

Singularities developed by the solutions of two Ostwald ripening models in reactive batch crystallizers

Jesús Ildefonso DÍAZ

(Universidad Complutense de Madrid)

The study of crystal precipitation attracted the attention of many specialists, specially after the pioneering works by the Nobel Prize F. W. Ostwald (1853-1932) on the so called *Ostwald ripening* in reactive batch crystallizers (persistency of a single crystal size for very large values of time). Several mathematical models can be introduced to this respect. The first one (a simplified model in which the number of crystals is assumed to be prescribed for any time) can be stated (after important simplifications) as the nonlinear ODEs system

$$\begin{cases} \frac{dx_1}{dt} + |f_1(x_1, x_2)|^{\delta-1} f_1(x_1, x_2) = 0 \\ \frac{dx_2}{dt} + |f_2(x_1, x_2)|^{\delta-1} f_2(x_1, x_2) = 0 \\ x_1(0) = x_{0,1} \\ x_2(0) = x_{0,2} \end{cases}$$

where $\delta > 0$ and $f_i(x_1, x_2) = \mu_1 x_1^3 + \mu_2 x_2^3 + e^{\Gamma/x_i} - \hat{c}$ for $i = 1, 2$ and for some positive constants μ_1, μ_2, Γ and \hat{c} . Here $x_i(t)$ represent the sizes of the crystals (which by simplicity we assume now only of two different types and in number, per unit volume, of μ_i). So, we assume $0 < x_{0,1} < x_{0,2}$. We shall show that (for any value $\delta > 0$) $x_1(t) \equiv 0$ after a finite time t_1^* and that $x_2(t) \rightarrow \xi_2$ when $t \rightarrow +\infty$ if $x_2(t_1^*) \in (\xi_1, +\infty)$ (with $x_2(t) = \xi_2$ after a finite time if $\delta \in (0, 1)$). Moreover, if $x_2(t_1^*) \in (0, \xi_1)$ then $x_2(t) \equiv 0$ after a finite time t_2^{**} (again, for any value $\delta > 0$). Here ξ_1 and ξ_2 are the two roots of the trascendent equation $f_2(0, x_{2,\infty}) = 0$. We also show that a singularity arises at time t_1^* : more precisely $\frac{dx_1}{dt}(t) \rightarrow -\infty$ as $t \rightarrow t_1^*$.

A more realistic model arises when the number of crystals of each size μ_j (now in number $N \geq 2$) is not prescribed but given by $n(x, t)$ the "solution" of the nonlinear and nonlocal hyperbolic problem

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

where

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

$$(3) \quad x^*(t) = \frac{\Gamma}{\log(c(t)/c^*)} \text{ and } c(t) = c_0 + \beta \int_0^{+\infty} x^3 n_0(x) dx - \beta \int_0^{+\infty} x^3 n(x, t) dx.$$

The natural modelling of the problem leads to the assumption $n_0(x) = \sum_{m=1}^N \mu_m \delta(x - x_{m,0})$, where μ_m are some given positive constants, $\delta(x)$ denotes the Dirac measure with unit mass at $x = 0$ and the values $0 < x_{1,0} < x_{2,0} < \dots < x_{N,0} < \infty$ are N given positive numbers representing the sizes of the initial crystals. Besides its relevance in the applications, which made specially interesting such a problem is that the corresponding solution is not a L^1 -valued function but a measure-valued function $n(\cdot, t)$. We shall prove that, under suitable additional conditions on G (for instance $\gamma, \delta \in (0, 1)$) the Ostwald ripening phenomenon takes place not only asymptotically (when $t \rightarrow +\infty$) but in a finite time.