believe that this is possible.

4. Quantitative results.

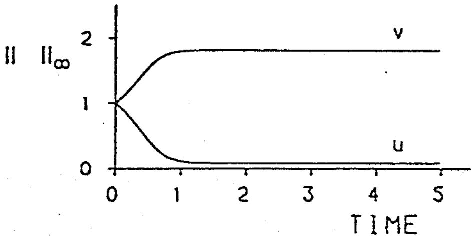
Numerical results: Figures 1–4 show the behaviour of $|u(\cdot,t)|_\infty$ and $|v(\cdot,t)|_\infty$ for $0 < t < 5$ for the system (1.2)–(1.5).

The solution was evaluated numerically using a finite-difference implicit scheme (Crank-Nicolson type).

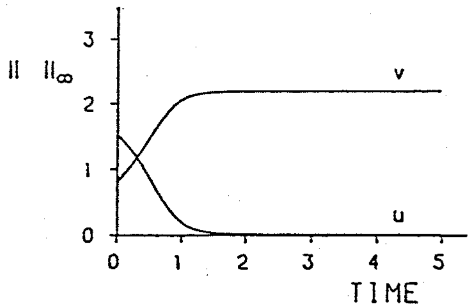
The diffusion parameters a, b, the initial data ϕ, ψ, the values of ϵ and m are indicated under each figures.



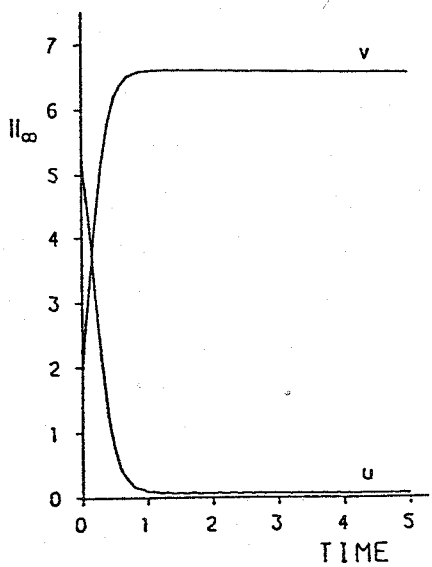
$m = 3 \quad \epsilon = 0.5$
$a = 0.1 \quad b = 0.001$
$\phi = 1 \quad \psi = 1$



$m = 3 \quad \epsilon = 0.05$
$a = 0.1 \quad b = 0.001$
$\phi = 1 \quad \psi = 1$



$m = 2 \quad \epsilon = 0.01$
$a = 0.1 \quad b = 1$
$\phi = 0.1(x - x^2) + 1.5,$
$\psi = 0.1(x - x^2) + 0.8$



$m = 1 \quad \epsilon = 0.01$
$a = 1 \quad b = 0.01$
$\phi = \sin(x - x^2) + 5$
$\psi = \cos(x - x^2) + 1$

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