Finite Difference Schemes for a Size Structured Coagulation-Fragmentation Model in the Space of Radon Measures

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Abstract

We develop and compare multiple finite difference schemes for a size structured coagulation-fragmentation model formulated in the space of Radon measures under the Bounded-Lipschitz norm. In particular, we develop a fully explicit scheme, a semi-implicit scheme, and an explicit scheme based on the mass conservation law governed by the model. We prove convergence for each scheme and test the schemes against multiple well-known examples. We analyze and compare important properties of each scheme such as mass conservation, order of convergence, and computation time.

Keywords: A Coagulation-Fragmentation Equation, Size Structured Populations, Radon Measures Equipped with Bounded-Lipschitz Norm, Finite Difference Schemes, Conservation of Mass

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1 Introduction

Coagulation equations have been studied in various forms since the pioneering work of Smoluchowski [64] where a system of differential equations was used to form a discrete coagulation model. This model was later taken into a continuous setting by Müller [51] where the system of differential equations was changed to an integro-differential equation. The history of fragmentation equations followed a similar development with Blatz and Tobolsky [13] introducing discrete fragmentation kernels which were extended to a continuous setting by Melzak [50].

Since their development, coagulation-fragmentation equations have had many uses in various applications in physics, chemistry, and biology. In particular, they have receive much attention in the study of population dynamics of oceanic phytoplanton [1, 4, 5, 11, 15, 36, 37, 60]. The idea of combining coagulation equations with size structured models was first introduced by Ackleh and Fitzpartick in [5]. Later, Ackleh extended this idea to include binary fragmentation in [1]. These models take the form of a first-order hyperbolic differential equation with nonlinear and nonlocal ingredients. The coagulation-fragmentation terms are useful in this application as phytoplankton populations tend to be modeled as collections of single cells adhered together via an organic glue. Through collisions, these groups of cells can either stick together to form an assemblage of greater size (coagulate) or split into groups of smaller sizes (fragment). The natural growth of assemblages due to single cell division is naturally modeled via a first order structured hyperbolic equation. As mentioned before, coagulation-fragmentation equations can be studied with either a discrete or continuous structure. In this paper, we make use of the setting of Radon measures to simultaneously study both cases. In this light, we consider the following size structured coagulation-fragmentation model presented in [7]:

$$\begin{cases} \partial_t \mu + \partial_x (g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu], & (t,x) \in (0,T) \times (0,\infty), \\ g(t,\mu)(0) D_{dx}\mu(0) = \displaystyle\int_{\mathbb{R}^+} \beta(t,\mu)(y)\mu(dy), & t \in [0,T], \\ \mu(0) = \mu_0 \in \mathcal{M}^+(\mathbb{R}^+), \end{cases} \quad . \tag{1}$$

where $\mu(t)$ belongs to $\mathcal{M}^+(\mathbb{R}^+)$, the set of finite nonnegative Borel measures on $\mathbb{R}^+ := [0,\infty)$. Here, given a Borel subset $A \subset \mathbb{R}^+$, $\mu_t(A) := \mu(t)(A)$ represents the number of individuals at time t of size x in A, and the functions g and d represent the growth and death rate of individuals at time t of size x, respectively. Likewise, the function β represents the reproduction rate of these individuals. More precisely, at time t and distribution $\mu(t)$, an individual with size x produces offspring at rate $\beta(t,\mu(t))(x)$. Finally, $D_{dx}\mu(0)$ denotes the Radon-Nikodym derivative of $\mu(t)$ with respect to the Lebesgue measure, dx, at the point $x = 0$. For more information about size structured models in a measure setting, we direct the reader to [6, 32]. Finally, K and F are the coagulation and fragmentation terms respectively that we will precisely define later.

As argued in [7], equation (1) in the framework of measure-valued solution allows naturally to unify both the discrete and continuous coagulation-fragmentation equation. In general the measure framework has proven to be useful in the modeling not only of biological phenomena but also of social and economical phenomena (see e.g. [54, 55, 56, 57, 58, 61] and references therein).

It is an important property of model (1) that the mass of the total population, $\int_0^\infty x\mu(dx)$, is conserved in the coagulation-fragmentation terms. With this in mind, this model can also be written in a conservation law like form as in [48, 66]:

$$\begin{cases} \partial_t(x\mu) + x\partial_x(g(t,\mu)\mu) + xd(t,\mu)\mu = \partial_x \mathcal{Q}_F[\mu] - \partial_x \mathcal{Q}_K[\mu], \\ g(t,\mu)(0)D_{dx}\mu(0) = \int_0^\infty \beta(t,\mu)(x)\mu(dx), \\ \mu_0 \in \mathcal{M}^+(\mathbb{R}^+), \end{cases} \tag{2}$$

for some integral kernels $\mathcal{Q}_F[\mu]$ and $\mathcal{Q}_K[\mu]$ satisfying $\partial_x \mathcal{Q}_F[\mu] = xF[\mu]$ in the sense of distributions.

Throughout literature, there are many assumptions on the kernels of the coagulation and fragmentation terms [10, 33, 38, 52, 19, 50, 49, 40, 28, 29]. Though these assumptions are important to many other applications, they tend to be nonsensical in the context of oceanic phytoplankton. In particular, the size of aggregates should be bounded as there is a maximum size aggregates can maintain. In light of this, we will stick to similar assumptions presented in [7] which will be explicitly stated later. We also include the additional assumption of the existence of a maximum size, $x_{\max}$, for which larger assemblages cannot be produced via the coagulation process. This assumption is natural in application as physical limits prevent the existence of arbitrarily large aggregates.

In this article, we develop and compare numerical schemes based on models (1) and (2) using similar finite-difference techniques discussed in [6]. Finite-difference techniques have many advantages including straight-forward implementation and accessibility. One main advantage of the finite-difference schemes is the ease of lifting schemes to higher-order accuracy as done in the aforementioned paper. Higher-order schemes are a necessity in optimal control and inverse problems where one is required to solve the equation in question multiple times. These methods have been well studied in both a smooth and integrable setting [46, 63]. However, there is currently little work done with finite-difference schemes in the space of measures.

As for the layout of the article, in section 2 we introduce notation that will be used throughout the paper and point out any proven results useful in our analysis. In section 3, we discuss the model in more detail and state the assumptions of the model ingredients. In section 4, we develop and study an explicit and semi-implicit scheme on model (1). We prove convergence of these schemes and discuss the advantages of each. In section 5, we derive model (2) in the setting of Radon measures. We then develop an explicit scheme on this model. In section 7, we test the schemes against well known examples. We display the computation time as well as numerical order of convergence. We leave the reader with some discussion and comments in section 8.

2 Preliminaries and Notation

In this section, we will provide some useful definitions and notation that will be used throughout the manuscript.

We denoted by $\mathcal{M}(\mathbb{R}^+)$ the space of finite Radon measures over $\mathbb{R}^+ := [0, \infty)$. Likewise, we denote its non-negative cone by $\mathcal{M}^+(\mathbb{R}^+)$. Both of these spaces will be equipped with the Bounded-Lipschitz (BL) norm defined by

$$\|\mu\|_{BL} := \sup_{\|\phi\|_{W^{1,\infty}} \le 1} \left\{ \int_{\mathbb{R}^+} \phi(x)\mu(dx) : \phi \in W^{1,\infty}(\mathbb{R}^+) \right\},$$

where $W^{1,\infty}(\mathbb{R}^+)$ is the usual Sobolev space over $\mathbb{R}^+$ with codomain $\mathbb{R}$ equipped with the usual norm $\|\phi\|_{W^{1,\infty}} := \|\phi\|_\infty + \|\phi'\|_\infty$. In contrast, the traditional norm associated with $\mathcal{M}(\mathbb{R}^+)$ is the total variation (TV) norm given by

$$\|\nu\|_{TV} = |\nu|(\mathbb{R}^+) = \sup_{\|f\|_\infty \le 1} \left\{ \int_{\mathbb{R}^+} f(x)\nu(dx) : f \in C_c(\mathbb{R}^+) \right\}.$$

These norms are well studied and compared in [31].

We remark that the BL and TV norms are equal on $\mathcal{M}^+(\mathbb{R}^+)$ but are different on $\mathcal{M}(\mathbb{R}^+)$, indeed,

$$\|\mu\|_{BL} \le \|\mu\|_{TV}$$

for $\mu \in \mathcal{M}(\mathbb{R}^+)$. It has also been shown in [31] that $\mathcal{M}(\mathbb{R}^+)$ is not complete under the BL norm. However, this problem is alleviated in closed balls under the TV norm. Indeed as shown in [30] sets of the form

$$S := \{\mu \in \mathcal{M}(\mathbb{R}^+) : \|\mu\|_{TV} < R\}$$

are complete under the BL norm. In $\mathcal{M}^+(\mathbb{R}^+)$, we additionally have that the BL-norm metrizes weak convergence. That is, a sequence $(\mu_n)_n$ converges weakly to $\mu \in \mathcal{M}^+(\mathbb{R}^+)$ if for every $f \in C_b(\mathbb{R}^+)$,

$$\int_{\mathbb{R}^+} f(x)(\mu_n(dx) - \mu(dx)) \longrightarrow 0,$$

as $n \longrightarrow \infty$. For more detail, we refer the reader to the aforementioned citations.

It is often convenient to use the operator notation in place of integration. That is for a function f, we say

$$(\mu, f) := \int_A f(x)\mu(dx),$$

where the set A is the support of the measure μ.

Finally, we say the flow of a Lipschitz vector field $g(t,x)$ is the function $T^g_{s,t}(x)$ which satisfies

$$\frac{d}{dt}T^g_{s,t}(x) = g(t, T_{s,t}(x)), \qquad T^g_{s,s}(x) = x. \tag{3}$$

In the case that $s = 0$, we often will write $T_t := T_{s,t}$.

3 Size Structured Coagulation-Fragmentation Model

In this section, we introduce and explain the size structured coagulation-fragmentation model (1). Well-posedness of this model is presented in [7]. We propose the following model:

$$\begin{cases} \partial_t \mu + \partial_x(g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu], & (t,x) \in (0,T] \times (0,\infty) \\ g(t,\mu)(0)D_{dx}\mu(0) = \displaystyle\int_{\mathbb{R}^+} \beta(t,\mu)(y)\mu(dy), & t \in [0,T]. \\ \mu(0) = \mu_0 \in \mathcal{M}^+(\mathbb{R}^+), \end{cases} \tag{4}$$

where

$$\begin{aligned} \mu &: [0,T] \longrightarrow \mathcal{M}^+(\mathbb{R}^+), \\ g, d, \beta &: [0,T] \times \mathcal{M}^+(\mathbb{R}^+) \longrightarrow W^{1,\infty}(\mathbb{R}^+), \\ K &: \mathcal{M}^+(\mathbb{R}^+) \longrightarrow \mathcal{M}(\mathbb{R}^+), \\ F &: \mathcal{M}^+(\mathbb{R}^+) \longrightarrow \mathcal{M}(\mathbb{R}^+). \end{aligned} \tag{5}$$

Here and from now on, the functions g, d, and β are nonnegative and represent the growth, death, and birth functions, respectively. They are assumed to be influenced by both time, t, and the solution to the population model, $\mu(t)$. In applications (e.g., see [2, 3, 18, 21]), it is common for these functions to depend on a weighted mean of the population in the following form:

$$\beta(t,\mu)(x) = B\left(t, x, \int_{\mathbb{R}^+} K_B(y)\mu(dy)\right)$$

and similar expressions for g and d, for given maps $B : [0,T] \times \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^+$ and $K_B : \mathbb{R}^+ \to \mathbb{R}^+$. Common physically motivated model functions utilize Beverton–Holt type [12] or Ricker type [59] nonlinearities with respect to the weighted mean of the population and of a Von Bertalanffy type [53] model with respect to structure x.

The coagulation term in model (1) is the measure given by

$$\begin{aligned} K[\mu](\cdot) &= \frac{1}{2}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \kappa(y,y')\delta_{y+y'}(\cdot)\mu(dy')\mu(dy) - \Big(\int_{\mathbb{R}^+} \kappa(y,\cdot)\mu(dy)\Big)\mu \\ &=: K^+[\mu] - K^-[\mu], \end{aligned} \tag{6}$$

where $\kappa(x,y)$ represents the rate at which individuals of size x coalesce with individuals of size y. The first term in (6), $K^+[\mu]$, represents the inflow of individuals due to coagulation. The second term in (6), $K^-[\mu]$, represents the number of individuals lost due to coagulation. Notice that $K^\pm[\mu]$ are measures which can be described in a distribution sense by

$$(K^+[\mu], \phi) = \frac{1}{2}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \kappa(y,x)\phi(x+y)\,\mu(dx)\,\mu(dy) \tag{7}$$

and

$$(K^-[\mu], \phi) = \int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \kappa(y,x)\phi(x)\,\mu(dy)\,\mu(dx), \tag{8}$$

for any bounded and measurable function $\phi : \mathbb{R}^+ \to \mathbb{R}$. Notice that if κ is symmetric, i.e. $\kappa(x,y) = \kappa(y,x)$, then

$$(K[\mu], \phi) = \frac{1}{2}\int_{\mathbb{R}^+}\int_{\mathbb{R}^+} \kappa(y,x)[\phi(x+y) - \phi(x) - \phi(y)]\,\mu(dx)\,\mu(dy). \tag{9}$$

In a similar light, the fragmentation term is the measure given by

$$F[\mu](\cdot) = \int_{\mathbb{R}^+} b(y,\cdot)a(y)\mu(dy) - a\mu =: F^+[\mu] - F^-[\mu]. \tag{10}$$

Here, $a(y)$ represents the global fragmentation rate of individuals of size y and $b(y,\cdot)$ is a measure supported on $[0,y]$ such that $b(y,A)$ represents the probability a particle of size y

fragments to a particle with size in the Borel set $A \subset \mathbb{R}$. The positive term, F^+, represents the inflow of individuals due to fragmentation, and the negative term, F^-, represents the number of individuals lost due to fragmentation. Similar to the coagulation terms, $F^{\pm}[\mu]$ are measures given explicitely by

$$(F^+[\mu], \phi) = \int_{\mathbb{R}^+} (b(y,\cdot), \phi) a(y)\, \mu(dy), \qquad \text{where} \qquad (b(y,\cdot),\phi) = \int_0^y \phi(x) b(y, dx),$$

and

$$(F^-[\mu], \phi) = \int_{\mathbb{R}^+} a(y)\phi(y)\mu(dy).$$

We impose the following assumptions on the growth, death and birth functions:

(A1) For any $R > 0$, there exists $L_R > 0$ such that for all $\|\mu_i\|_{TV} \leq R$ and $t_i \in [0, \infty)$ $(i = 1, 2)$ the following hold

$$\|g(t_1, \mu_1) - g(t_2, \mu_2)\|_\infty \leq L_R(|t_1 - t_2| + \|\mu_1 - \mu_2\|_{BL}),$$

$$\|d(t_1, \mu_1) - d(t_2, \mu_2)\|_\infty \leq L_R(|t_1 - t_2| + \|\mu_1 - \mu_2\|_{BL}),$$

$$\|\beta(t_1, \mu_1) - \beta(t_2, \mu_2)\|_\infty \leq L_R(|t_1 - t_2| + \|\mu_1 - \mu_2\|_{BL}),$$

(A2) There exists $\zeta > 0$ such that for all $T > 0$

$$\sup_{t\in[0,T]} \sup_{\mu\in\mathcal{M}^+(\mathbb{R}^+)} \|g(t,\mu)\|_{W^{1,\infty}} + \|d(t,\mu)\|_{W^{1,\infty}} + \|\beta(t,\mu)\|_{W^{1,\infty}} < \zeta,$$

(A3) For all $(t, \mu) \in [0, \infty) \times \mathcal{M}^+(\mathbb{R}^+)$,

$$g(t,\mu)(0) > 0 \quad \text{and} \quad g(t,\mu)(x_{\max}) = 0$$

for some large $x_{\max} > 0$.

We assume that the coagulation kernel κ satisfies the following assumption:

(K1) κ is symmetric, nonnegative, bounded by a constant C_κ, and globally Lipschitz with Lipschitz constant L_κ.

(K2) $\kappa(x, y) = 0$ whenever $x + y > x_{\max}$.

We assume that the fragmentation kernel satisfies the following assumptions:

(F1) $a \in W^{1,\infty}(\mathbb{R}^+)$ is non-negative,

(F2) for any $y \geq 0$, $b(y, dx)$ is a measure such that

(i) $b(y, dx)$ is non-negative and supported in $[0, y]$, and there exist a $C_b > 0$ such that $b(y, \mathbb{R}^+) \leq C_b$ for all $y > 0$,

(ii) there exists L_b such that for any $y, \bar{y} \geq 0$,

$$\|b(y,\cdot) - b(\bar{y},\cdot)\|_{BL} \leq L_b|y - \bar{y}|$$

(iii) for any $y \geq 0$,

$$(b(y,dx),x) = \int_0^y x\, b(y,dx) = y.$$

It follows from (F2) that for any ϕ, with $\|\phi\|_{W^{1,\infty}} \leq 1$, the function $\Phi[\phi](y) = (b(y,\cdot),\phi)$ is bounded Lipschitz with $\|\Phi[\phi](y)\|_{W^{1,\infty}} \leq \bar{C}_b = \max\{C_b, L_b\}$.

With the above assumptions, we have the following useful propositions proven in [7]:

Proposition 3.1. *For every $\mu \in \mathcal{M}(\mathbb{R}^+)$, we have*

$$\|K[\mu]\|_{TV} \leq \frac{3}{2} C_\kappa \|\mu\|_{TV}^2. \tag{11}$$

For every $\mu, \nu \in \mathcal{M}(\mathbb{R}^+)$ with $\|\mu\|_{TV}, \|\nu\|_{TV} \leq R$,

$$\|K[\mu] - K[\nu]\|_{BL} \leq \bar{L}_{\kappa,R}\|\mu - \nu\|_{BL}, \tag{12}$$

where $\bar{L}_{\kappa,R}$ is a constant depending only on C_κ, L_κ, and R.

Proposition 3.2. *For any $\mu \in \mathcal{M}(\mathbb{R}^+)$, we have*

$$\|F[\mu]\|_{TV} \leq (\bar{C}_b + 1)\|a\|_\infty \|\mu\|_{TV} \tag{13}$$

and

$$\|F[\mu] - F[\nu]\|_{BL} \leq C_{a,b}\|\mu - \nu\|_{BL}. \tag{14}$$

Given $T \geq 0$, we say a function $\mu \in C([0,T], \mathcal{M}^+(\mathbb{R}^+))$ is a weak solution to (1) if for all $\phi \in (C^1 \cap W^{1,\infty})([0,T] \times \mathbb{R}^+)$ and for all $t \in [0,T]$, the following holds:

$$\begin{aligned} &\int_0^\infty \phi(t,x)\mu_t(dx) - \int_0^\infty \phi(0,x)\mu_0(dx) = \\ &\quad \int_0^t \int_0^\infty \left[\partial_t \phi(s,x) + g(s,\mu_s)(x)\partial_x\phi(s,x) - d(s,\mu_s)(x)\phi(s,x)\right]\mu_s(dx)ds \\ &\quad + \int_0^t (K[\mu_s] + F[\mu_s], \phi(s,\cdot))\,ds + \int_0^t \int_0^\infty \phi(s,0)\beta(s,\mu_s)(x)\mu_s(dx)ds. \end{aligned} \tag{15}$$

Notice that we can also write model (1) with the boundary condition as a source term:

$$\partial_t \mu + \partial_x(g(t,\mu)\mu) + d(t,\mu)\mu = K[\mu] + F[\mu] + S(t)[\mu_t], \tag{16}$$

where $S(t)[\mu] = \Big(\int_0^\infty \beta(t,\mu)(y)\mu(dy)\Big)\delta_{x=0}$.

Remark 3.1. *Well-posedness for equation (4) under assumptions (A1)-(A3), (K1)-(K2), (F1)-(F2) is established in [7]. We note that if μ_0 is supported on the finite domain $[0, x_{\max}]$, then assumptions (A3) and (K2) guarantee the solution remains supported in this interval for all $t > 0$. This allows any integration against $\mu_t(dx)$ listed above to collapse to integration over $[0, x_{\max}]$.*

4 An explicit and a semi-implicit numerical scheme

In this section, we introduce two numerical schemes to approximate equation (4) assuming the initial condition μ_0 is a non-negative measure supported on $[0, x_{\max}]$. The first scheme is fully explicit and the second, semi-implicit. We prove the convergence of the numerical solution toward the solution of (4) in both cases.

We discretize the space domain $[0, x_{\max}]$ by introducing the points $x_j := j\Delta x$, $j = 0, 1, 2, 3, \ldots, J$, with $x_J = x_{\max}$, and the time domain $[0, T]$ considering the points $t_k := k\Delta t$, where $k = 0, 1, 2, \ldots, \bar{k}$ and $t_{\bar{k}} = T$. Denote $\Lambda_j := (x_{j-1}, x_j]$, $j \geq 1$. We then approximate the initial condition μ_0 by the following combination of Dirac delta measures placed at the nodes x_j:

$$\mu_0 \approx \sum_{j=1}^{J} m_j^0 \delta_{x_j} \qquad \text{where} \qquad m_j^0 := \mu_0(\Lambda_j).$$

We will then approximate the solution μ_{t_k} of (4) by measures $\mu_{\Delta x}^k$ of the form

$$\mu_{\Delta x}^k = \sum_{j=1}^{J} m_j^k \delta_{x_j}, \tag{17}$$

where the coefficients m_j^k are obtained through some numerical scheme.

To formulate the numerical scheme we introduce the following discretization of the model coefficients:

- for the functions $f = g, \beta, d$:
$$f_j^k := f(t_k, \mu_{\Delta x}^k)(x_j),$$
- for the coagulation kernel $\kappa(x, y)$:
$$\kappa_{j,l} := \kappa(x_j, x_l),$$
- for the fragmentation measure $b(x, \cdot)$:
$$b_{\Delta x}(x_i) := \sum_{j=1}^{i} b_{i,j} \delta_{x_j} \qquad \text{where} \qquad b_{j,l} := b(x_j, \Lambda_l).$$

4.1 Explicit Scheme

In this section, we define the coefficient m_j^k in (17) through the following fully explicit scheme:

$$\begin{cases} \dfrac{m_j^{k+1} - m_j^k}{\Delta t} + \dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + d_j^k m_j^k = \dfrac{1}{2} \displaystyle\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{i=1}^{J} \kappa_{i,j} m_i^k m_j^k \\ \qquad\qquad\qquad\qquad + \displaystyle\sum_{i=j}^{J} b_{i,j} a_i m_i^k - a_j m_j^k \qquad j = 1, .., J, . \\ g_0^k m_0^k = \Delta x \displaystyle\sum_{j=1}^{J} \beta_j^k m_j^k \end{cases} \tag{18}$$

We can rewrite this equation so as to express m^{k+1} in function of m^k as follows:

$$\begin{cases} m_j^{k+1} = \Big(1 - \dfrac{\Delta t}{\Delta x} g_j^k - \Delta t \displaystyle\sum_{i=1}^{J} \kappa_{i,j} m_i^k - \Delta t d_j^k - \Delta t a_j\Big) m_j^k + \dfrac{\Delta t}{\Delta x} g_{j-1}^k m_{j-1}^k \\ \qquad\qquad + \dfrac{1}{2}\Delta t \displaystyle\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k + \Delta t \sum_{i=j}^{J} b_{i,j} a_i m_i^k \qquad j = 1, ..., J, \\ g_0^k m_0^k = \Delta x \displaystyle\sum_{j=1}^{J} \beta_j^k m_j^k. \end{cases} \tag{19}$$

For this scheme, we impose the following Courant–Friedrichs–Lewy (CFL) condition

$$\Delta t\Big(C_\kappa \|\mu_0\|_{TV} \exp((\zeta + C_b C_a)T) + C_a \max\{1, C_b\} + (1 + \frac{1}{\Delta x})\zeta\Big) \leq 1. \tag{20}$$

where the constants C_a, C_b, C_κ are defined in assumptions (A1), (F1), (F2).

The proof of the convergence of this explicit scheme is done through a series of lemmas. We first prove that the approximate solutions $\mu_{\Delta x}^k$, defined in (17), are non-negative and bounded in the TV-norm uniformly in Δt and Δx:

Lemma 4.1. *For each $k = 1, \dots, \bar{k}$, the measure $\mu_{\Delta x}^k$ is non-negative and satisfies*

$$\|\mu_{\Delta x}^k\|_{TV} \leq \|\mu_0\|_{TV} \exp((\zeta + C_b C_a)T). \tag{21}$$

Proof. We show via induction that for any $k = 1, \dots, \bar{k}$,

(i) $\mu_{\Delta x}^k \in \mathcal{M}^+(\mathbb{R}^+)$ i.e. $m_j^k \geq 0$ for all $j = 1, \dots, J$,

(ii) $\|\mu_{\Delta x}^k\|_{TV} \leq \|\mu_{\Delta x}^0\|_{TV}(1 + (\zeta + C_b C_a)\Delta t)^k$.

The TV-bound stated in the Lemma then follows using that $(1 + x) \leq e^x$ and $k\Delta t \leq T$.

Let us first verify that $m_j^{k+1} \geq 0$. Since g, β, κ, a, and b are non-negative, it is enough, in view of (19), to verify that

$$\frac{1}{\Delta x} g_j^k + \sum_{i=1}^{J} \kappa_{i,j} m_i^k + d_j^k + a_j \leq \frac{1}{\Delta t}. \tag{22}$$

Notice that in view of assumptions (A2) and (F1) we have $g_j^k, d_j^k \leq \zeta$ and $a_j \leq C_a$. Moreover by the induction hypothesis and (K1),

$$\sum_{i=1}^{J} \kappa_{i,j} m_i^k \leq C_\kappa \sum_{i=1}^{J} m_i^k = C_\kappa \|\mu_{\Delta x}^k\|_{TV} \leq C_\kappa \|\mu_{\Delta x}^0\|_{TV} \exp((\zeta + C_b C_a)T).$$

We thus obtain (22) using the CFL condition (20).

Concerning the total variation bound, notice first that since $m_j^{k+1} \geq 0$ for all j, we have $\|\mu_{\Delta x}^{k+1}\|_{TV} = \sum_{j=1}^J m_j^{k+1}$. Then from rearranging (18) we obtain

$$\begin{aligned}\|\mu_{\Delta x}^{k+1}\|_{TV} \leq \sum_{j=1}^J m_j^k + \frac{\Delta t}{\Delta x}\sum_{j=1}^J \Big(g_{j-1}^k m_{j-1}^k - g_j^k m_j^k\Big) + \Delta t \sum_{j=1}^J \sum_{i=j}^J b_{i,j} a_i m_i^k \\ + \Delta t\Big(\frac{1}{2}\sum_{j=1}^J \sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{j=1}^J \sum_{i=1}^J \kappa_{i,j} m_i^k m_j^k\Big).\end{aligned} \tag{23}$$

Since $g_J^k = 0$ by (A3),

$$\sum_{j=1}^J \Big(g_{j-1}^k m_{j-1}^k - g_j^k m_j^k\Big) = g_0^k m_0^k - g_J^k m_J^k = \Delta x \sum_{j=1}^J \beta_j^k m_j^k \leq \zeta \Delta x \sum_{j=1}^J m_j^k. \tag{24}$$

Moreover, $\sum_{j=1}^i b_{i,j} = b(x_i, \mathbb{R}^+) \leq C_b$ by (F2) so that

$$\sum_{j=1}^J \sum_{i=j}^J b_{i,j} a_i m_i^k = \sum_{i=1}^J \sum_{j=1}^i b_{i,j} a_i m_i^k \leq C_b C_a \sum_{i=1}^J m_i^k. \tag{25}$$

Finally, due to assumption (K2), we have $\kappa_{ij} = \kappa_{ji} \geq 0$. Together with $m_i^k \geq 0$, we obtain

$$\sum_{j=1}^J \sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k = \sum_{i=1}^{J-1} \sum_{j=i+1}^J \kappa_{i,j-i} m_i^k m_{j-i}^k = \sum_{i=1}^J \sum_{l=1}^J \kappa_{i,l} m_i^k m_l^k \tag{26}$$

Thus,

$$\frac{1}{2}\sum_{j=1}^J \sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{j=1}^J \sum_{i=1}^J \kappa_{i,j} m_i^k m_j^k \leq -\frac{1}{2}\sum_{i=1}^J \sum_{l=1}^J \kappa_{i,l} m_i^k m_l^k \leq 0.$$

Therefore, (23) yields

$$\|\mu_{\Delta x}^{k+1}\|_{TV} \leq (1 + (\zeta + C_a C_b)\Delta t) \sum_{j=1}^J m_j^k = (1 + (\zeta + C_a C_b)\Delta t)\|\mu_{\Delta x}^k\|_{TV}.$$

Using the induction hypothesis, we obtain $\|\mu_{\Delta x}^{k+1}\|_{TV} \leq \|\mu_{\Delta x}^0\|_{TV}(1 + (\zeta + C_b C_a)\Delta t)^{k+1}$ as desired. □

Lemma 4.2. *There exists an $L > 0$ independent of Δx and Δt such that for any p, q,*

$$\|\mu_{\Delta x}^q - \mu_{\Delta x}^p\|_{BL} \leq L|q - p|\Delta t.$$

Proof. For $\phi \in W^{1,\infty}(\mathbb{R}^+)$ with $\|\phi\|_{W^{1,\infty}} \leq 1$, and denoting $\phi_j := \phi(x_j)$, we have thanks to Lemma 4.1 that for any k,

$$
\begin{aligned}
(\mu_{\Delta x}^{k+1} - \mu_{\Delta x}^k, \phi) =& \sum_{j=1}^J (m_j^{k+1} - m_j^k)\phi_j \\
\leq& \Delta t \sum_{j=1}^J \phi_j \Big(\frac{1}{\Delta x}(g_{j-1}^k m_{j-1}^k - g_j^k m_j^k) - d_j^k m_j^k - a_j m_j^k \\
&+ \frac{1}{2}\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{i=1}^J \kappa_{i,j} m_i^k m_j^k + \sum_{i=j}^J b_{i,j} a_i m_i^k \Big).
\end{aligned}
$$

Denoting C^* the right-hand side of the TV-bound (21), we obtain

$$
(\mu_{\Delta x}^{k+1} - \mu_{\Delta x}^k, \phi) \leq \frac{\Delta t}{\Delta x} \sum_{j=1}^J \phi_j (g_{j-1}^k m_{j-1}^k - g_j^k m_j^k) + \Delta t(\zeta + C_a + C_b C_a + \frac{3}{2} C_\kappa C^*)C^*.
$$

Moreover since $g_J^k = 0$, the sum in the right-hand side can be written as

$$
\phi_1 g_0^k m_0^k + \sum_{j=1}^{J-1} (\phi_{j+1} - \phi_j) g_j^k m_j^k = \Delta x \phi_1 \sum_{j=1}^J \beta_j^k m_j^k + \sum_{j=1}^{J-1} (\phi_{j+1} - \phi_j) g_j^k m_j^k \leq 2\Delta x \zeta C^*.
$$

We thus obtain

$$
(\mu_{\Delta x}^{k+1} - \mu_{\Delta x}^k, \phi) \leq L\Delta t, \qquad L := (3\zeta + C_a + C_b C_a + \frac{3}{2} C_\kappa C^*)C^*.
$$

Taking the supremum over ϕ gives $\|\mu_{\Delta x}^{k+1} - \mu_{\Delta x}^k\|_{BL} \leq L\Delta t$ for any k. The result follows. □

We define continuous curves $\mu_{\Delta x}^{\Delta t} : [0, T] \to \mathcal{M}^+(\mathbb{R}_+)$ by linearly interpolating the $\mu_{\Delta x}^k$, $k = 1, \ldots, \bar{k}$:

$$
\mu_{\Delta x}^{\Delta t}(t) = \mu_{\Delta x}^0 \chi_0(t) + \sum_{k=0}^{\bar{k}-1} \left[\Big(1 - \frac{t - t_k}{\Delta t}\Big) \mu_{\Delta x}^k + \frac{t - t_k}{\Delta t} \mu_{\Delta x}^{k+1} \right] \chi_{(t_k, t_{k+1}]}(t).
$$

We deduce from Lemmas 4.1 and 4.2 that the measures $\mu_{\Delta x}^{\Delta t}(t)$ satisfy

$$
\|\mu_{\Delta x}^{\Delta t}(t)\|_{TV} \leq \|\mu_0\|_{TV} \exp((\zeta + C_b C_a)T) \qquad t \in [0, T], \tag{27}
$$

and

$$
\|\mu_{\Delta x}^{\Delta t}(t) - \mu_{\Delta x}^{\Delta t}(t')\|_{BL} \leq L|t - t'|\Delta t \qquad t, t' \in [0, T]. \tag{28}
$$

We can now prove that the family of numerical approximations $\mu_{\Delta x}^{\Delta t}$ converge to the unique solution of (1):

Theorem 4.1. *As $\Delta t, \Delta x \to 0$ while the CFL condition* (20) *holds, the whole family $\mu_{\Delta x}^{\Delta t}$ converges to the solution of* (1) *in $C([0, T], \mathcal{M}^+([0, x_{\max}]))$.*

Proof. Recall that any set of the form

$$X_R := \{\mu \in C([0,T], \mathcal{M}^+([0,x_{max}])) : \sup_{0\le t\le T} \|\mu(t)\|_{TV} \le R\} \qquad R>0,$$

where $\mathcal{M}^+([0,x_{max}])$ is endowed with the BL-norm, is complete. In view of (27) and (28) we can thus apply Arzel-Ascoli Theorem to $\mu_{\Delta x}^{\Delta t} \in X_R$, $R = \|\mu_0\|_{TV}\exp((\zeta + C_b C_a)T)$, to obtain that the family $\mu_{\Delta x}^{\Delta t}$ is relatively compact. The Theorem will thus follow if we can prove that any convergent subsequence of $\mu_{\Delta x}^{\Delta t}$ converges to the unique solution of (1).

We thus consider a subsequence $\mu_{\Delta x}^{\Delta t}$, which we still denote $\mu_{\Delta x}^{\Delta t}$ for notational convenience, converging to some μ. Take some $\phi \in C^1([0,T]\times[0,x_{\max}])$. Multiplying equation (18) by $\phi_j^k := \phi(k\Delta t, j\Delta x)$ and rearranging we have

$$\begin{aligned}&\sum_{k=1}^{\bar{k}-1}\sum_{j=1}^{J}\left((m_j^{k+1}-m_j^k)\phi_j^k + \frac{\Delta t}{\Delta x}(g_j^k m_j^k - g_{j-1}^k m_{j-1}^k)\phi_j^k + \Delta t\phi_j^k d_j^k m_j^k\right) = \\ &\Delta t\sum_{k=1}^{\bar{k}-1}\sum_{j=1}^{J}\phi_j^k\left(\frac{1}{2}\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^k m_{j-i}^k - \sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^k + \sum_{i=j}^{J} b_{i,j}a_i m_i^k - a_j m_j^k\right).\end{aligned} \tag{29}$$

We point out the terms on the left-hand side of the above equations are identical to Theorem 4.2 of [6] where we proved that

$$\begin{aligned}&\sum_{k=1}^{\bar{k}-1}\sum_{j=1}^{J}\left((m_j^{k+1}-m_j^k)\phi_j^k + \frac{\Delta t}{\Delta x}(g_j^k m_j^k - g_{j-1}^k m_{j-1}^k)\phi_j^k + \Delta t\phi_j^k d_j^k m_j^k\right) \\ &= \int \phi(T,x)d\mu_{\Delta x}^{\Delta t}(T)(x) - \int \phi(0,x)d\mu_{\Delta x}^{0}(x) \\ &- \int_0^T \Big(\int \Big[\partial_x\phi(t,x)g(t,\mu_{\Delta x}^{\Delta t})(x) + \partial_t\phi(t,x) - d(t,\mu_{\Delta x}^{\Delta t}(t))(x)\phi(t,x)\Big]d\mu_{\Delta x}^{\Delta t}(t)(x) \\ &\qquad + \phi(t,0)\int \beta(t,\mu_{\Delta x}^{\Delta t}(t))(x)d\mu_{\Delta x}^{\Delta t}(t)(x)\Big)dt + o(1),\end{aligned} \tag{30}$$

where $o(1)\to 0$ as $\Delta x, \Delta t \to 0$.

We now focus on the terms on the right-hand side of (29). We have with assumption (K2)

$$\begin{aligned}\sum_{j=1}^{J}\left(\frac{1}{2}\sum_{i=1}^{j-1}\phi_j^k\kappa_{i,j-i}m_i^k m_{j-i}^k - \sum_{i=1}^{J}\phi_j^k\kappa_{i,j}m_i^k m_j^k\right) &= \frac{1}{2}\sum_{i=1}^{J}\sum_{j=i+1}^{J}\phi_j^k\kappa_{i,j-i}m_i^k m_{j-i}^k - \sum_{j=1}^{J}\sum_{i=1}^{J}\phi_j^k\kappa_{i,j}m_i^k m_j^k \\ &= \frac{1}{2}\sum_{i=1}^{J}\sum_{l=1}^{J}(\phi_{l+i}^k - \phi_l^k - \phi_i^k)\kappa_{i,l}m_i^k m_l^k \\ &= (K[\mu_{\Delta x}^k], \phi^k).\end{aligned} \tag{31}$$

As for the fragmentation terms, we first notice that

$$\sum_{j=1}^{J}\sum_{i=j}^{J} b_{i,j}\phi_j^k a_i m_i^k = \sum_{i=1}^{J}\sum_{j=1}^{i} b_{i,j}\phi_j^k a_i m_i^k = \sum_{i=1}^{J}(b_{\Delta x}(x_i,\cdot),\phi^k)a_i m_i^k. \tag{32}$$

Moreover, denoting $Lip(\phi)$ the Lipschitz constant of ϕ,

$$|(b_{\Delta x}(x_i,\cdot),\phi^k)-(b(x_i,\cdot),\phi^k)| \;=\; |\sum_{j=1}^{i}(b(x_i,\cdot)(\phi^k(x_j)-\phi^k)1_{\Lambda_j})| \le C_b\Delta x Lip(\phi).$$

It follows that

$$\sum_{j=1}^{J}\sum_{i=j}^{J} b_{i,j}\phi_j^k a_i m_i^k - \sum_{j=1}^{J} a_j\phi_j^k m_j^k = (F[\mu_{\Delta x}^k],\phi^k) + O(\Delta x),$$

where $O(\Delta x) \le C_b\Delta x Lip(\phi)$. Thus the right-hand side of (29) is

$$\begin{aligned}
&\Delta t\sum_{k=1}^{\bar{k}-1}\Big\{(K[\mu_{\Delta x}^k],\phi^k) + (F[\mu_{\Delta x}^k],\phi^k)\Big\} + O(\Delta x)\\
&= \Delta t\sum_{k=1}^{\bar{k}-1}\Big\{(K[\mu_{\Delta x}^{\Delta x}(t_k)],\phi(t_k,\cdot)) + (F[\mu_{\Delta x}^{\Delta x}(t_k)],\phi(t_k,\cdot))\Big\} + O(\Delta x).
\end{aligned}$$

Making use of (12) and (14), it is easily seen that $(K[\mu_{\Delta x}^{\Delta x}(t)],\phi(t,\cdot))$ and $(F[\mu_{\Delta x}^{\Delta x}(t)],\phi(t,\cdot))$ are continuous in t. Thus the right-hand side of (29) is

$$\int_0^T (K[\mu_{\Delta x}^{\Delta x}(t)],\phi(t,\cdot)) + (F[\mu_{\Delta x}^{\Delta x}(t)],\phi(t,\cdot))\,dt + o(1).$$

The result follows. □

4.2 Semi-Implicit Scheme

We present now a slight modification of the explicit scheme of the previous section where we approximate the coagulation term by $\frac{1}{2}\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k - \sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^{k+1}$. We thus obtain the following scheme

$$\begin{cases}
\dfrac{m_j^{k+1}-m_j^k}{\Delta t} + \dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + d_j^k m_j^k = \dfrac{1}{2}\displaystyle\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k - \sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^{k+1}\\
\qquad\qquad\qquad\qquad + \displaystyle\sum_{i=j}^{J} b_{i,j}a_i m_i^k - a_j m_j^k,\\
g_0^k m_0^k = \Delta x\displaystyle\sum_{j=1}^{J}\beta_j^k m_j^k.
\end{cases} \tag{33}$$

It will be useful to rewrite it as follows

$$\begin{cases} (1+\Delta t\sum_{i=1}^{J}\kappa_{i,j}m_i^k)m_j^{k+1} = (1-\frac{\Delta t}{\Delta x}g_j^k - \Delta t d_j^k - \Delta t a_j)m_j^k + \frac{\Delta t}{\Delta x}g_{j-1}^k m_{j-1}^k \\ \qquad\qquad + \frac{1}{2}\Delta t\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k + \Delta t\sum_{i=j}^{J}b_{i,j}a_i m_i^k, \qquad . \\ g_0^k m_0^k = \Delta x\sum_{j=1}^{J}\beta_j^k m_j^k. \end{cases} \tag{34}$$

Notice that this scheme is well-defined since m_j^{k+1} is computed from the previous m_i^k, $i = 1,\dots,J$, and $m_1^{k+1},\dots,m_{j-1}^{k+1}$.

We assume the following Courant-Friedrichs-Lewy (CFL) condition on our mesh:

$$\bar{\zeta}(2\Delta t + \frac{\Delta t}{\Delta x}) \le 1 \qquad \text{where } \bar{\zeta} = \max\{\zeta, \|a\|_{W^{1,\infty}}\}. \tag{35}$$

We point out that contrary to the CFL condition (20) we assumed for the explicit scheme, this CFL condition does not involve the total initial mass $\|\mu_0\|_{TV}$. This is the main justification for the introduction of this semi-implicit scheme.

Lemma 4.3. *For every $k = 1,2,\dots,\bar{k}$, $\mu_{\Delta x}^k$ is a non-negative measure supported in $[0, x_{max}]$:*

$$m_j^k \ge 0 \qquad \textit{for any } j \ge 1,$$

and

$$m_j^k = 0 \qquad \textit{for } j > J.$$

Proof. This can be proved by induction using (34). Indeed if $m^k \ge 0$, then notice that

$$1 - \frac{\Delta t}{\Delta x}g_j^k - \Delta t d_j^k - \Delta t a_j \ge 1 - \frac{\Delta t}{\Delta x}\zeta - \Delta t(\zeta + \|a\|_\infty) \ge 1 - \bar{\zeta}(2\Delta t + \frac{\Delta t}{\Delta x})$$

which is ≥ 0 by the CFL condition. We easily deduce that $m^{k+1} \ge 0$.

Next if $m_j^k = 0$ for $j > J$, it follows from (34) that $m_{J+1}^{k+1} = 0$ recalling that $g_J^K = g(t_k, x_{max}) = 0$ by (A3) and $\kappa_{i,J+1-i} = 0$ by (K2). We then deduce that $m_j^{k+1} = 0$ for any $j > J$. □

We next proceed as in the study of the explicit scheme by proving that the measures $\mu_{\Delta x}^k$ are uniformly bounded in the TV-norm and are Lipschitz in time for the BL-norm.

Lemma 4.4. *For any $k = 0,1,\dots,\bar{k}$,*

$$\|\mu_{\Delta x}^k\|_{TV} \le \|\mu_0\|_{TV}\exp((C_aC_b+\zeta)T).$$

Proof. Notice that $\|\mu^{k+1}_{\Delta x}\|_{TV} = \sum_{j=1}^J m_j^{k+1}$ since $m_j^{k+1} \geq 0$ for any j. With (33) we obtain

$$\begin{aligned}\|\mu^{k+1}_{\Delta x}\|_{TV} \leq & \sum_{j=1}^{J}(1-\Delta t d_j^k - \Delta t a_j)m_j^k + \frac{\Delta t}{\Delta x}\sum_{j=1}^{J}(g_{j-1}^k m_{j-1}^k - g_j^k m_j^k) + \Delta t \sum_{j=1}^{J}\sum_{i=j}^{J} b_{i,j}a_i m_i^k \\ & + \frac{1}{2}\Delta t \sum_{j=1}^{J}\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k - \Delta t\sum_{j=1}^{J}\sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^{k+1}.\end{aligned} \tag{36}$$

The 1st term in the right-hand side is clearly less than $\|\mu^k\|_{TV}$. According to (24)-(25), the sum of the 2nd and 3rd terms is less than $(\zeta + C_a C_b)\Delta t \|\mu^k\|_{TV}$. Moreover through changing the order of integration and a substitution as in (26), we can see

$$\frac{\Delta t}{2}\sum_{j=1}^{J}\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k - \Delta t\sum_{j=1}^{J}\sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^{k+1} = -\frac{1}{2}\Delta t\sum_{j=1}^{J}\sum_{i=1}^{J}\kappa_{i,j}m_i^k m_j^{k+1}.$$

Combining the above results, we obtain

$$\|\mu^{k+1}_{\Delta x}\|_{TV} \leq (1+\Delta t(\zeta + C_b C_a)\|\mu^k_{\Delta x}\|_{TV}.$$

Therefore, for each $k = 1, 2, \ldots \bar{k}$ we have

$$\|\mu^{k}_{\Delta x}\|_{TV} \leq (1+\Delta t(\zeta + C_b C_a)^k\|\mu_0\|_{TV} \leq \|\mu_0\|_{TV}\exp((C_a C_b + \zeta)T).$$

∎

Lemma 4.5. *There exists an $L > 0$ independent of Δx and Δt such that for any p, q,*

$$\|\mu^q_{\Delta x} - \mu^p_{\Delta x}\|_{BL} \leq L|q-p|\Delta t.$$

Proof. Same proof as that of Lemma 4.1. ∎

As before, we define the family of continuous curves $\mu^{\Delta t}_{\Delta x} : [0,T] \to \mathcal{M}^+(\mathbb{R}_+)$ by linearly interpolating the $\mu^k_{\Delta x}$:

$$\mu^{\Delta t}_{\Delta x}(t) = \mu^0_{\Delta x}\chi_{\{t_0\}}(t) + \sum_{k=0}^{K-1}\left[\left(1-\frac{t-t_k}{\Delta t}\right)\mu^k_{\Delta x} + \frac{t-t_k}{\Delta t}\mu^{k+1}_{\Delta x}\right]\chi_{(t_k,t_{k+1}]}(t).$$

Theorem 4.2. *As $\Delta t, \Delta x \to 0$ while the CFL condition* (35) *holds, the whole family $\mu^{\Delta t}_{\Delta x}$ converges to the solution of* (1) *in $C([0,T], \mathcal{M}^+([0, x_{\max}]))$.*

Proof. Due to the similarity of the semi-implicit scheme and the fully explicit scheme (4.1), we need only show

$$\frac{1}{2}\sum_{j=1}^{J}\sum_{i=1}^{j-1}\phi_j^k\kappa_{i,j-i}m_i^{k+1}m_{j-i}^k - \sum_{j=1}^{J}\sum_{i=1}^{J}\phi_j^k\kappa_{i,j}m_i^k m_j^{k+1} = (K[\mu^k_{\Delta x}], \phi(t_k,\cdot)) + O(\Delta t) \tag{37}$$

for $\phi \in W^{1,\infty}([0,T]\times[0,x_{\max}])$, where $O(\Delta t)$ depends only on the model parameters and $\|\phi\|_{W^{1,\infty}}$. Indeed, through a change of variables the right-hand side of (37) can be written as

$$\frac{1}{2}\sum_{i=1}^{J}\sum_{l=1}^{J}\kappa_{i,l}(\phi_{i+l}^k-\phi_i^k-\phi_l^k)m_l^k m_i^{k+1}$$
$$=\frac{1}{2}\int_0^{x_{\max}}\int_0^{x_{\max}}\kappa(x,y)(\phi(t_k,x+y)-\phi(t_k,x)-\phi(t_k,y))\mu_{\Delta x}^k(dx)\mu_{\Delta x}^{k+1}(dy).$$

Since κ and ϕ are bounded Lipschitz, the inner integral seen as a function of y is also bounded Lipschitz with norm bounded by a constant depending on C_κ, L_κ, $\|\phi\|_{W^{1,\infty}}$ and $\|\mu_0\|_{TV}\exp((C_aC_b+\zeta)T)$ due to Lemma (4.4). Owing to Lemma 4.5, we deduce that

$$\frac{1}{2}\int_0^{x_{\max}}\int_0^{x_{\max}}\kappa(x,y)(\phi(x+y)-\phi(x)-\phi(y))\mu_{\Delta x}^k(dx)\mu_{\Delta x}^{k+1}(dy)-(K[\mu_{\Delta x}^k],\phi(t_k,\cdot))\leq C\Delta t.$$

Thus, we obtain (37) and the result follows as in Theorem 4.1. □

5 Size Structured coagulation-fragmentation equation as conservation law

In this section, we derive equation (2), prove it is well-posed in a new topology, and develop an explicit scheme based on this equation.

5.1 Reformulation of (1) as a conservation law.

It was shown in [14] (proposed in [48, 66]) that a coagulation-fragmentation equation (i.e. model (1) with $g\equiv d\equiv\beta\equiv 0$) set in the space $L^1(\mathbb{R}^+)$ can be written as a conservation law in the following form:

$$x\partial_t u=-\partial_x\mathcal{Q}_K[u]+\partial_x\mathcal{Q}_F[u], \tag{38}$$

where, for $u\in L^1(\mathbb{R}^+)$,

$$\mathcal{Q}_K[u](x)=\int_0^x\int_{x-z}^{\infty}z\,\kappa(z,y)u(z)u(y)dydz, \tag{39}$$

and

$$\mathcal{Q}_F[u](x)=\int_0^x\int_{x-z}^{\infty}z\,\tilde{b}(z,y)u(z+y)dydz. \tag{40}$$

Here, $\tilde{b}(x,y)$ represents the rate at which a particle of size $x+y$ fragments into two particles of size x and y. Notice that $\partial_x\mathcal{Q}_K[\mu]=-xK[\mu]$ and $\partial_x\mathcal{Q}_F[\mu]=xF[\mu]$.

We wish to extend terms (39) and (40) to accommodate a measure setting while maintaining the properties $\partial_x\mathcal{Q}_K[\mu]=-xK[\mu]$ and $\partial_x\mathcal{Q}_F[\mu]=xF[\mu]$ in a weak sense. To deal with the coagulation term, multiply (39) by a test function $\phi \in C_b(\mathbb{R}^+)$ and integrate over $\mathbb{R}^+$ to obtain

$$
\begin{aligned}
(\mathcal{Q}_K[u], \phi) &= \int_0^\infty \int_0^x \int_{x-z}^\infty \phi(x)\, z\, \kappa(z,y) u(z) u(y) dy dz dx \\
&= \int_0^\infty \int_0^\infty \Big(\int_z^{z+y} \phi(x)\, dx \Big) z\kappa(z,y) u(y) u(z) dy dz.
\end{aligned}
$$

This can be generalized for an arbitrary measure $\mu(dx)$ considering $\mathcal{Q}_K[\mu]$ defined by

$$
(\mathcal{Q}_K[\mu], \phi) = \int_0^\infty \int_0^\infty \left[\int_z^{z+y} \phi(x) dx \right] z\, \kappa(z,y)\, \mu(dz)\, \mu(dy). \tag{41}
$$

Since κ is symmetric, we then have

$$
\begin{aligned}
(\partial_x \mathcal{Q}_K[\mu], \phi) &= -\left(\mathcal{Q}_K[\mu], \partial_x \phi\right) = -\int_0^\infty \int_0^\infty \left[\phi(z+y) - \phi(z)\right]\, z\, \kappa(z,y)\, \mu(dz)\, \mu(dy) \\
&= -\left(K[\mu], x\phi\right) = -\left(xK[\mu], \phi\right),
\end{aligned}
$$

as desired.

We can generalize the fragmentation term (40) in the same way. Multiplying (40) by ϕ and integrating gives

$$
(\mathcal{Q}_F[u], \phi) = \int_0^\infty \int_0^x \int_{x-z}^\infty z\tilde{b}(z,y) u(z+y) \phi(x) dy dz dx.
$$

The change of variables $y := t - z$ yields

$$
\begin{aligned}
(\mathcal{Q}_F[u], \phi) &= \int_0^\infty \int_0^x \int_x^\infty z\tilde{b}(z, t-z) u(t) \phi(x) dt dz dx \\
&= \int_0^\infty \int_0^\infty \tilde{b}(z, t-z) z \Big(\int_z^t \phi \Big)\, dz\, u(t) dt.
\end{aligned}
$$

Introducing the measure $b(t, dz)$ defined by

$$
(b(t,dz), \psi) = a(t)^{-1} \int_0^\infty \tilde{b}(z, t-z) \psi(z)\, dz, \qquad a(t) = \int_0^\infty z\tilde{b}(z, t-z)\, dz,
$$

we finally obtain

$$
(\mathcal{Q}_F[u], \phi) = \int_0^\infty \Big(b(t,dz), z \int_z^t \phi\, dx \Big) a(t)\, u(t) dt.
$$

We can now replace the measure $u(t)dt$ by an arbitrary measure μ wich results in the measure $\mathcal{Q}_F[\mu]$ defined by

$$
(\mathcal{Q}_F[\mu], \phi) = \int_0^\infty \left(b(y, dx), x \int_x^y \phi(z) dz \right) a(y) \mu(dy). \tag{42}
$$

Recalling that $(b(y,dx),x)=y$, we then have

$$\begin{aligned}(\partial_x \mathcal{Q}_F[\mu],\phi) &= -(\mathcal{Q}_F[\mu],\partial_x\phi)\\ &= \int_0^\infty (b(y,dx),x\phi(x))a(y)\mu(dy) - \int_0^\infty (b(y,dx),x)\phi(y)a(y)\mu(dy)\\ &= (xF[\mu],\phi),\end{aligned}$$

as desired.

With these generalizations, we can write equation (38) in the space of Radon measures as

$$x\partial_t\mu = \partial_x\mathcal{Q}_F[\mu] - \partial_x\mathcal{Q}_K[\mu]. \tag{43}$$

We add to this equation the biological processes of growth, birth, and death to obtain a similar expression of equation (1)

$$\begin{cases}\partial_t(x\mu) + x\partial_x(g(t,\mu)\mu) + xd(t,\mu)\mu = \partial_x\mathcal{Q}_F[\mu] - \partial_x\mathcal{Q}_K[\mu]\\ g(t,\mu)(0)D_{dx}\mu(0) = \displaystyle\int_0^\infty \beta(t,\mu)(x)\mu(dx)\\ \mu_0\in\mathcal{M}^+(\mathbb{R}^+)\end{cases}. \tag{44}$$

We take the time to point out this equation can be written in the form:

$$\begin{cases}\partial_t(x\mu) + \partial_x(xg(t,\mu)\mu + \mathcal{Q}_K[\mu] - \mathcal{Q}_F[\mu]) = g(t,\mu)\mu - xd(t,\mu)\mu\\ g(t,\mu)(0)D_{dx}\mu(0) = \displaystyle\int_0^\infty \beta(t,\mu)(x)\mu(dx)\\ \mu_0\in\mathcal{M}^+(\mathbb{R}^+)\end{cases}. \tag{45}$$

Given $T\geq 0$, we say a function $\mu\in C([0,T],\mathcal{M}^+(\mathbb{R}^+))$ is a weak solution to (44) if for all $\phi\in(C^1\cap W^{1,\infty})([0,T]\times\mathbb{R}^+)$, and for all $t\in[0,T]$ the following holds:

$$\begin{aligned}&\int_0^\infty x\phi(t,x)\mu_t(dx) - \int_0^\infty x\phi(0,x)\mu_0(dx) =\\ &\quad\int_0^t\int_0^\infty \left[x\partial_t\phi(s,x) + g(s,\mu_s)(x)(\phi(s,x)+x\partial_x\phi(s,x)) - xd(s,\mu_s)(x)\phi(s,x)\right]\mu_s(dx)ds\\ &\qquad + \int_0^t \left(\mathcal{Q}_K[\mu_s]-\mathcal{Q}_F[\mu_s],\partial_x\phi(s,\cdot)\right)ds\end{aligned} \tag{46}$$

Remark 5.1. *As in Remark 3.1, we can reduce the integrals above over the finite domain* $[0,x_{\max}]$ *if the initial measure* μ_0 *is supported in* $[0,x_{\max}]$.

Remark 5.2. *It is clear from* (46) *that the boundary condition in* (44) *is superfluous. However, this is only the case when the minimum size of the model is taken to be zero. In the case of some positive minimum size, the term*

$$\int_0^t\int_{x_{\min}}^{x_{\max}} x_{\min}\phi(s,x_{\min})\beta(s,\mu_s)(x)\mu_s(dx)ds$$

will be present in the weak formulation (46)*. In this case, it is clear solutions* (15) *and* (46) *are equivalent as the functions* $x\phi(x)$ *and* $\frac{1}{x}\phi(x)$ *are bounded-Lipschitz over* $[x_{\min}, x_{\max}]$ *for* $\phi \in W^{1,\infty}(\mathbb{R}^+)$*. It is straight forward to include a positive minimum size into the following numerical scheme.*

Continuing with (44) which assumes zero minimum size, it is clear that we can write this equation in the form

$$\partial_t(x\mu) + x\partial_x(g(t,\mu)\mu) + xd(t,\mu)\mu = \partial_x\mathcal{Q}_F[\mu] - \partial_x\mathcal{Q}_K[\mu], \tag{47}$$

or equivalently

$$\partial_t(x\mu) + \partial_x(xg(t,\mu)\mu) = N[\mu], \qquad N[\mu] := g(t,\mu)\mu - xd(t,\mu)\mu + xF[\mu] + xK[\mu], \tag{48}$$

with initial condition $\mu_0 \in \mathcal{M}^+((0,\infty))$.

It remains to be shown that (48) is well–posed. To this end, we introduce the following norm on $\mathcal{M}^+((0,\infty))$:

$$\|\mu\|_{BL_0} := \sup_{\|\phi\|_{W^{1,\infty}}\le 1} \{(\mu,\phi) :\ \phi \in W^{1,\infty}(\mathbb{R}^+),\ \phi(0) = 0\}. \tag{49}$$

This norm essentially gives us no information of the measures at the left boundary while maintaining structure on $(0,\infty)$ similar to the BL norm.

Given a measure $\mu \in \mathcal{M}^+((0,\infty))$, we denote $\tilde{\mu} \in \mathcal{M}^+(\mathbb{R}^+)$ its extension by 0 in the sense that $\tilde{\mu}(A) = \mu(A \cap (0,\infty))$ for any $A \subset \mathbb{R}^+$ Borel. It then follows that

$$(\tilde{\mu},\phi) = (\mu, \phi 1_{(0,\infty)}) \tag{50}$$

for any measurable function ϕ either non-negative or bounded. From equation (50), the following Lemma is immediate:

Lemma 5.1. *For any* $\mu \in \mathcal{M}^+((0,\infty))$*, we have*

$$\|\mu\|_{TV} = \|\tilde{\mu}\|_{TV}.$$

We also have the following estimation:

Lemma 5.2. *For any* $\mu \in \mathcal{M}((0,\infty))$*, we have*

$$\|\mu\|_{BL_0} \le \|\mu\|_{BL} \le \|\tilde{\mu}\|_{BL}.$$

Proof. The inequality $\|\mu\|_{BL_0} \le \|\mu\|_{BL}$ follows from the inclusion

$$\{\phi \in W^{1,\infty}(\mathbb{R}^+) :\ \|\phi\|_{W^{1,\infty}} \le 1,\ \phi(0) = 0\} \subset \{\phi \in W^{1,\infty}((0,\infty)) :\ \|\phi\|_{W^{1,\infty}} \le 1\}.$$

Finally, to prove $\|\mu\|_{BL} \le \|\tilde{\mu}\|_{BL}$, given some $\varepsilon > 0$, we take $\phi \in W^{1,\infty}((0,\infty))$, $\|\phi\|_{W^{1,\infty}} \le 1$ such that $\|\mu\|_{BL} \le (\mu,\phi) + \varepsilon$. Notice that ϕ can be extended to a function $\tilde{\phi} \in W^{1,\infty}(\mathbb{R}^+)$, with $\|\tilde{\phi}\|_{W^{1,\infty}} \le 1$. Then $(\mu,\phi) = (\tilde{\mu},\tilde{\phi}) \le \|\tilde{\mu}\|_{BL}$ and the result follows. □

In the same way, given a measure $\tilde{\mu} \in \mathcal{M}^+(\mathbb{R}^+)$, denote by $\mu = \tilde{\mu}_{|(0,\infty)}$ its restriction to $(0, \infty)$, i.e. $\mu(A) = \tilde{\mu}(A)$ for any Borel set $A \subset (0, \infty)$. Then, $\tilde{\mu} = \mu + \tilde{\mu}(\{0\})\delta_0$. In particular, $(\tilde{\mu}, \phi) = (\mu, \phi)$ for any ϕ with $\phi(0) = 0$. It follows that

Lemma 5.3. *For any $\tilde{\mu} \in \mathcal{M}^+(\mathbb{R}^+)$,*

$$\|\tilde{\mu}\|_{BL_0} = \|\tilde{\mu}_{|(0,\infty)}\|_{BL_0}. \tag{51}$$

We now claim equation (47) is well–posed under this framework. We begin with the following important proposition

Proposition 5.1. *For any $R > 0$ the set*

$$\{\mu \in \mathcal{M}^+((0, \infty)) : \|\mu\|_{TV} \leq R\}$$

is complete for the BL_0 norm. Moreover for any $M, R > 0$ the set

$$\{\mu \in \mathcal{M}^+((0, M]) : \|\mu\|_{TV} \leq R\}$$

is compact for the BL_0 norm.

Proof. Let us first prove that $\mathcal{S} := \{\mu \in \mathcal{M}^+((0, M]) : \|\mu\|_{TV} \leq R\}$ is compact for the BL_0 norm. Given a sequence μ_n of measures belonging to $\mathcal{S}$, denote $\tilde{\mu}_n$ their extension to $[0, \infty)$ as before. Since $\|\tilde{\mu}_n\|_{TV} = \|\mu_n\|_{TV} \leq R$, and the set $\{\mu \in \mathcal{M}^+([0, M]) : \|\mu\|_{TV} \leq R\}$ is compact for the BL norm by Theorem 2.7 in [32], we can extract a subsequence, still denoted $\tilde{\mu}_n$, converging to some $\tilde{\mu} \in \mathcal{M}^+([0, M])$, $\|\tilde{\mu}\|_{TV} \leq R$. Define μ to be the restriction of $\tilde{\mu}$ to $(0, M]$ i.e. $\mu(A) = \tilde{\mu}(A)$ for $A \subset (0, M]$. Then using Lemmas 5.1 and 5.3, we have $\mu \in \mathcal{S}$ and

$$\|\mu_n - \mu\|_{BL_0} = \|\tilde{\mu}_n - \tilde{\mu}\|_{BL_0} \leq \|\tilde{\mu}_n - \tilde{\mu}\|_{BL} \to 0.$$

Now let us prove that $\mathcal{S} := \{\mu \in \mathcal{M}^+((0, \infty)) : \|\mu\|_{TV} \leq R\}$ is complete. Let $(\mu_n)_n \subset \mathcal{S}$ be a Cauchy sequence for the BL_0 norm, and $\tilde{\mu}_n$ be their extensions to $[0, \infty)$. Since it is not true that $\|.\|_{BL} \leq \|.\|_{BL_0}$, we cannot a priori assert that $(\tilde{\mu}_n)_n$ is Cauchy for the BL norm. Instead, we split μ_n into a measure on $(0, 2]$ and a measure on $[1, \infty)$ and will rely on the fact that the BL and BL_0 norm are comparable on $[1, \infty)$. Take two smooth functions $u, v : \mathbb{R}^+ \to [0, 1]$ such that $u + v = 1$ and $u = 0$ in $[2, \infty)$, $v = 0$ in $[0, 1]$. We can then write $\tilde{\mu}_n = u\tilde{\mu}_n + v\mu_n =: \tilde{\mu}_n^1 + \mu_n^2$ with $\tilde{\mu}_n^1$ and μ_n^2 supported in $[0, 2]$ and $[1, \infty)$ respectively. Notice that $\|\tilde{\mu}_n^1\|_{TV}, \|\mu_n^2\|_{TV} \leq \|\tilde{\mu}_n\|_{TV} = \|\mu_n\|_{TV} \leq R$. Moreover, $(\mu_n^2)_n$ is Cauchy for the BL_0 norm. Indeed, taking $C > 0$ such that $\|v\phi\|_{W^{1,\infty}} \leq C$ if $\|\phi\|_{W^{1,\infty}} \leq 1$, we have $(\mu_n^2 - \mu_m^2, \phi) = (\mu_n - \mu_m, v\phi)$ so that $\|\mu_n^2 - \mu_m^2\|_{BL_0} \leq C\|\mu_n - \mu_m\|_{BL_0} \to 0$ as $m, n \to \infty$. Clearly, the BL and BL_0 norms are equivalent on $\mathcal{M}^+([1, \infty))$. In particular, $(\mu_n^2)_n$ is Cauchy for the BL norm. Since the set $\{\mu \in \mathcal{M}^+([1, \infty)), \|\mu\|_{TV} \leq R\}$ is complete for the BL norm, we obtain that μ_n^2 converges to some μ^2 for the BL norm, and thus also for the BL_0 norm. Moreover, $\tilde{\mu}_n^1$ converges up to a subsequence to some $\tilde{\mu}^1 \in M^+([0, 2])$. Denote μ^1 the restriction of $\tilde{\mu}^1$ to $(0, 2]$. As in the first part of the proof, we have $\mu_n^1 \to \mu^1$ in the BL_0 norm and thus $\mu_n \to \mu^1 + \mu^2$ for the BL_0 norm. Moreover,

$$R \geq \|\tilde{\mu}_n\|_{TV} = (\tilde{\mu}_n^1) = (\tilde{\mu}_n^1, 1) + (\mu_n^2, 1) \to (\tilde{\mu}^1, 1) + (\mu^2, 1) = \|\tilde{\mu}^1 + \mu^2\|_{TV} = \|\mu\|_{TV}.$$

Thus, $(\mu_n)_n$ has a convergent subsequence for the BL_0 norm. We conclude with the classical fact that if a Cauchy sequence has a convergent subsequence, then it converges. $\square$

With this result, we are ready to prove (48) is well-posed under the BL_0 norm.

Theorem 5.1. *Given an initial condition $\mu_0 \in \mathcal{M}^+((0,\infty))$, there exists a unique continuous global solution to* (48) $\mu : [0,\infty) \longrightarrow (\mathcal{M}^+((0,\infty)), \|\cdot\|_{BL_0})$ *which satisfies* (46)*.*

Proof. Well–posedness of (47) under $\|\cdot\|_{BL_0}$ follows from the results in [8]. Indeed, by considering first the linear equation

$$\partial_t(x\mu) + \partial_x(g(t,x)\,x\mu) = 0,$$

we see that this is the usual transport equation on the measure $x\mu$. Therefore, we have the unique solution given by $x\mu_t = T_t\sharp(x\mu_0)$ i.e. $(\mu_t, \phi) = \int_0^\infty \phi(T_t(x))\frac{x}{T_t(x)}\,\mu_0(dx)$, where $\phi \in C_b((0,\infty))$. Here T_t is the flow of the g (definition (3)). Notice, since $g \geq 0$ by assumption (A1), $|x/T_t(x)| \leq 1$ for $t > 0$, which allows us to check that the integral is well defined using the Dominated Convergence Theorem.

Next, by writing the solution to (48) as the mapping

$$\mu_t = P_t\mu_0 + \int_0^t P_{t-s}(N[\mu_s])\,ds, \tag{52}$$

where for any $\nu \in M_+((0,\infty))$, $P_t\nu$ is the measure $\frac{1}{x}(T_t^{g(t,\mu)}\sharp(x\nu))$ with $T_t^{g(t,\mu)} = T_t$ the flow of $(t,x) \to g(t,\mu_t)(x)$. Explicitly,

$$(\mu_t,\phi) = \int_0^\infty \phi(T_t(x))\frac{x}{T_t(x)}\,\mu_0(dx) + \int_0^t \Big(\int_0^\infty \phi(T_{t-s}(x))\frac{x}{T_{t-s}(x)}\,N[\mu_s](dx)\Big)\,ds.$$

Notice the function $f(x) := \phi(T_t(x))\frac{x}{T_t(x)}$ is bounded by $\|\phi\|_\infty$ as $\frac{x}{T_t(x)} \leq 1$ and has derivative

$$f'(x) = \phi'(T_t(x))\partial_x T_t(x)\frac{x}{T_t(x)} + \frac{\phi(T_t(x))}{T_t(x)} - \frac{\phi(T_t(x))}{T_t(x)}\frac{x}{T_t(x)}\partial_x T_t(x).$$

Taking ϕ as in (49), we have $|\phi(x)| = |\phi(x) - \phi(0)| \leq Lip(\phi)|x|$ and so

$$|f'(x)| \leq \|\phi'\|_\infty\|\partial_x T_t\|_\infty + Lip(\phi)(1 + \|\partial_x T_t\|_\infty) \leq C Lip(\phi).$$

Following the arguments from [8], we have for a small enough T, the mapping

$$\Gamma[\mu_t] = P_t\mu_0 + \int_0^t P_{t-s}(N[\mu_s])\,ds$$

is a contraction on

$$X_T := \{\mu \in C([0,T], (\mathcal{M}^+((0,\infty)), \|\cdot\|_{BL_0}) \,:\, \mu(0) = \mu_0, \quad \|\mu_t\|_{TV} \leq 2\|\mu_0\|_{TV}\}.$$

We can then extend this to $T = \infty$ as $\|\mu_t\|_{TV} \leq \|\mu_0\|_{TV}\exp(\zeta t)$. Indeed from (52),

$$\begin{aligned}(\mu_t, 1) &= (P_t\mu_0, 1) + \int_0^t (P_{t-s}N[\mu_s], 1)ds \\ &\leq (\mu_0, 1) + \int_0^t\int_0^\infty g(t,\mu_s)(x)\mu_s(dx)ds \\ &\leq (\mu_0, 1) + \zeta\int_0^t \|\mu_s\|_{TV}ds.\end{aligned}$$

The Gronwall inequality then gives the result. □

5.2 Finite Difference Schemes

In this section, we follow the ideas set in [6] applied to model (44). We assume that the initial measure μ_0 is supported in $[0, x_{\max}]$ and follow the notations defined at the beginning of Section 4 with the following exception concerning the definition of the node x_j for which we follow [14]: we denote $x_{j+\frac{1}{2}} := j\Delta x$, $j = 1, \dots, J$, with $x_{J+\frac{1}{2}} = x_{\max}$, $x_{\frac{1}{2}} = 0$, and $x_j = (x_{j-\frac{1}{2}} + x_{j+\frac{1}{2}})/2 = (j - \frac{1}{2})\Delta x$. The cell remains $\Lambda_j := (x_{j-\frac{1}{2}}, x_{j+\frac{1}{2}}]$. The others notations remain the same, in particular the discretizaton of the initial condition

$$\mu_0 \approx \sum_{j=1}^{J} m_j^0 \delta_{x_j} \quad \text{where} \quad m_j^0 := \mu_0(\Lambda_j),$$

of the solution

$$\mu_{\Delta x}^k = \sum_{j=1}^{J} m_j^k \delta_{x_j},$$

and of the functions $f = g, \beta, d$, κ and b:

$$f_j^k = f(t_k, \mu_{\Delta x}^k)(x_j), \qquad \kappa_{j,l} = \kappa(x_j, x_l), \qquad b_{j,l} = b(x_j, \Lambda_l).$$

Concerning the discretization of the coagulation and fragmentation kernel $\mathcal{Q}_K$ and $\mathcal{Q}_F$ defined in (41) and (42), we consider

$$\mathcal{Q}_{K,j}^k := \sum_{i=1}^{j} \sum_{l=j-i}^{J} \Delta x \, x_i \kappa_{i,l} m_l^k m_i^k$$

and

$$\mathcal{Q}_{F,j}^k := \sum_{i=j+1}^{J} \sum_{l=1}^{j} x_l \Delta x \, b_{i,l} a_i m_i^k.$$

Where we take $\mathcal{Q}_{F,0}^k = Q_{F,J}^k = 0$ and $\mathcal{Q}_{K,0}^k = \mathcal{Q}_{K,J}^k = 0$.

There is a useful result of these approximations which reads as follows:

Proposition 5.2. *Assuming $\sum_{j=1}^{J} m_j^k$ is bounded, for $\phi \in C^1([0, x_{\max}])$,*

$$\big(\mathcal{Q}_K[\mu_{\Delta x}^k], \phi\big) = \sum_{j=1}^{J} \phi(x_j) \mathcal{Q}_{K,j}^k + O(\Delta x)$$

and

$$\big(\mathcal{Q}_F[\mu_{\Delta x}^k], \phi\big) = \sum_{j=1}^{J} \phi(x_j) \mathcal{Q}_{F,j}^k + O(\Delta x).$$

Proof. We have from (41)

$$(\mathcal{Q}_K[\mu_{\Delta x}^k], \phi) = \sum_{l=1}^{J} \sum_{i=1}^{J} \int_0^{x_l} \phi(x_i + x_j - y) dy x_i k_{i,l} m_i^k m_l^k.$$

Using a right-hand approximation of the integral and a change of variables we arrive at

$$\begin{aligned}(\mathcal{Q}_K[\mu^k_{\Delta x}],\phi) &= \sum_{j=1}^{J}\sum_{i=1}^{j}\sum_{l=j-i}^{J}\phi(x_j)x_i\Delta x\kappa_{i,l}m_i^k m_l^k + O(\Delta x)\\ &= \sum_{j=1}^{J}\phi(x_j)\mathcal{Q}^k_{K,j} + O(\Delta x).\end{aligned}$$

Using a similar strategy, we arrive at the same result for $\mathcal{Q}_F$. □

From these terms, we propose the following upwind scheme based on (44):

$$\begin{cases} x_j\dfrac{m_j^{k+1}-m_j^k}{\Delta t} + x_j\dfrac{g_j^k m_j^k - g_{j-1}^k m_{j-1}^k}{\Delta x} + x_j d_j^k m_j^k = \dfrac{\mathcal{Q}^k_{F,j}-\mathcal{Q}^k_{F,j-1}-\mathcal{Q}^k_{K,j}+\mathcal{Q}^k_{K,j-1}}{\Delta x} \\ g_0^k\dfrac{m_0^k}{\Delta x} = \displaystyle\sum_{j=1}^{J}\beta_j^k m_j^k \end{cases}, \quad (53)$$

on which, we impose the following Courant–Friedrichs–Lewy (CFL) condition

$$\Delta t(C_\kappa\|\mu_0\|_{TV}\exp(\zeta + C_bC_a) + C_bC_a + (1+\frac{1}{\Delta x})\zeta) \leq 1. \quad (54)$$

Lemma 5.4. *For each $k = 1,\dots,\bar{k}$, the measure $\mu^k_{\Delta x}$ is a positive Radon measure with*

$$\|\mu^k_{\Delta x}\|_{TV} \leq \|\mu_0\|_{TV}\exp(CT)$$

for some C independent of Δx and Δt.

Proof. We show this proof via induction. Assume the following induction hypothesis:

(i) $\mu^k_{\Delta x} \in \mathcal{M}^+(\mathbb{R}^+)$. In other words, $m_j^k \geq 0$ for all $j = 1,\dots,J$.

(ii) $\|\mu^k_{\Delta x}\|_{TV} \leq \|\mu^0_{\Delta x}\|_{TV}\exp((\zeta + C_bC_a)T)$

It will be helpful to point out the following results on $\mathcal{Q}^k_{K,j}$ and $\mathcal{Q}^k_{F,j}$ which follow analogously from the proof of proposition 3.1 in [14]:

$$\begin{aligned}\mathcal{Q}^k_{K,j-1}-\mathcal{Q}^k_{K,j} &= \sum_{i=1}^{j-1}\sum_{l=j-i-1}^{J}\Delta x\, x_i\,\kappa_{i,l}m_l^k m_i^k - \sum_{i=1}^{j}\sum_{l=j-i}^{J}\Delta x\, x_i\,\kappa_{i,l}m_l^k m_i^k\\ &= \sum_{i=1}^{j}\left(\sum_{l=j-i-1}^{J}\Delta x\, x_i\,\kappa_{i,l}m_l^k m_i^k - \sum_{l=j-i}^{J}\Delta x\, x_i\,\kappa_{i,l}m_l^k m_i^k\right) - \sum_{l=1}^{J}\Delta x\, x_j\,\kappa_{j,l}m_l^k m_j^k\\ &= \sum_{i=1}^{j}\Delta x\, x_i\,\kappa_{i,j-i-1}m_{j-i-1}^k m_i^k - \sum_{l=1}^{J}\Delta x\, x_j\,\kappa_{j,l}m_l^k m_j^k \quad (55)\end{aligned}$$

and

$$\begin{aligned}
\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}^k &= \sum_{i=j+1}^{J}\sum_{l=1}^{j} \Delta x\, x_l\, b_{i,l} a_i m_i^k - \sum_{i=j}^{J}\sum_{l=1}^{j-1} \Delta x\, x_l\, b_{i,l} a_i m_i^k \\
&= \sum_{i=j+1}^{J}\sum_{l=1}^{j} \Delta x\, x_l\, b_{i,l} a_i m_i^k - \sum_{i=j}^{J}\sum_{l=1}^{j} \Delta x\, x_l\, b_{i,l} a_i m_i^k + \sum_{i=j}^{J} \Delta x\, x_j\, b_{i,j} a_i m_i^k \\
&= -\sum_{l=1}^{j} \Delta x\, x_l\, b_{j,l} a_j m_j^k + \sum_{i=j}^{J} \Delta x\, x_j\, b_{i,j} a_i m_i^k. \qquad (56)
\end{aligned}$$

Then from (53) we have

$$\begin{aligned}
m_j^{k+1} &= m_j^k - \frac{\Delta t}{\Delta x}(g_j^k m_j^k - g_{j-1}^k m_{j-1}^k) - \Delta t d_j^k m_j^k + \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}_{K,j-1}^k - \mathcal{Q}_{k,j}^k) + \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}) \\
&= (1 - \frac{\Delta t}{\Delta x} g_j^k - \Delta t d_j^k) m_j^k + \frac{\Delta t}{\Delta x} g_{j-1}^k m_{j-1}^k + \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}_{K,j-1}^k - \mathcal{Q}_{k,j}^k + \mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}).
\end{aligned}$$

From (55) and (56) we see

$$\mathcal{Q}_{K,j-1}^k - \mathcal{Q}_{K,j}^k \geq -\sum_{i=1}^{J} \Delta x\, \kappa_{i,j}\, m_i^k\, x_j\, m_j^k$$

and

$$\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}^k \geq -\sum_{i=1}^{J} \Delta x\, b_{j,i} a_i\, x_j m_j^k.$$

With this, assumptions (i) and (ii), and the CFL condition (54), we have

$$\begin{aligned}
m_j^{k+1} &\geq (1 - \frac{\Delta t}{\Delta x} g_j^k - \Delta t d_j^k - \Delta t \sum_{i=1}^{J} \kappa_{i,j}\, m_i^k - \Delta t \sum_{i=1}^{J} b_{j,i} a_i) m_j^k + \frac{\Delta t}{\Delta x} g_{j-1}^k m_{j-1}^k \\
&\geq 0.
\end{aligned}$$

Now, taking that m_j^k is positive for all j and k, we see that

$$\begin{aligned}
\sum_{j=1}^{J} m_j^{k+1} &= \sum_{j=1}^{J} (1 - \Delta t d_j^k) m_j^k - \frac{\Delta t}{\Delta x} \sum_{j=1}^{J} (g_j^k m_j^k - g_{j-1}^k m_{j-1}^k) \\
&\quad + \sum_{j=1}^{J} \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}_{K,j-1}^k - \mathcal{Q}_{K,j}^k) + \sum_{j=1}^{J} \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}^k) \\
&\leq \sum_{j=1}^{J} m_j^k + \Delta t \zeta \sum_{j=1}^{J} m_j^k + \Delta t \sum_{j=1}^{J}\sum_{i=j}^{J} b_{i,j} a_i m_i^k + \frac{\Delta t}{\Delta x} \sum_{j=1}^{J} Q_{K,j}^k (\frac{1}{x_{j+1}} - \frac{1}{x_j}) \\
&\leq (1 + \Delta t \zeta) \|\mu_{\Delta x}^k\|_{TV} + \Delta t \sum_{i=1}^{J}\sum_{j=1}^{i} b_{i,j} a_i m_i^k \\
&\leq (1 + \Delta t(\zeta + C_b C_a)) \|\mu_{\Delta x}^k\|_{TV}.
\end{aligned}$$

Therefore, we arrive at $\|\mu^k_{\Delta x}\|_{TV} \leq \|\mu^0_{\Delta x}\|_{TV} \exp((\zeta + C_b C_a)T) := C^*$.

□

Lemma 5.5. *There exists an $\mathcal{L} > 0$ such that for any $p, q \in \{1, 2, \dots, \bar{k}\}$*

$$\|\mu^q_{\Delta x} - \mu^p_{\Delta x}\|_{BL} \leq \mathcal{L}|q - p|\Delta t.$$

Proof. The proof of this Lemma is very similar to the proof of Lemma 4.4 in [6]. In this particular case, we only need to handle the addition of the coagulation and fragmentation terms. To this end, assume $q > p$ and for nonnegative $\phi \in W^{1,\infty}(\mathbb{R}^+)$ with $\|\phi\|_{W^{1,\infty}} = 1$ let $\phi_j := \phi(x_j)$. Then we have

$$\begin{aligned}
(\mu^q_{\Delta x} - \mu^p_{\Delta x}, \phi) &= \sum_{j=1}^{J} \phi_j (m^q_j - m^p_j) \\
&= \sum_{j=1}^{J} \sum_{k=p}^{q-1} \phi_j (m^{k+1}_j - m^k_j) \\
&= \sum_{j=1}^{J} \sum_{k=p}^{q-1} \phi_j \Big(\frac{\Delta t}{\Delta x}(g^k_{j-1} m^k_{j-1} - g^k_j m^k_j) - d^k_j m^k_j \Delta t\Big) \\
&\quad + \sum_{j=1}^{J} \sum_{k=p}^{q-1} \phi_j \frac{\Delta t}{x_j \Delta x}(\mathcal{Q}^k_{F,j} - \mathcal{Q}^k_{F,j-1} - \mathcal{Q}^k_{K,j} + \mathcal{Q}^k_{K,j}).
\end{aligned}$$

The first term in the last equality is identical to [6]. Therefore, notice due to Theorem 5.4 and (56)

$$\sum_{j=1}^{J} \frac{\Delta t}{x_j \Delta x} \phi_j (\mathcal{Q}^k_{F,j} - \mathcal{Q}^k_{F,j-1}) \leq \Delta t C_b C_a C^*$$

and from (55)

$$\sum_{j=1}^{J} \frac{\Delta t}{x_j \Delta x} \phi_j (\mathcal{Q}^k_{K,j-1} - \mathcal{Q}^k_{K,j}) \leq \Delta t C_\kappa C^{*2}.$$

Therefore, following the remaining argument from [6] we arrive at

$$(\mu^q_{\Delta x} - \mu^p_{\Delta x}, \phi) \leq (3\zeta C^* + C_b C_a C^* + C_\kappa C^{*2})(q - p)\Delta t.$$

□

Through similar arguments as before, Ascoli-Arzela's Theorem provides us with the existence of a convergence subsequence of the family $\{\mu^{\Delta t}_{\Delta x}\}$ in $C([0, T], \mathcal{M}^+([0, x_{\max}]))$. We are then ready to state the following Theorem:

Theorem 5.2. *Any convergent subsequence of the family $\mu^{\Delta t}_{\Delta x}$ converges to a solution of* (44) *in $C([0, T], \mathcal{M}^+([0, x_{\max}]))$.*

Proof. Rearranging (53), multiplying by ϕ_j^k, and summing over j and k, we arrive at the equation

$$\sum_{k=1}^{\bar{k}-1}\sum_{j=1}^{J}\left((m_j^{k+1}-m_j^k)x_j\phi_j^k+\frac{\Delta t}{\Delta x}(g_j^k m_j^k-g_{j-1}^k m_{j-1}^k)x_j\phi_j^k+\Delta t x_j\phi_j^k d_j^k m_j^k\right)=$$
$$\frac{\Delta t}{\Delta x}\sum_{k=1}^{\bar{k}-1}\sum_{j=1}^{J}\phi_j^k\left(\mathcal{Q}_{F,j}^k-\mathcal{Q}_{F,j-1}^k+\mathcal{Q}_{K,j-1}^k-\mathcal{Q}_{K,j}^k\right). \tag{57}$$

Notice that the function $x\phi(x)$ is bounded Lipschitz on $[0,x_{max}]$ so that we can deal with the left-hand side of equation (57) as before. We thus focus on the right-hand side of the above equation. First for any k, using that $\mathcal{Q}_{F,0}^k=\mathcal{Q}_{F,J}^k=0$, and (56), we have

$$\begin{aligned}\frac{1}{\Delta x}\sum_{j=1}^{J}\phi_j^k\left(\mathcal{Q}_{F,j}^k-\mathcal{Q}_{F,j-1}^k\right)&=\frac{1}{\Delta x}\sum_{j=1}^{J}\phi_j^k\left(\sum_{i=j}^{J}\Delta x\,x_j\,b_{i,j}a_i m_i^k-\sum_{l=1}^{j}\Delta x\,x_l\,b_{j,l}a_j m_j^k\right)\\&=\sum_{j=1}^{J}\sum_{i=j}^{J}\phi_j^k\,x_j\,b_{i,j}a_i m_i^k-\sum_{j=1}^{J}\sum_{l=1}^{j}\phi_j^k\,x_l\,b_{j,l}a_j m_j^k.\end{aligned}$$

Making use of $\sum_{l=1}^{j}x_l b_{j,l}=x_j+O(\Delta x)$ proven in [7] and Lemma 5.4, we have

$$\begin{aligned}\frac{1}{\Delta x}\sum_{j=1}^{J}\phi_j^k\left(\mathcal{Q}_{F,j}^k-\mathcal{Q}_{F,j-1}^k\right)&=\sum_{j=1}^{J}\sum_{i=j}^{J}\phi_j^k\,x_j\,b_{i,j}a_i m_i^k-\sum_{j=1}^{J}\phi_j^k\,x_j a_j m_j^k+O(\Delta x)\\&=\sum_{i=1}^{J}\sum_{j=1}^{i}\phi_j^k\,x_j\,b_{i,j}a_i m_i^k-\sum_{j=1}^{J}\phi_j^k\,x_j a_j m_j^k+O(\Delta x)\\&=\left(F[\mu_{\Delta x}^k],x\phi(t_k,x)\right)+O(\Delta x)\\&=\left(\partial_x\mathcal{Q}_F[\mu_{\Delta x}^k],\phi(t_k,\cdot)\right)+O(\Delta x).\end{aligned}$$

As for the coagulation term, summation-by-parts and recalling that $\mathcal{Q}_{K,0}^k=\mathcal{Q}_{K,J}^k=0$ yields

$$\begin{aligned}\frac{1}{\Delta x}\sum_{j=1}^{J}\phi_j^k(\mathcal{Q}_{K,j-1}^k-\mathcal{Q}_{K,j}^k)&=\frac{1}{\Delta x}\sum_{j=1}^{J}(\phi_{j+1}^k-\phi_j^k)\mathcal{Q}_{K,j}^k=\sum_{j=1}^{J}(\phi_{j+1}^k-\phi_j^k)\sum_{i=1}^{j}\sum_{l=j-i}^{J}x_i\kappa_{i,l}m_l^k m_i^k\\&=\sum_{i=1}^{J}\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k m_i^k\sum_{j=i}^{i+l}(\phi_{j+1}^k-\phi_j^k)\\&=\sum_{i=1}^{J}m_i^k\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k\phi_{i+l+1}^k-\sum_{i=1}^{J}m_i^k\phi_i^k\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k\\&=\sum_{i=1}^{J}m_i^k\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k\phi(t_k,x_i+x_l)-\sum_{i=1}^{J}m_i^k\phi(t_k,x_i)\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k+O(\Delta x).\end{aligned}$$

Using (K1), we can write

$$\frac{1}{\Delta x}\sum_{j=1}^{J}\phi_j^k(\mathcal{Q}_{K,j-1}^k-\mathcal{Q}_{K,j}^k)=\sum_{i=1}^{J}m_i^k\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k\phi(t_k,x_i+x_l)-\sum_{i=1}^{J}m_i^k\phi(t_k,x_i)\sum_{l=1}^{J}x_i\kappa_{i,l}m_l^k+O(\Delta x)$$
$$=\frac{1}{2}\sum_{i=1}^{J}\sum_{l=1}^{J}\kappa_{i,l}m_i^km_l^k(x_i+x_l)\phi(t_k,x_i+x_l)$$
$$-\sum_{i=1}^{J}\sum_{j=1}^{J}\kappa_{i,l}m_i^km_l^kx_i\phi(t_k,x_i)+O(\Delta x)$$
$$=\big(K[\mu_{\Delta x}^k],x\phi(t_k,x)\big)+O(\Delta x)$$
$$=-\big(\partial_x\mathcal{Q}_K[\mu_{\Delta x}^k],\phi(t_k,\cdot)\big)+O(\Delta x).$$

Therefore, the right-hand side of equation (57) becomes

$$\Delta t\sum_{k=1}^{\bar{k}-1}\big(\mathcal{Q}_K[\mu_{\Delta x}^k]-\mathcal{Q}_F[\mu_{\Delta x}^k],\partial_x\phi(t_k,\cdot)\big)+O(\Delta x).$$

Following the arguments in Theorem 4.1 and [6], we can pass through the limit to arrive at (46). □

Remark 5.3. *Borrowing the uniqueness of solutions from Theorem 5.1, we can lift convergence from a subsequence in $\|\cdot\|_{BL}$ to the whole sequence in $\|\cdot\|_{BL_0}$. Also, since solutions to (44) are taken to be absolutely continuous at the boundary, we can measure the error of the numerical sequence in the BL norm.*

6 Mass Conservation

In the study of coagulation-fragmentation equations, one desired property of numerical schemes is the conservation of mass, namely with our notation

$$\sum_{j=1}^{J}x_jm_j^k=\sum_{j=1}^{J}x_jm_j^0\qquad\text{for all } k=1,2,\dots,\bar{k}.\tag{58}$$

We examine in this section to what extent the numerical schemes we introduced so far conserve mass. We will consider separately the impact of the coagulation term and of the fragmentation term.

Notice the growth term g and the birth and death terms β and d naturally modify mass. We will thus assume in all this section that $g=\beta=d\equiv 0$. The fully explicit, semi-implicit and conservation law scheme then read:

- *fully-explicit:*

$$\frac{m_j^{k+1}-m_j^k}{\Delta t}=\frac{1}{2}\sum_{i=1}^{j-1}\kappa_{i,j-i}m_i^km_{j-i}^k-\sum_{i=1}^{J}\kappa_{i,j}m_i^km_j^k+\sum_{i=j}^{J}b_{i,j}a_im_i^k-a_jm_j^k\tag{59}$$

- *semi-implicit:*

$$\frac{m_j^{k+1} - m_j^k}{\Delta t} = \frac{1}{2}\sum_{i=1}^{j-1} \kappa_{i,j-i} m_i^{k+1} m_{j-i}^k - \sum_{i=1}^{J} \kappa_{i,j} m_i^k m_j^{k+1} + \sum_{i=j}^{J} b_{i,j} a_i m_i^k - a_j m_j^k \tag{60}$$

- *conservation law:*

$$x_j \frac{m_j^{k+1} - m_j^k}{\Delta t} = \frac{\mathcal{Q}_{F,j}^k - \mathcal{Q}_{F,j-1}^k - \mathcal{Q}_{K,j}^k + \mathcal{Q}_{K,j-1}^k}{\Delta x} \tag{61}$$

6.1 Coagulation Terms

Theorem 6.1. *Suppose $a \equiv 0$. Then the fully explicit scheme* (59) *and the conservation law scheme* (61) *conserve mass i.e.* (58) *holds true for both schemes.*

Proof. In the case of the fully explicit scheme, it is enough to show

$$\frac{1}{2}\sum_{j=1}^{J}\sum_{i=1}^{j-1} x_j \kappa_{i,j-i} m_i^k m_{j-i}^k - \sum_{j=1}^{J}\sum_{i=1}^{J} x_j \kappa_{i,j} m_i^k m_j^k = 0. \tag{62}$$

First we can rewrite the first term in the left-hand side using (K1)-(K2) as

$$\begin{aligned}\sum_{j=1}^{J}\sum_{i=1}^{j-1} x_j \kappa_{i,j-i} m_i^k m_{j-i}^k &= \sum_{i=1}^{J}\sum_{j=i+1}^{J} x_j \kappa_{i,j-i} m_i^k m_{j-i}^k = \sum_{i=1}^{J}\sum_{l=1}^{J} x_{l+i} \kappa_{i,l} m_i^k m_l^k \\ &= \sum_{i=1}^{J}\sum_{l=1}^{J} (x_l + x_i) \kappa_{i,l} m_i^k m_l^k\end{aligned}$$

where we used that $x_{l+i} = (l+i)\Delta x = x_l + x_i$. Equation (62) follows.

Concerning the conservation law scheme, notice that $\mathcal{Q}_{F,j}^k = 0$ for any j,k since $a = 0$. It is thus enough to show that

$$\sum_{j=1}^{J} (\mathcal{Q}_{K,j-1}^k - \mathcal{Q}_{K,j}^k) = 0.$$

Using (55), this is

$$\sum_{j=1}^{J}\sum_{i=1}^{j} x_i\, \kappa_{i,j-i-1} m_{j-i-1}^k m_i^k - \sum_{j=1}^{J}\sum_{l=1}^{J} x_j\, \kappa_{j,l} m_l^k m_j^k = 0. \tag{63}$$

Using assumption (K2) we can rewrite the first term in the left-hand side as

$$\sum_{j=1}^{J}\sum_{i=1}^{j} x_i\, \kappa_{i,j-i-1} m_{j-i-1}^k m_i^k = \sum_{i=1}^{J}\sum_{j=i}^{J} x_i\, \kappa_{i,j-i-1} m_{j-i-1}^k m_i^k = \sum_{i=1}^{J}\sum_{l=1}^{J} x_j\, \kappa_{j,l} m_l^k m_j^k$$

and (63) follows. □

Remark 6.1. *We point out that due to the implicit coagulation terms in the semi-implicit scheme (4.2), we cannot arrive at the analogous result. This is confirmed numerically in Section 7 below.*

6.2 Fragmentation Terms

In this section, we will analyze the mass conservation property of the fragmentation terms of each scheme. With this in mind, we first examine the fully explicit and semi implicit schemes. We point out that these schemes are equivalent when $\kappa \equiv 0$. As shown in [7],

$$(b_{\Delta x}(x_i, \cdot), x) = x_i + O(\Delta x).$$

This introduces a source of error from the mesh side. However, in the case of a positive minimum size $x_{\min} > 0$, this problem can be fixed with a different approximation of $b(y, \cdot)$ given by

$$b_{\Delta x}(x_i, \cdot) = \sum_{j=1}^{i} \alpha_j(x_i)\delta_{x_j} \quad \text{where} \quad \alpha_j(x_i) = \frac{1}{x_j}\int_{\Lambda_j} xb(x_i, dx).$$

This guarantees

$$(b_{\Delta x}(x_i, \cdot), x) = x_i$$

and thus mass conservation of the fragmentation terms follows directly from equation (4.1). Proof of convergence of this approximation in the BL norm can be found in the aforementioned paper.

In the context of the conservation law scheme (53), we have the following:

Theorem 6.2. *Let $\kappa \equiv 0$. Then the conservation law scheme* (61) *conserves mass i.e.* (58) *holds.*

Proof. As before, it is enough to show

$$\sum_{j=1}^{J}(\mathcal{Q}^k_{K,j-1} - \mathcal{Q}^k_{K,j}) = 0.$$

Using (56) this is

$$\sum_{j=1}^{J}\sum_{i=j}^{J} x_j\, b_{i,j} a_i m_i^k - \sum_{j=1}^{J}\sum_{l=1}^{j} x_l b_{j,l}\, a_j m_j^k = 0.$$

Swapping the order of summation in the first term gives the result. □

7 Numerical Results

In this section we implement the schemes in MATLAB and test them against some well known problems. The error in the BL norm is approximated with the algorithm presented in [34] and the order of convergence is given by

$$q = \log\left(\frac{\|\mu^{2\Delta t}_{2\Delta x} - \mu_{exact}\|_{BL}}{\|\mu^{\Delta t}_{\Delta x} - \mu_{exact}\|_{BL}}\right).$$

Example 1 For the first example, we take the coagulation kernel $\kappa(x, y) \equiv 1$ with $\mu_0 = e^{-x}dx$ and all other model ingredients are set to 0. This problem has an exact solution

$$\mu_t = \left(\frac{2}{2+t}\right)^2 \exp\left(-\frac{2}{2+t}x\right) dx$$

see [39] for more details. Simulation are performed over the finite domain $x \in [0, 20]$. We present the BL error, numerical order, and computation times for each scheme in Table 1. We plot the solutions, point-wise error, and relative mass of each scheme in Figure 1. As stated before, the semi-implicit scheme does not conserve mass through coagulation as demonstrated in this example.

Nx	**Nt**	**Explicit**			**Semi-Implicit**		
		BL Error	**Order**	**Time (secs)**	**BL Error**	**Order**	**Time (secs)**
50	100	0.046406			0.059118		
100	200	0.024121	0.94401	1.2972	0.029972	0.97997	1.9879
200	400	0.012296	0.97209	27.511	0.015119	0.98727	41.505
400	800	0.0062079	0.98605	455.73	0.0075973	0.99281	645.54
800	1600	0.0031190	0.99301	5942.6	0.0038088	0.99616	10370

Nx	**Nt**	**Conservation Law**		
		BL Error	**Order**	**Time (secs)**
50	100	0.076986		
100	200	0.040102	0.94091	19.83
200	400	0.020535	0.96561	338.35
400	800	0.010408	0.98042	6223.8
800	1600	0.0052438	0.98897	88950

Table 1: The BL error, numerical order, and computation time (in seconds) for the three schemes. We point out that for these simulations $\Delta x = \Delta t$ for all trials.

Example 2 In this example we consider fragmentation. We let $b(y, \cdot) = \frac{2}{y}dx$ and $a(x) = x$. As given in [62], this problem has an exact solution of

$$\mu_t = (1+t)^2 \exp(-x(1+t))dx.$$

We note that for fragmentation only equations, the fully explicit and semi-implicit are identical. We present the BL error, numerical order, and computation times for each scheme in Table 2. We plot the solutions, point-wise error, and relative mass of each scheme in Figure 2.

Example 3 In this example, we take the model ingredients $g(t, x) = 2 - 2e^x$, $d(x) = 1$, $\beta = 2$, $\kappa(x, y) = 1$, $b(y, \cdot) = \frac{2}{y}dx$, and $a(x) = x$ over the domain $x \in [0, 1]$. The initial condition for this problem is given by $\mu_0 = e^{-x}dx$. Since the solution to this equation is unknown, we compare the approximate solutions to a reference solution generated by the fully explicit scheme at $Nx = 3200$ and $Nt = 6400$ (See Table 3).

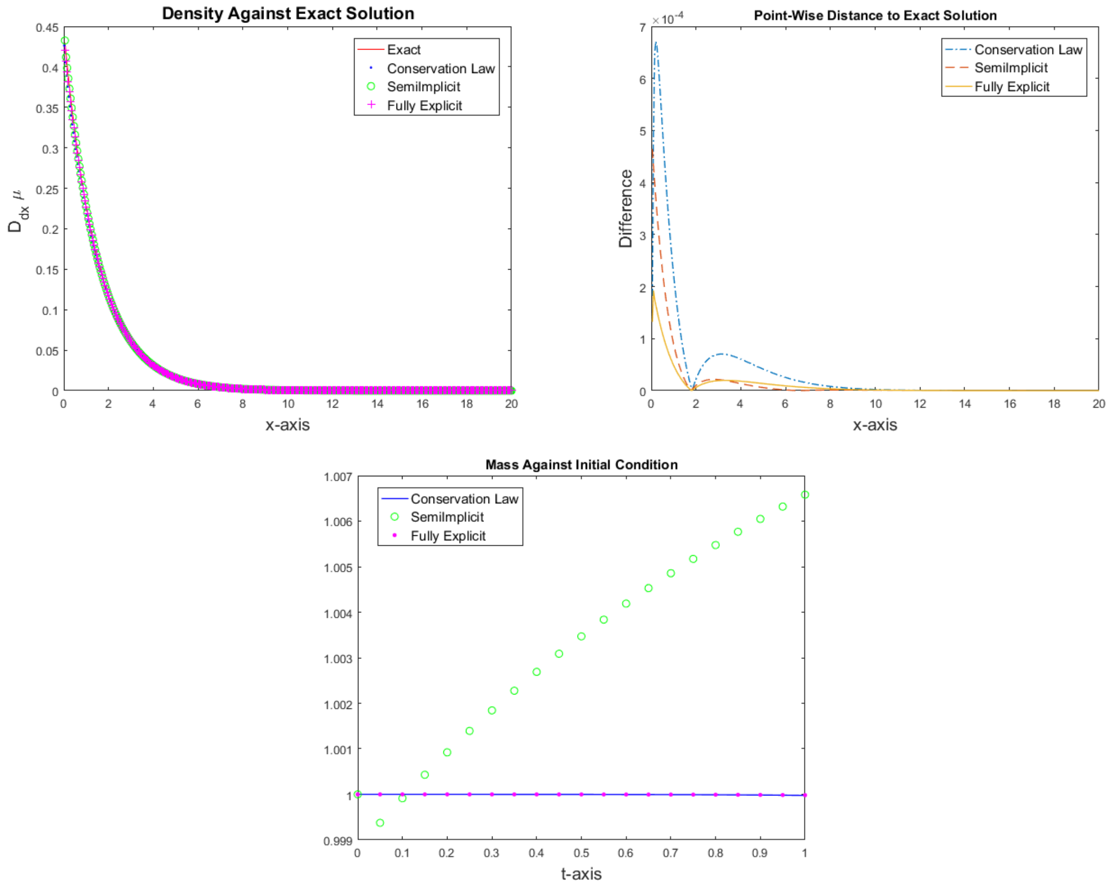

Figure 1: For Example 1 we present on the left side the numerical solution at time $T = 1$. On the right side we present the point-wise difference between the approximate solutions and exact solution. On the bottom, we present the relative mass according to the initial condition over $[0, 20]$.

Example 4 In this example, we provide a visualization of Theorem 4.1 from [7]. To this end we take the model ingredients of example 3 from before as well as the initial condition $\mu_0 = \delta_{0.2} + \delta_{0.4}$. Since $g(1) = 0$ and $g(x) > 0$ for $x \in [0, 1)$, Theorem 4.1 of [7] guarantees the steady-state solution will be absolutely continuous on the interval $[0, 1)$. This can be seen in Figure 3 as the solution gradually becomes absolutely continuous to the left of the characteristic curve of the 0.2 Dirac point.

8 Conclusion

In summary, there are a few differences between the three presented numerical schemes. One of the more striking discrepancy is in the computation time of each scheme. In all examples presented in Section 7, the conservation law scheme was much slower in comparison to both the explicit and semi-implicit schemes. This is mainly due to the double summations required to compute the $\mathcal{Q}^k_{K,j}$ and $\mathcal{Q}^k_{F,j}$ terms. This drastic difference in computation time seemingly

Nx	Nt	Explicit/SemiImplicit			Conservation Law		
		BLError	Order	Time (secs)	BLError	Order	Time (secs)
200	10	0.27759			0.51684		
400	20	0.15055	0.88275	2.4223	0.28095	0.87941	23.5
800	40	0.078274	0.94362	49.012	0.14664	0.93804	376.07
1600	80	0.03989	0.97251	765.21	0.074949	0.96829	6957.5
3200	160	0.020133	0.98644	11721	0.037898	0.98379	107980

Table 2: The BL error, numerical order, and computation time (in seconds) for the three schemes. We point out that for these simulations $\Delta x = \Delta t$ for all trials.

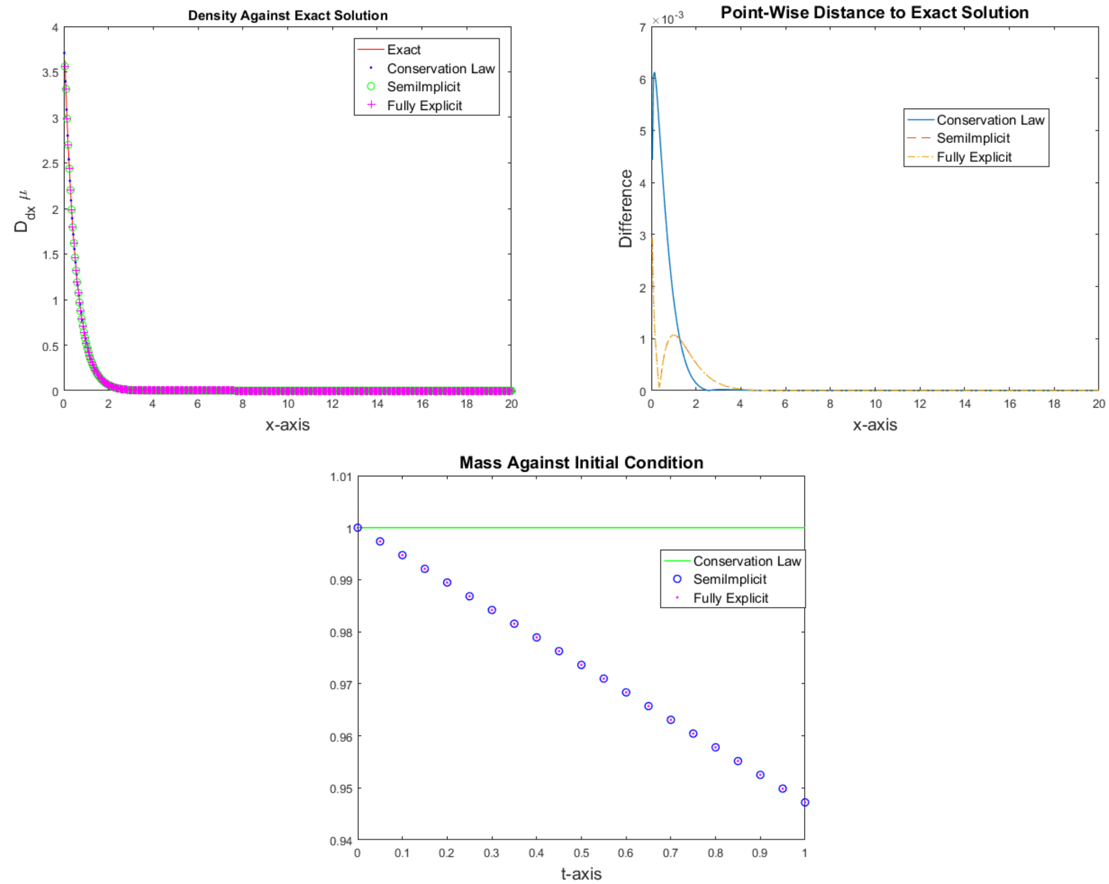

Figure 2: For Example 2 we present on the left side the numerical solution at time $T = 1$. On the right side we present the point-wise difference between the approximate solutions and exact solution. On the bottom, we present the relative mass according to the initial condition over $[0, 20]$.

has no real pay off as in all mesh sizes in the above example the explicit and semi-implicit schemes provide a more accurate approximation in a much shorter time. The main benefit of the conservation law scheme is its mass conservation property. This is the only scheme we have were the initial mass is conserved through fragmentation when the minimum size is zero.

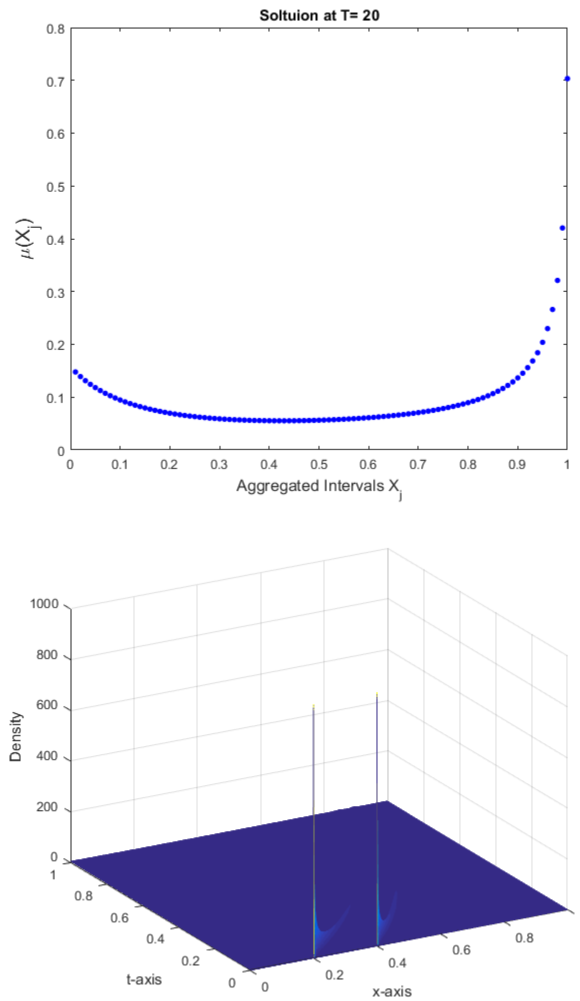

Figure 3: We present here the solution of example 4 at $T = 20$ over aggregated intervals of size 0.01 and a section of the mesh. Here $\Delta x = 0.001$ and $\Delta t = 0.0005$.

Nx	Nt	Explicit			Semi-Implicit		
		BL Error	**Order**	**Time (secs)**	**BL Error**	**Order**	**Time (secs)**
50	100	0.0039469		0.14104	0.025025		0.1243
100	200	0.0024508	0.68746	0.69537	0.012305	1.0242	0.60872
200	400	0.0013093	0.90442	4.4399	0.0061127	1.0093	3.585
400	800	0.0006399	1.0329	56.799	0.0030613	0.99766	55.39
800	1600	0.00028044	1.1902	1438.1	0.0015471	0.98462	1437.5

Nx	Nt	Conservation Law		
		BL Error	**Order**	**Time (secs)**
50	100	0.03332		0.48656
100	200	0.016804	0.98754	3.142
200	400	0.0084538	0.99115	48.925
400	800	0.0042551	0.99042	824.51
800	1600	0.0021498	0.98499	14165

Table 3: The BL error, numerical order, and computation time (in seconds) for the three schemes compared to the reference solution generated by the fully explicit scheme.

In application, this will not be the case; therefore, to this end we provide the adjustments to the explicit and semi-implicit schemes in Section 6.

The biggest benefit of the semi-implicit scheme is found in the CFL condition. Both the explicit and conservation law schemes have CFL conditions which are dependent on the initial condition. This dependency would be troublesome in sensitivity analysis on such a model where changing parameters such as the initial condition is commonplace. The main drawback of the semi-implicit scheme is the lack of mass conservation in both the coagulation and fragmentation terms. In the case of a positive minimum size, the adjustments provided in Section 6 alleviate this concern for fragmentation equations, however, there is currently no adjustment for the coagulation terms.

The examples provided above help illustrate multiple results proven elsewhere. For instance, example 4 illustrates the regularity theorem proven in [7] which has an analogous result proven in [35] for size structured population models (i.e. with no coagulation or fragmentation). This property shows the different effects each term has on the solution. For instance, the coagulation terms do not seem to affect the regularity of the solution. In other words, a coagulation equation with discrete initial condition will remain discrete (e.g. example 6 in [7]). In contrast, the regularity of the fragmentation kernel will affect the regularity of the solution. Indeed, in a fragmentation equation, a discrete fragmentation kernel will introduce point-masses throughout the population.

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