XXI Congreso de Ecuaciones Diferenciales y Aplicaciones
XI Congreso de Matemática Aplicada
Ciudad Real, 21-25 septiembre 2009
(pp. 1–5)

Measure-valued solutions to a nonlocal conservation law arising in crystal precipitation

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Key words: Measure-valued solutions to a nonlocal conservation law, crystal precipitation, extinction in finite time

Resumen

We study the so-called Oswald ripening in reactive batch crystallizer by means of the mathematical models proposed in by N.S. Tavare in 1985. Such a model takes into account not only crystal growth but also the decrease of crystals when they have small dimensions. The model can be stated in terms of a nonlocal and nonlinear conservation law. Besides its relevance in the applications, which made specially interesting such a problem, from the mathematical point of view, is that it can be proved that when the initial datum is a measure (for instance, the addition of a finite number of "Dirac deltas" located in some points $\{x_i\}_{i=1,..,m}$) then the corresponding solution is not a L^1-valued function but a measure-valued function $n(\cdot,t)$.The main goal of this communication is to present some improvements on the previous mathematical treatment made by A. Friedman, B. Ou and D.S. Ross in 1989 (see also the treatment made on photographic films in the book by A. Friedman and W. Littman of 1994).

1. Introduction

The study of crystal precipitation attracted the attention of many specialists since the XIX century. Phenomena as the so-called Oswald ripening in reactive batch crystallizer was the main object of some mathematical models (Tavare [11]) since they have a great relevance in many different contexts (see the treatment made on photographic films in the book by Friedman and Littman [9]). The Tavare's model take into account not only crystal growth but also the decrease of crystal when they have small dimensions (in fact, it does not consider the "nucleation processs̈in order to simplify the formulation). The model can be stated in terms of a conservation law

$$\begin{cases} \frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(Gn) = 0 & x>0, t>0, \\ n(x,0) = n_0(x) & x>0, \end{cases}$$

where G denotes a suitable nonlocal term (depending on n) which will be detailed at the presentation.Besides its relevance in the applications, which made specially interesting such a problem, from the mathematical point of view, is that it can be proved that when $n_0(x)$ is a measure (for instance, the addition of a finite number of "Dirac deltas" located in some points $\{x_i\}_{i=1,..,m}$) then the corresponding solution is not a L^1-valued function but a measure-valued function $n(\cdot, t)$.The main goal of this communication is to present some improvements on the previous mathematical treatment made in [8]. In particular, we prove that such type of solution satisfies the equation in a suitable weak sense and prove that, under suitable additional conditions on G, the Oswald ripening phenomenon (persistency of a single crystal size for very large values of time) takes play not only asymptotically (when $t \to +\infty$) but in a finite time.

We follows the formulation introduced in [8] but in a more general framework which allow us to prove the finite time Oswald ripening phenomena. So, our problem can be stated in the following terms: Find a function $u(x,t)$ satisfying the nonlinear and nonlocal problem

$$\begin{cases} \frac{\partial n}{\partial t} + \frac{\partial}{\partial x}(Gn) = 0 & x > 0, t > 0, \\ n(x,0) = n_0(x) & x > 0, \end{cases} \tag{1}$$

where

$$G(x,t) = \begin{cases} k_\gamma (c(t) - c^* e^{\Gamma/x})^\gamma & \text{if } x > x^*(t), \\ -k_\delta (c^* e^{\Gamma/x} - c(t))^\delta & \text{if } x < x^*(t), \end{cases} \tag{2}$$

$$x^*(t) = \frac{\Gamma}{\log(c(t)/c^*)} \tag{3}$$

$$c(t) = c_0 + \beta \int_0^{+\infty} x^3 n_0(x) dx - \beta \int_0^{+\infty} x^3 n(x,t) dx, \tag{4}$$

where the main changes, with respect to the formulation proposed in [8], concerns the assumptions

$$\gamma > 0 \text{ and } \delta > 0 \tag{5}$$

instead to impose

$$\gamma \geq 1\text{and } \delta \geq 1 \tag{6}$$

as done in [8]. We mention that it is well known (see, e.g. Aris [2]) that in many chemical reactions the kinetics leads to exponents $\gamma \in (0,1)$ and $\delta \in (0,1)$. As a matter of fact, the limit cases $\gamma = 0$ and $\delta = 0$ are also relevant in the applications (Aris) but they must be suitably formulated in terms of multivalued functions (Diaz [3]) and we shall not discus them in this communication. On the rest of parameters we assume that k_γ, k_δ, Γ, c_0, c^* and β are given positive numbers , with

$$c_0 > c^*.$$

Which made specially interesting the problem from the mathematical point of view is that the natural modelling of the problem leads to the assumption

$$n_0(x) = \sum_{m=1}^{N} \mu_m \delta(x - x_{m,0}) \tag{7}$$

where μ_m are given positive constants, $\delta(x)$ denotes the Dirac measure with unit mass at $x = 0$ and the values

$$0 < x_{1,0} < x_{2,0} < ... < x_{N,0} < \infty,$$

are N given positive numbers representing the sizes of the initial crystals. We mention that the case in which $n_0(x)$ is a continuous nonnegative function with compact support was considered in [7] but it looks less realist from the point of view of applications (see [11]).

2. On measure-valued solutions of the nonlocal and nonlinear conservation law

As mentioned, our approach follows closely the pioneering paper by A. Friedman, B. Ou and D.S. Ross [8] (see also the simplified exposition made in [9]). In this section we extend the results of [8] proving the existence and uniqueness of a solution of problem 1, 2, 3, 4, for the initial datum 7 under the general assumption 5.

Theorem 1. *Assume 5. Then, given $n_0(x)$ defined by (7), there exists a unique entropy solution $n(x,t)$ of problem 1, 2, 3, 4, $n \in C([0,+\infty) : M(0,+\infty))$. More precisely, we have the representation formula*

$$n(x,t) = \sum_{m=1}^{N} \mu_m \delta(x - x_m(t)) \tag{8}$$

for some functions $x_m(t)$ satisfying that $x_m(0) = x_{m,0}$.

As it is natural, we start by approximating the initial datum by

$$n_{0,j}(x) = \sum_{m=1}^{N} \mu_m \rho_j(x - x_{m,0})$$

where $\rho_j(x)$ is a smooth function such that

$$\rho_j \geq 0, \;\; \rho_j(x) = 0 \text{ if } \; |x| > \frac{1}{j} \text{ and } \int_{-\infty}^{+\infty} \rho_j(x)dx = 1.$$

The existence of a solution $(n_j(x,t), c_j(t))$ for this class of initial datum is an easy modification of the arguments of [7] since the *local existence* is built through the solution of the ordinary differential equation

$$\begin{cases} \frac{dx}{dt} = G_j(x,t) & t > 0, \\ x(0) = x_0. \end{cases}$$

It is clear that under assumption 5 function G is not globally Lipschitz continuous but it is locally Lipschitz continuous and monotone near the singular points. So, by well known results (see, e.g. [5]) we know the existence of a global solution $x(t)$. Then, as in [7],

$$\frac{d}{dt} n_j(x_j(t),t) = -\frac{\partial G_j(x_j(t),t)}{\partial x} n_j(x_j(t),t)$$

and thus

$$n_j(x_j(t),t) = n_{0,j}(x)e^{-\int_0^t \frac{\partial G_j(x_j(s),s)}{\partial x}ds}.$$

The rest of the arguments remain unchanged. Then we get that

$$c_j(t) = c_{1,j} - \beta \int_0^{+\infty} x^3 n_j(x,t)dx,$$

$$\frac{dc_j(t)}{dt} = -3\beta \int_0^{+\infty} x^3 n_j(x,t)\widehat{G}_j(x,t)dx,$$

where

$$\widehat{G}_j(x,t) = \begin{cases} k_\gamma(c_j(t) - c^* e^{\Gamma/x})^\gamma & \text{if } x > x_j^*(t), \\ -k_\delta(c^* e^{\Gamma/x} - c_j(t))^\delta & \text{if } x < x_j^*(t), \end{cases}$$

with

$$x_j^*(t) = \frac{\Gamma}{\log(c_j(t)/c^*)}.$$

If we denote by $x_j(t) \equiv x_j(t;x)$ the solution of

$$\begin{cases} \frac{dx_j}{dt} = \widehat{G}_j(x,t) & t > 0, \\ x_j(0) = x_0. \end{cases} \tag{9}$$

we obtain that $x_j(t)$ is well defined (even under 5) and that

$$\widehat{G}_j(x,t) \le C,\ \frac{dx_j}{dt} \le C \text{ and } \int_0^{+\infty} n_j(x,t)dx \le \int_0^{+\infty} n_{0,j}(x)dx \le C,$$

for a suitable positive constant C. Then we can extract a subsequence $c_j(t)$, $x_j(t)$ and $n_j(x,t)$ which are pointwise convergent to the searched solution satisfying the representation formula (8). Once more, the uniqueness of such a solution is consequence of the uniqueness of solution of the Cauchy problem obtaines passing to the limit in (9). The details will be given in [4].

Remark. It is possible to prove (see [4]) something which is not analyzed in [8] and it is the fact that the obtained solution $n(x,t)$ satisfies the hyperbolic equation in the weak entropy sense, $n \in C([0,+\infty) : \mathcal{M}(0,+\infty))$ as introduced by R. Di Perna [6] (see also, e.g., the exposition made in [10]) but here on the measure space $\mathcal{M}(0,+\infty)$ the bounded Radon measure space on the domain $(0,+\infty)$.

3. The extinction in finite time of all, except one, crystal sizes

Thanks to an extra assumption, we can prove that the Oswald ripening phenomenon (persistency of a single crystal size for very large values of time) takes play not only asymptotically (when $t \to +\infty$) but in a finite time.

Theorem 2. *Assume that*

$$\gamma \in (0,1) \text{ and } \delta \in (0,1). \tag{10}$$

Then there exts $\widehat{t} > 0$ *such that* $n(x,t) = \mu_N \delta(x - x_N(t))$ *for any* $t > \widehat{t}$. *Moreover,* $n(x,t) \to \mu_N \delta(x - \xi_2)$ *as* $t \to +\infty$, *where* ξ_2 *is one of the zeros of the trascendental equation*

$$\beta \mu_N \xi^3 + c^* e^{\Gamma/\xi} = c_0 + \beta \sum_{m=1}^{N} \mu_m x_m^3 \equiv c_1.$$

Idea of the proof. We use an energy method, similar to Lemma 2.2 of Chapter 1 of [1] to show that the solutions of the limit problem associated to (9) wanishes in a finite time (except for the last size x_N), thanks to the condition 10. The asymptotic behaviour follows similar arguments to the ones introduced in [8] (see also the simplified presentation made in [9])). The details will be given in [4].

Acknowledgments

The work of J.I. Diaz was supported by the research projects MTM2008-06208 of the Ministerio de Ciencia e Innovación, Spain and CCG07-UCM/ESP-2787 of the DGUIC of the CAM and the UCM.

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