ON AN INITIAL-VALUE PROBLEM FOR A NONLINEAR TRANSPORT EQUATION IN POLYMER CHEMISTRY

Herbert Gajewski and Klaus Zacharias
Berlin, GDR

We consider a mathematical model of emulsion polymerization. This model describes the time evolution of the particle size distribution function of a polymer within a chemical reactor. For the physico-chemical details we refer to /6,7,10/. The mathematical details and the proofs of our results, ensuring global existence, unicity, positivity and some regularity of the distribution function, will be published in /3/.

1. The model equation. We assume the particle size distribution to be governed by the following equation

$$(1)\quad \frac{\partial f}{\partial t}(t,v)+\frac{\partial}{\partial v}(r(t,v,M_0 f,M_1 f)f(t,v))=\frac{1}{2}\int_0^v k(v-w,w)f(t,v-w)f(t,w)dw - f(t,v)\int_0^\infty k(v,w)f(t,w)dw$$

with the initial condition

$$(2)\qquad f(0,v)=f_0(v)\ .$$

Here denotes $t\in S=[0,T]$, the time variable, $v\geq 0$ the particle volume variable. The physical meaning of the unknown function f is such that $f(t,v)dv$ is (proportional to) the average particle number per unit emulsion volume at time t with volume between v and $v+dv$. The function r is a given particle growth rate, depending on t, v and the moments of order zero and one

$$(M_0 f)(t)=\int_0^\infty f(t,v)dv\quad,\quad (M_1 f)(t)=\int_0^\infty vf(t,v)dv$$

of the distribution function, which can be interpreted as particle number and particle volume, respectively. The kernel $k=k(v,w)$ describes the rate of coalescence between particles of size v and w. The general assumption on k is symmetry and positivity.

Equation (1) may be looked at as a non-local first order partial integro- differential equation for f. We do not know any mathematical results concerning the full equation (1). Equation (1) with $r=0$ is the classical coagulation equation which describes (with varying signification of the variable v and with different assumptions on the kernel k) e. g. Brownian coagulation in plants and gravitational coagulation in clouds. Especially for meteorological applications see /9/, as to the mathematical side of the problem, see /1,2,4,5,8/.

2. Some a priori informations about the solution. By physical reasons we claim $f(t,v) \geq 0$ for $t \geq 0$, $v \geq 0$; $f(t,0) = 0$, $f(t,v) \to 0$ as $v \to \infty$. Integration of equation (1) gives in our situation

$$\frac{d}{dt} M_0 f = -\frac{1}{2} \int_0^\infty \int_0^\infty k(v,w) f(t,v) f(t,w) \, dv\, dw \leq 0 \ .$$

Multiplication by v and integration yields

$$\frac{d}{dt} M_1 f = \int_0^\infty r f \, dv \geq 0 \ .$$

So by coalescence the particle number $M_0 f$ decreases with time whereas the particle volume $M_1 f$ increases due to polymerization. Further in the special case that $r = r(t, M_0 f, M_1 f)$ we have

$$\text{(3)} \qquad \operatorname{supp} f \subset \{(t,v) \,/\, v \geq h(t)\} \ , \quad h(t) = \int_0^t r \, ds \ .$$

3. Assumptions. Our theorem formulated in the next section holds under the following assumptions on the rate functions r and k .

A1.

(i) $r = r_0(v) r_1(t, M_0 f, M_1 f)$;

(ii) r_0 is twice continuously differentiable in $R^+ = [0,\infty)$ so such

$$0 \leq r_0(v) \leq c_0 \ , \quad |r_0'(v)| + |r_0''(v)| \leq \text{const} \ , \quad v \in R^+ \ ;$$

(iii) r_1 is nonnegative on $S \times (0,\infty) \times (0,\infty)$; $r_1(\cdot, x, y)$ is μ-Hölder continuous for a $\mu > 0$, uniformly with respect to x, y in bounded sets of $(0,\infty) \times (0,\infty)$; $r_1(t,\cdot,\cdot)$ is locally Lipschitz-continuous, uniformly with respect to $t \in S$; for each strictly positive and continuous function a on S the initial value problem

$$b'(t) = c_0 a(t) r_1(t, a(t), b(t)) \ , \quad b(0) = b_0 > 0 \ , \quad t \in S$$

has a bounded solution b .

A2.

The function k is continuously differentiable on $R^+ \times R^+$ such that

$$0 \leq k(v,w) = k(w,v) \leq \text{const}(1 + (vw)^{-\beta}) \ ; \quad \beta \geq 0 \ ,$$

$$0 \geq \frac{\partial k}{\partial v}(v,w) \geq -\text{const}\left(1 + \frac{1}{v}\right) k(v,w) \ .$$

Remark 1. A for applications relevant example of rates r and k satisfying A1 and A2 is given by

$$r = r(M_0, M_1) = R_1 \left(R_2 \frac{M_1}{M_0^2} + R_3 \frac{M_1^{2/3}}{M_0^{5/3}}\right)^{1/2} ,$$

$$k = k(v,w) = K(v,w)^{-1/3} ,$$

(R_1, R_2, R_3, K given constants).

4. The main result. For a Banach space X we denote by $C_w^l(S;X)$ the space of l-times weakly continuously differentiable functions on S with values in X. We introduce the weigth functions

$$q(v) = (1+v)^{\nu} v^{-2\beta} , \quad \nu > 2\beta + \tfrac{3}{2} ,$$

$$p^2(v) = (1+v)^{\lambda} + v^{-2(1+\beta)} , \quad \lambda > 1 .$$

Let

$$H = \{ f \in L^2(R^+) \, / \, \|f\|^2 = \int_0^\infty q^2 f^2 dv < \infty \} , \quad H^+ = \{ f \in H \, / \, f \geq 0, \text{ a. e. in } R^+ \} .$$

For sufficiently large $\gamma > 0$ the operator A defined by

$$A f = \left(\frac{\gamma}{v^2} + p^2\right) f - \frac{1}{q^2}(q^2 f')' , \quad f' = \frac{df}{dv} ,$$

$$D(A) = \{ f \in H \, / \, f = v^{1+2\beta+\alpha} h , \; h \in C_0^\infty(R^+) \} , \; \alpha^2 = \gamma + 2\beta(2\beta+1) ,$$

turns out to be essentially selfadjoint in H. Let $E = D(A^{1/2})$ be the energetic space of A.

Theorem 1. Suppose A1, A2. Let in addition $f_0 \in E \cap H^+$, $f_0 \neq 0$. Then the initial-value problem (1), (2) has a unique solution $f \in C_w(S; E \cap H^+) \cap C_w^1(S;H)$. Moreover, the moments M_0 and M_1 satisfy the estimates

$$0 < M_0 f(t) \leq M_0 f_0 , \quad 0 < M_1 f_0 \leq M_1 f(t) \leq b(t) ,$$

where b is the solution of the initial-value problem

$$b' = c_0 M_0 f r_1(t, M_0 f, b) , \quad b(0) = M_1 f_0 .$$

5. Galerkin's method. Let $(h_n) \subset E$ be a system of functions complete in E and $H^n = \mathrm{span}(h_1, \ldots, h_n)$. Further let (f_{0n}) be a sequence such that $f_{0n} \in H^n$, $f_{0n} \to f_0$ in E. According to Galerkin's method we define approximate solutions f_n of f of the form

$$f_n = \sum_{i=1}^{n} a_i(t)h_i(v) \quad .$$

The coefficient functions $a_i(t)$ we determine by solving the following system of ordinary differential equations

$$(f_{nt} + R\, f_n, h_l) = (K\, f_n, h_l) \quad , \quad l = 1,\dots,n, \quad f_n(0,v) = f_{on}(v) \ .$$

Here $(.,.)$ denotes the scalar product in H , R and K are some regularizations of the operators generated by the transport term and the coalescence term in (1), respectively /3/.

Theorem 2. Under the hypotheses of Theorem 1 the Galerkin approximates f_n converge in H uniformly with respect to time to the solution f of the initial-value problem (1), (2).

Remark 2. Examples of appropriate basis functions are given in /3/.

Remark 3. In our numerical computations it turned out to be useful to introduce a new independent variable x according to a transformation $v=h(t)+g(t)\exp(cx)$, c=const, where h is the function defined in (3) and g is an appropriate scaling function. By means of such transformation we could overcome up to a certain extent numerical difficulties due to the fact, that in relevant cases the support of f essentially increases and travels to the right as time increases.

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