Absence of Gelation for Models of Coagulation-Fragmentation with Degenerate Diffusion

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Summary. — We show in this work that gelation does not occur for a class of discrete coagulation-fragmentation models with size-dependent diffusion. With respect to a previous work by the authors, we do not assume here that the diffusion rates of clusters are bounded below. The proof uses a duality argument first devised by M. Pierre and D. Schmitt for reaction-diffusion systems with a finite number of equations.

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1. – Introduction

We consider in this paper a discrete coagulation-fragmentation-diffusion model for the evolution of clusters, such as described for example in [12]. Denoting by $c_i := c_i(t, x) \geq 0$ the density of clusters with integer size $i \geq 1$ at position $x \in \Omega$ and time $t \geq 0$, the corresponding system writes (with homogeneous Neumann boundary conditions):

$$\partial_t c_i - d_i \Delta_x c_i = Q_i + F_i \qquad \text{for } x \in \Omega, t \geq 0, i \in \mathbb{N}^*, \tag{1a}$$

$$\nabla_x c_i \cdot n = 0 \qquad \text{for } x \in \partial\Omega, t \geq 0, i \in \mathbb{N}^*, \tag{1b}$$

$$c_i(0, x) = c_i^0(x) \qquad \text{for } x \in \Omega, i \in \mathbb{N}^*, \tag{1c}$$

where $n = n(x)$ represents a unit normal vector at a point $x \in \partial\Omega$, d_i is the diffusion constant for clusters of size i, and the terms Q_i, F_i due to coagulation and fragmentation, respectively, are given by

$$
(2)\qquad
\begin{aligned}
Q_i \equiv Q_i[c] := Q_i^+ - Q_i^- &:= \frac{1}{2}\sum_{j=1}^{i-1} a_{i-j,j}\, c_{i-j}\, c_j - \sum_{j=1}^{\infty} a_{i,j}\, c_i\, c_j,\\
F_i \equiv F_i[c] := F_i^+ - F_i^- &:= \sum_{j=1}^{\infty} B_{i+j}\, \beta_{i+j,i}\, c_{i+j} - B_i\, c_i.
\end{aligned}
$$

These terms are the result of assuming that the rates of aggregation and fragmentation reactions are proportional to the concentrations of the reacting clusters; see the reviews [13, 14] for a more detailed motivation of the model. The rates B_i, $\beta_{i,j}$ and $a_{i,j}$ appearing in (2) are assumed to satisfy the following natural properties (the last one expresses the conservation of mass):

$$
\text{(3a)}\qquad a_{i,j} = a_{j,i} \geq 0, \qquad \beta_{i,j} \geq 0 \quad (i,j \in \mathbb{N}^*),
$$
$$
\text{(3b)}\qquad B_1 = 0 \qquad B_i \geq 0 \quad (i \in \mathbb{N}^*),
$$
$$
\text{(3c)}\qquad i = \sum_{j=1}^{i-1} j\, \beta_{i,j}, \qquad i \geq 2 \quad (i \in \mathbb{N}).
$$

Existence of weak solutions to system (1)–(2) is proven in [12] under the following (sublinear growth) estimate on the parameters:

$$
(4)\qquad \lim_{j\to+\infty} \frac{a_{i,j}}{j} = \lim_{j\to+\infty} \frac{B_{i+j}\, \beta_{i+j,i}}{i+j} = 0, \qquad \text{(for fixed } i \geq 1\text{)},
$$

and provided that all $d_i > 0$.

In a previous paper (cf. [2]), we gave a new estimate for system (1)–(2) which basically stated that if $\sum_i i\, c_i(0,\cdot) \in L^2(\Omega)$, then for all $T \in \mathbb{R}_+$, $\sum_i i\, c_i \in L^2([0,T]\times\Omega)$. As a consequence, it was possible to show (under a slightly more stringent condition than (4)) that the mass $\int_\Omega \sum_i i\, c_i(t,x)\, dx$ is rigorously conserved for solutions of system (1)–(2): that is, no phenomenon of gelation occurs. However, these results were shown to hold only under the restrictive assumption on the diffusion coefficients d_i that $0 < \inf_i d_i \leq \sup_i d_i < +\infty$. Such an assumption is unfortunately not realistic, since large clusters are expected to diffuse more slowly than smaller ones, so that in reality one expects that $\lim_{i\to\infty} d_i = 0$. In the case of continuous, diffusive coagulation-fragmentation systems, for instance, typical example of diffusion coefficients include $d(y) = d_0 y^{-\gamma}$ for a constant d_0 and an exponent $\gamma \in (0,1]$, see [16]. For example, $d_i \sim i^{-1}$ if clusters are modelled by balls diffusing within a liquid at rest in dimension 3 (see [8, 11]).

Note that in system (1)–(2), mass is always conserved at the formal level. This can be seen by taking $\varphi_i = i$ in the following weak formulation of the kernel (which holds at the formal level for all sequence $(\varphi_i)_{i\in\mathbb{N}^*}$ of numbers):

$$\sum_{i=1}^{\infty} \varphi_i Q_i = \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{i,j} c_i c_j (\varphi_{i+j} - \varphi_i - \varphi_j), \tag{5}$$

$$\sum_{i=1}^{\infty} \varphi_i F_i = - \sum_{i=2}^{\infty} B_i c_i \left(\varphi_i - \sum_{j=1}^{i-1} \beta_{i,j} \varphi_j \right). \tag{6}$$

2. – Main results

This paper is devoted to the generalization of the results obtained in [2] to the case of degenerated diffusion coefficients d_i scaling like $i^{-\gamma}$ with $\gamma > 0$.

Therefore, we replace the first estimate in [2] (L^2 bound on $\sum i\, c_i$) by the following result:

Proposition 2.1. *Assume that* (3), (4) *hold, and that* $d_i > 0$ *for all* $i \in \mathbb{N}^*$. *Assume moreover that* $\sum_{i=1}^{\infty} i\, c_i(0,\cdot) \in L^2(\Omega)$, *and that* $\sup_{i\in\mathbb{N}^*} d_i < +\infty$. *Then, for all* $T > 0$, *the weak solutions to system* (1)–(2) *(obtained in [12]) satisfy the following bound:*

$$\int_0^T \int_\Omega \left[\sum_{i=1}^{\infty} i\, d_i\, c_i(t,x) \right] \left[\sum_{i=1}^{\infty} i\, c_i(t,x) \right] dx\, dt \le 4\, T \Big(\sup_{i\in\mathbb{N}^*} d_i \Big) \Big\| \sum_{i=1}^{\infty} i\, c_i(0,\cdot) \Big\|^2_{L^2(\Omega)}. \tag{7}$$

Note that as in [2], condition (4) and the fact that the diffusion rates are strictly positive are assumptions which are used in Proposition **2**.1 only in order to ensure the existence of solutions. The bound (7) still holds for solutions of an approximated (truncated) system, uniformly w.r.t. the approximation, when (4) is not satisfied, or when some of the d_i are equal to 0.

The proof of this estimate is based on a duality method due to M. Pierre and D. Schmitt [15], and is a variant of the proof of a similar estimate in the context of systems of reaction–diffusion with a finite number of equations (cf. [7]), or in the context of the Aizenman-Bak model of continuous coagulation and fragmentation [4, 6]. In those systems, the degeneracy occurs when one of the diffusions is equal to 0 (a general study for equations coming out of reversible chemistry with less than four species and possibly vanishing diffusion can be found in [5]).

When the sequence of diffusion coefficients d_i is not bounded below, estimate (7) is much weaker than what was obtained in [2] (that is, $\sum_i i\, c_i \in L^2([0,T]\times\Omega)$ for all $T > 0$). It is nevertheless enough to provide a proof of absence of gelation for coefficients $a_{i,j}$ which do not grow too rapidly (the maximum possible growth being related to the way in which d_i tends to 0 at infinity). More precisely, we can show the

Theorem 2.2. *Assume that* (3), (4) *hold, and that* $\sum_{i=1}^{\infty} i\, c_i(0,\cdot) \in L^2(\Omega)$. *Assume also that the following extra relationship between the coefficients of coagulation and diffusion holds:*

$$d_i \ge Cst\, i^{-\gamma}, \qquad a_{i,j} \le Cst \Big(i^\alpha\, j^\beta + i^\beta\, j^\alpha \Big), \tag{8}$$

with $\alpha + \beta + \gamma \le 1$, $\alpha, \beta \in [0,1)$, $\gamma \in [0,1]$.

Then, the mass is rigorously conserved for weak solutions of system (1)–(2) *given by the existence theorem in [12], that is: for all* $t \in \mathbb{R}_+$,

$$\int_\Omega \left[\sum_{i=1}^{\infty} i\, c_i(t,x) \right] dx = \int_\Omega \left[\sum_{i=1}^{\infty} i\, c_i(0,x) \right] dx,$$

so that no gelation occurs.

The conditions on α, β ensure that gelation (loss of mass in finite time) does not take place [9, 10], while the assumption that diffusion coefficients decay with the size is reasonable from a physical point of view: larger clusters are heavier, and hence feel less the influence of the surrounding particles. This result must be compared with previous results about mass conservation without presence of diffusion, which extend up to the critical linear case $a_{i,j} \leq \mathrm{Cst}\,(i+j)$ (see for instance [1, 3]) and, on the other hand, with results which ensure the appearance of gelation [9, 10]. In presence of diffusion, a recent result of Hammond and Rezakhanlou [11] proves mass conservation for the system (1) without fragmentation as a consequence of L^∞ bounds on the solution: they show that if $a_{i,j} \leq C_1(i^\lambda + j^\lambda)$ and $d_i \geq C_2 i^{-\gamma}$ for some $\lambda, \gamma, C_1, C_2 > 0$ and all $i, j \geq 1$, with $\lambda + \gamma < 1$, then under some conditions on L^∞ norms and moments of the initial condition, mass is conserved for the system without fragmentation; see [11, Theorems 1.3 and 1.4] and [11, Corollary 1.1] for more details.

The rest of the paper is devoted to the proofs of Proposition **2**.1 and Theorem **2**.2.

3. – Proofs

We begin with the

Proof of proposition **2***.1.* Since this proof is close to the proof of Theorem 3.1 in [7], we only sketch it. Denoting $\rho(t,x) = \sum_{i=1}^{\infty} i\, c_i(t,x)$ and $A(t,x) = \rho(t,x)^{-1} \sum_{i=1}^{\infty} i\, d_i\, c_i(t,x)$, we first observe that $\|A\|_{L^\infty} \leq \sup_{i \in \mathbb{N}^*} d_i$, and that (thanks to (3c) and (5), (6) with $\varphi_i = i$), the following local conservation of mass holds:

$$\partial_t \rho - \Delta_x (A\, \rho) = 0. \tag{9}$$

We now consider an arbitrary smooth function $H := H(t,x) \geq 0$. Multiplying inequality (9) by the function w defined by the following dual problem:

$$-\,(\partial_t w + A\, \Delta_x w) = H\, \sqrt{A}, \tag{10a}$$

$$\nabla_x w \cdot n(x)|_{\partial\Omega} = 0, \qquad w(T, \cdot) = 0 \tag{10b}$$

and integrating by parts on $[0,T] \times \Omega$, we end up with the identity

$$\int_0^T \int_\Omega H(t,x)\, \sqrt{A(t,x)}\, \rho(t,x)\, dx dt = \int_\Omega w(0,x)\, \rho(0,x)\, dx. \tag{11}$$

Multiplying now eq. (10a) by $-\Delta_x w$, integrating by parts on $[0,T]\times\Omega$ and using the Cauchy-Schwarz inequality, we end up with the estimate

$$\int_0^T\int_\Omega A\,(\Delta_x w)^2\,dxdt \le \int_0^T\int_\Omega H^2\,dxdt.$$

Recalling eq. (10a), we obtain the bound

$$\int_0^T\int_\Omega \frac{|\partial_t w|^2}{A}\,dxdt \le 4\int_0^T\int_\Omega H^2\,dxdt.$$

Using once again Cauchy-Schwarz inequality,

$$|w(0,x)|^2 \le \left(\int_0^T \sqrt{A(t,x)}\,\frac{|\partial_t w(t,x)|}{\sqrt{A(t,x)}}\,dt\right)^2 \le \int_0^T A(t,x)\,dt\int_0^T \frac{|\partial_t w|^2}{A}\,dt,$$

which leads to the following estimate of the L^2 norm of $w(0,\cdot)$:

$$\int_\Omega |w(0,x)|^2\,dx \le 4\,T\,\|A\|_{L^\infty(\Omega)}\int_0^T\int_\Omega H(t,x)^2\,dxdt. \tag{12}$$

Recalling now (11) and using Cauchy-Schwarz inequality one last time, we see that

$$\begin{aligned}\int_0^T\int_\Omega H\,\sqrt{A}\,\rho\,dxdt &\le \|\rho(0,\cdot)\|_{L^2(\Omega)}\,\|w(0,\cdot)\|_{L^2(\Omega)}\\ &\le 2\,\sqrt{T\,\|A\|_{L^\infty(\Omega)}}\,\|H\|_{L^2([0,T]\times\Omega)}\,\|\rho(0,\cdot)\|_{L^2(\Omega)}.\end{aligned}$$

Since this estimate holds true for all (nonnegative smooth) functions H, we obtain by duality that

$$\|\sqrt{A}\,\rho\|_{L^2(\Omega)} \le 2\,\sqrt{T\,\|A\|_{L^\infty(\Omega)}}\,\|\rho(0,\cdot)\|_{L^2(\Omega)}.$$

This is exactly estimate (7) of Proposition **2**.1. □

We now turn to the

Proof of theorem **2**.*2.* As $\sum_i i\,c_i(0,\cdot)\in L^1(\Omega)$, we may choose a nondecreasing sequence of positive numbers $\{\lambda_i\}_{i\ge 1}$ which diverges as $i\to+\infty$, and such that

$$\int_\Omega \sum_{i=1}^{\infty} i\,\lambda_i c_i^0 < +\infty. \tag{13}$$

(This is a version of de la Vallée-Poussin's Lemma; see [2, proof of Theorem 3.1] for details). We can also find a nondecreasing sequence of positive numbers $\{\psi_i\}$ such that

$$\lim_{i \to +\infty} \psi_i = +\infty, \tag{14}$$

$$\psi_i \le \lambda_i, \qquad \psi_{i+1} - \psi_i \le \frac{1}{i+1}, \qquad (i \in \mathbb{N}^*). \tag{15}$$

Roughly, this says that ψ_i grows more slowly than $\log i$ and than λ_i, and still diverges; we refer again to [2, proof of Theorem 3.1] and [2, Lemma 4.1] for the construction of such a sequence. Note that (15) implies that

$$\psi_{i+j} - \psi_i \le \log(i+j) - \log i, \qquad \text{for } i, j \in \mathbb{N}^*. \tag{16}$$

Using the weak formulation (5)–(6) of the coagulation and fragmentation operators with $\varphi_i = i\,\psi_i$, we see that for a weak solution $c_i := c_i(t,x) \ge 0$ of system (1)–(2), the following identity holds:

$$\begin{aligned}
\frac{d}{dt}\int_\Omega \sum_{i=1}^\infty i\,\psi_i\,c_i(t,x)\,dx &= \frac{1}{2}\int_\Omega \sum_{i=1}^\infty\sum_{j=1}^\infty \Big((i+j)\psi_{i+j} - i\,\psi_i - j\,\psi_j\Big)\,a_{i,j}\,c_i(t,x)\,c_j(t,x)\,dx \\
&\quad - \int_\Omega \sum_{i=2}^\infty \Big(i\,\psi_i - \sum_{j=1}^{i-1}\beta_{i,j}\,j\,\psi_j\Big) B_i\,c_i(t,x)\,dx \\
&\le \int_\Omega \sum_{i=1}^\infty\sum_{j=1}^\infty i\,\Big(\psi_{i+j} - \psi_i\Big)\,a_{i,j}\,c_i(t,x)\,c_j(t,x)\,dx \\
&\le \mathrm{Cst}\int_\Omega \sum_{i=1}^\infty\sum_{j=1}^\infty i\,\Big(\log(i+j) - \log i\Big)\,\Big(i^\alpha\,j^\beta + i^\beta\,j^\alpha\Big) c_i(t,x)\,c_j(t,x)\,dx,
\end{aligned}$$

where we have used the symmetry $i \to j, j \to i$ in the coagulation part, omitted the fragmentation part, which is non-negative for the superlinear test function $i \mapsto i\,\psi_i$, and used (16).

Then, observing that for any $\delta \in]0,1]$, there exists a constant $C_\delta > 0$ such that $\log(1 + j/i) \le C_\delta\,(j/i)^\delta$, we see that (for δ_1, δ_2 to be chosen in $]0,1]$),

$$\begin{aligned}
\sup_{t\in[0,T]}\Big(\int_\Omega \sum_{i=1}^\infty i\,\psi_i\,c_i(t,x)\,dx\Big) &\le \int_\Omega \sum_{i=1}^\infty i\,\psi_i\,c_i(0,x)\,dx \\
&\quad + \mathrm{Cst}\int_0^T\int_\Omega \sum_{i=1}^\infty\sum_{j=1}^\infty \Big(i^{\alpha+1-\delta_1}\,j^{\beta+\delta_1} + i^{\beta+1-\delta_2}\,j^{\alpha+\delta_2}\Big)\,c_i(t,x)\,c_j(t,x)\,dxdt.
\end{aligned}$$

The r.h.s in this estimate can be bounded by

$$\int_0^T\int_\Omega \Big[\sum_{i=1}^\infty i\,d_i\,c_i(t,x)\Big]\Big[\sum_{j=1}^\infty j\,c_j(t,x)\Big]\,dxdt$$

provided that

$$\alpha + 1 - \delta_1 \le 1 - \gamma, \qquad \beta + \delta_1 \le 1,$$

and

$$\beta + 1 - \delta_2 \le 1 - \gamma, \qquad \alpha + \delta_2 \le 1.$$

We see that it is possible to find δ_1, δ_2 in $]0,1]$ satisfying those inequalities under our assumptions on α, β, γ. Using then Proposition **2**.1, we see that for all $T > 0$, the quantity

$$\int_\Omega \sum_{i=1}^{\infty} i\, \psi_i\, c_i(t,x)\, dx$$

is bounded on $[0,T]$, and this ensures that it is possible to pass to the limit in the equation of conservation of mass for solutions of a truncated system. $\square$

We now provide (in the following remark) for the interested reader some ideas on how to get Theorem **2**.2 without assuming that $\sum_i i\, \log i\, c_i(0,\cdot) \in L^1(\Omega)$.

Remark **3**.1 (Absence of gelation via tightness). It is in fact possible to follow the lines of the proof of [2, Remark 4.3]: one introduces the superlinear test sequence $i\phi_k(i)$ with $\phi_k(i) = \frac{\log i}{\log k} 1_{i<k} + 1_{i\ge k}$ for all $k \in \mathbb{N}^*$, and uses the weak form of the kernels (5), (6). Then, using that the weak formulation of the fragmentation part is nonnegative for superlinear test sequences, and using the symmetry of the $a_{i,j}$ to only sum over the indices $i \ge j \in \mathbb{N}^*$ leads (as in [2]) to the expression

$$\frac{d}{dt} \int_\Omega \sum_{i=1}^{\infty} c_i\, i\phi_k(i) \le \int_\Omega \sum_{i\ge j}^{\infty} \sum_{j=1}^{\infty} a_{i,j} [ic_i][c_j] \left(\frac{\log(1+\frac{j}{i})}{\log(k)}\, \mathbb{I}_{i<k} \right.$$
$$\left. + \frac{j}{i} \left(\frac{\log(1+\frac{i}{j})}{\log(k)}\, \mathbb{I}_{i+j<k} + \frac{\log(\frac{k}{j})}{\log(k)}\, \mathbb{I}_{j<k\le i+j} \right) \right).$$

The first term is now estimated like $\log(1+j/i) \le \mathrm{Cst}\, (j/i)^{1-\beta}$ (or the same with α replacing β). In order to estimate the second and the third term, we distinguish the cases $i/j \le \log k$ and $i/j > \log k$. In the first case of the second and third terms (that is, when $i/j \le \log k$), one must estimate j by $i^\beta\, j^{1-\beta}$ (or the same with α replacing β). Finally, in the second part of the second and third terms (that is, when $i/j > \log k$), one must estimate j by $\frac{i^\beta\, j^{1-\beta}}{(\log k)^\beta}$ (or the same with α replacing β). The case when $\beta = 0$ (or $\alpha = 0$) and $\gamma > 0$ deserves a special treatment: in the second part of the second and last terms, on can use the following estimate: $j\, i^{1-\gamma} \le (\log k)^{-\gamma}\, j^{1-\gamma}\, i$.

Once those estimates have been used, it is possible to conclude that the mass is conserved as in [2], thanks to an argument using tightness.

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