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A DIFFUSION REACTION SYSTEM MODELLING SPATIAL PATTERNS

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1. Introduction

The system of differential equations discussed in this paper came up in modelling phenomena in chemistry known as Liesegang phenomena. Experiments show [6], [7] that diffusing ions (in the classical experiment silver and chromate ions) may form spatial structures like rings and bonds. Similar growth patterns have recently been observed and experimentally analysed by Hoppensteadt, Roth, Schmid and the author in bacterial cultures [3]. Here growth activating substances are replacing the ions, the growing bacterias correspond to the precipitating complex. In both cases the diffusion is slow and the reaction is fast. Furthermore, the tendency to pattern formation is increased by a threshold effect. The reaction is switched on (off) if the concentrations of the reacting substances are large (small) enough. Mathematically the assumption of such an effect can be described by a Volterra functional. In connection with Liesegang phenomena, systems showing slow diffusion and fast reaction have been studied by Keller and Rubinow [4],[5]. Switch on - switch off functionals arise also in the mathematical treatment of thermostats. The reader is referred to the recent publications of Glashoff and Sprekels on this subject [1],[2]. The results reported have been obtained jointly with Hoppensteadt, University of Utah.

2. The system of equations, analytic results

The following system, a simplified version of a more general one, shows at least numerically the structure formation observed in the experiment. Let $u=(u^1,u^2)$ be the concentrations of the diffusing substance ("nutrients"), b the concentration of the growing substance ("bacteria"). Then we look for solutions of the following system

$$
(1) \qquad \begin{aligned} \partial_t u^i &= D_i \Delta_x u^i - \rho c_i s(u) \\ \partial_t b &= \rho c_o s(u) \end{aligned}
$$

in a disc (petridish), where D_i, c_j are positive constants of the same size, ρ is a large positive number. s is a Volterra functional (switching functional) having only value 0 or 1. At the boundary the no-flux condition

$$
(2) \qquad \partial_\nu u^i = 0
$$

holds. For the study of pattern formation we assume that the initial values depend only on the radius r, $u^1(0,\cdot)$ and $b(0,\cdot)$ are constant and $\partial_r u^2(0,\cdot) \leq 0$. The threshold effect is formulated with help of switching curves Γ_{on} and Γ_{off} , defined for instance as level curve of a real function φ on the positive quadrant Q (example $\varphi(u) = u^1 \cdot u^2$), which we compose as sketched in figure 1a,b

$$Q = M_{off} \cup \Gamma_{off} \cup M_{on\,off} \cup \Gamma_{on} \cup M_{on}$$

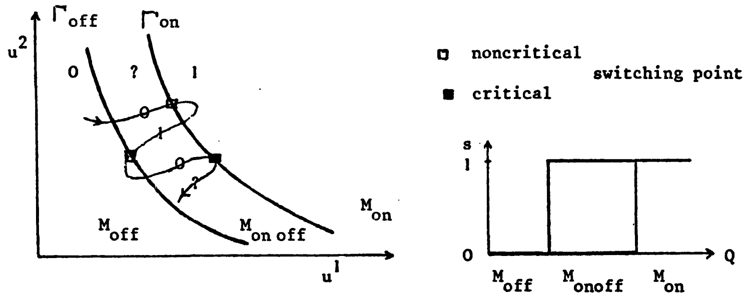

Figure 1 a, b

The switching functional cannot be uniquely defined if as in figure 1a the curve $t \to u(t,x)$, where x is fixed, has a critical switching point (touching point, no crossing). Therefore, we choose setvalued mappings for the analytical treatment.

Definition: Let $w: [0,\infty[\to Q$ be a continuous function. Define

$$\underline{s}(w)(t) := \begin{cases} 1 & \text{if there exists a } t_o < t \text{ such that } w(t_o) \in M_{on} \\ & \text{and } w(\tau) \notin \overline{M}_{off} \text{ for all } \tau, t_o < \tau \leq t\,; \\ 0 & \text{otherwise.} \end{cases}$$

$$\overline{s}(w)(t) := \begin{cases} 1 & \text{if there exists a } t_o \leq t \text{ such that } w(t_o) \in \overline{M}_{on} \\ & \text{and } w(\tau) \notin M_{off} \text{ for all } \tau, t_o \leq \tau < t\,; \\ 0 & \text{otherwise.} \end{cases}$$

These (extremally defined) Volterrafunctionals are used to reformulate the problem such that it can be solved by the Kakutani fixpoint theorem. The following analytic result is obtained.

Theorem. Let $\Omega \subset \mathbb{R}^2$ be an open, bounded set with $C^{1,\alpha}$ boundary, $u_o: \overline{\Omega} \to Q$ continuous and continuously differentiable at $\partial\Omega$. Then there exists a continuous function $u: [0,\infty[x\bar{\Omega} \to Q$ and a measurable function $\sigma:]0,\infty[x\Omega \to [0,1]$ satisfying

(3) $\partial_t u^i = D_i \Delta_x u^i - \rho c_i \sigma$

in $]0,\infty[x\Omega$ in distributional sense and

(4) $\sigma(t,x) \in [\underline{s}(u(\cdot,x)), \bar{s}(u(\cdot.x))](t)$ a.e.

$u(t,\cdot) \in C^1(\bar{\Omega})$ for $t > 0$; (2) is fulfilled as well as the initial condition

$$u(0,\cdot) = u_o .$$

Remark

(i) Instead of using a fixpoint theorem for setvalued compact mappings a more direct approximation can be applied. Let s be either $\underline{s}$ or $\bar{s}$ and replace in (1) s by the approximating functional

$$s_\varepsilon(w) = \frac{1}{\varepsilon} \int_0^\varepsilon s(w + e\delta)d\delta \quad , e = (1,1) ,$$

which is Lipschitz continuous with respect to the sup-norm.

(ii) Replace $s(u)$ in (1) by a function v satisfying an equation of the type

$$\varepsilon \partial_t v = p(u,v)$$

where $p(u,\cdot)$ is a polynomial of degree 3 and $p(u,v) = 0$ defines a surface in $Q \times [0,\infty[$ having a fold just over $\bar{M}_{onoff}$. The problem if for $\varepsilon \downarrow o$ the solutions of the corresponding system converge to those of problem considered here will be studied later.

(iii) The problem of finding sufficient conditions for uniqueness of the solution of the theorem is connected with the problem of measuring the set of critical switching points and still open.

3. Numerical results

Despite of the unsolved analytic problems Hoppensteadt, the author and Poeppe have shown that discretisations of the equation (1) can be treated numerically and show the qualitative behavior observed in the experiments. Whereas for the diffusion part a method of lines solver or a hopscotch technique has been used, the functional has been discretised as follows

$$s_{n,m} := \begin{cases} 1 & \text{if } s_{n-1,m} = 1 \text{ and } u_{n-1,m} \notin M_{off} , \\ & \text{or} \\ & s_{n-1,m} = 0 \text{ and } u_{n-1,m} \in \overline{M}_{on} ; \\ 0 & \text{otherwise} , \end{cases}$$

(n.m) is the (time, space) index.

The computer plots show the expected effect of a fast reaction and a slow diffusion which cannot keep up the supply of reacting substances necessary for the reaction. The following figure shows the typical distribution of b gotten for realistic parameters for large t .

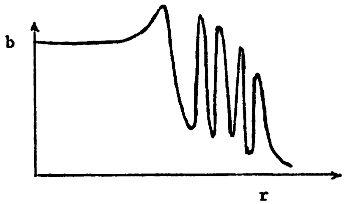

Figure 2

4. References

[1] K. Glashoff, J. Sprekels: The regulation of temperature by thermostats and set-valued integral equations. Integral Equations (to appear).

[2] K. Glashoff, J. Sprekels: An application of Glickberg's theorem to set valued integral equations arising in the theory of thermostats. Siam J. Math. Anal. 12, 477-486 (1981).

[3] F.C. Hoppensteadt, W. Jäger: Pattern formation by bacteria. Lecture Notes in Biomathematics 38, 69-81 (1980).

[4] J.B. Keller: Liesegang rings and a theory of fast reaction and slow diffusion. Proceedings of the Sympossium on Chemical Reactions, Mathematical Research Center, Madison, Wisconsin (1980).

[5] J.B. Keller, S.I. Rubinow: Recurrent precipitation and Liesegang rings. Preprint (1980).

[6] R.E. Liesegang: Naturw. Wochenschr. 11, 353 (1896).

[7] P.M. Noyes: Oscillations in homogenous systems. Ber. Bunsenges. Phys. Chem. 84, 295-303 (1980).