Coagulation-Fragmentation Models

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International Symposium on Particle Hierarchy

Tohoku University

March 2004

We consider **mathematical models** for

a **very large number of particles** (suspended in a fluid)

which can

- **coagulate** to form clusters
- the clusters can **merge** to form larger clusters
- the clusters can **fragment** (break apart) into smaller clusters
- the particles can **diffuse** in the carrier fluid
- the carrier fluid can be in motion

AIM

description of the temporal development of the particle size (volume or mass) distribution function coagulation-fragmentation models occur in

- aerosol physics
- atmospheric physics
- astrophysics
- polymer chemistry
- colloidal chemistry
- biology

$\vdots$

first models: M. v. Smoluchowski (1916/17), H. Müller (1928)

more recent reference: S.K. Friedlander: *Smoke, Dust and Haze*, Wiley (1977)

Smoluchowski-Müller coagulation equations

$\{y\}$ particle of size $\quad y \in \{1, 2, \dots\} \quad$ or $\quad y \in (0, \infty)$

binary coagulation: $\quad \{y\} + \{y'\} \xrightarrow[K(y,y')]{} \{y + y'\}$

$u(t, y)$ particle size distribution function

$$[\partial_t u]_{\mathrm{coag}} = Q_1(u) - Q_2(u)$$

$$Q_1(u)(y) = \frac{1}{2} \int_0^y K(y', y - y')u(y')u(y - y')\, dy'$$

$$Q_2(u)(y) = u(y) \int_0^\infty K(y, y')u(y')\, dy'$$

$$K(y, y') = K(y', y) \geq 0$$

fragmentation

$$\{y\} \xrightarrow[F(y,y')]{} \{y'\} + \{y - y'\}, \qquad 0 < y' < y$$

$$[\partial_t u]_{\text{frag}} = \int_y^\infty F(y', y)u(y')\,dy' - u(y)\int_0^y F(y, y')\frac{y'}{y}\,dy'$$

$$F(y', y) \geq 0$$

diffusive coagulation-fragmentation equations

$u(x,t,y)$ number of clusters of size $y \in Y$ at the place $x \in \Omega \subset \mathbb{R}^3$ at time $t \geq 0$

time evolution law:

$$\partial_t u + \mathrm{div}_x\, \vec{\jmath}(u) = [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}} \qquad \text{in } \Omega, \quad t > 0$$

$\vec{\jmath}(u)$ diffusive flux

Fick's law $\vec{\jmath}(u) = -a(y)\nabla_x u, \quad a(y) > 0$

$+$ boundary conditions $\big($e.g., no flux $\partial_\nu u = 0$ on $\Gamma = \partial\Omega\big)$

$+$ initial distribution $u(x,0,y) = u^0(x,y) \geq 0$

pure coagulation equations

discrete case $Y := \{1, 2, \dots\}$

$$\partial_t u(k) - a(k)\Delta u(k)$$

$$= \frac{1}{2}\sum_{j=1}^{k-1} K_{k-j,j}u(k-j)u(j) - u(k)\sum_{j=1}^{\infty} K_{k,j}u(j)$$

$k = 1, 2, \dots$

Bénilan-Wrzosek (1997); Laurençot, Wrzosek ($\geq$ 1997)

continuous case $Y = (0, \infty)$

$$\partial_t u - a(y)\Delta u$$

$$= \frac{1}{2}\int_0^y K(y-y', y')u(y-y')u(y')\,dy' - u(y)\int_0^\infty K(y, y')u(y')\,dy'$$

Amann (2000), Laurençot-Mischler (2002)

evolution law

$$\partial_t u + \mathrm{div}_x \vec{\jmath}(u) = [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}} \qquad \text{in } \Omega, \quad t > 0$$

$$+ \text{ BC} \qquad + \text{ IC}$$

general structure (with Fick's law and no flux boundary conditions)

$$\begin{array}{rll} \partial_t u - a(y)\Delta u = r(y,u) & \text{in } \Omega, & \\ \partial_\nu u = 0 & \text{on } \Gamma, & t > 0 \\ u(\cdot, 0) = u^0 & & \end{array}$$

consideration of the **carrier fluid**

Amann-Weber (2001)

incompressible mixture of (countably or uncountably many) immiscible fluids

$y \in Y_0$	type of the fluid $\big(y = 0$ carrier fluid, $\quad Y_0 = \{0\} \cup Y\big)$
$\vec{\omega}(y)$	velocity of fluid y
$\rho(y)$	density of fluid y
ρ	constant density of the mixture
$\vec{v} = \frac{1}{\rho}\int_{Y_0} \rho(y)\vec{\omega}(y)\,dy$	barycentric velocity of the mixture
$\vec{\jmath}(y) = \rho(y)\big(\vec{\omega}(y) - \vec{v}\big)$	diffusive flux of fluid y
$\vec{\varphi}(y)$	exterior force on fluid y

constitutive assumptions

$$\rho(y) = \eta y u(y)$$

$$\vec{j}(y) = -a(y)\nabla_x u(y)$$

$(\eta > 0)$ mass $\doteqdot$ volume

Fick's law, no cross-diffusion effects

$$\vec{f}(u) := \left[1 - \frac{\eta}{\rho}\int_Y u(y)y\,dy\right]\vec{\varphi}(0) + \frac{\eta}{\rho}\int_Y u(y)y\vec{\varphi}(y)\,dy$$

resulting exterior force on the mixture

conservation of mass and momentum

$$\nabla \cdot \vec{v} = 0$$

$$\rho\Big(\partial_t \vec{v} + (\vec{v} \cdot \nabla)\vec{v}\Big) - \nu \Delta \vec{v} = -\nabla p + \rho \vec{f}(u)$$

$$\partial_t u + \vec{v} \cdot \nabla u - a(y)\Delta u = [\partial_t u]_{\mathrm{coag}} + [\partial_t u]_{\mathrm{frag}}$$

volume scattering

Fasano, Rosso (2000); Fasano (2001, 2002), Walker (2003)

maximal cluster size $y_0 > 0$

$$[\partial_t u]_{\text{scatt}} = S_1(u) - S_2(u)$$

$$S_1(u)(y) = \frac{1}{2}\int_{y_0}^{2y_0}\int_{y'-y_0}^{y_0} K(y'', y'-y'')\beta(y', y)u(y'')u(y'-y'')\, dy''\, dy'$$

$$S_2(u)(y) = u(y)\int_{y_0-y}^{y_0} K(y, y')u(y')\, dy'$$

$$0 < y \leq y_0$$

$[\partial_t u]_{\text{coal}}$ needs also modification

Basic properties of all models

- $$u \geq 0$$

- $$\int_\Omega \int_Y u(y) y \, dy \, dx = \text{const}$$ conservation of mass

- $$\int_\Omega \int_Y u(y) \, dy \, dx < \infty$$ finiteness of the number of clusters *consequence*

mass $+$ # of clusters $= \displaystyle\int_\Omega \int_Y u(y)(1{+}y)\,dy\,dx = \|u\|_{L_1(\Omega,F)}$

$$F := L_1\big(Y, (1+y)\,dy\big)$$

$\Longrightarrow \quad E = L_1(\Omega, F)$ is the natural space for the study of the evolution problem

abstract setting: semilinear parabolic equation

$$\begin{array}{|c|}\hline \quad \dot{u} + Au = R(u), \quad t > 0 \quad \\ u(0) = u^0 \\ \hline \end{array} \qquad \text{in} \quad E = L_1(\Omega, F)$$

difficulties:

- A elliptic differential operator acting on infinite-dimensional (F-)valued functions
- R unbounded nonlinearity

solution:

study problems in vector-valued Besov spaces $B^s_{1,1}(\Omega, F)$ and use embedding results based on an extension of Mikhlin's multiplier theorem to vector-valued Besov spaces, Amann (1997)

Main results

All models are locally well-posed

(under reasonable assumptions)

i.e., for each $u^0 \geq 0$ there exists a unique local positive solution and
it satisfies the principle of conservation of mass

Amann (2000), Amann-Weber (2001), Walker (2003)

Global existence

models without carrier fluid (i.e., no coupling to the Navier-Stokes equations)

either $n = 1$

or diffusion coefficients independent of cluster size

Amann (2000), Walker (2003)

Laurençot-Mischler (2002)

restricted class of models (no scattering, special structure)

global existence of a weak solution

- no uniqueness

weak and strong compactness methods in L_1

Amann-Walker (2004)

global existence for small u^0

(no fragmentation)

idea of the proof $\big(\Omega$ bounded$\big)$

$-A$ generates an analytic contraction semigroup on $E = L_1(\Omega, F)$

$E = E_0 \oplus E_1$ with $E_0 = F\mathbf{1}_\Omega$

$A = \quad 0 \oplus A_1$

$u = \quad v \oplus w$

$\dot{u} + Au = R(u)$ is equivalent to $\begin{cases} \dot{v} = R_0(v, w) \\ \dot{w} + A_1 w = R_1(v, w) \end{cases}$

$\|v(t)\|_{E_0} \le \|v^0\|_{E_0} \le \|u^0\|_E$

$\|R_1(v, w)\|_{E_1} \le c\left(\|v\|_{E_0}^2 + \|w\|_{E_1}^2\right)$

e^{-tA_1} is exponentially decaying on E_1

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