AN ASYMPTOTICALLY STABLE SCHEME FOR DIFFUSIVE COAGULATION-FRAGMENTATION MODELS *

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Abstract. This paper is devoted to the analysis of a numerical scheme for the coagulation and fragmentation equation with diffusion in space. A finite volume scheme is developed, based on a conservative formulation of the spatially nonhomogeneous coagulation-fragmentation model. It is shown that the scheme preserves positivity, total volume and global steady states. Finally, several numerical simulations are performed to investigate the long time behavior of the solution.

Key words. coagulation-fragmentation equation, finite volume method

AMS subject classifications. 65R20, 82C05

1. Introduction

Coagulation and fragmentation processes occur in the dynamics of cluster growth and describe the mechanisms by which clusters can coalesce to form larger clusters or fragment into smaller ones. Models of this type have found important applications in areas ranging over polymer kinetics [35], aerosols [20], cluster formation in astrophysics [30] and animal grouping in biology.

This paper is devoted to the numerical simulation of the dynamics of the density function $f = f(t,x,y) \geq 0$ of particles (polymers, clusters) with position $x \in \Omega \subset \mathbb{R}^N$ ($N \geq 1$), volume $y \in \mathbb{R}^+ := (0, \infty)$, and time $t \geq 0$. The distribution function f is subject to coagulation and fragmentation phenomena with respect to the volume variable y and diffusion with respect to the space $x \in \Omega$ and is governed by the following equation

$$\frac{\partial f}{\partial t} - d(y)\Delta_x f = \mathcal{Q}(f), \tag{1.1}$$

where $\mathcal{Q}(f)$ is the coagulation-fragmentation operator acting on the volume variable $y \in \mathbb{R}^+$ and these particles diffuse in the environment Ω, which is assumed to be a smooth bounded domain with normalized volume $|\Omega| = 1$. Moreover, the model (1.1) is supplemented with an initial datum

$$f(0,x,y) := f^{\text{in}}(x,y), \tag{1.2}$$

and in the following analysis we will consider homogeneous Neumann boundary conditions on $\partial\Omega$

$$\nabla_x f(t,x,y) \cdot \nu(x) = 0, \quad (t,x,y) \in \mathbb{R}^+ \times \partial\Omega \times \mathbb{R}^+, \tag{1.3}$$

with ν the outward unit normal to Ω. We also assume the diffusion coefficient $d(y)$ to be non-degenerate in the sense that there exists $d_* \in \mathbb{R}^+$ such that

$$d(y) \geq d_* > 0, \quad y \in \mathbb{R}^+. \tag{1.4}$$

Let us first describe precisely the coagulation and fragmentation process. In the simplest coagulation-fragmentation models the clusters are usually assumed to be

fully identified by their size (or volume, or number of particles). The coagulation-fragmentation models we consider in this paper describe the time evolution of the cluster size distribution as the system of clusters undergoes binary coagulation and binary fragmentation events. More precisely, denoting by C_y the clusters of size y with $y \in \mathbb{R}^+$, the basic reactions taken into account herein are

$$C_y + C_{y'} \xrightarrow{a(y,y')} C_{y+y'}, \text{ (binary coagulation)} \tag{1.5}$$

$$C_y \xrightarrow{b(y-y',y')} C_{y-y'} + C_{y'}, \text{ (binary fragmentation)}, \tag{1.6}$$

where a and b denote the coagulation and fragmentation rates respectively, and are assumed to depend only on the size of the clusters involved in these reactions.

Thus, the coagulation-fragmentation operator is defined by

$$\mathcal{Q}(f) = \mathcal{Q}_{\mathsf{c}}(f) - \mathcal{Q}_{\mathsf{f}}(f), \tag{1.7}$$

where the coagulation operator only acts on the volume variable and is given by

$$\mathcal{Q}_{\mathsf{c}}(f)(y) = \frac{1}{2} \int_0^y a(y', y-y') f(y') f(y-y') \, dy' - \int_0^\infty a(y,y') f(y) f(y') \, dy', \tag{1.8}$$

whereas the fragmentation mechanism by which a single particle splits into two pieces is given by

$$\mathcal{Q}_{\mathsf{f}}(f)(y) = \frac{1}{2} \int_0^y b(y', y-y') \, dy' \, f(y) - \int_0^\infty b(y,y') f(y+y') \, dy'. \tag{1.9}$$

The coagulation coefficient, $a = a(y,y')$, characterizes the rate at which the coalescence of two particles with respective volumes y and y' produces a particle of volume $y+y'$, whereas the fragmentation coefficient, $b = b(y,y')$, represents the rate at which the fragmentation of one particle with volume $y+y'$ produces two particles of volume y and y'. Both coefficients a and b are nonnegative functions and

$$\begin{cases} a(y,y') = a(y',y), \, b(y,y') = b(y',y), \\ a, \, b \in L^\infty_{loc}\left(\mathbb{R}^+ \times \mathbb{R}^+\right). \end{cases} \tag{1.10}$$

For symmetric kernels, we observe that during the microscopic coagulation and fragmentation processes, as depicted in equations (1.5)–(1.6), the number of particles varies with time while the total volume of particles is conserved.

In terms of f, the total number of particles and the total volume of particle at time $t \geq 0$ are respectively given by

$$M_0(t,x) := \int_{\mathbb{R}^+} f(t,x,y) \, dy, \quad M_1(t,x) := \int_{\mathbb{R}^+} y f(t,x,y) \, dy.$$

Besides existence and uniqueness results, little is known of the qualitative behavior of solutions of coagulation-fragmentation equations except when coagulation and fragmentation coefficients are linked by the so-called "detailed balance condition": there exists a nonnegative function $\mathcal{M} \in L^1(\mathbb{R}^+, (1+y)dy)$ such that $\mathcal{M}(y) > 0$ and

$$a(y,y')\mathcal{M}(y)\mathcal{M}(y') = b(y,y')\mathcal{M}(y+y'), \quad (y,y') \in \mathbb{R}^+ \times \mathbb{R}^+. \tag{1.11}$$

This condition implies that $\mathcal{M}$ is a stationary solution to the coagulation-fragmentation equation and satisfies more precisely

$$d(y)\Delta_x\mathcal{M} = \mathcal{Q}(\mathcal{M}) = 0.$$

Furthermore, we observe that for any constant $\alpha \in \mathbb{R}$,

$$\mathcal{M}_\alpha(y) := e^{-\alpha y}\mathcal{M}(y), \quad y \in \mathbb{R}^+ \tag{1.12}$$

is still an equilibrium of the coagulation-fragmentation equation.

An additional and interesting feature of the detailed balance condition is that there exists an entropy H given by

$$H(f|\mathcal{M}) = \int_{\Omega \times \mathbb{R}^+} \left[f(x,y)\left(\ln\left(\frac{f(x,y)}{\mathcal{M}(y)} \right) - 1 \right) + \mathcal{M}(y) \right] dy\, dx,$$

which satisfies the following H theorem

$$\frac{dH(f)}{dt} \leq 0.$$

A natural conjecture would be that

$$f(t) \longrightarrow \mathcal{M}_\alpha, \quad \text{as} \quad t \to \infty,$$

where the value of $\alpha \in \mathbb{R}$ is fully determined by the initial total volume $M_1(0)$, conserved with time, such that

$$M_1(0) = \frac{1}{|\Omega|}\int_{\Omega \times \mathbb{R}^+} y\,\mathcal{M}_\alpha(y)\,dy\,dx = \int_{\mathbb{R}^+} y\,\mathcal{M}_\alpha(y)\,dy.$$

We refer to [8, 25, 27, 33] for a proof of convergence to equilibrium for the diffusive coagulation-fragmentation equation.

However, for this result to be true, the total volume of f^{in} and $\mathcal{M}_\alpha$ should be the same, and in particular the total volume should be conserved throughout time evolution. In addition, there are cases for which there is no equilibrium $\mathcal{M}_\alpha$ with the same total volume as f^{in}, and the above convergence cannot hold. Finally, a proof of the convergence of $f(t)$ to a single equilibrium is not available in all cases.

The main purpose of this work is to present a numerical scheme to solve (1.1) built upon a finite volume discretization with respect to the space variable $x \in \Omega$ and volume variable $y \in \mathbb{R}^+$. The analysis of the so-obtained scheme would allow to prove the convergence of the discretized particle density towards a solution to the continuous problem on a fixed time interval $[0,T]$ ($T > 0$), see for instance [6], but here our aim is different. It will consist in the study of the long time behavior of the numerical solution on a fixed mesh in space and volume variables. Indeed, often in applications we are interested in are steady states or the long time behavior of the solution. It is then important to design a numerical scheme which has good stability properties uniformly in time and remains consistent with respect to the exact solution for long time. Thus, the scheme proposed in this paper is designed such that it preserves qualitative properties of the exact solution, such as steady states of the coagulation-fragmentation operators (1.8)–(1.9). Moreover, an estimate of the entropy dissipation due to an appropriate finite volume approximation with respect to space and volume

variables is given and the scheme is shown to give a consistent approximation of the continuous problem in the long time asymptotic limit $t \to \infty$.

Before describing more precisely our results, let us recall that the coagulation and fragmentation equations (1.1) with (1.8)–(1.9) have been the object of several recent studies.

On the one hand, among the various approaches for the approximation of co-agulation and fragmentation models, we may distinguish between deterministic and Monte-Carlo methods. We refer for instance to [12, 17, 29] for deterministic methods, [3, 21] for stochastic methods, and the references therein. Concerning the convergence analysis of numerical methods for coagulation and fragmentation models, we refer to [28] for a rigorous study of quasi-Monte-Carlo methods. For deterministic approximations, the situation is different; the relationship between discrete and continuous models has been considered by some authors, see the survey paper [11] and [1]. A rigorous setting for the formal analysis performed in [1] under general assumptions on the coagulation and fragmentation coefficients has been given in [26]. Similar techniques are used to prove convergence of discrete schemes to the exact solution in [6].

However, little is known concerning the stability and the analysis of the numerical solution in the long time asymptotic limit. For the continuous model, in reference [25], the authors are able to apply the techniques of weak compactness, as in the paper by R.J. DiPerna and P.-L. Lions [10] about the Boltzmann equation, to prove the weak stability of weak solutions. In the case when an H-theorem holds, they can obtain some partial information about the large-time behavior of solutions. More recently, using entropy dissipation methods developed by L. Desvillettes and C. Villani [9], J. A. Carrillo *et al.* prove exponential decay of the solution towards equilibrium for the inhomogeneous Aizenman-Bak model [7] assuming restrictive conditions : constant kernels a and b and either constant diffusion coefficient or space dimension one. Our analysis for discrete models will be inspired by these works.

We now briefly outline the content of the paper. In the next section, we introduce the numerical approximation of (1.1) and state the stability result which we prove in Section 3. In the final section (Section 5), some numerical simulations are performed with the numerical scheme presented in Section 2 and the long time behavior of the solution is investigated.

2. Numerical scheme and main results

In order to compute an approximation of this model using a finite volume method in space variable $x \in \Omega$ and volume variable $y \in \mathbb{R}^+$, we observe that the coagulation-fragmentation operator can be written in a conservative form. Indeed, writing Equation (1.1) in a "conservative" form, as proposed in [30, 32], enables to describe precisely the time evolution of the total volume. Also, this formulation is particularly well adapted to a finite volume discretization, which in turn is expected to give a precise account of volume conservation. Precisely, the coagulation and fragmentation terms can be written in divergence form:

$$\begin{cases} y\,\mathcal{Q}_{\mathsf{c}}(f)(x,y) = -\dfrac{\partial \mathcal{C}(f)}{\partial y}(x,y), \\[4mm] y\,\mathcal{Q}_{\mathsf{f}}(f)(x,y) = -\dfrac{\partial \mathcal{F}(f)}{\partial y}(x,y), \end{cases}$$

where the operator $\mathcal{C}(f)$ is given by

$$\mathcal{C}(f)(x,y) := \int_0^y \int_{y-u}^\infty u\, a(u,v)\, f(x,u)\, f(x,v)\, dv du, \quad (x,y) \in \Omega \times \mathbb{R}^+, \qquad (2.1)$$

and $\mathcal{F}(f)$ is

$$\mathcal{F}(f)(x,y) := \int_0^y \int_{y-u}^\infty u\, b(u,v)\, f(x,u+v)\, dv du, \quad (x,y) \in \Omega \times \mathbb{R}^+. \qquad (2.2)$$

Finally, the coagulation-fragmentation equation reads

$$\begin{cases} y\, \dfrac{\partial f}{\partial t} - d(y)\, y\, \Delta_x f = -\dfrac{\partial \mathcal{C}(f)}{\partial y} + \dfrac{\partial \mathcal{F}(f)}{\partial y}, \\[4mm] f(0,x,y) = f^{\mathrm{in}}(x,y), \ \ (x,y) \in \Omega, \times \mathbb{R}^+ \end{cases} \qquad (2.3)$$

and we assume that the initial datum f^{in} is a nonnegative function which satisfies:

$$f^{\mathrm{in}} \in L^1(\Omega \times \mathbb{R}^+, (1+y)dx dy). \qquad (2.4)$$

Here and below, the notation $L^1(\Omega \times \mathbb{R}^+, (1+y)dx\, dy)$ stands for the space of the Lebesgue measurable real-valued functions on $\Omega \times \mathbb{R}^+$ which are integrable with respect to the measure $(1+y)dx\, dy$. When designing the volume discretization of the coagulation and fragmentation terms, it is necessary to truncate the infinite integrals in formulae (2.1)–(2.2). But this means restricting the domain of action of kernels a and b to a bounded set of volumes y, that is, preventing coagulation from occurring among particles with volume exceeding a fixed value. The discretization we propose is based on the conservative truncation method for the coagulation and fragmentation terms. Given a positive real number R, for $(x,y) \in \Omega \times (0,R)$ define

$$\mathcal{C}^R(f)(x,y) := \int_0^y \int_{x-u}^{R-u} u\, a(u,v)\, f(x,u)\, f(x,v)\, dv du,$$

$$= \int_0^y \int_y^R u\, a(u,w-u)\, f(x,u)\, f(x,w-u)\, dw du. \qquad (2.5)$$

In this case, $\mathcal{C}^R(f)(x,0) = \mathcal{C}^R(f)(x,R) = 0$ for each $x \in \Omega$ so that the total volume of the solution is now constant with respect to time. Using the same idea, we introduce a conservative truncation of the fragmentation terms: for $(x,y) \in \Omega \times (0,R)$ define

$$\mathcal{F}^R(f)(x,y) := \int_0^y \int_{y-u}^{R-u} u b(u,v) f(x,u+v)\, dv du,$$

$$= \int_0^y \int_y^R u b(u,w-u) f(x,w)\, dw du. \qquad (2.6)$$

Then, the conservative coagulation-fragmentation operator satisfies exactly the conservation of total volume, so that the following equation is indeed a conservative truncated coagulation and fragmentation equation:

$$\begin{cases} y\dfrac{\partial f_R}{\partial t} - d(y)\, y\, \Delta_x f_R = -\dfrac{\partial \mathcal{C}^R(f_R)}{\partial y}(x,y) + \dfrac{\partial \mathcal{F}^R(f_R)}{\partial y}(x,y) \\[4mm] f(0,x,y) = f^{\mathrm{in}}(x,y), \quad (x,y) \in \Omega \times (0,R), \end{cases} \qquad (2.7)$$

since

$$\frac{d}{dt}\int_0^R \int_\Omega y\, f_R(t,x,y)\, dx\, dy = 0.$$

Under the detailed balance condition (1.11), model (2.7) has also a steady state $\mathcal{M}_R$, depending only on y and such that

$$\mathcal{M}_R(y) = \mathcal{M}(y), \quad y \in [0,R]$$

and

$$\frac{1}{|\Omega|}\int_0^R \int_\Omega f^{\mathtt{in}}(x,y)\, dx\, dy = \int_0^R \mathcal{M}_R(y)\, dy.$$

Convergence for large values of R has been thoroughly studied in the recent past in the spatially homogeneous case [26]. However, an additional difficulty arises in the spatially inhomogeneous case. Indeed, convergence as $R \to \infty$ is still true, but it is unclear whether one obtains conservation of the total volume in the limit $R \to \infty$ (for kernels for which it is expected to hold, of course). We refer for instance to [22, 31, 34] for global weak solutions and [2] for local smooth solutions. Thus, in this paper we will focus only on the convergence of a sequence built on a numerical scheme towards a solution to Equation (2.7) when the truncature R is fixed. In the remainder of the paper, for the sake of clarity, we drop the subscript R and write f instead of f_R for a solution of Equation (2.7). The parameter R being fixed, this should raise no confusion. We now turn to the discretization of Equation (2.7). Having reduced the computation to a bounded interval, the second step is to introduce the space and volume discretizations. To this end, we fix $\Delta y \in (0,1)$ and N_y a large integer, and denote by $(y_{i-1/2})_{i \in \{0,\dots,N_y\}}$ a mesh of $(0,R)$, where $y_{i-1/2} = i\Delta y$, and $\Lambda_i = [y_{i-1/2}, y_{i+1/2})$ for $i \geq 0$.

Concerning the space variable, we choose an admissible mesh of Ω given by a family $\mathcal{T}$ of control volumes (open and convex polygons in 2-D), a family $\mathcal{E}$ of edges and a family of points $(x_K)_{K \in \mathcal{T}}$ which satisfy Definition 5.1 in [15]. This definiton implies that the straight line between two neighboring centers of cells (x_K, x_L) is orthogonal to the edge $\sigma = K|L$. In the set of edges $\mathcal{E}$, we distinguish the interior edges $\sigma \in \mathcal{E}_{int}$ and the boundary edges $\sigma \in \mathcal{E}_{ext}$. For a control volume $K \in \mathcal{T}$, we denote by $\mathcal{E}_K$ the set of its edges, by $\mathcal{E}_{int,K}$ the set of its interior edges, and by $\mathcal{E}_{ext,K}$ the set of edges of K included in $\Gamma = \partial\Omega$.

In the sequel, we denote by d the distance in $\mathbb{R}^N$, and by m the Lebesgue measure in $\mathbb{R}^N$. We assume that the family of meshes considered satisfies the following regularity constraint: there exists $\xi > 0$ such that

$$\mathrm{d}(x_K,\sigma) \geq \xi\, \mathrm{d}(x_K,x_L), \quad \text{and for } K \in \mathcal{T}, \text{ for } \sigma \in \mathcal{E}_{int,K},\ \sigma = K|L. \qquad (2.8)$$

The size of the mesh is defined by

$$\delta = \max_{K \in \mathcal{T}}(\mathrm{diam}(\mathrm{K})). \qquad (2.9)$$

For all $\sigma \in \mathcal{E}$, we define the transmissibility coefficient:

$$\tau_\sigma = \begin{cases} \dfrac{\mathrm{m}(\sigma)}{\mathrm{d}(x_K,x_L)}, & \text{for } \sigma \in \mathcal{E}_{int},\ \sigma = K|L, \\[2ex] \dfrac{\mathrm{m}(\sigma)}{\mathrm{d}(x_K,\sigma)}, & \text{for } \sigma \in \mathcal{E}_{ext,K}. \end{cases}$$

Next, $X(\mathcal{T})$ will be the set of functions from Ω to $\mathbb{R}$ which are constant over each control volume $K \in \mathcal{T}$.

We define the approximation $f^h(0)$ of the initial datum f^{in} as usual by

$$f^h(0) = \sum_{i=0}^{N_y} \sum_{K \in \mathcal{T}} f_{K,i}^{\text{in}} \mathbf{1}_{K \times \Lambda_i}, \tag{2.10}$$

with

$$f_{K,i}^{\text{in}} = \frac{1}{\text{m}(K)\Delta y} \int_{\Lambda_i} \int_K f^{\text{in}}(x,y) \, dx \, dy,$$

where $\mathbf{1}_E$ denotes the characteristic function of the subset E of $\Omega \times \mathbb{R}^+$ and converges strongly to f^{in} in $L^1(\Omega \times \mathbb{R}^+)$ as $h = (\Delta y, \delta)$ goes to 0.

Let us now introduce the numerical scheme itself. For each integer $i \in \{0, \ldots, N_y\}$ and each $K \in \mathcal{T}$, we define the approximation of $f(t,x,y)$ for $t \in \mathbb{R}^+$ and $(x,y) \in K \times \Lambda_i$ as $f_{K,i}(t)$. The sequence $(f_{K,i}(t))_{K,i}$ is defined by the following discretization of the coagulation-fragmentation equation: for $K \in \mathcal{T}$, $i \in \{0, \ldots, N_y\}$, we solve the ordinary differential system

$$\begin{cases} \text{m}(K) \dfrac{df_{K,i}(t)}{dt} - d(y_{i-1/2}) \displaystyle\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} f_{K,i}(t) = \text{m}(K) \mathcal{Q}_{K,i}, \\[2mm] f_{K,i}(0) := f_{K,i}^{\text{in}}. \end{cases} \tag{2.11}$$

We have set

$$\mathcal{Q}_{K,i} = -\frac{\mathcal{C}_{K,i+1/2} - \mathcal{C}_{K,i-1/2}}{y_{i-1/2}\Delta y} + \frac{\mathcal{F}_{K,i+1/2} - \mathcal{F}_{K,i-1/2}}{y_{i-1/2}\Delta y} \tag{2.12}$$

where the flux $\mathcal{C}_{K,i+1/2}$ in (2.12) represents an approximation of the coagulation operator (2.5), $\mathcal{F}_{K,i+1/2}$ is the approximation of the fragmentation part (2.6) and both are defined by

$$\mathcal{C}_{K,i+1/2} = \sum_{j=0}^{i} \sum_{l=i+1}^{N_y-1} \Delta y^2 \, y_{j-1/2} \, a_{j,l-j} \, f_{K,j}(t) \, f_{K,l-j}(t), \tag{2.13}$$

where $a_{i,j} := a(y_i, y_j)$ with $y_i = (i+1/2)\Delta y$ and

$$\mathcal{F}_{K,i+1/2} = \sum_{j=0}^{i} \sum_{l=i+1}^{N_y-1} \Delta y^2 \, y_{j-1/2} \, b_{j,l-j} \, f_{K,l}(t), \tag{2.14}$$

where $b_{i,j} := b(y_i, y_j)$ whereas the fluxes at the boundary are

$$\mathcal{C}_{K,-1/2} = \mathcal{F}_{K,-1/2} = \mathcal{C}_{K,N_y+1/2} = \mathcal{F}_{K,N_y+1/2} = 0, \quad K \in \mathcal{T}. \tag{2.15}$$

Concerning the approximation of the diffusion in space, we let $\nu_{K,\sigma}$ denote the unit normal to σ outward from K and define an approximation of $\nabla_x f \cdot \nu_{K_\sigma}$ on σ by

$$D_{K,\sigma} f_{K,i} = \begin{cases} f_{L,i} - f_{K,i} \text{ if } \sigma = K|L \in \mathcal{E}_{int,K}, \\ 0 \text{ if } \sigma \in \mathcal{E}_{ext,K}, \end{cases} \tag{2.16}$$

for all $K \in \mathcal{T}$. This discretization obviously relies on a simple finite volume approach for the space and volume variables (see, *e.g.* [6]).

The following function f^h defined on $\mathbb{R}^+ \times \Omega \times [0,R]$ will be useful in the sequel.

$$f^h(t,x,y) = \sum_{K \in \mathcal{T}} \sum_{i=0}^{N_y} f_{K,i}(t) \mathbf{1}_{K \times \Lambda_i}. \tag{2.17}$$

We may now state our main result.

THEOREM 2.1. *Assume that the coagulation and fragmentation kernels satisfy (1.4), (1.10) and (1.11) and f^{in} satisfies (2.4). We consider a uniform volume mesh in y and require the mesh $\mathcal{T}$ in space to satisfy conditions (2.8), (2.9). Then there exists a unique solution f^h to the finite volume scheme (2.11)–(2.16) which satisfies*

  (i) *nonnegativity*

$$f_{K,i}(t) \geq 0, \quad (K,i) \in \mathcal{T} \times \{0,\ldots,N_y\}, \quad t \in \mathbb{R}^+,$$

  (ii) *conservation of total volume*

$$\frac{d}{dt}\left[\sum_{K,i} \mathrm{m}(K) \Delta y\, y_{i-1/2} f_{K,i}(t) \right] = 0, \quad \forall t \in \mathbb{R}^+,$$

  (iii) *entropy dissipation*

$$\frac{dH(f^h|\mathcal{M})}{dt} + \Delta y \sum_{K,i} \sum_{\sigma \in \mathcal{E}_K} d(y_{i-1/2}) \tau_\sigma D_{K,\sigma} f_{K,i} \ln\left(\frac{f_{K,i}}{\mathcal{M}_i} \right) = -D(f^h),$$

where

$$H(f^h|\mathcal{M}) = \sum_{K,i} \mathrm{m}(K) \Delta y \left[f_{K,i}\left(\ln\left(\frac{f_{K,i}}{\mathcal{M}_i} \right) - 1 \right) + \mathcal{M}_i \right]$$

and

$$D(f^h) = \frac{1}{2} \sum_{K,i} \sum_{l=0}^{i} \Delta y^2 \mathrm{m}(K) \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right) \left[\ln\left(\frac{a_{l,i-l} f_{K,l} f_{K,i-l}}{b_{l,i-l} f_{K,i}} \right) \right].$$

  (iv) *Moreover, the finite volume scheme is asymptotic-preserving, i.e.,*

$$f^h(t) \longrightarrow \mathcal{M}_\alpha^h \quad as \ t \longrightarrow \infty,$$

where

$$\mathcal{M}_\alpha^h(x,y) = \mathcal{M}_{\alpha,i} := e^{-\alpha y_i} \mathcal{M}(y_i), \quad \forall (x,y) \in K \times [y_{i-1/2}, y_{i+1/2})$$

and $\alpha \in \mathbb{R}^+$ is such that

$$\sum_{K \in \mathcal{T}} \sum_{i=0}^{N_y} \mathrm{m}(K) y_{i-1/2} \mathcal{M}_{\alpha,i} = \sum_{K \in \mathcal{T}} \sum_{i=0}^{N_y} \mathrm{m}(K) y_{i-1/2} f_{K,i}^{in}.$$

3. A priori estimates

As we mentioned in the introduction, our goal is not to prove that the sequence of functions $(f^h)_h$ converges in some sense to a function f as $h = (\Delta y, \delta)$ goes to 0, but to study the long time behavior of the numerical solution and to prove its uniform stability with respect to time. First, we prove that the solution f^h to the scheme (2.11)–(2.15) enjoys properties similar to those of function f given by (2.7) which we gather in Prop. 3.1 below.

On the one hand, we first rewrite the discrete coagulation-fragmentation obtained from the conservative form (2.7) in a new form which is consistent with the classical formulation (1.7)–(1.9). On the other hand, we find a discrete version of the weak formulation from which we prove *a priori* estimates.

PROPOSITION 3.1. *Assume the approximation of the coagulation-fragmentation model (2.5)–(2.7) given by the finite volume scheme (2.11)–(2.16). Then the discrete operator satisfies*

$$\mathcal{Q}_{K,i} = \frac{1}{2} \sum_{j=0}^{i} \Delta y \left(a_{j,i-j} f_{K,j} f_{K,i-j} - b_{j,i-j} f_{K,i} \right)$$
$$- \sum_{j=i}^{N_y-1} \Delta y \left(a_{i,j-i} f_{K,i} f_{K,j-i} - b_{i,j-i} f_{K,j} \right). \tag{3.1}$$

Proof. Starting from the definition of the fluxes (2.13) and (2.14), we set

$$\mathcal{Q}_{K,i} = -\frac{\mathcal{C}_{K,i+1/2} - \mathcal{C}_{K,i-1/2}}{y_{i-1/2} \Delta y} + \frac{\mathcal{F}_{K,i+1/2} - \mathcal{F}_{K,i-1/2}}{y_{i-1/2} \Delta y}$$

and by construction

$$y_{i-1/2} \mathcal{Q}_{K,i} = -\sum_{j=0}^{i} \sum_{l=i+1}^{N_y-1} \Delta y \, y_{j-1/2} \left(a_{j,l-j} f_{K,j} f_{K,l-j} - b_{j,l-j} f_{K,l} \right)$$
$$+ \sum_{j=0}^{i-1} \sum_{l=i}^{N_y-1} \Delta y \, y_{j-1/2} \left(a_{j,l-j} f_{K,j} f_{K,l-j} - b_{j,l-j} f_{K,l} \right),$$

which can be easily simplified into

$$y_{i-1/2} \mathcal{Q}_{K,i} = -\sum_{l=i+1}^{N_y-1} \Delta y \, y_{i-1/2} \left(a_{i,l-i} f_{K,i} f_{K,l-i} - b_{i,l-i} f_{K,l} \right)$$
$$+ \sum_{l=0}^{i-1} \Delta y \, y_{l-1/2} \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right).$$

Then, adding and subtracting the term $y_{i-1/2} \left(a_{i,0} f_{K,0} f_{K,0} - b_{i,0} f_{K,i} \right)$, we get

$$y_{i-1/2} \mathcal{Q}_{K,i} = \sum_{l=0}^{i} \Delta y \, y_{l-1/2} \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right)$$
$$- \sum_{l=i}^{N_y-1} \Delta y \, y_{i-1/2} \left(a_{i,l-i} f_{K,i} f_{K,l-i} - b_{i,l-i} f_{K,l} \right).$$

Hence, it only remains to treat the first term of the right hand side: we compute for a symmetric sequence $g_{i,j}$ such that $g_{i,j} = g_{j,i}$ for each $(i,j) \in \{0,\dots,N_y\}^2$ that

$$\sum_{l=0}^{i} l\, g_{l,i-l} = \sum_{l=0}^{i} i\, g_{l,i-l} - \sum_{l=0}^{i} (i-l)\, g_{l,i-l}$$
$$= \sum_{l=0}^{i} i\, g_{l,i-l} - \sum_{l=0}^{i} l\, g_{i-l,l}.$$

Thus, using the symmetry $g_{i-l,l} = g_{l,i-l}$, we finally get

$$\frac{1}{2} \sum_{l=0}^{i} i\, g_{l,i-l} = \sum_{l=0}^{i} l\, g_{l,i-l}.$$

Therefore, with $y_{i-1/2} = i\Delta y$ and taking successively $g_{i,j} = a_{i,j}\, f_{K,i}\, f_{K,j}$ and $g_{i,j} = b_{i,j}$, we obtain the result

$$\mathcal{Q}_{K,i} = \frac{1}{2} \sum_{l=0}^{i} \Delta y \left(a_{l,i-l}\, f_{K,l}\, f_{K,i-l} - b_{l,i-l}\, f_{K,i} \right)$$
$$- \sum_{l=i}^{N_y-1} \Delta y \left(a_{i,l-i}\, f_{K,i}\, f_{K,l-i} - b_{i,l-i}\, f_{K,l} \right).$$

$$\square$$

Next, we prove the following estimates:

PROPOSITION 3.1. *Assume the approximation of the coagulation-fragmentation operator (2.5)–(2.6) is given by the finite volume scheme (2.13)–(2.14). Then, for each $K \in \mathcal{T}$ the discrete operator $(\mathcal{Q}_{K,i})_{0 \le i \le N_y}$ satisfies a discrete weak formulation: for any sequence $(\varphi_i)_{0 \le i \le N_y}$ and for each $K \in \mathcal{T}$*

$$\sum_{i=0}^{N_y-1} \Delta y\, \mathcal{Q}_{K,i}\, \varphi_i = -\frac{1}{2} \sum_{i=0}^{N_y-1} \sum_{l=0}^{i} \Delta y^2 \left(a_{l,i-l}\, f_{K,l}\, f_{K,i-l} - b_{l,i-l}\, f_{K,i} \right) (\varphi_l + \varphi_{i-l} - \varphi_i). \tag{3.2}$$

Proof. We multiply (3.1) by $\Delta y\, \varphi_i$ and sum over $i \in \{0,\dots,N_y-1\}$ to get

$$\sum_{i=0}^{N_y-1} \Delta y\, \mathcal{Q}_{K,i}\, \varphi_i = \Delta y^2 \left(I_1 - I_2 \right), \tag{3.3}$$

with

$$I_1 = \frac{1}{2} \sum_{i=0}^{N_y-1} \sum_{j=0}^{i} \left(a_{j,i-j}\, f_{K,j}\, f_{K,i-j} - b_{j,i-j}\, f_{K,i} \right) \varphi_i,$$

$$I_2 = \sum_{i=0}^{N_y-1} \sum_{j=i}^{N_y-1} \left(a_{i,j-i}\, f_{K,i}\, f_{K,j-i} - b_{i,j-i}\, f_{K,j} \right) \varphi_i.$$

We keep the first term I_1 as it is and only treat the term I_2. First, we commute indexes (i,j) and then perform a change of index on I_2 which yields

$$
I_2 = \sum_{j=0}^{N_y-1} \sum_{i=0}^{j} (a_{i,j-i} f_{K,i} f_{K,j-i} - b_{i,j-i} f_{K,j}) \varphi_i
$$
$$
= \sum_{i=0}^{N_y-1} \sum_{l=0}^{i} (a_{i-l,l} f_{K,i-l} f_{K,l} - b_{i-l,l} f_{K,i}) \varphi_{i-l}. \tag{3.4}
$$

Using the symmetry $a_{i,j} = a_{j,i}$ and $b_{i,j} = b_{j,i}$ for each $(i,j) \in \{0,\dots,N_y-1\}$, we also have that

$$
I_2 = \sum_{i=0}^{N_y-1} \sum_{l=0}^{i} (a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i}) \varphi_l. \tag{3.5}
$$

Finally, gathering (3.3)–(3.5), we get the result

$$
\sum_{i=0}^{N_y-1} \Delta y \, \mathcal{Q}_{K,i} \varphi_i = -\frac{1}{2} \sum_{i=0}^{N_y-1} \sum_{l=0}^{i} \Delta y^2 \, (a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i})(\varphi_l + \varphi_{i-l} - \varphi_i).
$$

$$\square$$

Now we are ready to prove Theorem 2.1.

4. Proof of Theorem 2.1

Let us first mention that using the structure of the discrete operator obtained in Prop. 3.1, the proof of the convergence to equilibrium starting at the bottom of page 14 resembles very much that of the same result in [25] or [8, 27, 33] and is even simpler since $y \in (0, R)$.

We assume that the kinetic and diffusion coefficients fulfill (1.4), (1.10) and (1.11), respectively, and that a and b are positive *a.e.* in $\mathbb{R}^+ \times \mathbb{R}^+$. We are also given an initial datum f^{in} satisfying (2.4) and denote by f^h the solution to (2.11) constructed in (2.12)–(2.14).

On the one hand, existence and uniqueness of a solution to

$$
\frac{df_{K,i}}{dt} - d(y_{i-1/2}) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} f_{K,i} = \mathrm{m}(K) \mathcal{Q}_{K,i} \tag{4.1}
$$

directly follows by applying the classical Cauchy-Lipschitz theorem for a finite set of ordinary differential equations. Existence of a global solution will be a consequence of the following uniform estimates with respect to time.

On the other hand, the discrete distribution function, solution to (4.1), satisfies the following estimates. Assuming that the initial distribution function f^{in} is nonnegative, we follow classical arguments and consider the modified equation

$$
\frac{df_{K,i}}{dt} - d(y_{i-1/2}) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} f_{K,i} = \mathrm{m}(K) \left[\mathcal{Q}_{K,i}^+ - L_{K,i} f_{K,i} \right],
$$

with

$$
\mathcal{Q}_{K,i}^+ = \Delta y \max \left(\left[\frac{1}{2} \sum_{j=0}^{i} a_{j,i-j} f_{K,j} f_{K,i-j} + \sum_{j=i}^{N_y-1} b_{i,j-i} f_{K,j} \right], 0 \right)
$$

and

$$L_{K,i} = \Delta y \left[\frac{1}{2} \sum_{j=0}^{i} b_{j,i-j} + \sum_{j=i}^{N_y-1} a_{i,j-i} f_{K,j-i} \right].$$

Then the nonnegativity of $f_{K,i}$ readily follows from the monotonicity of the discrete operator $\sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} f_{K,i}$ and the comparison principle for all K and i. This in turn implies the nonnegativity of the gain operator $\mathcal{Q}_{K,i}^+$ and thus that $f_{K,i}$ solves the desired equation (4.1).

Next, we prove the total volume conservation

$$\frac{d}{dt} \sum_{i=0}^{N_y-1} \sum_{K \in \mathcal{T}} m(K) \Delta y\, y_{i-1/2} f_{K,i}(t) = 0. \tag{4.2}$$

Indeed, we multiply (4.1) by $\Delta y\, y_{i-1/2}$ and sum over $(K,i) \in \mathcal{T} \times \{0,\dots,N_y-1\}$:

$$\frac{d}{dt} \sum_{K,i} m(K) \Delta y\, y_{i-1/2} f_{K,i}(t) = -\frac{1}{2} \sum_{K,i} \Delta y\, d(y_{i-1/2}) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D_{K,\sigma} f_{K,i} D_{K,\sigma}(y_{i-1/2})$$
$$+ \sum_{K,i} m(K) \Delta y\, \mathcal{Q}_{K,i} y_{i-1/2}.$$

Thus, using a discrete integration by parts, we prove that the first term of the right hand side is zero, whereas applying Prop. 3.1 with $\varphi_i = y_{i-1/2}$ also gives that

$$\sum_{K,i} m(K) \Delta y\, \mathcal{Q}_{K,i} y_{i-1/2} = 0,$$

which concludes the proof of (ii).

Now, let us prove the stabilization towards an equilibrium in the long time when the kinetic coefficients a and b satisfy the detailed balance condition (1.11). As mentioned in the introduction, the detailed balance condition (1.11) ensures an analogue of the Boltzmann H-theorem for the coagulation-fragmentation equations which we derive now for the discrete solution to (2.11). We set

$$H(f^h | \mathcal{M}^h) = \sum_{K,i} m(K) \Delta y \left(f_{K,i} \left(\ln \left(\frac{f_{K,i}}{\mathcal{M}_i} \right) - 1 \right) + \mathcal{M}_i \right)$$

and take in the discrete weak formulation (3.2) the test function φ such as $\varphi_i = \ln(f_{K,i}/\mathcal{M}_i)$ with $\mathcal{M}_i = \mathcal{M}(y_i) > 0$, and noticing that

$$\frac{dH(f^h)}{dt} = \sum_{K,i} m(K) \Delta y \frac{df_{K,i}}{dt} \ln \left(\frac{f_{K,i}}{\mathcal{M}_i} \right)$$

and recalling (3.2) with $\varphi_i = \ln(f_{K,i}/\mathcal{M}_i)$, we obtain

$$\frac{dH(f^h)}{dt} + \Delta y \sum_{K,i} \sum_{\sigma \in \mathcal{E}_K} d(y_{i-1/2}) \tau_\sigma D_{K,\sigma} f_{K,i} \ln \left(\frac{f_{K,i}}{\mathcal{M}_i} \right)$$
$$= -\Delta y \sum_{K,i} m(K) \mathcal{Q}_{K,i} \ln \left(\frac{f_{K,i}}{\mathcal{M}_i} \right),$$

which yields

$$\frac{dH(f^h)}{dt} + \Delta y \sum_{K,i} \sum_{\sigma \in \mathcal{E}_K} d(y_{i-1/2}) \tau_\sigma \frac{(D_{K,\sigma} f_{K,i})^2}{f_{K|L,i}} = -D(f^h), \qquad (4.3)$$

with $f_{K|L,i} = (f_{K,i} - f_{L,i})/(\ln(f_{K,i}/f_{L,i})) > 0$. We then treat the right hand side using the detailed balance condition (1.11) and get

$$D(f^h) = \frac{1}{2} \sum_{K,i} \sum_{l=0}^{i} \Delta y^2 \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right) \left[\ln \left(\frac{a_{l,i-l} f_{K,l} f_{K,i-l}}{b_{l,i-l} f_{K,i}} \right) \right],$$

which proves (iii).

Now, we study the long-time asymptotic behavior of the numerical solution f^h. To this aim we establish the following estimates:

LEMMA 4.1. *The numerical solution f^h satisfies the following uniform estimates with respect to time $t \in \mathbb{R}^+$: there exists $\kappa_0 > 0$ such that*

$$\sum_{K,i} \mathrm{m}(K) \Delta y (1 + y_{i-1/2}) f_{K,i}(t) + H(f^h(t)|\mathcal{M}^h) \le \kappa_0.$$

Moreover, for all $t \in \mathbb{R}^+$, we have

$$\Delta y \int_0^t \left[\sum_{i=0}^{N_y} \sum_{\sigma \in \mathcal{E}_{int}} d(y_{i-1/2})^{1/2} \mathrm{m}(\sigma) |D f_{K,i,\sigma}(s)| \right]^2 ds \le \kappa_0 \qquad (4.4)$$

and

$$\Delta y^2 \int_0^t \sum_{K,i} \sum_{l=0}^{i} \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right) \left[\ln \left(\frac{a_{l,i-l} f_{K,l} f_{K,i-l}}{b_{l,i-l} f_{K,i}} \right) \right] ds \le \kappa_0. \quad (4.5)$$

Proof. Using total volume conservation and entropy dissipation, we have already proven that

$$\sum_{K,i} \mathrm{m}(K) \Delta y \, y_{i-1/2} f_{K,i}(t) + H(f^h(t)|\mathcal{M}^h) \le C_0.$$

It remains to show that there exists a constant $C_0 > 0$, only depending on the initial datum $f^{\mathtt{in}}$ and $\mathcal{M}$, such that

$$\sum_{K,i} \mathrm{m}(K) \Delta y f_{K,i}(t) \le C_0. \qquad (4.6)$$

Indeed, on the one hand we notice that

$$\sum_{K,i} \mathrm{m}(K) \Delta y f_{K,i}(t) \le e^2 \sum_{K,i} \mathrm{m}(K) \Delta y \mathbf{1}_{\{f_{K,i}(t) \le e^2 \mathcal{M}_i\}} \mathcal{M}_i$$

$$+ \frac{1}{2} \sum_{K,i} \mathrm{m}(K) \Delta y \mathbf{1}_{\{f_{K,i}(t) > e^2 \mathcal{M}_i\}} f_{K,i} \left| \ln \left(\frac{f_{K,i}(t)}{\mathcal{M}_i} \right) \right|$$

$$\le e^2 \sum_{K,i} \mathrm{m}(K) \Delta y \mathcal{M}_i$$

$$+ \frac{1}{2} \sum_{K,i} \mathrm{m}(K) \Delta y f_{K,i}(t) \left| \ln \left(\frac{f_{K,i}(t)}{\mathcal{M}_i} \right) \right|.$$

On the other hand, observing that $r\ln(r) \geq r|\ln(r)| - 2/e$ for $r > 0$, we have

$$f_{K,i}(t)\ln\left(\frac{f_{K,i}(t)}{\mathcal{M}_i}\right) \geq f_{K,i}(t)\left|\ln\left(\frac{f_{K,i}(t)}{\mathcal{M}_i}\right)\right| - \frac{2\mathcal{M}_i}{e};$$

hence we get

$$\sum_{K,i}\mathrm{m}(K)\Delta y\, f_{K,i}(t)\left|\ln\left(\frac{f_{K,i}(t)}{\mathcal{M}_i}\right)\right| \leq \sum_{K,i}\mathrm{m}(K)\Delta y\, f_{K,i}(t)\ln\left(\frac{f_{K,i}(t)}{\mathcal{M}_i}\right)$$
$$+ \frac{2}{e}\sum_{K,i}\mathrm{m}(K)\Delta y\,\mathcal{M}_i$$
$$\leq H(f^h(t)|\mathcal{M}^h) + \sum_{K,i}\mathrm{m}(K)\Delta y\left(f_{K,i}(t) + \frac{2}{e}\mathcal{M}_i\right).$$

Combining the two inequalities yields

$$\frac{1}{2}\sum_{K,i}\mathrm{m}(K)\Delta y\, f_{K,i}(t) \leq \left(e^2 + \frac{1}{e}\right)\sum_{K,i}\mathrm{m}(K)\Delta y\,\mathcal{M}_i + \frac{1}{2}H(f^h(t)|\mathcal{M}^h)$$
$$\leq \left(e^2 + \frac{1}{e}\right)\sum_{K,i}\mathrm{m}(K)\Delta y\,\mathcal{M}_i + \frac{1}{2}H(f^h(0)|\mathcal{M}^h) =: C_0.$$

Next, let us prove (4.5). We start with the entropy estimates (4.3), which we integrate with respect to time $t \in \mathbb{R}^+$, giving

$$H(f^h(t)|\mathcal{M}^h) + \int_0^t \Delta y \sum_{K,i}\sum_{\sigma\in\mathcal{E}_K} d(y_{i-1/2})\tau_\sigma \frac{(D_{K,\sigma}f_{K,i}(t))^2}{f_{K|L,i}(t)}ds + \int_0^t D(f^h(s))ds$$
$$\leq H(f^h(0)|\mathcal{M}^h).$$

Then, since H is a convex function, we know that $H(f^h(t)|\mathcal{M}^h)$ is bounded from below and we get the result (4.5).

Finally, we show there exists $C_0 > 0$, only depending on f^{in} and $\mathcal{M}$, such that

$$\int_0^t \left[\sum_{\substack{i=0 \\ \sigma=K|L}}^{N_y}\sum_{\sigma\in\mathcal{E}_{int}} \mathrm{m}(\sigma)d(y_{i-1/2})^{1/2}|Df_{K,i,\sigma}(s)|\right]^2 ds \leq C_0 \qquad \forall t \in \mathbb{R}^+. \tag{4.7}$$

To this aim, we start with the Cauchy-Schwarz inequality

$$\sum_{\substack{i=0 \\ \sigma=K|L}}^{N_y}\sum_{\sigma\in\mathcal{E}_{int}} \mathrm{m}(\sigma)d(y_{i-1/2})^{1/2}|Df_{K,i,\sigma}|$$
$$\leq \left(\sum_{\substack{i=0 \\ \sigma=K|L}}^{N_y}\sum_{\sigma\in\mathcal{E}_{int}} \tau_\sigma d(y_{i-1/2})\frac{|Df_{K,i,\sigma}|^2}{f_{K|L,i}}\right)^{1/2}\left(\sum_{\substack{i=0 \\ \sigma=K|L}}^{N_y}\sum_{\sigma\in\mathcal{E}_{int}} \mathrm{m}(\sigma)\mathrm{d}(x_K,x_L)\, f_{K|L,i}\right)^{1/2}.$$

Applying (2.8) and (4.2), (4.3), it follows that

$$
\left(\sum_{i=0}^{N_y} \sum_{\substack{\sigma \in \mathcal{E}_{int} \\ \sigma = K|L}} \Delta y \, \mathrm{m}(\sigma) d(y_{i-1/2})^{1/2} |Df_{K,i,\sigma}| \right)^2
$$

$$
\leq \frac{2}{\xi} \left(\sum_{i=0}^{N_y} \sum_{\substack{\sigma \in \mathcal{E}_{int} \\ \sigma = K|L}} \Delta y \, \tau_\sigma d(y_{i-1/2}) \frac{|Df_{K,i,\sigma}|^2}{f_{K|L,i}} \right) \left(\sum_{i=0}^{N_y} \sum_{K \in \mathcal{T}} \Delta y \, \mathrm{m}(K) f_{K,i} \right)
$$

$$
\leq \frac{2C_0}{\xi} \left(\sum_{i=0}^{N_y} \sum_{\substack{\sigma \in \mathcal{E}_{int} \\ \sigma = K|L}} \Delta y \, \tau_\sigma d(y_{i-1/2}) \frac{|Df_{K,i,\sigma}|^2}{f_{K|L,i}} \right).
$$

Then, for each $t \in \mathbb{R}^+$ we integrate the latter inequality with respect to time over the interval $[0,t]$ and use the entropy dissipation (4.3) which guarantees that the right hand side is uniformly bounded with respect to time. $\qquad\square$

We now prove that the numerical solution converges to a steady state. Let $(t^n)_{n \geq 0}$ be a sequence of positive real numbers such that $t^n \to +\infty$ and set $f^n(t) = f^h(t^n + t)$ for $n \geq 1$ and $t \in \mathbb{R}^+$. Owing to the construction of f^n, it is easily seen that f^n is a weak solution to (2.11)–(2.15) on $[0,+\infty)$ with initial datum $f^h(t^n)$. We fix $T \in \mathbb{R}^+$ and infer from above that

$$
\sup_{t \in [0,T]} \sum_{K,i} m(K) \Delta y (1+y_i) f^n_{K,i}(t) + H(f^n(t)|\mathcal{M}^h) \leq \kappa_0.
$$

Moreover, by construction of f^n and applying Lemma 4.1, this implies that

$$
\Delta y \int_0^T \sum_{i=0}^{N_y} \sum_{\sigma \in \mathcal{E}_{int}} d(y_{i-1/2})^{1/2} \mathrm{m}(\sigma) |Df^n_{K,i,\sigma}(t)| \, dt
$$

$$
\leq \Delta y \int_{t^n}^{t^n+T} \sum_{i=0}^{N_y} \sum_{\sigma \in \mathcal{E}_{int}} d(y_{i-1/2})^{1/2} \mathrm{m}(\sigma) |Df_{K,i,\sigma}(t)| \, dt \longrightarrow 0 \quad \text{as} \quad n \to \infty \quad (4.8)
$$

and

$$
\Delta y^2 \int_0^T \sum_{K,i} \sum_{l=0}^{i} \left(a_{l,i-l} f^n_{K,l} f^n_{K,i-l} - b_{l,i-l} f^n_{K,i} \right) \left[\ln\left(\frac{a_{l,i-l} f^n_{K,l} f^n_{K,i-l}}{b_{l,i-l} f^n_{K,i}} \right) \right] dt
$$

$$
\leq \Delta y^2 \int_{t^n}^{t^n+T} \sum_{K,i} \sum_{l=0}^{i} \left(a_{l,i-l} f_{K,l} f_{K,i-l} - b_{l,i-l} f_{K,i} \right) \left[\ln\left(\frac{a_{l,i-l} f_{K,l} f_{K,i-l}}{b_{l,i-l} f_{K,i}} \right) \right] dt
$$

$$
\longrightarrow 0 \quad \text{as} \quad n \to \infty. \tag{4.9}
$$

Thus, from the bounds established in Lemma 4.1 and the scheme (2.11), we deduce that $(\partial_t f^n)_{n \in \mathbb{N}}$ is bounded in $L^\infty(0,T)$, so that the sequence $(f^n)_{n \in \mathbb{N}}$ is also bounded (even if the bounds depend on h and R) in $W^{1,\infty}(0,T)$ and so by the Ascoli theorem is compact in $\mathcal{C}([0,T])$. Therefore, there is a subsequence of $(f^n)_{n \in \mathbb{N}}$ (not relabeled) and a weak solution $\bar{f}$ to (2.11)–(2.15) such that

$$
f^n \longrightarrow \bar{f} \quad \text{in } \mathcal{C}([0,T]) \quad \text{as} \quad n \longrightarrow +\infty. \tag{4.10}
$$

Moreover, passing to the limit in (3.1), it easily follows that

$$\mathcal{Q}_{K,i}(f^n) \longrightarrow \mathcal{Q}_{K,i}(\bar{f}) \quad \text{in } L^1(0,T) \quad \text{as} \quad n \longrightarrow +\infty, \tag{4.11}$$

and passing to the limit in the discrete diffusion operator, we get

$$d(y_{i-1/2}) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D f^n_{K,i,\sigma} \longrightarrow d(y_{i-1/2}) \sum_{\sigma \in \mathcal{E}_K} \tau_\sigma D \bar{f}_{K,i,\sigma} \quad \text{in } L^1(0,T) \quad \text{as} \quad n \longrightarrow +\infty. \tag{4.12}$$

On the one hand, we use (4.9) and (4.10) to conclude that

$$D(\bar{f}) = 0, \quad a.e. \quad \text{in } (0,T).$$

Consequently, $\bar{f}$ satisfies

$$a_{i,j}\,\bar{f}_{K,i}(t)\,\bar{f}_{K,j}(t) = b_{i,j}\,\bar{f}_{K,i+j}(t)$$

for almost every $t \in (0,T)$ and each $(K,i,j) \in \mathcal{T} \times \{0,\dots,N_y\}^2$. In particular, this implies that

$$\mathcal{Q}_{K,i}(\bar{f}(t)) = 0 \quad \forall (K,i,j) \in \mathcal{T} \times \{0,\dots,N_y\}^2.$$

On the other hand, (4.8) and (4.12) ensure that

$$D_{K,\sigma}\bar{f}_{K,i} = 0 \quad \forall (K,i,\sigma) \in \mathcal{T} \times \{0,\dots,N_y\} \times \mathcal{E} \tag{4.13}$$

for almost every $t \in (0,T)$. Therefore, $\bar{f}(t)$ does not depend on time and satisfies the steady-state equation (2.11). Moreover, using the zero flux boundary conditions (1.3) and (4.13), $\bar{f}$ does not depend on $K \in \mathcal{T}$; the steady state is thus uniquely determined by the initial total volume. Recalling that the differential equation (2.11) conserves global volume, we conclude that there is $\alpha \in \mathbb{R}^+$ such that

$$\bar{f}_{K,i} := \mathcal{M}_{\alpha,i}\,a.e.\,\text{in } (0,T),$$

where

$$\sum_{i=0}^{N_y-1} \sum_{K \in \mathcal{T}} \Delta y\,\mathrm{m}(K)\,y_{i-1/2}\mathcal{M}_i = \sum_{i=0}^{N_y-1} \sum_{K \in \mathcal{T}} \Delta y\,\mathrm{m}(K)\,y_{i-1/2}f^{\mathrm{in}}_{K,i}.$$

Finally, since the limit is uniquely determined and the trajectory compact, the whole trajectory converges towards the equilibrium.

5. Numerical simulations

This section is devoted to the numerical study of convergence to equilibrium under the detailed balance condition and when this condition is not satisfied. We also investigate numerically the case with non-homogeneous Dirichlet boundary conditions.

5.1. Detailed balance kernels and convergence to equilibrium.

We assume that the coagulation and fragmentation coefficients fulfill the following detailed balance condition: there exists a nonnegative function $\mathcal{M} \in L^1(\mathbb{R}^+,(1+y)\,dy)$ such that

$$a(y,y')\mathcal{M}(y)\mathcal{M}(y') = b(y,y')\mathcal{M}(y+y') \quad \forall (y,y') \in \mathbb{R}^+ \times \mathbb{R}^+. \tag{5.1}$$

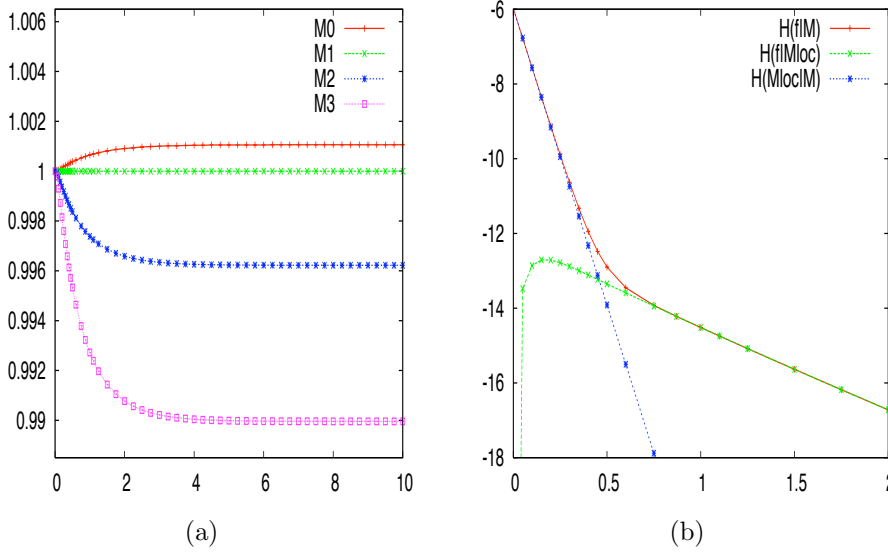FIG. 5.1. *Evolution of (a) the total number of particles M_0, the total volume M_1, M_2 and M_3 (b) the functional $H(f|\mathcal{M})$, $H(f|\mathcal{M}_{loc})$ and $H(\mathcal{M}_{loc}|\mathcal{M})$ in log scale.*

Since in that case there exists a Lyapunov functional H at the discrete level, we have proven that the numerical solution f^h converges to a discrete equilibrium $\mathcal{M}^h$. Here, we choose kernels a and b as follows:

$$a(y,y') = b(y,y') = 1,$$

which yields $\mathcal{M}(y) = \exp(-y/\sqrt{M_1})$. This is the Aizenman-Bak model for reacting polymers which diffuse in space with a constant coefficient $d(y) = d > 0$. In [7], the authors demonstrate that the entropy-entropy dissipation method developed by Desvillettes and Villani for the Boltzmann equation [9] applies directly and gives exponential convergence with explicit rates towards global equilibrium for a constant diffusion coefficient in any spatial dimension or for non-degenerate diffusion in dimension one. Therefore, the global equilibrium is given by

$$\mathcal{M}(y) = \exp(-y/\sqrt{M_1}), \quad y \in \mathbb{R}^+,$$

where the number M_1 is given by

$$M_1 := \frac{1}{|\Omega|} \int_\Omega \int_{\mathbb{R}^+} y\, f^{\mathtt{in}}(x,y)\, dx\, dy,$$

and $\mathcal{M}$ satisfies

$$d(y)\Delta_x\mathcal{M} = \mathcal{Q}(\mathcal{M}) = 0.$$

On the other hand, the local equilibrium $\mathcal{M}_{loc}$ is

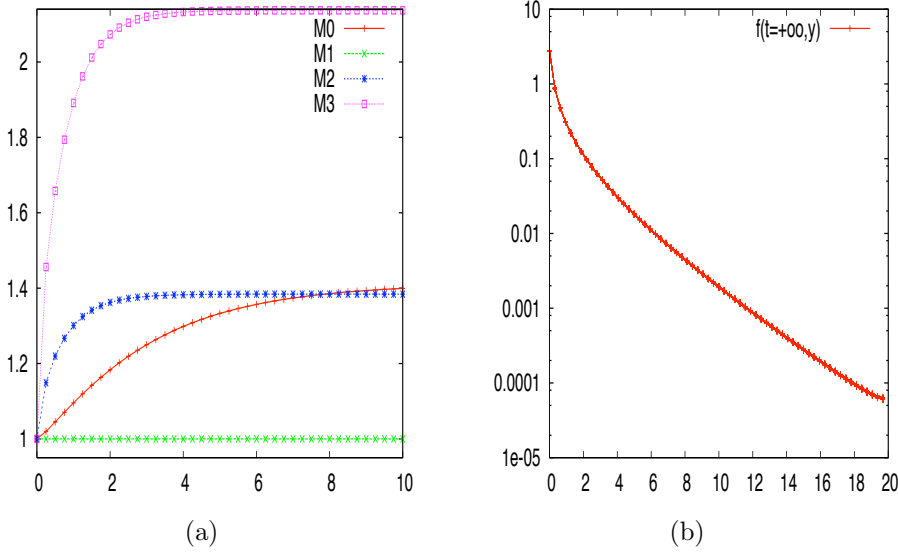$$\mathcal{M}_{loc}(x,y) = \exp(-y/\sqrt{M_1(x)}),$$

FIG. 5.2. *Evolution of (a) the total number of particles M_0, the total volume M_1, M_2 and M_3 (b) the functional $H(f|\mathcal{M})$, $H(f|\mathcal{M}_{loc})$ and $f^h(t \simeq \infty, y)$ in log scale.*

where the function $x \in \Omega \to M_1(x) \in \mathbb{R}^+$ is given by

$$M_1(x) := \int_{\mathbb{R}^+} y f(t,x,y) \, dy,$$

and $\mathcal{M}_{loc}$ satisfies

$$\mathcal{Q}(\mathcal{M}_{loc}) = 0.$$

The relative entropy $H(f|\mathcal{M})$ can be split in two different parts:

$$H(f|\mathcal{M}) = H(f|\mathcal{M}_{loc}) + H(\mathcal{M}_{loc}|\mathcal{M}), \tag{5.2}$$

where the first term in the right-hand side represents the "distance" between f and the local equilibrium, whereas the second term evaluates the distance between the local and global equilibria and only depends on the macroscopic quantity M_1. In the following we present some numerical results. As an initial datum, we take

$$f^{\texttt{in}}(x,y) = \exp(-\alpha(x)y),$$

with $\alpha(x) = 1 + 0.1 \cos(2\pi x_1) \cos(2\pi x_2)$ and $x = (x_1, x_2) \in (-1/2, 1/2)^2$. The diffusion is $d(y)$ is the constant $d(y) = 0.1$, the truncation is $R = 20$, the number of points used to discretize the volume variable is first $N_y = 64$ and next $N_y = 128$ and the time step is taken to be $\Delta t = 0.002$.

Let us first mention that in [18, 19] a similar problem, the trend to equilibrium of the solution to the nonhomogeneous Boltzmann equation, is investigated numerically. It is shown that the relative entropy with respect to the local equilibrium oscillates with time when the solution becomes close to the equilibrium. Here we will show that the situation is completely different and much simpler.
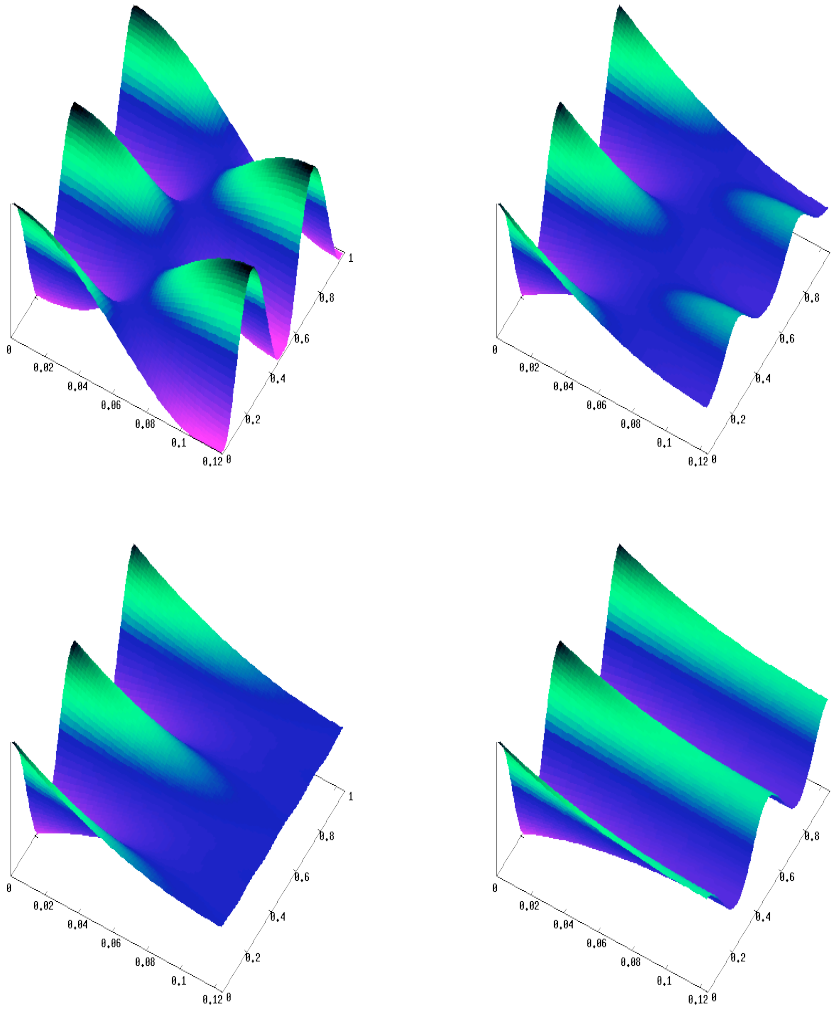
FIG. 5.3. *Time evolution of the density $M_0(x)$ at time $t = 0$, 0.33, 0.66 and 4*

In Figure 5.1 we report the evolution of the total number of particles M_0, the high-order moments in y of f^h with respect to time and the Lyapunov functional $H(f|\mathcal{M})$. As expected, the total volume $M_1(t)$ remains constant throughout time evolution and the moments stabilize to a fixed value. Regarding the asymptotic profile, our numerical results are in fair agreement with the equilibrium $\mathcal{M}(x) = \exp(-x)$. Moreover, we observe that the scheme is able to give the correct behavior of the numerical entropy $H(f|\mathcal{M})$, which converges exponentially fast to zero [7]. However, we observe that the trend to equilibrium for the coagulation-fragmentation with diffusion is much simpler than the trend to equilibrium for the Boltzmann equation [18], since no oscillation occurs for the relative entropy $H(f|\mathcal{M}_{loc})$. Indeed, after a short transient regime, the solution f converges to equilibrium exponentially with respect to
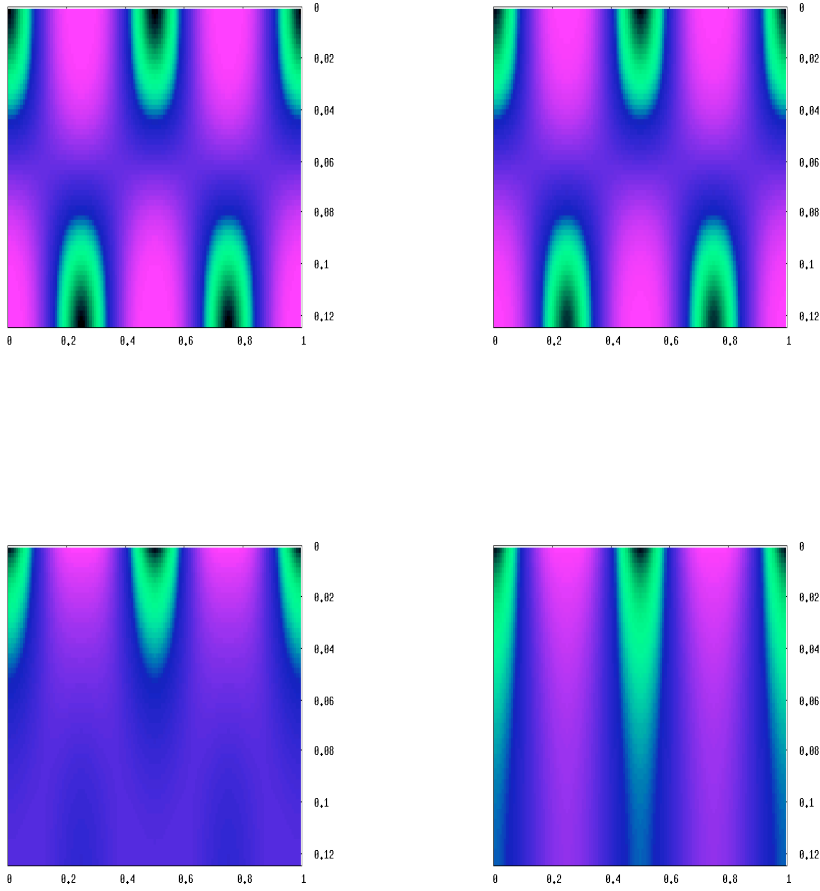
FIG. 5.4. *Time evolution of the volume density $M_1(x)$ at time $t = 0$, 0.33, 0.66 and 4*

time. Let us mention that here the situation is slightly different from the Boltzmann equation, since the entropy is strongly dissipative both in space (from the diffusion) and in volume (from the coagulation-fragmentation operator); this could explain why no oscillation occurs.

5.2. Convergence to equilibrium without the detailed balance condition. After this first result, we now explore a different situation where nothing is known about equilibrium and entropy dissipation. Indeed, we choose kernels a and b as follows:
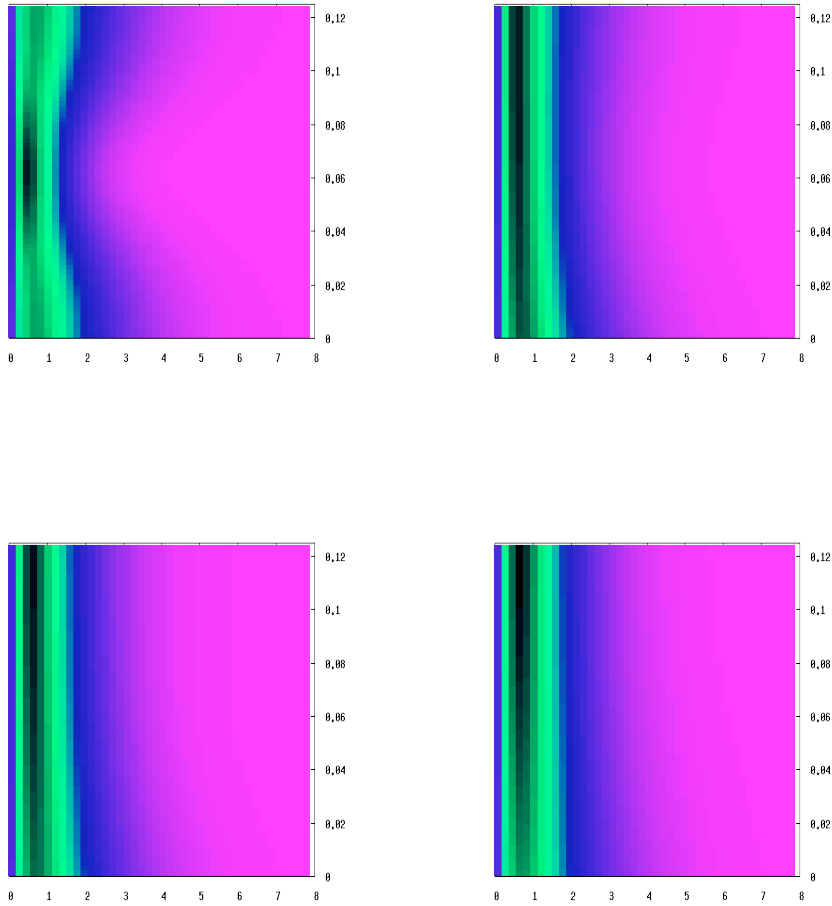
$$a(y, y') = (y y')^{1/2}, \quad b(y, y') = 1.$$

Fɪɢ. 5.5. *2D projection (x_1,y) of the density $y f(t,x,y)$ at time $t=0$, 0.33, 0.66 and 4*

The situation becomes much more complicated since there is no detailed balance condition, but it is proven in [14] that there exists a steady state solution to the coagulation-fragmentation operator. However, there is proof neither of convergence to a stationary solution nor of existence of entropy. As an initial datum, we take

$$f^{\mathtt{in}}(x,y) = \exp(-\alpha(x)y),$$

with $\alpha(x) = 1 + 0.5\cos(4\pi x_1)\cos(4\pi x_2)$ and $x = (x_1,x_2) \in [-1/2,1/2]^2$. Moreover, the diffusion is taken to be

$$d(y) = 0.1/(1+y), \quad y \in (0,R),$$

which becomes degenerate when R goes to infinity. We performed several numerical simulations in order that the solution is no longer sensitive to the trunctation R or the

number of grid points. To generate the following figures, we have taken $R = 20$, the number of points to discretize the volume variable $N_y = 64$, and the time step to be $\Delta t = 0.002$. In Figure 5.2, we still report the evolution of the total number of particles M_0 and other high-order moments in y of f^h, that is, M_1, M_2 and M_3. As expected, the total volume $M_1(t)$ remains constant throughout time evolution, whereas high-order moments vary and then stabilize to a fixed value, which means that the solution converges to a steady state. In the same figure (right hand side), we also report the distribution function with respect to y in a log scale for large time, which indicates that the tail with respect to y of the steady state $\bar{f}$ is still exponentially decreasing and $\bar{f}$ is of course constant in $x \in \Omega$.

5.3. Convergence to equilibrium for nonhomogeneous boundary conditions.   In this last section, we study the coagulation-fragmentation operator with diffusion in space and mixed boundary conditions in $x \in \Omega$. More precisely, we aim to approximate the solution in $\Omega = (0, 1/8) \times (0, 1)$ to

$$
\begin{cases}
\dfrac{\partial f}{\partial t} - d(y)\Delta_x f = \mathcal{Q}(f), \\[2ex]
f(t=0, x, y) = f^{\mathrm{in}}(x, y), \quad (x, y) \in \Omega \times \mathbb{R}^+, \\[2ex]
f(t, x_1=0, x_2, y) = \exp(-\alpha(0, x_2) y), \quad (x_2, y) \in \partial\Omega \times \mathbb{R}^+, \\[2ex]
\nabla_x f \cdot \vec{n}(x) = 0, \quad \text{if } x_1 = 1/8, x_2 \in (0, 1), \\
\nabla_x f \cdot \vec{n}(x) = 0, \quad \text{if } x_1 \in (0, 1/8), x_2 = 0 \\
\nabla_x f \cdot \vec{n}(x) = 0, \quad \text{if } x_1 \in (0, 1/8), x_2 = 1,
\end{cases}
$$

with $\vec{n}$ the external unit normal to $\partial\Omega$.

We consider an initial condition which is at equilibrium for the coagulation fragmentation operator

$$
f^{\mathrm{in}}(x, y) = exp(-\alpha(x) y), \quad (x, y) \in \Omega \times \mathbb{R}^+,
$$

with $\alpha(x) = 2/(1 + \cos(32\pi x_1)\cos(4\pi x_2))$. We perform numerical simulations using the finite volume scheme with diffusion coefficient $d(y) = 0.01/(1+y)$ and $a = b \equiv 1$.

We then define the moment of order $\ell \geq 0$ of the numerical approximation by

$$
M_\ell^h(t) = \sum_{K \in \mathcal{T}} \sum_{i=0}^{I^h} \mathrm{m}(K) \Delta y \, y_i^\ell \, f_{K,i}(t),
$$

and we plot in Figure 5.3 the time evolution of the moments of order 0, 1, 2, and 3.

The following figures (Figures 5.3, 5.4 and 5.5) are illustrations of the profile of the number of particles $M_0(t, x)$ and total volume $M_1(t, x)$ for $t \in \mathbb{R}^+$ and $x \in \Omega$ and also the projections

$$
P(t, x_2, y) = \int_0^{1/8} y f(t, x, y) dx_1, \quad x_2 \in (0, 1), y \in \mathbb{R}^+.
$$

This allows us to observe the qualitative behavior of the system. The profiles are in this case smooth and also converge to an equilibrium. For such computations we have taken $N_y = 64$ and have used a 128×128 grid points for the space variable

$x \in \Omega$. In this situation, we cannot characterize explicitly the equilibrium in space, since the diffusion coefficient is not constant and H is not valid here due to the Dirichlet boundary conditions for $x_1 = 0$ and hence the total volume is not preserved at all. However, we still observe that the numerical solution converges to a discrete equilibrium (see Figures 5.3–5.5).

6. Conclusion

In this paper, we make use of different principles (volume conservation, entropy dissipation, existence of steady states) which allow to build a stable and accurate numerical scheme for the nonlinear dynamics of coagulation, fragmentation and diffusion equations. Such an algorithm is able to recover the main properties of the exact solution, and in some particular cases, it is proven that the method is asymptotically stable, in the sense that the numerical solution converges to an equilibrium which is consistent with the exact equilibrium of the system. Numerical simulations illustrate the efficiency of the algorithm even when we cannot prove convergence to equilibrium.

Here we have only considered the time evolution of a distribution function, but the method can be easily coupled with Euler or Navier-Stokes equations after some adaptations. Typical applications are transport problems (including linear and nonlinear diffusion or fluid dynamics), which are coupled with population balance dynamics represented by a distribution function f depending on space $x \in \Omega$ and a "size" variable $y \in \mathbb{R}^+$.

On the other hand, for some coagulation and fragmentation kernels [16, 6], total volume is not conserved at all and then a nonconservative formulation can be used to discretize the coagulation and fragmentation operators using the same kind of finite volume scheme. Then the finite volume approach allows to use non-uniform meshes for the volume variable $y \in \mathbb{R}^+$, which is particularly well-suited in this case [16].

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