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Duality- and entropy methods in coagulation-fragmentation models

Abstract. This article presents a selected overview of the existence theory and qualitative analysis of coagulation-fragmentation models describing the formation and break-up of clusters/particles/polymers in various applications in physics, chemistry, astronomy and biology.

In particular, we shall discuss recent results on spatially inhomogeneous coagulation-fragmentation models, which are obtained by duality methods and/or entropy methods.

We shall show how a duality argument provides e.g. global-in-time L^2 -bounds, while the entropy method implies entropy related a priori estimates and explicit convergence to equilibrium.

Keywords. Coagulation-fragmentation model, gelation, saturation, duality method, entropy method, global weak solution, large-time-behaviour, fast-reaction limit.

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1 - Introduction

Starting from the pivotal works of Smoluchowski [54, 55], coagulation-fragmentation models have been widely used to describe the formation and the break-up of a wide range of clusters/polymers in as many areas as physics (aerosols, raindrops, smoke, sprays), chemistry (polymerisation processes), astronomy (formation of galaxies) and biology (hematology, animal grouping).

A detailed description of both processes, coagulation and fragmentation, will often reveal highly complex mechanisms, which will make realistic model very complicated. Speaking of fragmentation and thinking of the break-up of droplets in particular, a detailed description would need to consider internal oscillations, viscosity- and surface-tension effects etc. in order to determine the number of subdroplets a single droplet is going to break up into (cf. [38] for instance).

Avoiding such a detailed description, the present review focuses on mathematical methods for coagulation-fragmentation models, which are based on the assumption that the *particles/clusters/polymers are entirely described by their mass/size*.

There are mainly three levels of description of coagulation-fragmentation processes:

First, there is the *microscopic description* of a finite ensemble of particles undergoing stochastic interaction events (e.g. the Marcus-Lushnikov process, see e.g. [33]) as originally proposed by Smoluchowski [54].

Secondly, and in the focus of this article, the *mesoscopic description* models coagulation and fragmentation in terms of a nonnegative density $f(t, x, y)$ depending on time t , possibly position x and the cluster size/mass y . The time evolution of this density is then given by a deterministic mean-field equation, [55].

A third level of description uses the macroscopic scales, which are directly linked to observations.

Linking limits between microscopic and mesoscopic descriptions involve the convergence of stochastic processes (like the Marcus-Lushnikov process converging to the Smoluchowski equation, [49]) or mean-field limits. An example for a limit from a mesoscopic mean-field equation to a macroscopic evolution equation are fast-reaction limits, see e.g. [29] and the last Section of this paper.

The article is organised as follows:

In the following Section 2, the Smoluchowski coagulation equation is presented along with formal properties, a discussion of the phenomenon of gelation and an example of the existence theory for the discrete Smoluchowski equation by using a limit of finite-dimensional approximating systems.

In Section 3, discrete coagulation-fragmentation models are presented, most importantly the Becker-Döring model. Moreover, the phenomenon of saturation is presented.

The final and main Section 4 focuses on spatial inhomogeneous coagulation-fragmentation models with diffusion: First, we revise the L^1 -existence theory as developed in [39, 40]. We then present a duality method for diffusive equations (see e.g. [36, 52, 21]), which allows to prove uniform-in-time L^2 -estimates. This global L^2 -bound can be used to show existence of generalised coagulation-fragmentation models as well as absence of gelation. Further, we present an entropy method, which allows to prove convergence to equilibrium with explicit rates. Finally, we shall demonstrate a fast-reaction-limit based on entropy-estimates and a duality argument.

2 - The Smoluchowski equation: a model for coagulation

The Smoluchowski coagulation equation (see [54, 55, 46]) models the evolution of a nonnegative mesoscopic density of clusters/polymers $0 \leq f(t, y)$ depending on time $t \geq 0$ and the size variable $y \in Y$. The case $Y = \mathbb{N}$ is called the *discrete Smoluchowski equation* while the *continuous Smoluchowski equation* considers $Y = [0, \infty)$. The governing evolution of both the discrete and the continuous Smoluchowski equation share the same structure:

$$(1) \quad \partial_t f(t, y) = Q_{\text{coag}}(f, f)(y) = Q_1(f, f) - Q_2(f, f).$$

On the right hand side of eq. (1), the quadratic terms $Q_1(f, f)$ and $Q_2(f, f)$ describe the gain and the loss of clusters of size y due to binary coagulation events. Coagulation events involving more than two particles are considered negligible in the Smoluchowski models.

The gain term $Q_1(f, f)$ accounts for the particles of size y being formed by the coagulation of two smaller particles

$$\{y'\} + \{y - y'\} \xrightarrow{a(y', y - y')} \{y\}, \quad \text{for all } y' < y.$$

Here, $a(y', y - y')$ denotes a nonnegative and symmetric coagulation rate/kernel:

$$(2) \quad 0 \leq a(y, y') = a(y', y).$$

In case of the continuous Smoluchowski model with size variable $y \in [0, \infty)$, the gain term Q_1 is an integral term

$$(3) \quad Q_1(f, f) = \frac{1}{2} \int_0^y a(y', y - y') f(y - y') f(y') dy',$$

where the stoichiometric coefficient $\frac{1}{2}$ reflects the fact that two clusters merge into one.

The lost term $Q_2(f, f)$ comprises the loss of particles of size y due to the formation of larger clusters:

$$\{y\} + \{y'\} \xrightarrow{a(y, y')} \{y + y'\}, \quad \text{for all } y' \in Y.$$

In the continuous Smoluchowski equation this leads to the following integral

$$(4) \quad Q_2(f, f) = f(y) \int_0^\infty a(y, y') f(y') dy'.$$

The physics/chemistry/biology of the considered coagulation process is expressed in the coagulation coefficients $a(y', y)$ as given in (2), see e.g. the survey of Drake [26].

The original works of Smoluchowski, for example, considered the coagulation of colloidal particles according to

$$a(y, y') = (y^\alpha + (y')^\alpha)^\beta (y^{-\gamma} + (y')^{-\gamma}), \quad \alpha, \beta, \gamma \geq 0, \quad \alpha\beta \leq 1,$$

where Smoluchowski studied in particular $\alpha = \gamma = 1/3, \beta = 1$, see [54]. Another class of coagulation rates are the ballistic kernels

$$a(y, y') = (y^\alpha + (y')^\alpha)^\beta |y^\gamma - (y')^\gamma|, \quad \alpha, \beta, \gamma \geq 0, \quad \alpha\beta + \gamma \leq 1,$$

or kernels of the type

$$a(y, y') = y^\alpha (y')^\beta + (y')^\alpha y^\beta, \quad \alpha, \beta \in [0, 1].$$

Amongst the latter, the Golovin kernel $(\alpha, \beta) = (0, 1)$ [35] has been used to describe cloud droplets while the Stockmeyer kernel $\alpha = \beta = 1$ [58] models branched-chain polymers.

2.1 - Formal properties of the continuous Smoluchowski equation

This Section summarises formal properties of the continuous Smoluchowski equation. Analog results for discrete coagulation (and coagulation-fragmentation) models will be stated below as needed.

At first, we derive a weak formulation of eq. (1): By multiplication with a suitable test-function $\varphi(y)$ and integration over $y \in [0, \infty)$, we obtain with Fubini's theorem

$$(5) \quad \begin{aligned} \frac{d}{dt} \int_0^\infty f(t, y) \varphi(y) dy &= \int_0^\infty Q_{coag}(f, f) \varphi(y) dy \\ &= \frac{1}{2} \int_0^\infty \int_0^\infty a(y, y') f(y) f(y') (\varphi'' - \varphi - \varphi') dy dy', \end{aligned}$$

where we have used the shorthand notation $\varphi = \varphi(y)$, $\varphi' = \varphi(y')$ and $\varphi'' = \varphi(y + y')$.

In particular, with the choice $\varphi(y) = y^k$ and $\text{sign}(\varphi'' - \varphi - \varphi') = \text{sign}(k - 1)$, it follows formally that

$$t \mapsto \int_0^\infty \varphi(y) f(t, y) dy = \begin{cases} \searrow & k < 1, \\ \text{constant} & k = 1, \\ \nearrow & k > 1. \end{cases}$$

The testfunction $\varphi = 1$ shows that the number of particles $\int_0^\infty f(t, y) dy$ is decreasing due to the coagulation process.

More importantly, testing with $\varphi(y) = y$ implies the formal conservation of mass

$$\frac{d}{dt} \int_0^\infty y f(t, y) dy = \int_0^\infty y Q_{coag}(f, f) dy = 0.$$

However, without further assumptions on the coagulation kernel, it is in general only possible to prove that the mass is non-increasing: Considering a cut off $R > 0$ and a sequence of test-functions $\varphi(y) = \min\{y, R\}$, which satisfies $\varphi'' - \varphi - \varphi' \leq 0$, we find that the map $t \mapsto \int_0^\infty \min\{y, R\} f(t, y) dy$ is non-increasing. Thus, by Fatou's lemma we

conclude that

$$t \mapsto \int_0^{\infty} y f(t, y) dy$$

is non-increasing.

It is indeed a well known phenomenon of mesoscopic coagulation models that the formal conservation of mass is violated for sufficiently growing coagulation coefficients. This phenomenon is called *gelation* and shall be discussed further in the following Section 2.2.

We conclude this Section by noting that for all kernels $a(y, y')$ satisfying

$$a(y, y') \leq a(y, y + y') + a(y', y + y'), \quad y, y' \in Y,$$

it follows formally from testing with $\varphi(y) = pf(t, y)^{p-1}$ that the L^p -Norm is non-increasing:

$$t \mapsto \|f(t, \cdot)\|_{L^p} \quad \text{non-increasing for } p \geq 1.$$

2.2 - Gelation, gelation time and gelation profiles

We shall consider in particular the product coagulation kernel $a(y, y') = y y'$. At first, we restate the weak formulation (5), i.e.

$$(6) \quad \frac{d}{dt} \int_0^{\infty} f(t, y) \varphi(y) dy = \frac{1}{2} \int_0^{\infty} \int_0^{\infty} yy' f(y) f(y') (\varphi'' - \varphi - \varphi') dy' dy.$$

Introducing the moments

$$M_0(t) = \int_0^{\infty} f(t, y) dy, \quad M_1(t) = \int_0^{\infty} y f(t, y) dy,$$

we test (6) with $\varphi(y) = 1$ and obtain

$$\frac{d}{dt} M_0(t) = -\frac{1}{2} \int_0^{\infty} \int_0^{\infty} yy' f(y) f(y') dy' dy = -\frac{1}{2} M_1^2(t).$$

Thus, integration over a time interval $[0, T]$ for any $T > 0$ yields

$$M_0(T) + \frac{1}{2} \int_0^T M_1^2 dt = M_0(0).$$

Since $0 \leq M_0(T) \leq M_0(0)$ is bounded for all $T > 0$ it follows that

$$\int_0^\infty M_1^2 dt < \infty \implies M_1 \in L^2((0, \infty)),$$

which implies that

$$M_1(t) < M_1(0) \quad \text{after some finite time } t \geq 0.$$

The phenomenon that the formal conservation of mass is violated within finite time is called *gelation* and

$$T_g = \inf\{t \geq 0 : M_1(t) < M_1(0)\}$$

is called *gelation time*. At gelation a phase transition occurs, which marks the formation of clusters of infinite/macroscopic size.

A more general result holds for coagulation kernel of the form

$$a(y, y') = y^\alpha (y')^\beta + (y')^\alpha (y)^\beta, \quad \alpha, \beta \in [0, 1].$$

For these kernels, gelation occurs provided that $\lambda = \alpha + \beta \in (1, 2]$. In fact, it has been shown in [31] that

$$M_k = \int_0^\infty y^k f(t, y) dy \in L^2((0, \infty)) \quad \text{for} \quad k \in \left(\frac{\lambda}{2}, \frac{1+\lambda}{2}\right),$$

which implies, in particular, that $M_1 \in L^2(0, \infty)$ for $\lambda > 1$.

An interesting question addresses the characterisation of the gelation time T_g . While constituting an open problem for many general coagulation coefficients, the product kernel $a(y, y') = y y'$ allows to answer it explicitly.

First, we calculate explicitly the blow-up time of second moment

$$M_2 = \int_0^\infty y^2 f(t, y) dy,$$

which evolves according to

$$\frac{d}{dt} M_2(t) = \frac{1}{2} \int_0^\infty \int_0^\infty y y' f(y) f(y') ((y + y')^2 - y^2 - (y')^2) dy' dy = M_2^2(t),$$

and therefore blows-up at time $T_2 = \frac{1}{M_2(0)}$ (recall the explicit solution $\frac{1}{M_2(t)} = \frac{1}{M_2(0)} - t$).

With gelation time marking the appearance of infinite size clusters, one can conjecture that gelation should correspond to the blow-up of higher order moments. In the case of the product kernel $a(y, y') = y y'$, this conjecture can be proven. In particular, we find that $T_g = T_2$: Defining the formal Laplace-type-transform

$$E(t, p) = \int_0^\infty e^{-py} y f(t, y) dy, \quad \partial_p E(t, p) = - \int_0^\infty e^{-py} y^2 f(t, y) dy,$$

we observe that $E(t, 0) = M_1(t)$ and $\partial_p E(t, 0) = -M_2(t)$. Next, by testing (6) with $\varphi(y) = e^{-py} y$ for $p \in [0, \infty)$, we calculate

$$\partial_t E(t, p) = \int_0^\infty e^{-py} y^2 f(y) dy \int_0^\infty e^{-py'} y' f(y') dy' - \int_0^\infty e^{-py} y^2 f(y) dy \int_0^\infty y' f(y') dy'$$

and obtain the following Burgers-type equation

$$\partial_t E(t, p) + (E(p) - E(0)) \partial_p E(t, p) = 0.$$

Since by construction $\partial_p E(t, p) \geq \partial_p E(t, 0) = -M_2(t)$ it follows that the above Burgers equation develops shocks at first at $p = 0$ at the same time as the second order moment blows up. As a results of the shock at $p = 0$, the value of $E(t, 0) = M_1(t)$ has to decrease, i.e.

$$E(t, 0) = M_1(t) < M_1(0), \quad t > T_2,$$

and we conclude that gelation occurs at the same time as the second order moment blows up, i.e. $T_g = T_2$. For general coagulation coefficients, the characterisation of the gelation time is often an open problem.

No gelation occurs for at most linearly growing kernels. Examples for which conservation of mass is proven rigorously (see e.g. [2] and Section 2.3 below) are

$$a(y, y') \leq C(1 + y + y'),$$

and

$$a(y, y') = y^\lambda (y')^\beta + (y')^\lambda (y)^\beta, \quad \lambda = \alpha + \beta \leq 1.$$

In the particular case of the linear kernel $a(y, y') = y + y'$, one can again explicitly calculate that no gelation occurs by using a Laplace transform: For $p \geq 0$, we define

$$F(t, p) = \int_0^\infty e^{-py} f(t, y) dy,$$

and observe that

$$F(t, 0) = \int_0^\infty f(t, y) dy = M_0(t), \quad \partial_p F(t, 0) = - \int_0^\infty y f(t, y) dy = -M_1(t).$$

First, we calculate for $a(y, y') = y + y'$ that as long as the mass is conserved, i.e. $M_1(t) = M_0(t)$, we have

$$\frac{d}{dt} M_0(t) = -M_0(t) M_1(0), \quad M_0(t) = M_0(0) e^{-M_1(0)t}.$$

Then, we compute

$$\begin{aligned} \partial_t F(t, p) &= \frac{1}{2} \int_0^\infty \int_0^\infty (y + y') [e^{-p(y+y')} - e^{-py} - e^{-py'}] f(t, y) f(t, y') dy' dy \\ &= -F(t, p) \partial_p F(t, p) - M_1(0) F(t, p) + M_0(t) \partial_p F(t, p). \end{aligned}$$

Thus, we have

$$\partial_t F(t, p) + (F(t, p) - M_0(0) e^{-M_1(0)t}) \partial_p F(t, p) = -M_1(0) F(t, p),$$

which implies

$$F\left(t, p_0 - \frac{1 - e^{-M_1(0)t}}{M_1(0)} [M_0(0) - F(0, p_0)]\right) = e^{-M_1(0)t} F(0, p_0),$$

and the function

$$p_0 \mapsto p_0 - \frac{1 - e^{-M_1(0)t}}{M_1(0)} [M_0(0) - F(0, p_0)]$$

is one-to-one because its derivative is

$$p_0 \mapsto 1 + \frac{1 - e^{-M_1(0)t}}{M_1(0)} \partial_p F(0, p_0)$$

and

$$\frac{-\partial_p F(0, p_0)}{M_1(0)} = \frac{\int_0^\infty e^{-p_0 y} y f(0, y) dy}{\int_0^\infty y f(0, y) dy} \leq 1.$$

The Smoluchowski coagulation process continuously decreases the number of particles. In [9], Carr and da Costa showed for the discrete Smoluchowski equation with $0 < a_{i,j} \leq C(j + K)$ with a constant $C > 0$ and for $(i, j) \in \mathbb{N} \times \mathbb{N}$ that provided

$$M_1(0) = \sum_{j=1}^{\infty} j c_j(0) < \infty:$$

$$c_j(t) \rightarrow 0, \quad \forall j \in \mathbb{N} \quad \text{as } t \rightarrow \infty.$$

Thus, even if the mass $M_1(t) = M_0(0)$ is conserved for all $t \geq 0$, there occurs a *loss of mass in infinite time* in the sense that particles of any fixed size j will have coalesced and

$$M_k(t) = \sum_{j=1}^{\infty} j^k c_j(t) \rightarrow 0 \quad \text{as } t \rightarrow \infty, \quad k \in [0, 1).$$

An analog results holds for the continuous Smoluchowski equation for $a(y, y') > 0$ for $y \neq y'$ on $(y, y') \in Y \times Y$, see [42]. Assuming in addition that $a(y, y') \geq (yy')^\lambda$ for $\lambda \in [0, 1]$ and $f^{in}(y) \equiv 0$ a.e. on $y \in (0, \delta)$ for $\delta > 0$, then $M_k(t) \leq C_k t^{-k}$ for all $k \in (0, 1)$ (see [42]).

Another interesting (and in general open) question concerns the profiles of the solution at gelation. For the kernel

$$(7) \quad a(y, y') = y^\alpha (y')^\beta + (y')^\alpha (y)^\beta, \quad \alpha, \beta \in [0, 1],$$

with $\lambda = \alpha + \beta \in (1, 2]$, there is the conjecture that at gelation time (see [31, 42])

$$f(T_g, y) \sim y^{-\frac{3+\lambda}{2}} \quad \text{as } y \rightarrow \infty.$$

The dynamical scaling hypothesis proposes (see e.g. [25]) that as a mean particle size $s(t) \rightarrow \infty$ as $t \rightarrow T_*$ (possible choices are e.g. $s(t) = M_1(t)/M_0(t)$, $s(t) = M_2(t)/M_1(t)$ or $s(t) = M_3(t)/M_2(t)$, see [25]) the particle density approaches a self-similar profile:

$$f(t, y) \sim \frac{1}{s(t)^\tau} \varphi\left(\frac{y}{s(t)}\right) \quad \text{as } t \rightarrow T_*.$$

In the case of the kernel (7) which satisfies $a(\xi y, \xi y') = \xi^\lambda a(y, y')$, it is conjectured that $\frac{1}{s(t)^\tau} \varphi\left(\frac{y}{s(t)}\right)$ is a self-similar solution with $\tau = 2$ for $T_* = \infty$ if $\lambda \in [0, 1]$ and with $\tau = (\lambda + 3)/2$ for $T_* = T_g$ if $\lambda \in (1, 2]$. The case $\lambda = 1$ with $\alpha > 0$ requires a modified ansatz, see [25].

Recently, Niethammer and Velázquez showed in [48] for continuous kernels with homogeneity $\gamma \in [0, 1]$, i.e. $a(\xi y, \xi y') = \xi^\gamma a(y, y')$, which satisfy the growth condition $a(y, y') \leq C(y^\gamma + (y')^\gamma)$ that solutions tend towards self-similar solutions of the form

$$f(t, y) \sim \frac{1}{t^\alpha} \varphi\left(\frac{y}{t^\beta}\right) \quad \text{with } \alpha = 1 + (1 + \gamma)\beta,$$

where the self-similar profile features so called fat tails, i.e. for any $\rho \in (\gamma, 1)$, there exists a continuous, self-similar profile

$$\varphi(t, y) \sim (1 - \rho)y^{-(1+\rho)}.$$

2.3 - Existence of weak solutions of the discrete Smoluchowski equation

The alternative to continuous-in-size models are discrete-in-size models with a size variable $i \in \mathbb{N} = Y$. By denoting the cluster density $c_i(t) \geq 0$ with $c = (c_i)$, we consider

$$(8) \quad \frac{d}{dt} c_i(t) = Q_{coag}(c, c) = \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} c_{i-j}(t) c_j(t) - \sum_{j=1}^{\infty} a_{i,j} c_i(t) c_j(t),$$

$$(9) \quad c_i(0) = c_i^{in},$$

for the coagulation coefficients $a_{i,j} = a_{j,i} \geq 0$.

The system (8) can be approximated by finite-dimensional systems of ODEs for (c_i) , $i = 1, \dots, N$ with a cutoff index N :

$$(10) \quad \frac{d}{dt} (c_i^N)(t) = \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} c_{i-j}^N(t) c_j^N(t) - c_i^N(t) \sum_{j=1}^N a_{i,j} c_j^N(t),$$

$$(11) \quad c_i^N(0) = c_i^{in}.$$

The weak formulation of the approximating cutoff models reads as:

$$(12) \quad \frac{d}{dt} \sum_{i=1}^N \varphi_i c_i^N = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_{i,j} (\varphi_{i+j} \mathbb{1}_{j \leq N-1} \mathbb{1}_{i \leq N-j} - \varphi_i - \varphi_j) c_i^N c_j^N.$$

The existence of solutions to the cutoff models (12) follows from the standard (Cauchy-Lipschitz) theory for autonomous systems of ODEs: Suppose $a = a(c^N) \in C^1(\mathbb{R}^N, \mathbb{R}^N)$ and $c^N(0) \in \mathbb{R}^N$, then, there exists a unique solution of the ODE system

$$\frac{d}{dt} c^N(t) = a(c^N(t)), \quad c^N(0) = c^{in},$$

on a maximal interval of existence $[0, T)$ for $T > 0$. Moreover, if $T < \infty$, then

$$\lim_{t \rightarrow T^-} \|c^N(t)\| = \infty.$$

While global-in-time solutions cannot be expected in general for superlinear ODEs, the system (10) satisfies the natural *a priori* estimate of non-increasing mass:

$$\frac{d}{dt} \sum_{i=1}^N i c_i^N = \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_{i,j} [(i+j) \mathbb{1}_{j \leq N-1} \mathbb{1}_{i \leq N-j} - i - j] c_i^N c_j^N \leq 0,$$

so that

$$(13) \quad \sum_{i=1}^N i c_i^N(t) \leq \sum_{i=1}^N i c_i^{in}.$$

Therefore, given nonnegative initial data c_i^m , $i \in \mathbb{N}$ and thus considering non-negative solutions $0 \leq c_i^N(t)$ for all $N > 0$, the *a priori* estimate (13) allows to extend solutions to global solutions (defined on $[0, \infty)$). Note that the global solutions of the coagulation system (10), (11) for any cutoff size N exist without any further restriction on the nonnegative coefficients $a_{i,j}$.

The uniform boundedness of the mass (13) and the nonnegativity of the solution c_i^N imply also the weak-* compactness of the sequence c_i^N : Assuming finite initial mass

$$M_{in} = \sum_{i=1}^{\infty} i c_i^m < \infty,$$

it follows from (13) that for all cutoff $N > 0$

$$\sum_{i=1}^N i c_i^N(t) \leq \sum_{i=1}^N i c_i^m \leq M_{in}.$$

Therefore, for all $i \in \mathbb{N}$, the approximating sequence $(c_i^N(t))_{N \in \mathbb{N}}$ is bounded in $L^\infty([0, +\infty))$ and converges in a diagonal argument, up to subsequences, towards a function $c_i(t)$ weakly-* in $L^\infty([0, +\infty))$:

$$(14) \quad c_i^N \rightharpoonup c_i \quad \text{in} \quad L^\infty([0, +\infty)) \text{ weak-*}.$$

Strong compactness of the sequence c_i^N can be shown under the assumption of sublinear coagulation coefficients:

$$(15) \quad 0 \leq a_{i,j} \leq K(i+j).$$

Then, for any $i = 1, \dots, N$, and using $c_i^N(t) \leq M_{in}$

$$\begin{aligned} \left| \frac{d}{dt} c_i^N(t) \right| &\leq \left| \frac{1}{2} \sum_{j=1}^{i-1} a_{j,i-j} c_j^N(t) c_{i-j}^N(t) \right| + c_i^N(t) \left| \sum_{j=1}^N a_{i,j} c_j^N(t) \right| \\ &\leq \frac{1}{2} M_{in}^2 \sum_{j=1}^{i-1} a_{j,i-j} + M_{in} K \sum_{j=1}^N (i+j) c_j^N(t) \\ &\leq \frac{1}{2} M_{in}^2 \sum_{j=1}^{i-1} a_{j,i-j} + M_{in} K(i+1) M_{in} \end{aligned}$$

so that (thanks to Ascoli's Theorem)

$$c_i^N(t) \xrightarrow{N \rightarrow \infty} c_i(t) \quad \text{for a.e. } t \geq 0.$$

The assumption of sublinear coagulation rates (15) allows also to prove the propagation of superlinear moments like in the following estimate of a logarithmic

moment: Assume that the initial first logarithmic moment is finite, i.e

$$L_{in} = \sum_{i=1}^{\infty} (i \ln i - i + 1) c_i^{in} < \infty,$$

and denote the approximating first logarithmic moment by

$$L^N(t) = \sum_{i=1}^N (i \ln i - i + 1) c_i^N(t).$$

Then, by the weak formulation (12) with the test-sequence $\varphi(i) = i \ln i - i + 1$, we estimate with

$$\varphi(i+j) \mathbb{1}_{j \leq N-1} \mathbb{1}_{i \leq N-j} - \varphi(i) - \varphi(j) \leq i \ln(1+j/i) + j \ln(1+i/j)$$

and with the assumption of sublinear moments (15) that

$$\begin{aligned} \frac{d}{dt} L^N(t) &\leq \frac{1}{2} \sum_{i=1}^N \sum_{j=1}^N a_{i,j} (i \ln(1+j/i) + j \ln(1+i/j)) c_i^N(t) c_j^N(t) \\ &\leq \sum_{i=1}^N \sum_{j=1}^N K(i+j) i \ln(1+j/i) c_i^N(t) c_j^N(t), \end{aligned}$$

where we have used a symmetry argument. Continuing by using $\ln(1+x) \leq x$ and $x \ln(1+x) \leq (x \ln x - x + 1) + x$, we estimate

$$\begin{aligned} \frac{d}{dt} L^N(t) &\leq \sum_{i=1}^N \sum_{j=1}^N K[i^2 \ln(1+j/i) + ij \ln(1+j/i)] c_i^N(t) c_j^N(t) \\ &\leq \sum_{i=1}^N \sum_{j=1}^N K[ij + ij \ln(1+j)] c_i^N(t) c_j^N(t) \\ &\leq \sum_{i=1}^N \sum_{j=1}^N K i [2j + (j \ln j - j + 1)] c_i^N(t) c_j^N(t) \\ &\leq K M_{in} (2 M_{in} + L^N(t)). \end{aligned}$$

Using Gronwall's lemma, for any $t \in [0, T]$, $N \in \mathbb{N}$, we obtain

$$(16) \quad L^N(t) \leq (2 M_{in} + L_{in}) e^{K M_{in} T}.$$

This implies in a first limit $c_i^N(t) \rightarrow c_i(t)$ that

$$\sup_{t \in [0, T]} \sum_{i=1}^N (i \ln i - i + 1) c_i(t) \leq C(K, T, L_{in}),$$

and, in a second limit $N \rightarrow \infty$ that

$$\sup_{t \in [0, T]} \sum_{i=1}^{\infty} (i \ln i - i + 1) c_i(t) \leq C(K, T, L_{in}).$$

Proposition 2.1 (Existence of mass conserving solutions). *Assume nonnegative at most linearly growing coagulation coefficients*

$$0 \leq a_{i,j} \leq K(i+j).$$

Consider nonnegative initial data $0 \leq c_i^{in}$ with finite first-logarithmic moment

$$L_{in} = \sum_{i=1}^{\infty} (i \ln i - i + 1) c_i^{in} < \infty.$$

Then, there exists a weak solution $c_i \in L_{loc}^{\infty}([0, +\infty))$ to the Smoluchowski equation with initial data c_i^{in}

$$\begin{aligned} \frac{d}{dt} c_i(t) &= \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} c_{i-j}(t) c_j(t) - c_i(t) \sum_{j=1}^{\infty} a_{i,j} c_j(t), \quad i \in \mathbb{N}, \\ c_i(0) &= c_i^{in}, \quad i \in \mathbb{N}. \end{aligned}$$

In particular, the term $\sum_{j \in \mathbb{N}} a_{i,j} c_j$ lies in $L_{loc}^1([0, +\infty))$ for all $i \in \mathbb{N}$.

Moreover, the total mass $\sum_{i \in \mathbb{N}} i c_i(t)$ is conserved for all $t \in [0, +\infty)$, i.e. no gelation occurs.

Proof. We pass to the limit $N \rightarrow \infty$ in the approximating cutoff system. Remembering the uniform bound $\sum_{i=1}^N i c_i^N(t) \leq M_{in}$ for all $t \geq 0$ and the strong convergence $c_i^N(t) \rightarrow c_i(t)$ for a.e. $t \geq 0$, it is clear that (for any given $i \in \mathbb{N}$)

$$\frac{d}{dt} c_i^N \rightharpoonup \frac{d}{dt} c_i \quad \text{in } \mathcal{D}'((0, +\infty)),$$

and

$$\sum_{j=1}^{i-1} a_{j,i-j} c_j^N(t) c_{i-j}^N(t) \rightarrow \sum_{j=1}^{i-1} a_{j,i-j} c_j(t) c_{i-j}(t), \quad \text{for a.e. } t \geq 0.$$

The crucial point is to prove that (for all $i \in \mathbb{N}$)

$$\sum_{j=1}^N a_{i,j} c_j^N(t) \rightarrow \sum_{j=1}^{\infty} a_{i,j} c_j(t), \quad L^1([0, T]),$$

for all $T > 0$ in order to be able to pass to the limit in the cutoff system (10) in the sense of distributions. We therefore estimate for any $i \in \mathbb{N}$ and $N_0 < N$:

$$\begin{aligned}
\left| \sum_{j=1}^N a_{i,j} c_j^N(t) - \sum_{j=1}^{\infty} a_{i,j} c_j(t) \right| &\leq \sum_{j=N+1}^{\infty} K(i+j) c_j(t) \\
&\quad + \sum_{j=1}^N K(i+j) |c_j^N(t) - c_j(t)| \\
&\leq \frac{K(i+N+1)}{(N+1)\ln(N+1) - (N+1) + 1} \sum_{j=N+1}^{\infty} (j \ln j - j + 1) c_j(t) \\
&\quad + K(i+N_0) \sum_{j=1}^{N_0} |c_j^N(t) - c_j(t)| + \frac{K(i+N_0+1)}{(N_0+1)\ln(N_0+1) - (N_0+1) + 1} \\
&\quad \times \sum_{j=N_0+1}^N (j \ln j - j + 1) |c_j^N(t) - c_j(t)| \\
&\leq K(i+N_0) \sum_{j=1}^{N_0} |c_j^N(t) - c_j(t)| + \frac{K(i+N_0+1)}{(N_0+1)\ln(N_0+1) - (N_0+1) + 1} \\
&\quad \times \sum_{j=N_0+1}^{\infty} (j \ln j - j + 1) \left(c_j^N(t) \mathbf{1}_{j \leq N} + c_j(t) \right) \\
&\leq K(i+N_0) \sum_{j=1}^{N_0} |c_j^N(t) - c_j(t)| + \frac{2KC(T, K, L_{in})(i+N_0+1)}{(N_0+1)\ln(N_0+1) - (N_0+1) + 1},
\end{aligned}$$

which proves the strong L^1 -convergence as N_0 can be taken arbitrarily large in the limit $N \rightarrow \infty$. \square

3 - Discrete coagulation-fragmentation models

In the previous Section, we have considered pure coagulation models and seen that superlinear coagulation coefficients lead to gelation. In this Section, we shall also take into account the opposing process of the break-up of clusters.

We shall first focus on discrete-in-size coagulation-fragmentation models, i.e. $i \in \mathbb{N} = Y$, $c_i(t) \geq 0$, $c = (c_i)$, and we consider the evolutionary problem

$$\begin{aligned}
\frac{d}{dt} c_i(t) &= Q_{coag}(c, c) + Q_{frag}(c) \\
&= Q_1(c, c) - Q_2(c, c) + Q_3(c) - Q_4(c).
\end{aligned}$$

Here, $Q_{frag}(c) = Q_3(c) - Q_4(c)$ denotes a linear fragmentation term consisting of a gain term $Q_3(c)$, which describes the creation of cluster of size i due to break-up of

larger clusters ($\beta_{i+j,i}$ is related to the number of clusters obtained after breakup):

$$\{i+j\} \xrightarrow{B_{i+j}\beta_{i+j,i}} \{i\} + \{j\}, \quad j > 1$$

and a loss term $Q_4(c)$, accounting for the fragmentation of clusters of size i :

$$\{i\} \xrightarrow{B_i} \text{all pairs } \{i-j\} + \{j\} \quad \text{with } j < i.$$

Altogether, we consider the following discrete-in-size coagulation-fragmentation model:

$$\begin{aligned} (17) \quad \frac{d}{dt} c_i(t) &= Q_{coag}(c, c) + Q_{frag}(c) \\ &= \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} c_{i-j} c_j - \sum_{j=1}^{\infty} a_{i,j} c_i c_j + \sum_{j=1}^{\infty} B_{i+j} \beta_{i+j,i} c_{i+j} - B_i c_i \end{aligned}$$

with the coagulation-fragmentation coefficients

$$\begin{aligned} (18) \quad a_{i,j} &= a_{j,i} \geq 0, \quad \beta_{i,j} \geq 0, \quad (i, j \in \mathbb{N}), \\ B_1 &= 0 \quad B_i \geq 0, \quad (i \in \mathbb{N}), \\ (\text{mass conservation}) \quad i &= \sum_{j=1}^{i-1} j \beta_{i,j}, \quad (i \in \mathbb{N}, i \geq 2). \end{aligned}$$

The last assumption on the fragmentation coefficients in (18) ensures the formal conservation of mass. This can be best seen in the weak formulation of the discrete coagulation-fragmentation problem: Given a test-sequence φ_i , we have

$$\begin{aligned} (19) \quad \sum_{i=1}^{\infty} \varphi_i Q_{coal}(c, c) &= \frac{1}{2} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} a_{i,j} c_i c_j (\varphi_{i+j} - \varphi_i - \varphi_j), \\ \sum_{i=1}^{\infty} \varphi_i Q_{frag}(c) &= - \sum_{i=2}^{\infty} B_i c_i \left(\varphi_i - \sum_{j=1}^{i-1} \beta_{i,j} \varphi_j \right). \end{aligned}$$

Thus, testing the weak formulation with the sequence $\varphi_i = i$, it follows analog to the Smoluchowski equation that the mass is non-increasing in time:

$$(20) \quad \rho(t) = \sum_{i=1}^{\infty} i c_i(t, x) dx \leq \sum_{i=1}^{\infty} i c_i^{in}(x) dx = \rho^{in}.$$

If gelation occurs in (20), then $\rho(t) < \rho^{in}$ for a finite time $t > 0$. We remark that although fragmentation can prevent gelation to occur in some situations this will not be possible in general, see e.g. [2, 17, 30, 31, 41]. Depending on the coefficients of coagulation and fragmentation, three cases are distinguished: i) weak coagulation (entailing the existence of a mass-conserving solution independently of the presence

of fragmentation), ii) strong fragmentation (entailing the existence of a mass-conserving solution due to the presence of fragmentation), and iii) strong coagulation, where gelation occurs depending on the initial mass and the growth behaviour of the coefficients of coagulation and fragmentation.

3.1 - The Becker-Döring model

The Becker-Döring model is a classical discrete coagulation-fragmentation model, which considers only interactions between monomers (i.e. clusters of size one) and polymers: First, the binary coagulation between monomers and polymers leads to the formation of particles of size i

$$Q_1(c, c) : \quad \{i-1\} + \{1\} \xrightarrow{a_{i-1}} \{i\}, \quad 1 < i,$$

and the consumption of particles of size i

$$Q_2(c, c) : \quad \{i\} + \{1\} \xrightarrow{a_i} \{i+1\}, \quad 1 \leq i.$$

Secondly, fragmentation of monomers from polymers leads to the gain of particles of size i

$$Q_3(c) : \quad \{i+1\} \xrightarrow{b_{i+1}} \{i\} + \{1\}, \quad 1 \leq i,$$

as well as the loss of particles of size i

$$Q_4(c) : \quad \{i\} \xrightarrow{b_i} \{i-1\} + \{1\}, \quad 1 < i.$$

The Becker-Döring model, in which all coagulation and fragmentation events involve monomers, can be rewritten as a coupled system of a monomer-equation and a hierarchy of polymer-equations:

$$\begin{aligned} \frac{d}{dt} c_1 &= -W_1(c) - \sum_{i=1}^{\infty} W_i(c), \\ \frac{d}{dt} c_i &= W_{i-1}(c) - W_i(c), \quad i \geq 2, \end{aligned}$$

where

$$W_i(c) = a_i c_1 c_i - b_{i+1} c_{i+1},$$

and we redefine (compared to (18)) $a_1 = \frac{a_{1,2}}{2}$, $b_2 = \frac{b_{1,1}}{2}$, and $a_i = a_{i,1}$, $b_i + 1 = b_{i,1}$ for $i \geq 2$.

The theory of coagulation-fragmentation models is in general much better developed when assuming a so called *detailed balance condition*, i.e. when assuming the

existence of a nonnegative *equilibrium* $E(y) \in L_1^1(Y) = L^1(Y, (1+y)dy)$ such that

$$a(y, y') E(y) E(y') = b(y, y') E(y + y'), \quad (y, y') \in Y \times Y.$$

The detailed balance condition is then also satisfied by all functions

$$E_z(y) = E(y) z^y, \quad y \in Y, \quad \text{for } z \geq 0,$$

yet E_z is not necessarily in $L_1^1(Y)$. One therefore defines

$$\begin{aligned} z_s &= \sup \{z \geq 0 : E_z \in L_1^1(Y)\}, & z_s &\in [1, \infty], \\ \rho_s &= M_1(E_{z_s}(y)) \in [0, \infty], & \rho_s &\in [0, \infty], \end{aligned}$$

and ρ_s is called the *saturation mass* and denotes the largest mass to be represented by a detailed balance equilibrium.

A most important consequence of assuming a detailed balance condition is the existence of a monotone entropy functional:

$$H(f|E) = \int_Y f \left(\ln \left(\frac{f}{E} \right) - 1 \right) dy,$$

satisfying the following H-Theorem:

$$\begin{aligned} \frac{d}{dt} H(f|E) &= -\frac{1}{2} D(f), \\ D(f) &= \int_Y \int_Y (aff' - bf'') (\ln(aff') - \ln(bf'')) dy dy', \end{aligned}$$

where we have used the shorthand notation $f = f(y)$, $f' = f(y')$ and $f'' = f(y + y')$. Note, that the entropy dissipation $D(f)$ vanishes only for detail-balance equilibria.

3.2 - Saturation phenomena and large-time asymptotics

Detailed balance equilibria of the Becker-Döring can only represent mass up to the saturation mass ρ_s . It is thus conjectured that in the large-time behaviour

$$f(t, y) \xrightarrow{t \rightarrow \infty} E_z(y) \quad \text{with} \quad \begin{cases} z : M_1(E_z) = M_1(f_{in}) & \text{if } M_1(f_{in}) \leq \rho_s, \\ z = z_s & \text{if } M_1(f_{in}) > \rho_s. \end{cases}$$

This conjecture has been proven for the Becker-Döring model as well as certain generalisations, and under certain assumptions of strong fragmentation, see e.g. [3, 56, 8, 9, 16].

In the following we shall illustrate the saturation phenomenon in the Becker-Döring model by assuming an initial mass $\rho^{in} = M_1(c^{in})$ larger than the saturation

mass $\rho_s = M_1(E_{z_s}) < \infty$:

$$\rho^{in} > \rho_s = M_1(E_{z_s}).$$

According to the conjecture, we expect that $c_i(t) \rightarrow E_i z_s^i$ as $t \rightarrow \infty$, while the remaining mass $\rho^{in} - \rho_s$ should go to larger and larger clusters as $t \rightarrow \infty$.

The following method of proving rigorously the large time behaviour of the Becker-Döring model was first developed by Penrose [51] and later extended by Niethammer [47] to coefficients of the type

$$a_i = a_1 i^\alpha, \quad b_i = a_i(z_s + q i^{-\gamma}), \quad i \geq 2,$$

with $\alpha \in (0, 1]$, $\gamma \in [0, 1)$, $a_1 > 0$, $z_s > 0$, $q > 0$. A first step applies the time rescaling $\tau = \varepsilon^{1-\alpha+\gamma} t$ and introduces a cutoff index i_ε such that $i_\varepsilon \rightarrow \infty$ and $\varepsilon i_\varepsilon \rightarrow 0$ as $\varepsilon \rightarrow 0$. In [3], it was shown that the solution of the above Becker-Döring model conserves mass $M_1(t) = M_1(0)$ for all $t \geq 0$.

The goal is thus to capture the saturation mass in $\sum_{i=1}^{i_\varepsilon} i c_i(\tau) \sim \rho_s$ while the excess mass $\rho^{in} - \rho_s$ is contained in even larger clusters.

Using mass conservation and the above rescaling, the Becker-Döring model can be written in the following alternative formulation:

$$\begin{aligned} \sum_{i=1}^{\infty} i c_i(\tau) &= \rho, \\ \frac{d}{d\tau} c_i &= \frac{1}{\varepsilon^{1-\alpha+\gamma}} (W_{i-1}(c) - W_i(c)), \quad i \geq 2, \end{aligned}$$

where

$$\begin{aligned} W_i(c) &= a_i \left(c_1 - \frac{b_i}{a_i} \right) c_i - (b_{i+1} c_{i+1} - b_i c_i) \\ &= a_1 i^\alpha (c_1 - z_s - q i^{-\gamma}) - (b_{i+1} c_{i+1} - b_i c_i). \end{aligned}$$

Next, one introduces the following continuum approximation in the study of the excess mass: For $(\tau, x) \in (0, \infty) \times ((i - 1/2)\varepsilon, (i + 1/2)\varepsilon)$, we consider

$$f(\tau, x) = \frac{1}{\varepsilon^2} c_i(\tau), \quad W(\tau, x) = \frac{1}{\varepsilon^2} W_i(f(\tau)),$$

and obtain

$$\partial_\tau f = -\partial_x W(f), \quad W(f)(\tau, x) \sim a_1(x^\alpha u(\tau) - q x^{\alpha-\gamma}),$$

where $u(\tau) = \varepsilon^{-\gamma}(c_1(\tau) - z_s)$. Then, using that $c_1(\tau) \rightarrow E_1 z_s$ and $\frac{E_i}{E_{i+1}} = \frac{z_s}{E_1}$ for large i , Niethammer [47] showed for a suitable choice of i_ε (e.g. $i_\varepsilon = -\ln(\varepsilon)$) and by applying the continuum approximation for $i \geq i_\varepsilon$, i.e. for $x \in ((i_\varepsilon - 1/2)\varepsilon, \infty)$ that

in the limit $\varepsilon \rightarrow 0$ with $i_\varepsilon \rightarrow \infty$ and $i_\varepsilon \varepsilon \rightarrow 0$:

$$\sum_{i=1}^{i_\varepsilon} i c_i(\tau) \sim \rho_s, \quad \int_0^\infty x f(\tau, x) dx = \rho - \rho_s.$$

For many general coagulation-fragmentation models, the characterisation of saturation remains an open problem.

4 - Spatially inhomogeneous coagulation-fragmentation models with diffusion

This Section is devoted to spatially inhomogeneous coagulation-fragmentation models with diffusion, i.e. we study the evolution of a polymer/cluster density $f(t, x, y) \geq 0$ depending on time $t \geq 0$, size $y \in Y = [0, \infty)$ and position $x \in \Omega \subset \mathbb{R}^d$ and subject to

$$\begin{aligned} (21) \quad \partial_t f - d(y) \Delta_x f &= Q_{coag}(f, f) + Q_{frag}(f) \\ &= Q_1(f, f) - Q_2(f, f) + Q_3(f) - Q_4(f), \end{aligned}$$

with a size-dependent diffusion coefficients $d(y)$ and diffusion is taking place within a bounded domain Ω with sufficiently smooth boundary $\partial\Omega$ (e.g. $\partial\Omega \in C^2$). W.l.o.g. we can assume a normalised volume $|\Omega| = 1$ after rescaling x accordingly. Together with (21), we assume non-flux homogeneous Neumann boundary conditions

$$(22) \quad \nabla_x f(t, x, y) \cdot \nu(x) = 0 \quad \text{on} \quad \partial\Omega,$$

and nonnegative initial data

$$(23) \quad 0 \leq f_{in}(x, y).$$

The existence theory of spatially inhomogeneous (or also homogeneous) coagulation-fragmentation models like eqs. (21)-(23) has applied two basic functional settings: The first is based on fixed-point and compactness methods in spaces of continuous functions (see e.g. [44, 45, 27, 34, 63]) while the second uses weak and strong compactness methods in $L^1(Y)$ (see, e.g. [3, 57, 14, 15, 30, 39, 40]). The latter approach has the advantage of only relying on a physically natural setting of nonnegative initial data with integrable number and mass densities, i.e. $0 \leq f_{in}(y) \in L^1_1(Y) = L^1(Y, (1+y)dy)$ and shall be presented in the following Section.

4.1 - Existence theory in L^1 via weak compactness

Following [39], we shall show in this Section the existence of (global) weak solutions of continuous coagulation-fragmentation models with diffusion based on weak compactness methods in $L^1(Y)$.

Definition 4.1 (Weak solutions of continuous coagulation-fragmentation models with diffusion). *Let $T \in (0, \infty]$. Assume nonnegative initial data with finite mass, i.e. $0 \leq f_{in} \in L^1(\Omega \times \mathbb{R}_+; (1+y)dxdy)$.*

Then, a weak solution of the coagulation-fragmentation model (21)-(23) on $[0, T]$ is a non-negative function

$$f \in C((0, T); L^1(\Omega \times \mathbb{R}_+)) \cap L^\infty(0, T; L^1(\Omega \times \mathbb{R}_+; ydydx))$$

satisfying $f(0) = f_{in}$ and $f \in L^1((0, T) \times (1/R, R); W^{1,1}(\Omega))$ for all $R \in \mathbb{R}_+$.

Moreover, the four gain- and loss terms of coagulation and fragmentation are integrable in the sense that

$$Q_{1,2,3,4} \in L^1((0, T) \times \Omega \times (0, R)).$$

Finally, f satisfies the following weak formulation

$$\begin{aligned} \int_{\Omega} \int_0^\infty (\psi(t)f(t) - \psi(0)f^{in}) dydx + \int_0^t \int_{\Omega} \int_0^\infty (-f \partial_t \psi + d(y) \nabla f \nabla \psi) dydxds \\ = \frac{1}{2} \int_0^t \int_{\Omega} \int_0^\infty Q(f) \psi dydxds, \quad \forall t \in (0, T), \end{aligned}$$

for all compactly supported (in y) test functions $\psi \in C^1([0, T] \times \Omega \times \mathbb{R}_+)$.

The crucial step of the proof is the following weak stability principle:

Proposition 4.1 (Stability principle for weak solutions in L^1 , [39]). *For $T \in (0, \infty)$ let (f_n) be a sequence of weak solutions of the coagulation-fragmentation model (21)-(23) with sequences of coefficients $a_n \rightarrow a$, $b_n \rightarrow b$ and $d_n \rightarrow d$ and a common initial data f_{in} . For all $n \in \mathbb{N}$ let $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ be a weakly compact set with*

$$f_n(t) \in \mathcal{K}_w, \quad \text{for each } t \in [0, T],$$

and suppose moreover for all $R > 0$ and $i \in \{1, 2, 3, 4\}$ that

$$\begin{aligned} \sup_{t \in [0, T]} \int_{\Omega} \int_0^\infty f_n(t)(1+y) dydx \leq C_T, \\ Q_{i,n}(f_n) \text{ weakly compact in } L^1((0, T) \times \Omega \times (0, R)). \end{aligned}$$

Then, there exists a subsequence (f_{n_k}) and a limiting function f such that

$$\begin{aligned} f_{n_k} \rightharpoonup f \quad \text{in } C([0, T]; w - L^1(\Omega \times \mathbb{R}_+)), \\ Q_{i,n_k}(f_{n_k}) \rightharpoonup Q_i(f) \quad \text{weakly in } L^1((0, T) \times \Omega \times (0, R)), \end{aligned}$$

for $R \in \mathbb{R}_+$, $i \in \{1, 2, 3, 4\}$. Thus, f is a weak solution of the coagulation-fragmentation problem (21)-(23) on $[0, T)$. Moreover,

$$\int_0^\infty \psi(y) f_{n_k} dy \rightarrow \int_0^\infty \psi(y) f dy \quad \text{in } L^1((0, T) \times \Omega)$$

for $\psi \in \mathcal{D}(\mathbb{R}_+)$. Finally, the total mass satisfies $\int_\Omega M_1(t) dx \leq \int_\Omega M_1(0) dx$

The above weak stability principle Lemma 4.1 can be proven, for instance, in a framework of coagulation-fragmentation models satisfying a detailed balance condition. In the following, we shall discuss how the associated entropy and entropy-dissipation functionals entail natural *a priori* estimates, which are sufficient to prove the weak compactness required by the weak stability principle Lemma 4.1 for solutions of eq. (21).

We consider a given detailed balance equilibrium $E(y)$ and the associated relative entropy functional

$$(24) \quad H(f|E(y)) = \int_\Omega \int_Y f \left(\ln \left(\frac{f}{E} \right) - 1 \right) dy,$$

which dissipates according to the following H-Theorem:

$$(25) \quad \frac{d}{dt} H(f|E) + \int_\Omega \int_Y d(y) \frac{|\nabla f|^2}{f} dy dx + \frac{1}{2} \int_\Omega \int_Y \int_Y (aff' - bf'') (\ln(aff') - \ln(bf'')) dy dy' dx = 0,$$

where we denote $f = f(y)$, $f' = f(y')$, $f'' = f(y + y')$.

Note that the entropy dissipation functional consists of two nonnegative integral terms, which express the entropy dissipation due to diffusion, the so called *Fisher information*, and the entropy dissipation due to coagulation and fragmentation.

Supposing initial data with finite entropy $H(f_{in}|E) \leq C < \infty$, the H-Theorem (25) implies formally a uniform-in-time bound of the relative entropy

$$(26) \quad \sup_{t \in [0, \infty)} H(f(t)|E) \leq H(f_{in}|E) \leq C < \infty.$$

In return, this implies also that the time-integral of the entropy dissipation functional is uniformly bounded for any time interval $[0, T]$. More precisely, we have that the time-integrated Fisher information

$$(27) \quad \int_0^T \int_\Omega \int_Y d(y) \frac{|\nabla f|^2}{f} dy dx ds \leq C, \quad \text{for all } T > 0,$$

and the time-integrated coagulation-fragmentation part of the entropy dissipation

$$(28) \quad \int_0^T \int_{\Omega} \int_Y \int_Y (aff' - bf'')(\ln(aff') - \ln(bf'')) dy dy' dx ds \leq C, \quad \text{for all } T > 0,$$

constitute a *natural set of a priori estimates* related to the entropy dissipation for various constants $C = C(\Omega, E(y), H(f^{in}|E))$ depending only on the domain Ω , the detailed balance equilibrium $E(y)$ and the initial relative entropy $H(f^{in}|E)$.

As a second natural *a priori estimate*, we shall use that the total mass is bounded uniformly in time if the initial mass $\int_{\Omega} \int_Y y f_{in}(x, y) dy dx$ is finite:

$$(29) \quad C_0 = \sup_{t \in [0, \infty)} \int_{\Omega} \int_Y y f(t, x, y) dy dx \leq \int_{\Omega} \int_Y y f_{in}(x, y) dy dx < \infty.$$

In the following, we shall always consider solutions subject to nonnegative initial data f_{in} (23) with finite mass and entropy.

The below two Lemmas establish additional *a priori* estimates, which allow to prove the weak compactness required by Proposition 4.1:

Lemma 4.1 (see [39] for the proof). *Let $\xi : \mathbb{R}_+ \times \Omega \times Y \mapsto \{0, 1\}$ be measurable and $\alpha \geq e^2$. Then, for $t \geq 0$*

$$\int_{\Omega} \int_Y \xi(t) f(t) dy dx \leq 2(\alpha + e^{-1}) \int_{\Omega} \int_Y \xi(t) E dy dx + \frac{2}{\ln(\alpha)} H(f(t)|E).$$

Lemma 4.2. *For $t \in \mathbb{R}_+$ holds with $f(t) \left| \ln \frac{f(t)}{E(y)} \right| \leq f(t) \ln \frac{f(t)}{E(y)} + \frac{2E}{e}$,*

$$(30) \quad \int_{\Omega} \int_Y f(t) \left(1 + \left| \ln \left(\frac{f(t)}{E(y)} \right) \right| \right) dy dx \leq C.$$

Proof. It follows from Lemma 4.1 with $\xi(t) = \mathbf{1}_{\Omega \times Y}$ that

$$\int_{\Omega} \int_Y f(t) dy dx \leq C|\Omega| \|E\|_1 + C \leq C,$$

for a constant $C = C(\Omega, E(y), H(f^{in}|E), C_0)$. □

Before proving the weak compactness Lemma 4.4 required for the weak stability principle in Proposition 4.1, we recall the Dunford-Pettis theorem on weak compactness in L^1 :

Lemma 4.3 (Dunford-Pettis theorem). *A sequence (f_n) is contained in a weakly compact subset $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ if (f_n) is bounded in $L^1(\Omega \times \mathbb{R}_+)$ and satisfies:*

$$\lim_{R \rightarrow \infty} \sup_{n \geq 1} \int_{\{f_n \geq R\}} f_n(x, y) dx dy = 0,$$

and if for all $\varepsilon > 0$, there exists a measurable $S \subset \Omega \times \mathbb{R}_+$ with $|S| < \infty$ such that

$$\sup_{n \geq 1} \int_{(\Omega \times \mathbb{R}_+) \setminus S} |f_n| \leq \varepsilon.$$

Lemma 4.4 (Weak compactness lemma, [39]). *Let $T \in \mathbb{R}_+$ and let $(f_n) \geq 0$ be a sequence such that for all $n \geq 1$*

$$(31) \quad \sup_{t \in [0, T]} \int_{\Omega} \int_Y f_n(t) \left(1 + y + \left| \ln \left(\frac{f_n(t)}{E(y)} \right) \right| \right) dy dx \leq C_T,$$

$$(32) \quad \int_0^T \int_{\Omega} \int_Y \int_Y (a_n f_n f'_n - b_n f''_n) (\ln(a_n f_n f'_n) - \ln(b_n f''_n)) dy dy' dx ds < C_T,$$

with constants $C_T = C(T, \Omega, E(y), H(f^{in}|E), C_0)$ not depending on n .

Then, the sequence (f_n) is weakly compact in $L^1((0, T) \times \Omega \times \mathbb{R}_+)$ and the sequences $(Q_i(f_n))$ are weakly compact in $L^1((0, T) \times \Omega \times (0, R))$ for $i \in 1, 2, 3, 4$ and $R \in \mathbb{R}_+$.

Moreover, there exists a weakly compact subset $\mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ such that $(f_n(t)) \in \mathcal{K}_w$ for all $t \in [0, T]$ and $n \geq 1$.

Proof (Sketch of the proof). At first, for $S \subset \Omega \times \mathbb{R}_+$ measurable, $|S| < \infty$ and $\alpha \geq e^2$, it follows from (31) and Lemma 4.1 that

$$(33) \quad \int_S f_n(t) dy dx \leq 4\alpha \int_S E(y) dy dx + \frac{2C_T}{\ln(\alpha)} \leq C_T(E, |S|, \alpha).$$

Eq. (31) implies moreover that

$$(34) \quad \int_{\Omega} \int_{\alpha}^{\infty} f_n(t) dy dx \leq \frac{C_T}{\alpha}.$$

Thus, $f_n(t) \in \mathcal{K}_w \subset L^1(\Omega \times \mathbb{R}_+)$ for all $n \geq 1$ with \mathcal{K}_w defined in the way that $g \in \mathcal{K}_w$ satisfies the above equations (33) and (34) for all measurable $S \subset \Omega \times \mathbb{R}_+$ with $|S| < \infty$ and $\alpha \geq e^2$. Moreover, since $E(y) \in L^1(0, \infty)$ and $|\Omega| = 1$, the Dunford-Pettis theorem shows that \mathcal{K}_w is weakly compact.

In the following, we sketch how to show the integrability of the coagulation and fragmentation integral $Q_{1,n}$, $Q_{2,n}$, $Q_{3,n}$ and $Q_{4,n}$ (see [39] for the details).

First, for all $R \in \mathbb{R}_+$

$$Q_{4,n}(f_n) = \frac{f_n(t, x, y)}{2} \int_0^y b_n(y', y - y') dy' \leq R \|b_n\|_\infty f_n.$$

Therefore, the sequence $(Q_{4,n}(f_n))$ (where $Q_{4,n}$ may be an approximation of Q_4 with coefficients $a_n \rightarrow a$, $b_n \rightarrow b$ and $d_n \rightarrow d$) is weakly compact in $L^1((0, T) \times \Omega \times (0, R))$ since (f_n) is weakly compact and $\|b_n\|_\infty$ is assumed bounded.

Secondly, we observe that for all $\alpha \geq e^2$, the elementary inequality $\eta \leq \alpha \xi + \frac{(\eta - \xi) \ln(\eta/\xi)}{\ln(\alpha)}$ for $(\eta, \xi) \in \mathbb{R}_+^2$ yields for measurable $S \subset (0, T) \times \Omega \times (0, R)$

$$\int_S a_n(y', y - y') f_n(y') f_n(y - y') dy dx dt \leq \alpha \sup_{n \geq 1} \int_S Q_4(f_n) dy dx dt + \frac{C_T}{\ln(\alpha)}.$$

Letting then $\alpha \rightarrow \infty$ shows that the sequence $(Q_{1,n}(f_n))$ is weakly compact in $L^1((0, T) \times \Omega \times (0, R))$ for all $R \in \mathbb{R}_+$.

In a third step, we have for all $\alpha \geq 2R \in \mathbb{R}_+$

$$\begin{aligned} \int_S Q_{3,n}(f_n) dy dx dt &\leq \int \int_0^\alpha b_n(y, y - y') f_n(y') dy' dy dx dt \\ &\quad + \|b_n\|_{L^\infty(a-R, \infty)} \int_S \int_\alpha^\infty f_n(y') dy' dy dx dt \\ &\leq C \int_S \int_0^\alpha f_n(y') dy' dx dt + \|b_n\|_{L^\infty(a-R, \infty)} C(T, R), \end{aligned}$$

and the sequence $(Q_{3,n}(f_n))$ is weakly compact in $L^1((0, T) \times \Omega \times (0, R))$ since (f_n) is weakly compact.

Finally, because of

$$\int_0^T \int_\Omega \int_Y \int_Y (a_n f_n f'_n - b_n f''_n) \ln \left(\frac{a_n f_n f'_n}{b_n f''_n} \right) dy dy' dx ds < C_T,$$

it follows also that $(Q_{2,n}(f_n))$ is weakly compact in $L^1((0, T) \times \Omega \times (0, R))$ from the weak compactness of $(Q_{3,n}(f_n))$ in a similar argument as above showing the weak compactness of $(Q_{1,n}(f_n))$.

The existence of weak solutions in L^1 to discrete inhomogeneous coagulation-fragmentation models with diffusion can be shown in a similar way to above, see [40]. More precisely, we consider for $c = (c_i)$, $i \in \mathbb{N}$ the system

$$(35) \quad \begin{aligned} \frac{d}{dt} c_i - d_i \Delta_x c_i &= Q_{coag}(c, c) + Q_{frag}(c) \\ &= \frac{1}{2} \sum_{j=1}^{i-1} a_{i-j,j} c_{i-j} c_j - \sum_{j=1}^{\infty} a_{i,j} c_i c_j + \sum_{j=1}^{\infty} B_{i+j} \beta_{i+j,i} c_{i+j} - B_i c_i, \end{aligned}$$

together with homogeneous Neumann boundary conditions

$$(36) \quad \nabla_x c_i(t, x) \cdot \nu(x) = 0 \quad \text{on} \quad \partial\Omega, \quad i \in \mathbb{N},$$

and nonnegative initial data

$$(37) \quad c_i^{in}(x, y) \geq 0, \quad i \in \mathbb{N}.$$

In eq. (35), the (d_i) denote a sequence of size-dependent diffusion coefficients and diffusion is taking place within a smoothly bounded (e.g. $\partial\Omega \in C^2$) domain Ω with normalised volume $|\Omega| = 1$.

Weak (global) solutions of the discrete coagulation-fragmentation model with diffusion (35)-(37) are defined as follows:

Definition 4.2 (Weak solutions of discrete inhomogeneous coagulation-fragmentation model with diffusion). *Let $T \in (0, \infty]$ and suppose initial data $0 \leq c_i^{in} \in L^1(\Omega)$ with finite total mass $\sum_{i=1}^{\infty} i \|c_i^{in}\|_1 < \infty$.*

Then, a weak solution of (35)-(37) on $[0, T)$ is a non-negative function

$$c_i \in C([0, T); L^1(\Omega)), \quad \sup_{t \in [0, T)} \sum_{i=1}^{\infty} i \|c_i\|_1 < C(c_i^{in}), \quad i \in \mathbb{N},$$

with $Q_{1,2,3,4}(c) \in L^1((0, T) \times \Omega)$. Moreover, c_i are mild solutions of

$$c_i(t) = e^{d_i \Delta_x t} c_i^{in} + \int_0^t e^{d_i \Delta_x (t-s)} (Q_{coag} + Q_{frag})(c(s)) ds, \quad i \in \mathbb{N},$$

and $e^{d_i \Delta_x t}$ is the C_0 -semigroup of $d_i \Delta_x$ in $L^1(\Omega)$ with homogeneous Neumann boundary conditions.

Remark 4.1. *We remark that weak L^1 -solutions require in particular the quadratic, infinite sum of the loss term of coagulation to be integrable, i.e.*

$$Q_2(c) = \sum_{j=1}^{\infty} a_{i,j} c_i c_j \in L^1((0, T) \times \Omega).$$

Proposition 4.2 (Global weak solutions, [40]). *Assume that the coefficients of (35) satisfy*

$$(38) \quad \lim_{j \rightarrow \infty} \frac{a_{i,j}}{j} = \lim_{j \rightarrow \infty} \frac{B_{i+j} \beta_{i+j,i}}{i+j} = 0, \quad (\text{for fixed } i \geq 1).$$

Then, there exists a global weak solutions $c_i \in C([0, T]; L^1(\Omega))$, $i \in \mathbb{N}$ for all $T > 0$ satisfying in particular that the total mass is non-increasing

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

and that the loss term of the coagulation $Q_2(c)$ is integrable

$$\sum_{j=1}^{\infty} a_{i,j} c_i c_j \in L^1([0, T] \times \Omega).$$

4.2 - Duality method and global L^2 -estimate

At the price of less general initial data with $\rho^{in} \in L^2(\Omega)$, a theory of existence and absence of gelation for discrete inhomogeneous coagulation-fragmentation models with diffusion was presented in [5] and extended to degenerate diffusion coefficients in [6].

The key lemma applies a duality method (see e.g. [36, 52, 21] and also [7] for a recent improvement) to establish a global-in-time $L^2(\Omega)$ -estimate, which can also be generalised to degenerate diffusion coefficients, see [5, 6, 21]:

Lemma 4.5 (Global $L^2(\Omega)$ -estimates via duality, see [5, 6]). *Assume coagulation-fragmentation coefficients satisfying (38) and suppose initial data with $\rho^{in}(x) = \sum_{i=1}^{\infty} i c_i^{in}(x) \in L^2(\Omega)$.*

Then, for all $T > 0$

$$(39) \quad \|\rho\|_{L^2(\Omega_T)} \leq \left(1 + \frac{\sup\{d_i\}}{\inf\{d_i\}} \right) T \|\rho^{in}\|_{L^2(\Omega)},$$

or for degenerate diffusion (i.e. $\inf_i \{d_i\} = 0$)

$$(40) \quad \int_0^T \int_{\Omega} \left[\sum_{i=1}^{\infty} i d_i c_i(t, x) \right] \left[\sum_{i=1}^{\infty} i c_i(t, x) \right] dx \leq 4 T \sup_{i \in \mathbb{N}} \{d_i\} \|\rho^{in}\|_{L^2(\Omega)}.$$

Proof (Proof of duality bounds). By denoting $A(t, x) = \frac{1}{\rho} \sum_{i=1}^{\infty} i d_i c_i$, it follows that $\|A\|_{\infty} \leq \sup_{i \in \mathbb{N}} \{d_i\}$ and that

$$\partial_t \rho - A_x(A \rho) = 0.$$

Then, multiplication with the nonnegative solution $w(t, x)$ of the dual problem:

$$(41) \quad \begin{aligned} -(\partial_t w + A A_x w) &= H \sqrt{A}, \\ \nabla_x w \cdot \nu(x)|_{\partial \Omega} &= 0 \\ w(T, \cdot) &= 0 \end{aligned}$$

for any smooth function $H = H(t, x) \geq 0$ leads to

$$(42) \quad \int_0^T \int_{\Omega} H(t, x) \sqrt{A(t, x)} \rho(t, x) dx dt = \int_{\Omega} w(0, x) \rho(0, x) dx.$$

Next, testing the dual problem (41) with $-A_x w$ (this can be made rigorous by a standard approximation procedure of solutions of parabolic problems, see [21]), we estimate

$$\begin{aligned} - \int_0^T \int_{\Omega} \partial_t (|\nabla w|^2 / 2) dx dt + \int_0^T \int_{\Omega} A (A_x w)^2 dx dt &\leq \int_0^T \int_{\Omega} H \sqrt{A} (-A_x w) dx dt \\ &\leq \frac{1}{4\varepsilon} \int_0^T \int_{\Omega} H^2 dx dt + \varepsilon \int_0^T \int_{\Omega} A (A_x w)^2 dx dt \end{aligned}$$

and obtain with $\nabla w(T) = 0$ and $\varepsilon = \frac{1}{2}$ that

$$\int_0^T \int_{\Omega} A (A_x w)^2 dx dt \leq \int_0^T \int_{\Omega} H^2 dx dt.$$

Therefore, in a second step, one can show that

$$\int_0^T \int_{\Omega} \frac{|\partial_t w|^2}{A} dx dt \leq 4 \int_0^T \int_{\Omega} H^2 dx dt,$$

and hence, with $|w(0, x)|^2 \leq \left(\int_0^T \sqrt{A} \frac{|\partial_t w|}{\sqrt{A}} dt \right)^2$ that

$$\int_{\Omega} |w(0, x)|^2 dx \leq 4 T \|A\|_{L^{\infty}(\Omega)} \int_0^T \int_{\Omega} H^2 dx dt.$$

Returning to eq. (42) above, we continue to estimate

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

for all nonnegative smooth functions H . Thus, by duality, we conclude that

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

which shows (40) and concludes the proof in case of degenerate diffusion coefficients. Finally, for bounded diffusion coefficients with $\inf_i \{d_i\} > 0$, the L^2 -bound (40) follows directly from (39). \square

4.3 - Global weak L^2 -solutions via duality method

The above duality Lemma 4.5 provides a uniform-in-time $L^2(\Omega)$ -bound without assumptions on the coagulation-fragmentation coefficients, in particular without any restriction on the growth of the coagulation coefficients $a_{i,j}$ which are responsible for gelation.

However, the construction of solutions of (35)-(37) requires a limit of suitable approximating solutions and in order to pass to the limit (similar to Section 2.3), we shall need the assumptions (38) as in the L^1 theory, i.e. as in Proposition 4.2 above. More precisely, for solutions c_i^N of approximating truncated systems, we need to pass to the limit in the lost term of coagulation

$$Q_2^N = c_i^N \sum_{j=1}^{\infty} a_{i,j} c_j^N.$$

Indeed, since c_i^N converges to c_i weak-* in $L^\infty((0, T) \times \Omega)$, we require that

$$\sum_{j=1}^{\infty} a_{i,j} c_j^N \rightarrow \sum_{j=1}^{\infty} a_{i,j} c_j \quad \text{strongly in } L^1((0, T) \times \Omega),$$

which can be shown under the assumption $\lim_{j \rightarrow \infty} \frac{a_{i,j}}{j} = 0$ by the following estimate

$$\int_0^T \int_{\Omega} \left| \sum_j a_{i,j} (c_j^N - c_j) \right| dx \, dt \leq 2 \sup_{j \geq j_0} \left| \frac{a_{i,j}}{j} \right| \|\rho\|_{L^2} + \sup_{j \leq j_0} \|c_j^N - c_j\|_{L^1}.$$

It is thus interesting to remark that the existence theory of the discrete coagulation-fragmentation model with diffusion (35)-(37) does not really benefit from

having a global L^2 -bound via the duality Lemma 4.5 in comparison to the L^1 theory developed in [39].

However, the L^2 approach succeeds in proving solutions for generalised coagulation-fragmentation models with quadratic fragmentation, for which the L^1 compactness theory can no longer be applied to, see [5]:

Theorem 4.1 (Existence theory for generalised quadratic models, [5]). *Consider the generalised quadratic coagulation-fragmentation model*

$$\begin{aligned} \partial_t c_i - d_i \Delta_x c_i &= \frac{1}{2} \sum_{k+l=i} a_{k,l} c_k c_l - \sum_{k=1}^{\infty} a_{i,k} c_i c_k \\ &+ \frac{1}{2} \sum_{k,l=1}^{\infty} \sum_{i < \max\{k,l\}} b_{k,l} c_k c_l \beta_{i,k,l} - \sum_{k=1}^{\infty} b_{i,k} c_i c_k. \end{aligned}$$

Then, global weak L^1 -solutions exist in 1D provided that

$$\lim_{l \rightarrow \infty} \frac{a_{k,l}}{l} = 0, \quad \lim_{l \rightarrow \infty} \frac{b_{k,l}}{l} = 0, \quad \lim_{l \rightarrow \infty} \sup_k \left\{ \frac{b_{k,l}}{kl} \beta_{i,k,l} \right\} = 0 \quad k, i \in \mathbb{N}.$$

4.4 - Absence of gelation

The following Theorem shows how the duality estimate 4.5 allows to prove absence of gelation. Provided bounded diffusion coefficients, this is done under almost as general assumptions on the coagulation coefficients as for space homogeneous models, see e.g. [2].

Theorem 4.2 (Absence of gelation, [5, 6]). *Assume an initial mass $\rho^{in}(x) \in L^2(\Omega)$. Moreover, in the case of bounded diffusion coefficients*

$$0 < \inf_{i \in \mathbb{N}} \{d_i\} \leq d_i \leq \sup_{i \in \mathbb{N}} \{d_i\} < \infty,$$

assume that there exists a bounded function $\theta : [0, +\infty) \rightarrow (0, +\infty)$ satisfying $\theta(x) \rightarrow 0$ as $x \rightarrow \infty$ such that

$$(43) \quad a_{i,j} \leq (i+j) \theta(\max\{j/i, i/j\}) \quad \text{for all } i, j \geq 1.$$

On the other hand, in the case of the degenerate diffusion coefficients

$$0 = \inf_{i \in \mathbb{N}} \{d_i\}, \quad Ci^{-\gamma} \leq d_i < \infty,$$

for an exponent $\gamma \in [0, 1]$ and a constant C , assume that

$$(44) \quad a_{i,j} \leq C(i^\alpha j^\beta + i^\beta j^\alpha) \quad \text{for all } i, j \geq 1,$$

with $\alpha + \beta + \gamma \leq 1$, $\alpha, \beta \in [0, 1]$ and a constant C .

Then, the weak solutions to the system (35)-(37) with coefficients (38) given by Proposition 4.2 and satisfying the global bounds of Lemma 4.5 have a bounded superlinear moment on bounded time intervals $[0, T]$ for all $T > 0$, i.e. there exists an increasing function $C = C(T) > 0$ and an increasing sequence of positive numbers $\{\psi_i\}_{i \geq 1}$ with $\lim_{i \rightarrow \infty} \psi_i \rightarrow \infty$ such that for all $T > 0$,

$$(45) \quad \int_{\Omega} \sum_{i=1}^{\infty} i \psi_i c_i \leq C(T) \quad \text{for all } t \in [0, T].$$

As a consequence, the total mass is conserved

$$\int_{\Omega} \rho(t, x) dx = \int_{\Omega} \rho^{in}(x) dx \quad \text{for all } t \geq 0.$$

Proof (Idea of the proof in a simplified case). We sketch the proof considering the special case of the sublinear kernel $a_{i,j} = \sqrt{ij}$ and by neglecting fragmentation $B_i = 0$ (w.l.o.g. since fragmentation counteracts gelation) and by assuming bounded diffusion coefficients. Moreover, to further simplify the argument, we shall assume initial data with a bounded first-logarithmic moment,

$$\int_{\Omega} \sum_{i=0}^{\infty} i \ln i c_i^{in}(x) dx < \infty.$$

For general initial data with bounded initial mass, one can construct a suitable superlinear initial moment using the De la Vallée-Poussin's lemma, see [10].

At first, we test the weak formulation with $\varphi_i = \ln i$ and use $\ln(1+x) \leq C\sqrt{x}$ to estimate

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} \sum_{i=1}^{\infty} i \ln i c_i dx &= \int_{\Omega} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} \sqrt{ij} c_i c_j \left(i \ln \left(1 + \frac{j}{i} \right) + j \ln \left(1 + \frac{i}{j} \right) \right) dx \\ &\leq 2 \int_{\Omega} \sum_{i=1}^{\infty} \sum_{j=1}^{\infty} ij c_i c_j dx \leq 2 \int_{\Omega} \rho(t, x)^2 dx. \end{aligned}$$

As a consequence, we have for all $T > 0$

$$\int_{\Omega} \sum_{i=0}^{\infty} i \ln i c_i(T, x) dx \leq \int_{\Omega} \sum_{i=0}^{\infty} i \ln i c_i(0, x) dx + 2 \int_0^T \int_{\Omega} \rho(t, x)^2 dx dt.$$

Then, the global L^2 -bounds of Lemma 4.5 ensure the propagation of the logarithmic moment $\int \sum_{i=0}^{\infty} i \ln i c_i(\cdot, x) dx$ and, thus, the mass conservation. \square

4.5 - Entropy method and convergence to equilibrium

In this Section, we prove explicit convergence to equilibrium for a continuous, spatially inhomogeneous coagulation-fragmentation model with diffusion and normalised coefficients.

The key lemma establishes a so called *entropy entropy-dissipation estimate*, an explicit bound of the relative entropy with respect to the global equilibrium in terms of the ongoing entropy dissipation.

This so called *entropy method* applies to evolutionary problems, which feature a monotone (e.g. nonincreasing) entropy functional E with an extremal (e.g. minimising) entropy E_{∞} , for which the entropy dissipates according to an entropy dissipation functional D , i.e.

$$(46) \quad \frac{d}{dt}E = \frac{d}{dt}(E - E_{\infty}) = -D \leq 0.$$

Moreover, the entropy dissipation functional is supposed to be non-degenerate in the sense that the global equilibrium can be uniquely identified for the set of states with zero entropy dissipation $D = 0$ by taking into account all the conservation laws of the system.

An entropy entropy-dissipation estimate is then a functional inequality of the form

$$(47) \quad D \geq \Phi(E - E_{\infty}), \quad \Phi(0) = 0, \quad \Phi \geq 0,$$

and a Gronwall lemma implies directly from the eqs. (46) and (47) the convergence to equilibrium in relative entropy. If $\Phi'(0) > 0$, then the obtained convergence is exponential.

The entropy method quantifies the large-time behaviour in terms of *functional inequalities*, which as such are not connected to the evolutionary problem. Thus, one advantage of the entropy method is a robustness in the sense that these functional entropy entropy-dissipation estimates may be reapplied in modified models. In fact, we shall give an example in the proof of Lemma 4.6 below.

Moreover, the entropy method avoids linearisation and/or compactness arguments and therefore yields global convergence with constants and rates, which can (in principle) be calculated explicitly.

Going back to ideas of Boltzmann and Grad, the entropy method has been successfully used in many situations ranging from (non)linear diffusion equations (see

e.g. [13]), integral equations (such as the spatially homogeneous Boltzmann equation [59, 60, 61]), over reaction-diffusion systems (see e.g. [18, 19, 20, 21]) to kinetic equations (see e.g. [23, 24], [32], [4]). The entropy method has also been applied to spatially homogeneous coagulation-fragmentation problem in [1] and [37].

Note, that convergence to equilibrium in the relative logarithmic Boltzmann entropy implies convergence in L^1 due to Csiszár-Kullback-Pinsker type inequalities.

In the following, we prove (faster-than-polynomial/exponential) convergence to equilibrium via the entropy method for a continuous, spatial inhomogeneous coagulation-fragmentation with diffusion and normalised coagulation-fragmentation coefficients. Generalising the homogeneous model discussed in [1], we consider a continuous-in-size cluster density $f(t, x, y)$ depending on time $t \geq 0$, position $x \in \Omega$ and size $y \in [0, \infty)$ satisfying the following coagulation-fragmentation model with normalised coefficients (e.g. $a(y, y') = 2$)

$$(48) \quad \begin{aligned} \partial_t f - d(y) \Delta_x f = Q(f, f) = & \int_0^y f(y - y') f(y') dy' - 2f(y) \int_0^\infty f(y') dy' \\ & + 2 \int_y^\infty f(y') dy' - y f(y), \end{aligned}$$

together with homogeneous Neumann boundary condition

$$\nabla_x f \cdot \nu = 0, \quad x \in \partial\Omega,$$

and nonnegative initial data $0 \leq f^{in}(x, y)$.

The size-dependent diffusion coefficient $d(y)$ is assumed bounded on intervals $[\delta, \delta^{-1}]$ for all $\delta > 0$, but may degenerate at most linearly for large sizes:

$$(49) \quad d(y) \leq d^*(\delta), \quad \forall y \in [\delta, \delta^{-1}], \quad 0 < \frac{d_*}{1+y} \leq d(y), \quad \forall y \in [0, \infty).$$

The weak formulation of the coagulation-fragmentation operator Q for a smooth test-function $\varphi = \varphi(y)$ and a function $f = f(y)$ (such that the integrals exist) reads (with $y'' = y + y'$) as

$$(50) \quad \begin{aligned} \int_0^\infty Q(f, f)(y) \varphi(y) dy = & \int_0^\infty \int_0^\infty [\varphi(y'') - \varphi(y) - \varphi(y')] f(y) f(y') dy dy' \\ & + 2 \int_0^\infty \Phi(y) f(y) dy - \int_0^\infty y \varphi(y) f(y) dy, \end{aligned}$$

where the function Φ denotes the primitive of φ ($\partial_y \Phi = \varphi$) with $\Phi(0) = 0$.

Then, by denoting the first and the zero moments

$$N = \int_0^\infty y' f(y') dy', \quad M = \int_0^\infty f(y') dy',$$

the mass density $N(t, x)$ and the number density $M(t, x)$, the evolutionary problem eq. (48) conserves formally the total mass

$$\partial_t N - \triangle_x \left(\int_0^\infty d(y') y' f(y') dy' \right) = 0,$$

while the number density satisfies

$$\partial_t M - \triangle_x \left(\int_0^\infty d(y') f(y') dy' \right) = N - M^2.$$

Next, by testing the weak formulation with $\ln(f)$, the entropy (free energy) functional

$$H(f)(t, x) = \int_0^\infty (f \ln f - f) dy,$$

dissipates according to

$$\begin{aligned} \frac{d}{dt} \int_{\Omega} H(f) dx &= -D_H(f) \leq 0, \\ D_H(f) &= \int_{\Omega} \int_0^\infty d(y) \frac{|\nabla_x f|^2}{f} dy dx \\ &\quad + \int_{\Omega} \int_0^\infty \int_0^\infty (f'' - ff') \ln \left(\frac{f''}{ff'} \right) dy dy' dx \geq 0, \end{aligned}$$

where $f = f(y)$, $f' = f(y')$ and $f'' = f(y + y')$.

For the spatially homogeneous model (48), Aizenman and Bak [1] found the following remarkable inequality

$$(51) \quad \int_0^\infty \int_0^\infty (f'' - ff') \ln \left(\frac{f''}{ff'} \right) dy dy' \geq M H(f|f_N) + 2(M - \sqrt{N})^2,$$

where $H(f|f_N) = H(f) - H(f_N)$ denotes the relative entropy with respect to a local/

intermediate detailed-balance equilibria of the coagulation-fragmentation process:

$$(52) \quad f_N(t, x) = e^{-\frac{1}{\sqrt{N(t, x)}} y},$$

which depends on space and time only through the macroscopic moment $N(t, x)$ and satisfies the relation $M = \sqrt{N}$.

The inequality (51) implies the following lower bound of the entropy dissipation

$$(53) \quad D_H(f) \geq D_1(f) = \int_{\Omega} \int_0^{\infty} d(y) \frac{|\nabla_x f|^2}{f} dy dx + M H(f|f_N) + 2(M - \sqrt{N})^2.$$

Eq. (53) shows that the entropy dissipation sums the two effects of diffusion and coagulation-fragmentation. The process of coagulation and fragmentation is only able to push the particle density $f(t, x, y)$ towards the class of intermediate equilibria (52) and it is a consequence of spatial diffusion and the homogeneous Neumann boundary conditions on the bounded domain Ω to select from the class of intermediate equilibria f_N the unique global equilibrium parametrised by the conserved total initial mass:

$$f_{\infty} = e^{-\frac{y}{\sqrt{N_{\infty}}}}, \quad N_{\infty} = \int_{\Omega} N(x) dx = \int_{\Omega} \int_0^{\infty} y f^{in}(x, y) dy dx.$$

The existence of global weak mass-conserving solutions to eq. (48) with a diffusion constant $d(y) \in L^{\infty}([1/R, R])$ for all $R > 0$ has been established in [39]. These solutions satisfy the entropy dissipation inequality

$$\int_{\Omega} H(f(t)) dx + \int_0^t \int_{\Omega} D_H(f(s)) ds \leq \int_{\Omega} H(f_0) dx.$$

Using the entropy method, the following convergence to equilibrium was obtained in [22] in the one-dimensional case $\Omega = [0, 1]$ by generalising a first result of exponential convergence assuming (not very physically) bounded diffusion coefficients [10]:

Theorem 4.3 (Faster-than-polynomial convergence to equilibrium). *Suppose nonnegative initial data $(1 + y + \ln f_0)f_0 \in L^1((0, 1) \times (0, \infty))$ with positive initial mass $\int_0^1 \int_{\Omega} N_0(x) dx = N_{\infty} > 0$ on $\Omega = (0, 1)$. Assume at most linearly degenerating diffusion coefficients (49).*

Then, for a constant $\beta < 2$ and $t > 0$

$$(54) \quad \|f(t, \cdot, \cdot) - f_\infty\|_{L^1_{x,y}} \leq C_\beta e^{-(\ln t)^\beta},$$

and for all $t \geq t_* > 0$, and $q > 0$,

$$\int_0^\infty (1+y)^q \|f(t, \cdot, y) - f_\infty(y)\|_{L^\infty_x} dy \leq C_{\beta,q} e^{-(\ln t)^\beta}.$$

The proof is based on the following entropy entropy-dissipation estimate:

Lemma 4.6 (Entropy entropy-dissipation estimate). *Assume that $0 \leq f = f(x, y)$ is measurable and satisfies the following moment estimates:*

$$(55) \quad 0 < \mathcal{M}_* \leq M(x) = \int_0^\infty f(x, y) dy \leq \|M\|_{L^\infty_x},$$

$$(56) \quad 0 < N_\infty = \int_\Omega \int_0^\infty y f(x, y) dy dx,$$

$$(57) \quad \int_\Omega \int_0^\infty y^{2p} f(x, y) dx dy \leq \mathcal{M}_{2p}.$$

Then, for all $A \geq 1$ and $p > 1$ the following entropy entropy-dissipation estimate holds:

$$(58) \quad D_1(f) \geq \frac{C}{A \|M\|_{L^\infty_x}} \int_\Omega H(f|f_\infty) dx - C \frac{\mathcal{M}_{2p}}{A^{2p+1}},$$

with a constant $C = C(\mathcal{M}_*, N_\infty, d_*, P(\Omega))$ depending only on \mathcal{M}_* , N_∞ , d_* , and the Poincaré constant $P(\Omega)$ of the domain Ω .

Proof (Sketch of the proof of Lemma 4.6). We remark that with the definition of the relative entropy $H(f|g) = H(f) - H(g)$, the following additivity property between global and local equilibria holds

$$(59) \quad H(f|f_\infty) = H(f|f_N) + H(f_N|f_\infty),$$

where the space integral of the relative entropy between f_N and f_∞ is non-negative:

$$\int_\Omega H(f_N|f_\infty) dx = 2 \left(\sqrt{\int_\Omega N dx} - \int_\Omega \sqrt{N} dx \right) \geq 0,$$

despite f_N and f_∞ not necessarily having the same L^1_y -norm.

Thus, in a first step we begin with the additivity properties (59) of the relative entropy:

$$(60) \quad \int_0^1 H(f|f_\infty) dx = \int_0^1 H(f|f_N) dx + 2\left(\sqrt{\overline{N}} - \overline{\sqrt{N}}\right),$$

where we have introduced the shorthand notation $\overline{N} = \int_{\Omega} N dx$ and $\overline{\sqrt{N}} = \int_{\Omega} \sqrt{N} dx$.

Secondly, we estimate the second term of the above equality by applying a functional inequality, which was derived in [19] as part of an entropy entropy-dissipation estimate for a reaction-diffusion system of two reacting species $M \leftrightarrow \sqrt{N}$ with degenerate diffusion. This functional inequality quantifies that diffusive effects are passed from one species onto another species via the ongoing reversible reaction between these two species. In the present context, it reads as the functional inequality

$$\sqrt{\overline{N}} - \overline{\sqrt{N}} \leq \frac{2}{\sqrt{N_\infty}} \left[\|M - \sqrt{N}\|_{L_x^2}^2 + \|M - \overline{M}\|_{L_x^2}^2 \right],$$

and formulates a control of a nonnegative measure for the spatial inhomogeneity of the moment N in terms of an L^2 -measure for the reaction of $M \leftrightarrow \sqrt{N}$ and an L^2 -measure for the spatial inhomogeneity of the moment M .

Assuming moreover a lower bound of the moment $M(t, x) > \mathcal{M}_* > 0$, we continue to estimate (60) as follows

$$(61) \quad \begin{aligned} \int_0^1 H(f|f_\infty) dx &\leq C \left[\int_0^1 MH(f|f_N) dx + 2\|M - \sqrt{N}\|_{L_x^2}^2 \right] + \frac{4\|M - \overline{M}\|_{L_x^2}^2}{\sqrt{N_\infty}} \\ &\leq C \int_0^1 \int_0^\infty \int_0^\infty (f'' - ff') \ln \left(\frac{f''}{ff'} \right) dy dy' dx + \frac{4\|M - \overline{M}\|_{L_x^2}^2}{\sqrt{N_\infty}}, \end{aligned}$$

where we have applied the Aizenman-Bak inequality (51).

In a third step, we estimate the L^2 -measure for the spatial inhomogeneity of the moment M , i.e. $\|M - \overline{M}\|_{L_x^2}^2$ in terms of the Fisher information term of (53). This can be done by assuming higher order moments of $f(\cdot, y)$ and a cutoff $A > 0$ in the size-variable y to bypass the degenerate diffusion coefficients $d(y)$ for large clusters. By denoting

$$M_A(t, x) := \int_0^A f(t, x, y) dy, \quad M_A^c(t, x) := \int_A^\infty f(t, x, y) dy,$$

we estimate for any $p > 1$

$$\begin{aligned} \|M - \overline{M}\|_{L_x^2}^2 &= \int_{\Omega} (M_A - \overline{M}_A + M_A^c - \overline{M}_A^c)^2 dx \\ &\leq 2\|M_A - \overline{M}_A\|_{L_x^2}^2 + \frac{4}{A^{2p}} \int_{\Omega} \left(\int_0^{\infty} y^p f(y) dy \right)^2 dx \\ &\leq C(P, d_*) A \|M\|_{L_x^{\infty}} \int_{\Omega} \int_0^{\infty} d(y) \frac{|\nabla_x f|^2}{f} dy dx + \frac{4}{A^{2p}} \|M\|_{L_x^{\infty}} \mathcal{M}_{2p}, \end{aligned}$$

where we have assumed an L^{∞} -bound $\|M\|_{L_x^{\infty}}$ and that the total number density is uniformly bound in time, i.e. $\|M\|_{L_t^{\infty}(L_x^1)} < \infty$. \square

Remark 4.2. *We remark that the entropy entropy-dissipation estimate of Lemma 4.6 holds in any space dimensions provided the necessary a-priori moment bounds hold. These moment bounds however, can so far be only proven in the one-dimensional case.*

The following lemma proves in the one-dimensional case *a priori* estimates, which are required for applying the entropy entropy-dissipation estimate:

Lemma 4.7 (*A priori estimates*). *Assume $\Omega = [0, 1]$.*

Then, the number density $M(t, x)$ satisfies a $(L^1 \cap L^2) + L^{\infty}$ bound, i.e.

$$\|M(t, \cdot)\|_{L_x^{\infty}} \leq m_{\infty} + m_2(t),$$

with a constant m_{∞} and a $L^1 \cap L^2(0, \infty)$ -function $m_2(t)$. Moreover, we have

$$\int_0^1 M(t, x) dx \geq \mathcal{M}_{0*} > 0.$$

Proof. Considering $f(t, x, y) - f(t, \tilde{x}, y) = 2 \int_{\tilde{x}}^x \sqrt{f}(t, \zeta, y) \partial_x \sqrt{f}(t, \zeta, y) d\zeta$, we integrate first in \tilde{x} and then in y and estimate

$$\begin{aligned} \int_0^{\infty} \left| f(t, x, y) - \int_0^1 f(t, \tilde{x}, y) d\tilde{x} \right| dy \\ \leq 2 \left[\int_0^{\infty} \int_0^1 \frac{f(t, x, y)}{d(y)} dx dy \right]^{\frac{1}{2}} \left[\int_0^{\infty} \int_0^1 d(y) |\partial_x \sqrt{f}(t, x, y)|^2 dx dy \right]^{\frac{1}{2}}, \end{aligned}$$

which implies

$$M(t, x) \leq \int_0^1 M(t, \tilde{x}) d\tilde{x} + d_*^{-1/2} (\mathcal{M}_0^* + N_\infty)^{1/2} D(f(t))^{1/2}.$$

and thus the first statement of Lemma 4.7.

Next, we estimate for $m_2(t) \in L^1 \cap L^2(0, \infty)$

$$\frac{d}{dt} \int_0^1 M(t, x) dx = \int_0^1 (N - M^2) dx \geq \int_0^1 N_{in}(x) dx - (m_\infty + m_2(t)) \int_0^1 M(t, x) dx,$$

and thus

$$\begin{aligned} \int_0^1 M(t, x) dx &\geq \int_0^1 M_{in}(x) dx e^{-\int_0^t (m_\infty + m_2(\sigma)) d\sigma} \\ &\quad + \int_0^1 N_{in}(x) dx \int_0^t e^{-\int_s^t (m_\infty + m_2(\sigma)) d\sigma} ds \\ &\geq e^{-\int_0^\infty m_2(\sigma) d\sigma} \left[e^{-m_\infty t} \|M_{in}\|_{L_x^1} + \frac{1 - e^{-m_\infty t}}{m_\infty} \|N_{in}\|_{L_x^1} \right]. \end{aligned}$$

□

The next Lemma establishes higher order moments of the solution of (48):

Lemma 4.8 (Higher moment estimates). *We denote*

$$M_p(f)(t) = \int_0^1 \int_0^\infty y^p f dy dx.$$

Then, the solutions of (48) satisfy for $p > 1$ and for a.a. $t \geq t_ > 0$*

$$M_p(f)(t) \leq (2^{2p} C)^p = \mathcal{M}_p^*,$$

with a constant $C = C(t_, f_{in})$ depending only on the initial data f_{in} and $t_* > 0$.*

Proof (Sketch of the proof of Lemma 4.8, [22]). The proof exploits that the fragmentation process of (48) produces moments. Testing the weak formulation with y^p with $p > 1$, we obtain

$$\frac{d}{dt} M_p(f)(t) \leq (2^p - 2) M_p(f)(t) [m_\infty + m_2(t)] - \frac{p-1}{p+1} M_{p+1}(f)(t).$$

Thus, the interpolation

$$-\frac{p-1}{p+1}M_{p+1}(f) \leq \frac{\varepsilon^{-p}}{p+1}N_\infty - \frac{p}{p+1}\varepsilon^{-1}M_p(f),$$

for $\varepsilon > 0$ and Duhamel's formula with the estimate $\int_0^t m_2 ds \leq \mu_2 \sqrt{t-t_*}$ (exploiting $m_2 \in L^2(0, \infty)$) allows to show that the moment $M_{p+1}^{t_*}$ is bounded for positive times $t \geq t_* > 0$ if the moment M_p is bounded for positive times $t \geq t_* > 0$. For initial data with bounded first order moment $(1+y)f_{in} \in L^1$, we apply then the de la Vallée-Poussin Lemma: for any $f \in L^1$ exists $\varphi \nearrow \infty$ such that $\varphi f \in L^1$, see [22] for the details.

Then, for a regularised version of $\varphi(y)$, we calculate the evolution of the $y \varphi(y)$ -moment and estimate $y \varphi(y) Q_{frag} \leq -C_1 y^{1+\delta}$, which leads to a bound of a moment M_p with $p > 1$ for positive times $t \geq t_* > 0$. \square

Lemma 4.9 (Positive lower bound on number density $M(t, x)$). *Let $t_* > 0$ be given.*

Then, there is a strictly positive constant \mathcal{M}_ (depending on t_* , d_* and $d^*(\delta)$) such that*

$$M(t, x) \geq \mathcal{M}_* > 0.$$

Proof (Sketch of the proof). By introducing a linear lower bound for the lost terms, we consider the equality

$$\partial_t f - d(y) \partial_{xx} f = g_1 - yf - \|M(t, \cdot)\|_{L_x^\infty} f,$$

where $g_1(t, x)$ is nonnegative. Therefore,

$$(\partial_t + d(y) \partial_{xx}) \left(f e^{\int_0^t \|M(s, \cdot)\|_{L_x^\infty} ds} \right) = g_2,$$

where g_2 is nonnegative.

Next, we apply Fourier series and Poisson's formula to the solution of $\partial_t h - d \partial_{xx} h = G \in L^1$ with homogeneous Neumann boundaries on $(0, 1)$ and obtain

$$\begin{aligned} h(t, x) &= \frac{1}{2\sqrt{\pi}} \int_{-1}^1 \tilde{h}(0, z) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d}t} e^{-\frac{(2k+x-z)^2}{4dt}} dz \\ &\quad + \frac{1}{2\sqrt{\pi}} \int_0^t \int_{-1}^1 \tilde{G}(s, z) \sum_{k=-\infty}^{\infty} \frac{1}{\sqrt{d}(t-s)} e^{-\frac{(2k+x-z)^2}{4d(t-s)}} dz ds, \end{aligned}$$

where \tilde{h} and \tilde{G} are mirrored evenly around $x = 0$.

Then, for $t_1 \geq 0$ and $t \in [t_*, 2t_*]$ for some $t_* > 0$, we estimate

$$f(t_1 + t, x, y) \geq C \int_0^1 f(t_1, z, y) e^{-(2t_* + \frac{1}{d_* t_*})y} dz,$$

and further

$$\begin{aligned} M(t_1 + t, x) &\geq C e^{-(2t_* + \frac{1}{d_* t_*})\frac{1}{\delta}} \int_0^1 \int_{\frac{1}{\delta}}^{\frac{1}{\delta}} f(t_1, z, y) dy dz \\ &\geq C e^{-(2t_* + \frac{1}{d_* t_*})\frac{1}{\delta}} \left(M_{0*} - \delta N_{\infty} - K\delta - \frac{\int_0^1 H(f) dx}{\ln K} \right), \end{aligned}$$

where we have used that $\int_{\frac{1}{\delta}}^{\infty} f(y) dy \leq \delta N$ and $\int_0^{\delta} f(y) dy \leq K\delta + \int_0^{\delta} f \frac{\ln f}{\ln K} dx$.

Choosing δ and K , we get that $M(t_1 + t, x) \geq \mathcal{M}_*$ and the statement follows since $\mathcal{M}_* = \mathcal{M}_*(d_*, d^*, m_{\infty}, \mu, H(f_{in}), t_*)$ does not depend on t_1 . \square

Proof (Proof of Theorem 4.3). We first prove the convergence to equilibrium (57) assuming that the entropy entropy-dissipation Lemma 4.6 can be applied. In fact, provided Lemma 4.6, we estimate that for any $A > 1$

$$(62) \quad \frac{d}{dt} \int_0^1 H(f|f_{\infty}) dx \leq - \frac{C}{\|M\|_{L_x^{\infty}}} \frac{1}{A} \int_0^1 H(f|f_{\infty}) dx + \frac{C_p 2^{8p^2}}{A^{2p+1}},$$

where $\|M(t, \cdot)\|_{L_x^{\infty}} \leq m_{\infty} + m_2(t)$ by Lemma 4.7.

Next, we chose $A = A(t) > 2$ by balancing the two r.h.s. terms (e.g. positive term = 1/2 negative term) and obtain

$$\frac{1}{A} \leq C^{-1/2} \left(\frac{C \int_0^1 H(f|f_{\infty}) dx}{\|M\|_{L_x^{\infty}} 2^{8p^2}} \right)^{\frac{1}{2p}},$$

which in return inserted into (62) yields via a Gronwall Lemma algebraic convergence of the relative entropy $\int_0^1 H(f|f_{\infty}) dx$ with rate $2p$ for all $p > 1$.

Then, in a second step we obtain faster-than-polynomial convergence by summing over $2p \in \mathbb{N}$ and calculate that

$$\int_0^1 H(f(t)|f_{\infty}) dx \leq L(t - C),$$

where (for all $1 < \alpha < 2$)

$$L^{-1}(t) = \sum_{2p \geq 1} \frac{t^{2p}}{(C 2p)^{2p} 2^{8p^2}} = \sum_{2p \geq 1} t^{2p} e^{-8p^2 \ln 2 - 2p \ln(2p C)} \geq C(\alpha) e^{\ln^{2(\alpha-1)}(t)},$$

for all t large enough and any $1 < \alpha < 2$.

Secondly, in order to prove the regularity estimate

$$\int_0^\infty (1+y)^q \|f(t, \cdot, y) - f_\infty(y)\|_{L_x^\infty} dy \leq C e^{-\alpha t},$$

we observe that the moment control of Lemma 4.8 implies

$$\int_0^T \int_0^1 \int_0^\infty (1+y)^q Q^+(f, f) dy dx dt \leq C_T.$$

We then use the regularising effect of 1D heat equation: i.e. that solutions to $\partial_t f - d(y)\partial_{xx}f = g$ satisfy for all $q \in [1, 3)$ with $\frac{1}{r} + 1 = \frac{1}{p} + \frac{1}{q}$ that

$$(63) \quad \|f\|_{L^r([0, T] \times \Omega)} \leq C_T d(y)^{\frac{1-q}{2q}} \|f_{in}\|_{L_x^p} + C_T d(y)^{\frac{1-q}{2q}} \|g\|_{L_{t,x}^p},$$

where $d(y)^{\frac{1-q}{2q}} \leq (1+y)^{1/3}$ for y large and C_T denotes various constants which depend polynomially on T . Thus,

$$\|f(\cdot, \cdot, y)\|_{L^{3-\varepsilon}([t_*, T] \times \Omega)} \leq C_T \left(\|f(0, \cdot, y)\|_{L_x^1} + \|Q^+(f, f)(\cdot, \cdot, y)\|_{L^1([0, T] \times \Omega)} \right),$$

which implies that the quadratic term $Q^+(f, f)$ of (48) is in $L^{3/2-\varepsilon}([t_*, T] \times \Omega)$. Then, by a bootstrap argument, one chooses in a next iteration step any $p < 3/2$ in (63), which implies $f(\cdot, \cdot, y) \in L^r([t_*, T] \times \Omega)$ for all $r < \infty$. Therefore, after a further iteration, we obtain $f(\cdot, \cdot, y) \in L^\infty([t_*, T] \times \Omega)$. Finally, a similar estimate like (63) (see [22]) shows that the parabolic H^1 -regularity of the solutions of $\partial_t f - d(y)\partial_{xx}f = g \in L^\infty$ depends also at most polynomially on T , i.e.

$$\int_0^\infty (1+y)^q \|f(T, \cdot, y)\|_{H_x^1} dy \leq C_T.$$

The statement follows then by interpolating the polynomially-in-time growing H^1 -norm with the faster-than-polynomially converging L^1 -norm, which follows from

(54) after applying a Csiszár-Kullback-Pinsker inequality

$$\begin{aligned} \int_0^\infty (1+y)^q \|f(T, \cdot, y) - f_\infty(y)\|_{L_x^\infty} dy \\ \leq \int_0^\infty \left((1+y)^q \|f(T, \cdot, y) - f_\infty(y)\|_{H_x^1}^{3/4} \|f(T, \cdot, y) - f_\infty(y)\|_{L_x^1}^{1/4} \right) dy \\ \leq C_T^{3/4} e^{-\alpha T}. \end{aligned}$$

□

4.6 - Fast-reaction limit towards a macroscopic diffusion equation

In this Section, we consider a family of inhomogeneous coagulation-fragmentation models with rescaled coagulation and fragmentation rates compared to (48), i.e.

$$(64) \quad \partial_t f^\varepsilon - d(y) \triangle_x f^\varepsilon = \frac{1}{\varepsilon} (Q_{\text{coag}}(f^\varepsilon, f^\varepsilon) + Q_{\text{frag}}(f^\varepsilon)).$$

We shall investigate the fast-reaction limit $\varepsilon \rightarrow 0$. Formally, we expect in the limit that

$$f^\varepsilon \xrightarrow{\varepsilon \rightarrow 0} e^{-\frac{y}{\sqrt{N^0(t,x)}}},$$

where the limiting mass density $N^0(t, x)$ satisfies the nonlinear diffusion equation

$$(65) \quad \partial_t N^0(t, x) - \triangle_x n(N^0(t, x)) = 0, \quad n(N) = \int_0^\infty d(y) y e^{-\frac{y}{\sqrt{N}}} dy.$$

In fact, assuming bounded diffusion coefficients $d(y)$, the nonlinear diffusion equation (65) is also nondegenerate due to

$$0 < \inf_{[0, \infty)} \{d(y)\} N \leq n(N) \leq \sup_{[0, \infty)} \{d(y)\} N.$$

The fast-reaction-limit of (64) without a rate of convergence was proven rigorously in [12] via a compactness argument. Here, we shall present an interesting approach based on a duality method, which allows to obtain also a rate of convergence. This duality-based argument was laid out in [11]. However, it assumes a uniform-in- ε lower bound on $M^\varepsilon(t, x)$, which, despite expected to hold, remains an open technical problem to prove rigorously.

First, we recall the lower bound of the entropy dissipation (53), which reads in the rescaled version as

$$-\varepsilon \frac{d}{dt} \int_\Omega H(f^\varepsilon) dx \geq \int_\Omega M^\varepsilon H(f^\varepsilon | f_{N^\varepsilon}) dx + 2 \int_\Omega ((M^\varepsilon) - \sqrt{N^\varepsilon})^2 dx,$$

where we have neglected the nonnegative diffusion term entirely. As a consequence, we have

$$\int_0^\infty \int_\Omega M^\varepsilon H(f^\varepsilon | f_{N^\varepsilon}) dx dt \leq \varepsilon C.$$

Assuming a uniform lower bound on the number density $M^\varepsilon(t, x) \geq \mathcal{M}_* > 0$, it follows from a Csiszár-Kullback-Pinsker inequality that

$$\|f^\varepsilon - e^{-\frac{y}{\sqrt{N^\varepsilon}}}\|_{L_t^2(L_{x,y}^1)}^2 \leq \varepsilon C(\mathcal{M}_*).$$

Next, by using an interpolation with bounds of higher order moments, one can show (see [11] for the details) that for an interpolation exponent $0 < \theta < 1$, there exists a remainder $f_1^\varepsilon \in L_{t,x}^2(L_y^1((1+y)dy))$ with

$$f^\varepsilon = e^{-\frac{y}{\sqrt{N^\varepsilon}}} + \varepsilon^\theta f_1^\varepsilon, \quad \text{with} \quad \nabla_x f_1^\varepsilon \cdot \nu(x) = 0 \text{ on } \partial\Omega.$$

As a consequence, we have

$$\partial_t N^\varepsilon - \Delta_x n(N^\varepsilon) = \varepsilon^\theta \Delta_x \int_0^\infty d(y) y f_1^\varepsilon dy = \varepsilon^\theta \Delta_x g^\varepsilon,$$

where $g^\varepsilon \in L_{t,x}^2$ with $\nabla_x g^\varepsilon \cdot \nu(x) = 0$ on $\partial\Omega$.

We apply then a duality method similar to Lemma 4.5 in order to show that provided initial data $N_{in} \in L_x^2$, then the solutions of the nonlinear diffusion equation

$$(66) \quad \partial_t N^\varepsilon - \Delta_x n(N^\varepsilon) = \varepsilon^\theta \Delta_x g^\varepsilon, \quad \nabla_x N^\varepsilon \cdot \nu(x)|_{\partial\Omega} = 0,$$

converge in $L_{t,x}^2$ as $\varepsilon \rightarrow 0$ to the solution $N(t, x)$ of

$$(67) \quad \partial_t N - \Delta_x n(N) = 0, \quad \nabla_x N \cdot \nu(x)|_{\partial\Omega} = 0.$$

In fact, one can prove analog to Lemma 4.5 that the nonnegative solution $w \geq 0$ of the dual problem

$$-\partial_t w - \frac{n(N^\varepsilon) - n(N)}{N^\varepsilon - N} \Delta_x w = H \geq 0, \quad \nabla_x w \cdot \nu(x)|_{\partial\Omega} = 0, \quad w(T) = 0,$$

satisfies

$$\|\Delta_x w\|_{L^2([0,T] \times \Omega)} \leq C \|H\|_{L^2([0,T] \times \Omega)}.$$

Thus, by testing the difference of eqs. (66) and (67), we estimate

$$\left| \int_0^T \int_{\Omega} (N^\varepsilon - N) H dx dt \right| \leq \varepsilon^\theta \|g^\varepsilon\|_{L^2_{t,x}} \|\triangle_x w\|_{L^2([0,T] \times \Omega)},$$

which implies by duality

$$\|N^\varepsilon - N\|_{L^2_{t,x}} \leq C \varepsilon^\theta \|g^\varepsilon\|_{L^2_{t,x}} \leq C \varepsilon^\theta,$$

since $H \geq 0 \in C_0^\infty([0, T] \times \Omega)$ is arbitrary.

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