From Chemistry to Mathematics & back

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Universidade de Lisboa, Faculdade de Ciências, CEMS.UL

CEMS Day

January 27, 2026

Plan

1. **From: a bit of my personal journey**
2. **Back: some of the science that keeps me busy**

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2. **Back: Some of the science that keeps me busy**

- I am a member of CEMS.UL since November 15, 2025

A bit of my personal journey

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but there was life before this date. . .

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...let us see some aspects of it:

A bit of my personal journey

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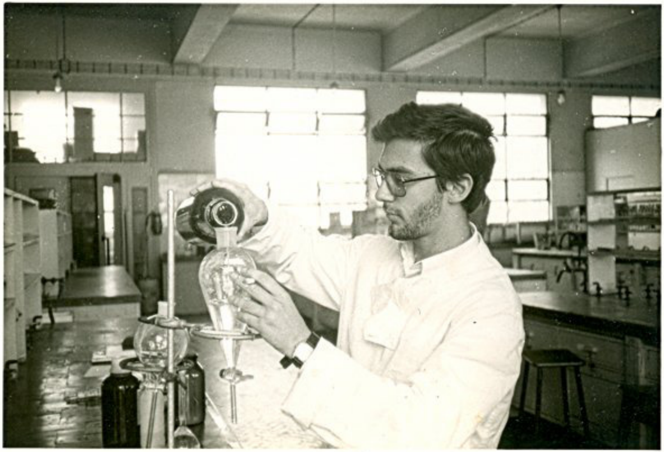

"The past is a different country: They do things differently there", L.P. Hartley

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Markus Kreer FPdC Gero Friesecke

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Rafael | Isabel André (or Tomás) | FPdC Tomás (or André) | Beatriz

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(DMIST, March 2019)
JT Pinto FPdC

A bit of my personal journey

. . . and **teaching**.

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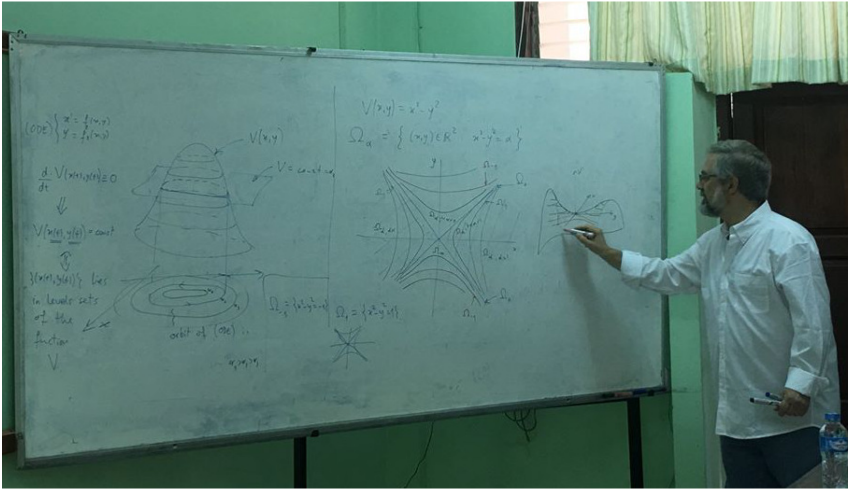

(National University of Laos, February 2018)

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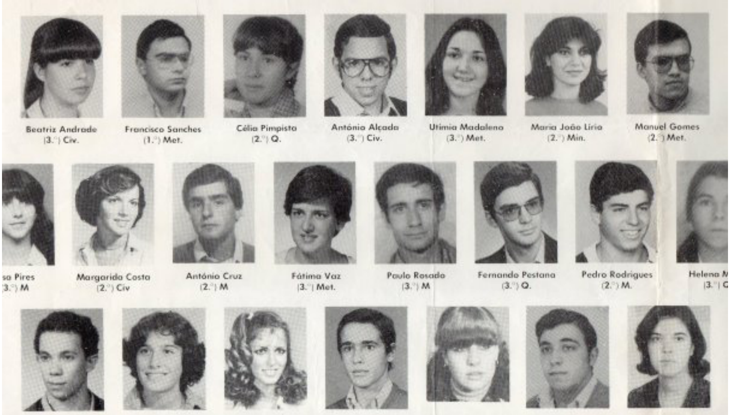

(Candidates to the Student's Union, IST, 1983)

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A bit of my personal journey

...in the present (UAb, 40 years later):

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(*Decano*'s speech at the inauguration of the rector, UAb, 2023)

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Presiding over the Portuguese Mathematical Society:

Presidents of the SPM, 2004–2016
N. Crato M. Abreu FPdC J. Buescu

A bit of my personal journey

Editorial work for the EMS Newsletter (2017–20) / Magazine (2020–24):

A bit of my personal journey

Helping to develop mathematics overseas (Laos, Mongolia, Africa, . . .)

(African Institute for Mathematical Sciences – South Africa, class of 2025/26)

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Now that you know me better, let us speak about...

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2. **Back: some of the science that keeps me busy**

Some of the science that keeps me busy

My research work is on (finite and infinite dimensional) ODEs.

Most (but by no means all) is about **coagulation-fragmentation** type equations, which are a kind of population balance equations for a population of different clusters made of identical particles.

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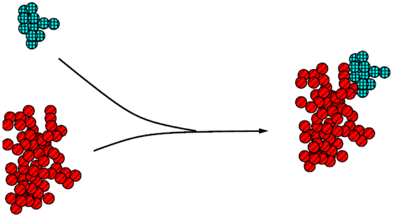
My research work is on (finite and infinite dimensional) ODEs.

Most (but by no means all) is about **coagulation-fragmentation** type equations, which are a kind of population balance equations for a population of different clusters made of identical particles.

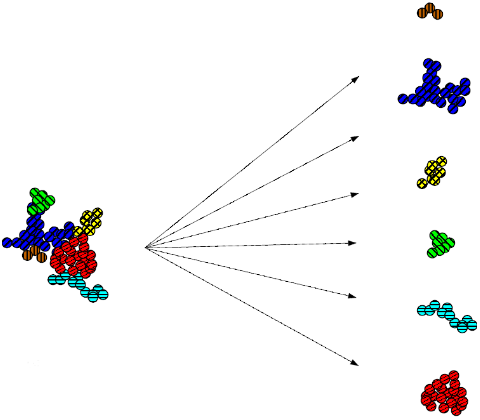
The basic processes are the following:

The **coagulation process**:



Some of the science that keeps me busy

The (spontaneous) **fragmentation process**:



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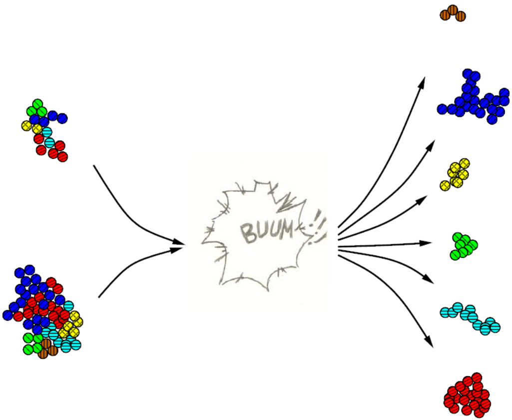
The (collisional) **fragmentation process**:



Some of the science that keeps me busy

How do we model these processes mathematically?

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The original idea is due to **Marian von Smoluchowski** (1916, 1917)

Some of the science that keeps me busy

It is based in a **chemical kinetics** approach:

For a chemical reaction schematically represented by

$$X + Y \underset{k_b}{\overset{k_f}{\rightleftharpoons}} Z$$

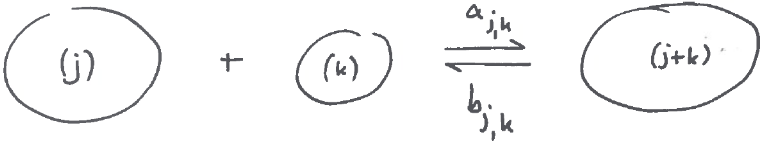
the rate of production of Z is given by

$$\frac{dc_Z(t)}{dt} = k_f c_X(t) c_Y(t) - k_b c_Z(t)$$

where $c_X(t)$ is the concentration of the species X at time t, etc.

Some of the science that keeps me busy

Consider the particular case schematically represented by



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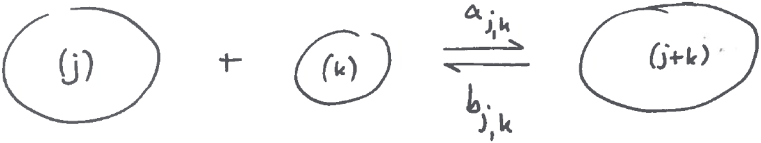

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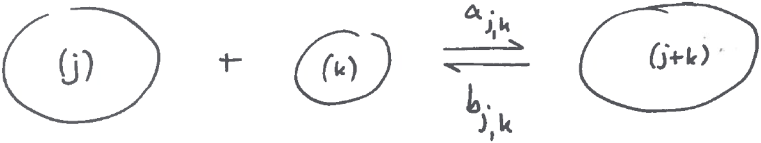

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The evolution of the clusters' concentrations is governed by

$$\frac{dc_i}{dt} = \frac{1}{2}\sum_{k=1}^{i-1} W_{i-k,k}(c) - \sum_{k=1}^{\infty} W_{i,k}(c), \qquad j \in \mathbb{N}^+,$$

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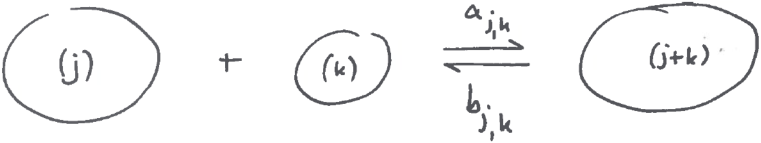

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This ∞-dim ODE is called the **discrete coagulation-fragmentation equation**.

Some of the science that keeps me busy

If the sizes of the clusters can vary continuously, then the corresponding **continuous coagulation-fragmentation equation** is the following integro-differential equation

$$\frac{\partial c(x,t)}{\partial t} = \frac{1}{2}\int_0^x W(x-y,y;c)dy - \int_0^\infty W(x,y;c)dy, \qquad x \in \mathbb{R}^+,$$

where

$$W(x,y;c) = a(x,y)c(x,t)c(y,t) - b(x,y)c(x+y,t).$$

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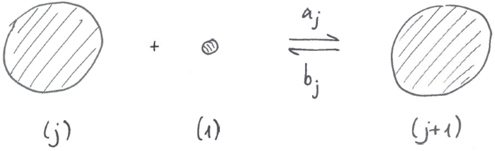
Some particular structures of the rate coefficients $a_{j,k}, b_{j,k}$ are relevant for some applications, giving rise to important special equations. For example:

- If the reactions must always involve a 1-cluster (=monomer)



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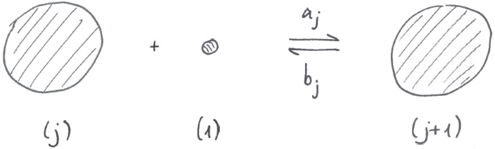

we have the **Becker-Döring equation**

$$\begin{cases} \dot{c}_i = \widetilde{W}_{i-1}(c) - \widetilde{W}_i(c), & i \geq 2 \\ \dot{c}_1 = -\widetilde{W}_1(c) - \sum_{j=1}^{\infty} \widetilde{W}_j(c) & \end{cases}$$

where $\widetilde{W}_j(c) := W_{j,1}(c) = a_j c_j c_1 - b_j c_{j+1}$.

Some of the science that keeps me busy

- If no fragmentation occurs we have the **Smoluchowski's coagulation equation**

$$\frac{dc_i}{dt} = \frac{1}{2}\sum_{k=1}^{i-1} a_{i-k,k}c_{i-k}(t)c_k(t) - c_i(t)\sum_{k=1}^{\infty} a_{i,k}c_k(t), \qquad j \in \mathbb{N}^+,$$

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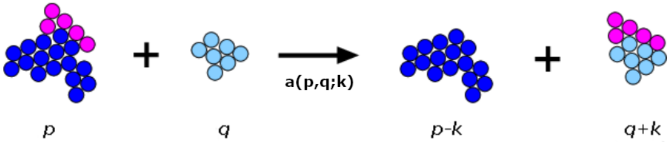
- If the processes consist of a coagulation instantaneously followed by a binary fragmentation we can see it as an exchange of a part of a cluster, as in



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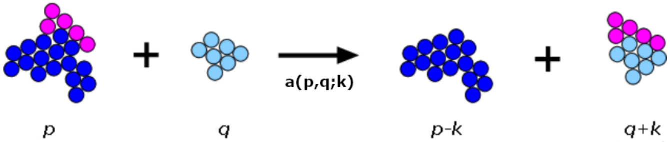

modelled by the **generalized exchange-driven** equation:

Some of the science that keeps me busy

$$\dot{c}_i = \sum_{k=1}^{i} W_{i-k;k}(c) - \sum_{k=1}^{\infty} W_{i;k}(c), \qquad i \in \mathbb{N}^+,$$

where

$$W_{p;k}(c) := \sum_{q=k}^{\infty} \omega(q,p;k)(c)$$

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Several other variants exist in the literature, modelling diverse phenomena such as **nucleation mechanisms** in Physics, **deposition models** in Materials Science, **polymerisation processes** in Chemistry, **aerosol formation** in Atmospheric Science, **prion dynamics** in Biology, **shoal distributions** in Ecology, etc.

Some of the science that keeps me busy

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- **Conserved quantities** or lack thereof: conservation of mass, "gelation". . .
- **Relations with other models**: particle systems, PDE. . .

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- controlled approximation by finite dimensional ODEs
- energy/energy dissipation bounds (*à la* Boltzmann equation studies)
- convenient topologies

Some of the science that keeps me busy

Examples of my recent work illustrate some of the tools used in the field:

- Travelling waves in a dissipative-dispersive approximation of a nonlinear coagulation-fragmentation equation, (in preparation), (with N. Bedjaoui, J. Correia, K. Vongsavang)
  [Approximating solutions by a diffusive-dispersive PDE, study of their travelling wave solutions by phase plane analysis methods]
- The discrete generalized exchange-driven system, Math. Methods Appl. Sci. (2026),(with P. Barik, J.T. Pinto, R. Sasportes)
  [Using typical coagulation-fragmentation tools: truncation, weak L^1-convergence, *a priori* and uniform bounds]
- a study of a toy model of silicosis (2020, 2021, 2024), (with P. Antunes, M. Drmota, M. Grinfeld, J.T. Pinto, R. Sasportes)
  [Asymptotic analysis, typical coagulation-fragmentation tools, and finite-dimensional ODE methods]

Some of the science that keeps me busy

Let's have a bird's-eye view of the study of the toy model for the silicosis desease, in which a number of diverse tools were used.

It was published in:

1. Modelling Silicosis: the Structure of Equilibria, *Euro. Jnl. Appl. Math.*, **31** (2020) 950–967
   (with Michael Drmota, Michael Grinfeld)
2. Modelling Silicosis: Existence, Uniqueness, and Basic Properties of Solutions, *Nonlinear Anal. Real World Appl.*, **60** (2021) 103299
   (with João Teixeira Pinto, Rafael Sasportes)
3. Modelling Silicosis: Dynamics of a Model with Piecewise Constant Coefficients, *J. Dyn. Diff. Equ.*, **36** (2), (2024) 1285–1310
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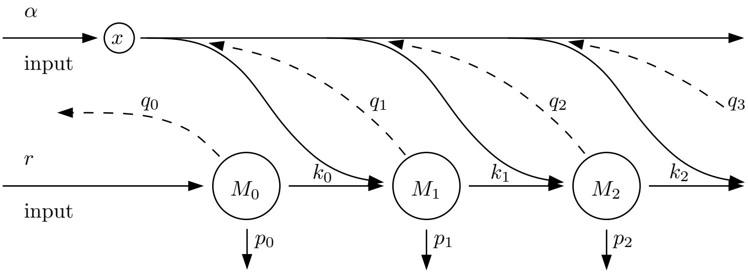
Some of the science that keeps me busy

The reaction scheme is as follows:



With

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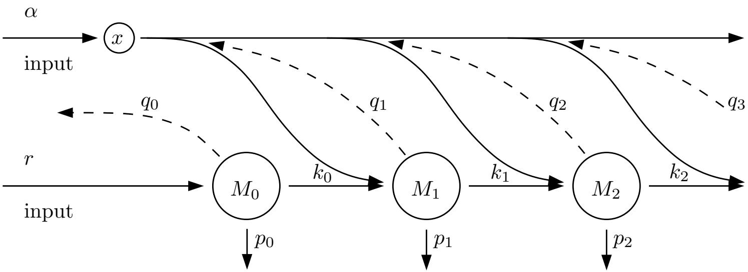

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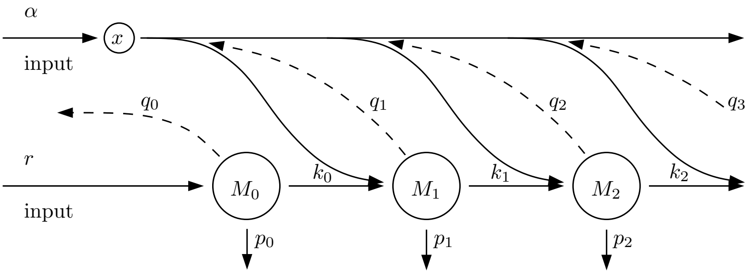

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- α input rate of silica particles *(environment)*;
- r input rate of new macrophages *(physiology)*;
- $(q_i)_{i\in\mathbb{N}_0}$ death rate (i-nondecrease);
- $(p_i)_{i\in\mathbb{N}_0}$ escape rate through the mucociliary escalator (i-nonincrease).

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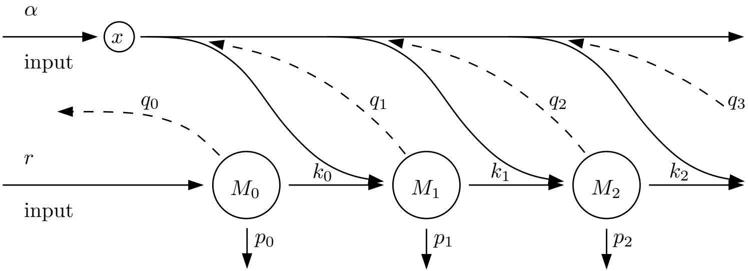

$$\begin{cases} \dot{M}_0 = r - k_0 x M_0 - (p_0 + q_0) M_0 \ , \\ \dot{M}_i = k_{i-1} x M_{i-1} - k_i x M_i - (p_i + q_i) M_i \ , \quad i \in \mathbb{N}^+ \\ \dot{x} = \alpha - x \sum_{i=0}^{\infty} k_i M_i + \sum_{i=0}^{\infty} i q_i M_i \ , \\ x(0) = x_0, \quad M_i(0) = M_{0i}, \quad i \in \mathbb{N}. \end{cases} \tag{1}$$

Some of the science that keeps me busy

The Banach spaces relevant to study this system are

$$X^\gamma := \left\{ y := (x, M_0, M_1, \dots) : \|y\|_\gamma := |x| + \sum_{j=0}^{\infty} (1+j)^\gamma |M_j| < \infty \right\}$$

(The space with $\gamma = 1$ is the space of "finite mass" sequences.)

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A caricature assumption about the rate coefficiente k_i, p_i and q_i allow us to conclude the existence of a saddle-node bifurcation and to say something about the dynamics [3]:

Some of the science that keeps me busy

If, for some fixed $N \in \mathbb{N}^+$, the rate coefficients satisfy

$$k_i \equiv k, \qquad p_i = \begin{cases} 1 & \text{if } i \leqslant N, \\ 0 & \text{if } i \geqslant N+1, \end{cases} \quad \text{and} \quad q_i = \begin{cases} 0 & \text{if } i \leqslant N, \\ 1 & \text{if } i \geqslant N+1, \end{cases}$$

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then, introducing the new variables

$$u := \sum_{i=0}^{\infty} M_i, \qquad v := \sum_{i=N+1}^{\infty} iM_i, \qquad w := \sum_{i=N}^{\infty} M_i,$$

the silicosis system (1) becomes

$$\begin{cases} \dot{x} &= \alpha - kxu + v \\ \dot{u} &= r - u \\ \dot{v} &= -v + kxw + kNM_N \\ \dot{w} &= -w + kxM_{N-1} \\ \dot{M}_0 &= r - M_0 - kxM_0 \\ \dot{M}_i &= -M_i - kxM_i + kxM_{i-1}, \quad i \in \mathbb{N}^+. \end{cases} \tag{2}$$

Some of the science that keeps me busy

System (2) consists of a $(N+5)$-dimensional ODE coupled with an ∞-dimensional lower triangular system.

We can prove the existence of a bifurcation point and study the dynamics of the finite dimensional ODE by a delicate analysis of the spectra of the linearization about the bifurcation point using a perturbation argument. Playing around with the time evolution of the norms $\|\cdot\|_0$ and $\|\cdot\|_1$ of the solutions. . .

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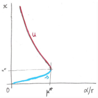
. . . we can actually prove the stable branch locally exponentially attracts solutions of the ∞-dimensional system (1) in the norm topology of X^1.



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If you want to know more, the following reviews are a good starting point:

- Ph. Laurençot, S. Mischler, *On Coalescence Equations and Related Models*, in: P. Degond et al (Eds.): Modelling and Computational Methods for Kinetic Equations, Birkhäuser, 2004, pp. 321–356.
- R. L. Pego, *Lectures on Dynamics in Models of Coarsening and Coagulation*, in: W. Bao, J.-G. Liu (Eds.): Dynamics in Models of Coarsening, Coagulation, Condensation and Quantization; Lecture Notes Series, Institute for Mathematical Sciences, National University of Singapore, vol. 9, World Scientific, 2007, pp. 1–61.
- F.P. da Costa, *Mathematical Aspects of Coagulation-Fragmentation Equations*, in: J.-P. Bourguignon et al. (Eds.): Mathematics of Planet Earth: Energy and Climate Change, Springer, 2015. pp. 83–162.

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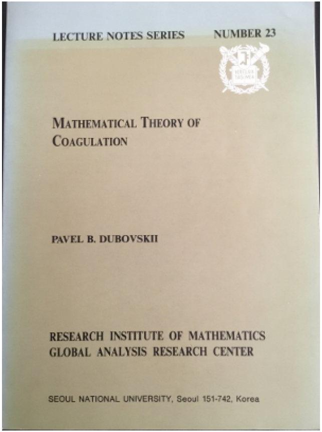
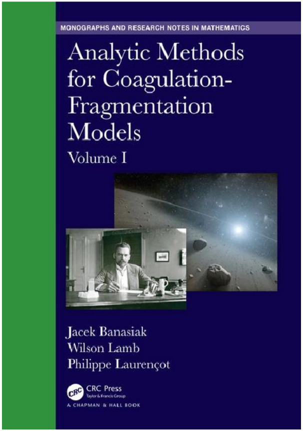
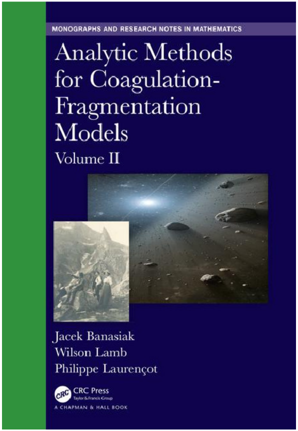
And for a deeper dive the following books are recommended:







Thank you!