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In: Michal Greguš (ed.): Equadiff 5, Proceedings of the Fifth Czechoslovak Conference on Differential Equations and Their Applications held in Bratislava, August 24-28, 1981. BSB B.G. Teubner Verlagsgesellschaft, Leipzig, 1982. Teubner-Texte zur Mathematik, Bd. 47. pp. 119--122.

Persistent URL: http://dml.cz/dmlcz/702273

DISSIPATION AND ASYMPTOTIC BEHAVIOR

OF SOME REACTION - DIFFUSION SYSTEMS

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1. Introduction

We shall deal with the behavior for large times of solutions $u = (u_1,u_2,u_3)$ to initial-boundary value problems of the form

$$(1) \qquad \begin{aligned} &u_{1t} - D\Delta u_1 = ku_2^2 - k'u_1u_3 = -\tfrac{1}{2}u_{2t} = u_{3t} \quad \text{on } [0,+\infty[\,\times G, \\ &\frac{\partial u_1}{\partial n}\Big|_{\partial G} = 0, \quad u_i\Big|_{t=0} = a_i, \ i=1,2,3. \end{aligned}$$

We assume that $G \subset \mathbb{R}^N$ is a bounded domain with a smooth boundary ∂G and that $D>0$, $k>0$, $k'>0$. The problem (1) is a model of certain polycondensation processes (cf. Pell-Davis [12]). We shall obtain information about the asymptotic behavior of such processes making use of their dissipation rate. For results on the asymptotic behavior of solutions to problems similar to (1) see Gajewski-Zacharias [6] and Gajewski-Gärtner [5].

We consider (1) as a special case of more general reaction-diffusion systems. Let n denote the total number of species involved and let r be the number of those species for which we have to take into account diffusion. We set

$$L^p:=L^p(G;\mathbb{R}^n),\ 1 \leq p \leq \infty,\ C:=C(\overline{G};\mathbb{R}^n),\ C_+:=\{v\in C \mid v \geq 0\},$$
$$V:=\{v=(v_1,\ldots,v_n)\in L^2 \mid v_i \in H^1(G),\ i=1,\ldots,r\}.$$

We define a linear operator A from V to its dual space V^* by

$$\forall v,\forall h\in V: \ \langle Av,h\rangle := \int_G \sum_{i=1}^{r} D_i \operatorname{grad} v_i \operatorname{grad} h_i \, dx,$$

where $D_1,\ldots,D_r$ are given positive numbers. If $\alpha = (\alpha_1,\ldots,\alpha_n)$ is a multi-index and $v\in V$ we set $v^\alpha = v_1^{\alpha_1}\cdot\ldots\cdot v_n^{\alpha_n}$. The reaction-diffusion problems we are interested in are of the form

$$(2) \qquad \begin{aligned} &\frac{du}{dt}(t) + Au(t) = F(u(t)) \text{ for a.e. } t\in S,\ u(0) = a, \\ &u\in L^2_{loc}(S;V)\cap C(S;C),\ \frac{du}{dt}\in L^2_{loc}(S;V^*), \end{aligned}$$

where $S = [0,T]$, $T < \infty$, or $S = [0,+\infty[$ and $F(v):=\sum_{\alpha,\beta} k_{\alpha\beta} v^\alpha(\beta-\alpha)$ ($k_{\alpha\beta} \geq 0$; $k_{\alpha\beta} > 0$ only for a finite number of multi-indices). For a detailed interpretation of the function F (which represents a "mass action kinetics") see Horn-Jackson [8] or Feinberg [4].

The problem obtained from (2) setting $S = [0,+\infty[$, $n = 3$, $r = 1$, $D_1 = D$ and $k_{\alpha\beta} = \begin{cases} k & \text{if } \alpha = (0,2,0),\ \beta = (1,0,1), \\ k' & \text{if } \alpha = (1,0,1),\ \beta = (0,2,0), \\ 0 & \text{otherwise} \end{cases}$
will be regarded as the precise formulation of problem (1).

2. Existence, uniqueness, regularity

The following theorem on existence and uniqueness local in time can be proved by standard arguments (cf. e.g. Martin [10], Ch. 8).

Theorem 1. For every $a \in C$ there exists $T > 0$ such that the problem (2) with $S = [0,T]$ has a unique solution.

Remark 1. Let u be the solution to (2). If $a \in C_+$ then $u(t) \in C_+$ for every $t \in S$. To prove this one can use the lattice structure of the space V (cf. Nečas [11], Ch. 7, §2).

Remark 2. Well known results on evolution equations (see e.g. Barbu [1], Tanabe [13]) along with the special form of F allow to prove that for the solution u to (2) (with $S=[0,T]$, $T < \infty$) we have

$$\forall t \in]0,T[\ : \ u \in C^1([t,T];C),\ Au \in C([t,T];C).$$

Further regularity results can be proved if the assumptions on the initial value a are strengthened.

Remark 3. It is easy to see that for a solution u to the special problem (1) we have $0 \leq u_2(t) + 2u_3(t) = a_2 + 2a_3$. Using these relations one can prove

Theorem 2. For every $a \in C_+$ $(n=3)$ there exists a unique solution to problem (1) (note that for (1) we have $S = [0,+\infty[$).

Remark 4. Let u be the solution to (1) corresponding to an initial value a such that $a_2(x) \geq d > 0$. It is easy to check that for every $t > 0$

$$u_2(t) \geq \frac{d}{1+2dkt},\quad \min_{x\in\overline{G}} u_1(t,x) > 0,\quad \min_{x\in\overline{G}} u_3(t,x) > 0.$$

3. Dissipation and asymptotic behavior

In this section we assume that we are given $e \in C$ such that

$$\forall \alpha,\beta:\quad k_{\alpha\beta}e^{\alpha} = k_{\beta\alpha}e^{\beta}, \tag{3}$$
$$Ae = 0,\quad \min_{x\in\overline{G}} e_i(x) > 0,\ i=1,\dots,n.$$

These relations mean that e is a (nontrivial) equilibrium state for the pure diffusion process and for all pairs of reactions $\alpha \rightleftharpoons \beta$ simultaneously. Obviously, (3) can be satisfied for the special problem (1). By means of e we define a function $H : C_+ \to [0,+\infty[$ as follows:

$$H(v) := \int_G \sum \Phi\left(\frac{v_i}{e_i}\right) e_i \, dx, \quad \text{where} \quad (q) := \begin{cases} q(\ln q - 1) + 1 & \text{for } q > 0, \\ 1 & \text{for } q = 0. \end{cases}$$

Using (3) we can prove

Theorem 3. Let $a \in C_+$ and let u denote the corresponding solution to problem (2). Then $H(u(t)) \leq H(u(s))$ if $t \geq s$ and $s, t \in S$. Moreover, if $\min_{x \in \bar{G}} u_i(t,x) > 0$, $i = 1, \ldots, n$, then

$$\frac{d}{dt} H(u(t)) = \int_G \sum_{i=1}^{n} \frac{du_i}{dt}(t) \ln \frac{u_i(t)}{e_i} \, dx = - \int_G \left\{ \sum_{i=1}^{r} D_i \frac{|\operatorname{grad} u_i(t)|^2}{u_i(t)} + \frac{1}{2} \sum_{\alpha,\beta} (k_{\alpha\beta} u^{\alpha}(t) - k_{\beta\alpha} u^{\beta}(t)) \ln \frac{k_{\alpha\beta} u^{\alpha}(t)}{k_{\beta\alpha} u^{\beta}(t)} \right\} dx .$$

Remark 5. In the case of pure reaction systems a Liapunov function similar to H has been used by Horn-Jackson [8]. Note that for mass action systems $\mu_i := \ln \frac{u_i}{e_i}$ is the (suitably scaled) chemical potential of the species with the concentration u_i and that $- \int_G \sum_{i=1}^{n} \frac{du_i}{dt}(t) \mu_i(t) dx$ is the dissipation rate of the process under consideration (see De Groot [2]). Condition (3) guarantees that the dissipation rate is nonnegative, i. e. that the model is in accordance with the Second Law of Thermodynamics (cf. the discussion of this point by Horn-Jackson [8]; see also Horn [7] and Feinberg [3]).

Remark 6. Let $L_H := \{ v \in L^1 \mid H(|v|) < \infty \}$. L_H can be considered as an Orlicz space (see Kufner-John-Fučík [9]). Theorem 3 shows that each trajectory of (2) originating at a point $a \in C_+$ is bounded in the space L_H.

The proof of the following theorem on the asymptotic behavior of the solution to the special problem (1) uses essentially the results of Theorem 3.

Theorem 4. Let $a \in C_+$ $(n=3)$ be chosen such that $a_2(x) \geq d > 0$. Then there exists a unique e such that

$$\text{(4)} \qquad \begin{aligned} & e \in C_+, \ \operatorname{grad} e_1 = 0, \ k e_2^2 = k' e_1 e_3, \ e_2 + 2e_3 = a_2 + 2a_3, \\ & \int_G (2e_1 + e_2) dx = \int_G (2a_1 + a_2) dx. \end{aligned}$$

If u is the solution to (1) then

$$\text{(5)} \qquad u(t) \longrightarrow e \text{ in } L_H \text{ as } t \longrightarrow \infty .$$

The result of this theorem can be improved if $G \subset R^1$. First one can show that in the statement (5) the space L_H may be replaced by the space C. Using this fact and a linearization of the problem in a neighbourhood of the point e one can prove

Theorem 5. Let $G \subset R^1$ and let u and e be the solutions to (1) and to (4), respectively (we assume the initial value to be chosen as in Theorem 4). Then

$$\|u(t) - e\|_C \leq \text{const} \exp(-\gamma t), \quad t \geq 0,$$

if $\gamma > 0$ is sufficiently small.

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