COAGULATION-FRAGMENTATION MODELS WITH DIFFUSION

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Consider systems of a very large number of particles, being suspended in a fluid, for example, which can diffuse and coagulate to form clusters that, in turn, can merge to form larger clusters or can break apart into smaller ones. Models of cluster growth arise in a variety of situations, for example in aerosol science, atmospheric physics, colloidal chemistry, or polymer science, etc. The theory originates in the work of M.V. Smoluchowski [9], [10] and has found various generalizations, extensions, and applications in the physical literature (e.g., [5], [6]).

The Model. The aim of the theory is the description of the particle size distribution function u as a function of time and space as the system undergoes changes due to various physical influences.

The equations under consideration are of the form

$$\partial_t u - \nabla \cdot (\boldsymbol{a} \nabla u + \vec{a} u) + a_0 u = [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}} \ , \tag{1}$$

where the coagulation term $[\partial_t u]_{\mathrm{coag}}$ is given by

$$[\partial_t u]_{\mathrm{coag}}(y) = \frac{1}{2} \int_0^y \gamma(y-y', y') u(y-y') u(y')\, dy' - u(y) \int_0^\infty \gamma(y, y') u(y')\, dy' \tag{2}$$

and the fragmentation term $[\partial_t u]_{\mathrm{frag}}$ has the form

$$[\partial_t u]_{\mathrm{frag}}(y) = \int_y^\infty \varphi(y', y) u(y')\, dy' - u(y) \int_0^y \varphi(y, y') \frac{y'}{y}\, dy' \tag{3}$$

for $y \in Y$, with y being the size of a cluster. Here it is assumed that either $Y = \mathbb{R}^+$ and dy is Lebesgue's measure on Y (the case of continuous coagulation-fragmentation equations) or $Y = \dot{\mathbb{N}} := \{1, 2, 3, \ldots\}$ and dy is the counting measure (the discrete case). In general, the coagulation and fragmentation kernels γ and φ, respectively, depend smoothly on $t \in \mathbb{R}^+$ and $x \in \mathbb{R}^n$, where $n = 1, 2, 3$. The diffusion matrix $\boldsymbol{a}$, the drift vector $\vec{a}$, and the absorption rate a_0 also depend smoothly on (t, x) and on $y \in Y$. In addition, $\boldsymbol{a}$ is supposed to be symmetric and uniformly positive definite.

The coagulation kernel has to satisfy

$$0 \leq \gamma(y, y') = \gamma(y', y) , \qquad y, y' \in Y , \tag{4}$$

(in this note we suppress the (t, x)-dependence throughout). Thus the first integral in (2) expresses the fact that a cluster of size y can come into existence only if two clusters of sizes $y - y'$ and y' collide. (Thus we neglect triple and higher collisions assuming them to be rare.) The factor $1/2$ guarantees that each combination is counted only once. The last term in (2) says that a cluster of size y disappears if it coagulates with a cluster of any size.

The fragmentation kernel is supposed to satisfy

$$0 \leq \varphi(y, y') , \qquad 0 < y' \leq y < \infty , \quad y, y' \in Y . \tag{5}$$

Thus the first integral in (3) accounts for the production of clusters of size y by the breakup of clusters of larger sizes. The second term takes care of the disappearance of y-clusters by their fragmentation into smaller ones. In particular, multiple fragmentation is allowed.

In order to understand the meaning of (1) we assume for a moment that $\vec{a}$ and a_0 are identically zero and $\boldsymbol{a}$ is independent of (t, x). Then, assuming also that no fragmentation occurs, (1) takes the form

$$\begin{aligned} \partial_t u(y) - \boldsymbol{a}(y) \triangle u(y) = \frac{1}{2} \int_0^y & \gamma(y - y', y') u(y - y') u(y') \, dy' \\ - u(y) \int_0^\infty & \gamma(y, y') u(y') \, dy' \end{aligned} \tag{6}$$

in $\mathbb{R}^n$ for $y \in \mathbb{R}^+$, in the continuous case. In the discrete case (1) reduces (with obvious notation) to the infinite system of coupled diffusion equations

$$\partial_t u_j - \boldsymbol{a}_j \triangle u_j = \frac{1}{2} \sum_{k=1}^{j} \gamma_{j-k,k} u_{j-k} u_k - u_j \sum_{k=1}^{\infty} \gamma_{j,k} u_k , \qquad j = 1, 2, \ldots ,$$

on $\mathbb{R}^n$. This shows that, loosely speaking, (1) is — in the continuous case — an uncountable system of coupled reaction-diffusion equations on $\mathbb{R}^n$.

The Theorem. Besides of (4), (5), and regularity we also assume that the coagulation and fragmentation kernels are bounded, that is, there exists a constant $\beta > 0$ such that

$$\gamma(y, y') \leq \beta , \quad \varphi(y, y') \leq \beta , \qquad y, y' \in Y ,$$

and the volume rate of change in the fragmentation process is also bounded, that is,

$$\frac{1}{y} \int_0^\infty \varphi(y, y') y' \, dy' \leq \beta , \qquad y \in Y .$$

Since u represents a density function we ought to have $u \geq 0$. The following theorem shows that this is true if the initial distribution u^0 is nonnegative.

Theorem. *Suppose that* $u^0 \geq 0$ *satisfies*

$$\int_{\mathbb{R}^n} \int_Y \left|\partial_x^\alpha u^0(x,y)\right| (1+y)\, dy\, dx < \infty \ , \qquad |\alpha| \leq 2 \ .$$

Then there exists a maximal $T > 0$ *such that the coagulation-fragmentation system* (1)–(3) *possesses a unique solution* u *on* $[0,T)$ *satisfying* $u \geq 0$ *and*

$$\int_{\mathbb{R}^n} \int_Y u(x,t,y)(1+y)\, dy\, dx < \infty \ . \tag{7}$$

It is a smooth function of x *for* $t > 0$ *and depends continuously on all data.*

If there is no absorption (*i.e.,* $a_0 = 0$) *then the total volume is conserved, that is,*

$$\int_{\mathbb{R}^n} \int_Y u(x,t,y) y\, dy\, dx = \int_{\mathbb{R}^n} \int_Y u^0(x,y) y\, dy\, dx$$

for $0 < t < T$*.*

Lastly, $T = \infty$*, that is,* u *is a global solution, if either* $n = 1$ *or* $\boldsymbol{a}$ *is independent of* y*, or coagulation does not take place.*

A few remarks are in order:

- Condition (7) means that the total number of particles, that is,

$$\int_{\mathbb{R}^n} \int_Y u(x,t,y)\, dy\, dx \ ,$$

as well as the total volume

$$\int_{\mathbb{R}^n} \int_Y u(t,x,y) y\, dy\, dx$$

stay finite during the time evolution.

- Our theorem comprises continuous and discrete coagulation models simultaneously.
- We consider the case where coagulation, fragmentation, and diffusion occur.

Most of the mathematical research on coagulation-fragmentation problems is concerned with the *kinetic* model

$$\dot{u} = [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}} \ ,$$

where no diffusion is admitted (e.g., [3] for the discrete case and [8] for the continuous one; see [1] for further references). The situation where diffusion is taken into consideration has been studied in the discrete case only (e.g., [4], [7], [11]; again see [1] for additional references and more precise information). Our theorem is the first existence result at all in the case of continuous coagulation-fragmentation models with diffusion. It is also the first general result, even in the discrete case, guaranteeing the existence of a unique solution preserving the total volume.

Remarks on the Proof. The basic idea consists in interpreting (1)–(3) as a vector-valued reaction-diffusion system, that is, as a reaction-diffusion equation for a density function u which takes values in an infinite-dimensional Banach space, namely in

$$\mathbb{F} := L_1\big(Y, (1+y)\,dy\big) \ .$$

This space occurs naturally. Indeed, if $u \geq 0$ then

$$\int_{t_0}^{t_1} \int_X \int_Y u(t,x,y)(1+y)\,dy\,dx\,dt = \int_{t_0}^{t_1} \int_X \|u(t,x,\cdot)\|_{\mathbb{F}}\,dx\,dt$$

is the sum of the number of particles and of the volume being contained during the times interval (t_0, t_1) in the domain X of $\mathbb{R}^n$ (where by the size of a cluster we mean its volume). Since this quantity should be finite for $X = \mathbb{R}^n$ during time evolution one is led to consider problem (1)–(3) in the Banach space $L_1(\mathbb{R}^n, \mathbb{F})$. Thus, denoting by $\mathcal{A}$ the linear differential operator

$$u \mapsto -\nabla \cdot (\boldsymbol{a}\nabla u + \vec{a}u) + a_0 u$$

on $\mathbb{R}^n$, operating on $L_1(\mathbb{R}^n, \mathbb{F})$-valued functions (i.e., $\mathbb{F}$-valued regular distributions), and putting

$$F(u) := [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}} \ ,$$

we arrive at the initial value problem

$$\dot{u} + \mathcal{A}u = F(u) \ , \quad t > 0 \ , \qquad u(0) = u^0 \tag{8}$$

in $L_1(\mathbb{R}^n, \mathbb{F})$, that is, $u(t) \in L_1(\mathbb{R}^n, \mathbb{F})$ for $t \geq 0$.

Formally, (8) is a semilinear parabolic evolution equation. The nonstandard feature, however, is the fact that $\mathcal{A}$ operates on vector-valued functions. If we knew that $-\mathcal{A}$ generated an analytic semigroup on $L_1(\mathbb{R}^n, \mathbb{F})$ then we could apply the abstract theory of semilinear parabolic evolution equations to (8) to prove local well-posedness, at least.

The standard way to establish the resolvent estimates guaranteeing that $-\mathcal{A}$ is the generator of an analytic semigroup on L_p (in the classical finite-dimensional case) is to look at constant coefficient operators first and to use Fourier analysis and Fourier multiplier theorems of Mikhlin type.

In our case, even in the simplest situation where $\mathcal{A}u = -a\triangle u$ for a smooth positive bounded function $a : Y \to \mathbb{R}$ (independent of $x \in \mathbb{R}^n$, which means 'constant coefficient') the symbol (i.e., $a\,|\xi|^2$ for $-a\triangle$) is operator-valued ($a\,|\xi|^2$ being an operator of point-wise multiplication). But it is known that an analogue to Mikhlin's theorem for operator-valued symbols is not valid, in general, on $L_p(\mathbb{R}^n, E)$ for any $p \in [1, \infty)$, if E is an infinite-dimensional Banach space not isomorphic to a Hilbert space.

However, in [2] it is proven that a Mikhlin-type Fourier multiplier theorem is valid for operator-valued symbols, provided $L_p(\mathbb{R}^n, E)$ is replaced by any Besov space $B^s_{p,q}(\mathbb{R}^n, E)$. In particular, we can take the vector-valued Slobodeckii spaces

$$W^s_1(\mathbb{R}^n, \mathbb{F}) = B^s_{1,1}(\mathbb{R}^n, \mathbb{F}) , \qquad s \in \mathbb{R}\backslash\mathbb{Z} .$$

More precisely, it follows from the results in [2] and standard arguments that $-\mathcal{A}$ generates a strongly continuous analytic semigroup on $W^s_1(\mathbb{R}^n, \mathbb{F})$ for $s \in \mathbb{R}\backslash\mathbb{Z}$ and that the domain of this generator equals $W^{s+2}_1(\mathbb{R}^n, \mathbb{F})$.

As for the right-hand side, we show that F is a smooth map from $W^\sigma_1(\mathbb{R}^n, \mathbb{F})$ into $W^\tau_1(\mathbb{R}^n, \mathbb{F})$ where $\sigma > \tau$ are suitably chosen so that $-1 < s < \tau < \sigma < s + 2$.

These facts and standard results from the theory of parabolic evolution equations guarantee the existence of a unique maximal solution

$$u \in C\big([0, T), W^{s+2}_1(\mathbb{R}^n, \mathbb{F})\big) \cap C^1\big([0, T), W^s_1(\mathbb{R}^n, \mathbb{F})\big) ,$$

provided $u^0 \in W^{s+2}_1(\mathbb{R}^n, \mathbb{F})$ and $s \in (-1, \infty)\backslash\mathbb{N}$. Furthermore, $u(t)$ is smooth if $t > 0$. Thanks to this regularizing effect and the fact that the semigroup generated by $-\mathcal{A}$ is positive, it is possible to show that $u(t) \geq 0$ if $u^0 \geq 0$.

Finally, solving (1) in $W^s_1(\mathbb{R}^n, \mathbb{F})$ with $s < 0$ and using the embedding

$$W^{s+2}_1(\mathbb{R}^n, \mathbb{F}) \hookrightarrow L_1(\mathbb{R}^n, \mathbb{F}) \hookrightarrow W^s_1(\mathbb{R}^n, \mathbb{F}) , \qquad -1 < s < 0 ,$$

it follows that $u(t) \in L_1(\mathbb{R}^n, \mathbb{F})$ for $0 \leq t < T$. Thus (7) is true.

Since our solution is smooth and nonnegative, it is not difficult, thanks to the special structure of the right-hand side, to verify that the total volume is conserved. This is an a priori estimate which is strong enough to imply a uniform bound if $n = 1$, by virtue of Sobolev-type embedding theorems. Then the growth properties of the nonlinearity and a Gronwall-type argument give global existence if $n = 1$.

If no coagulation occurs then (1) is linear and global existence is immediate. Finally, if $\boldsymbol{a}$ is independent of $y \in Y$ then integration of (8) with respect to dy reduces our problem to a standard parabolic differential inequality for $\overline{u} := \int_Y u\, dy$ on $\mathbb{R}^n$. In this case the parabolic maximum principle implies the bounds which are needed to show that $T = \infty$. For details we refer to [1].

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