Derivation and mathematical study of a sorption-coagulation equation

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Abstract
This paper deals with the derivation and mathematical study of a new model of interactions between chemical polymers and metal ions. The equation describes the evolution of the distribution $f(t, p, q)$ of all polymers at time $t \geq 0$ in a given configuration $(p, q)$, belonging to a set of admissible configurations $S$. Variable $p$ being the size of the polymer and $q$ the number of metal ions they captured through sorption. The model consists of a nonlinear transport term in the $q$ variable and a quadratic source term, a two-dimensional coagulation operator in both variables $p$ and $q$. We formally derive the model from considerations on microscopic chemical processes. Next, we prove the existence of solutions for all time and we build a finite volume scheme. We prove that the sequence of approximated solutions is convergent, thanks to a $L^1$ -- weak stability principle. Finally, we illustrate and discuss the long-time behaviour of the solutions.

Keywords: polymers, metal ions, coagulation equation, existence of solutions, finite volume scheme, weak stability, partial differential equation

Mathematics Subject Classification numbers: 65R20, 82C05, 35Q82, 35Q92

(Some figures may appear in colour only in the online journal)

1. Introduction

1.1. Motivations

In this paper, we aim to derive and study a sorption-coagulation equation modelling interactions between chemical polymers and metal ions. Among the applications, chemical polymers able to ‘catch’ metal ions are used either to obtain purified water or to clear contaminated...
water after some industrial process, e.g. [39, 44]. The principle is the following: chemical polymers are introduced into an aqueous solution (water) containing metal ions (e.g. copper ions, lead ions); metal ions bind on specific polymers; then the solution is filtered through a porous membrane. As a result, we get, on one side of the membrane, (heavy) polymers with the ions, while, above the membrane, it remains a clean solution, free of ions. We refer the reader to the reviews [40, 41] for a precise description of this process. Nevertheless, the development of these applications and their improvement give rise to some technical difficulties. Indeed, various phenomena remain unclear, such as the role of the fouling effect (adhesion of polymers to the membrane), the aggregation phenomenon, the concentration effect and interaction with the wall of the cell (recipient) or else the interaction with the fluid. For recent findings, techniques and models on the subject we refer to [33–38, 42].

Here, to go further into a better understanding of this process, we focus on the first part (before filtration) and design a model accounting for the interactions between polymers and ions in the solution. Specifically, we propose a new model that takes both polymer–metal ions (sorption) and polymer–polymer (coagulation) interactions into account. In existing models, e.g. [33, 34, 39], the authors consider macroscopic quantities and equilibrium theory. In the present work, we propose a new approach, based on the observation of chemical reactions at a microscopic scale. The resulting equations are related to a family of well-known models on interacting particles, such as the coagulation–fragmentation equation or Lifschitz–Slyozov (LS) equation. However, to the best of our knowledge, this is the first time such an approach has been applied to this type of interactions (polymer–ion and polymer–polymer). Consequently, the model we derive below addresses novel mathematical issues about well-posedness, numerical approximation and long-time behaviour, questions we start to answer here. Before doing so, let us briefly describe the chemical background needed as well as the existing literature on the subject.

1.2. Chemical background for the mathematical modelling

A polymer is a macromolecule made of many repeat units called monomers. To illustrate this definition, let us give an example of a polymer: polyacrylic acid. Acrylic acid identified by the molecular formula \( \text{C}_2\text{H}_3\text{O}_2 \) plays the role of the monomer and polyacrylic acid is a chain of acrylic acids with the molecular formula \(- \text{C}_2\text{H}_3\text{O}_2\text{n} -\), where \( n \) stands for the number of occurrences of acrylic acid.

1.2.1. Polymer–ion interaction. The interactions between polymers and ions take place in specific sites of the chain called functional groups. The latter is a (repeat) subunit of the polymer, able to hold one metal ion. The composition or the location of the functional group fluctuates according to: the structure of the chain; the metal ions at stake; and the 'type' of interaction. In the case of polyacrylic acid, each monomer loses a proton (\( H^+ \)) in solution leading to a negatively charged polymer so that positively charged ions can bind on the chain. We refer the reader to [39, 40] for more examples.

In the present work, we follow [39] and assume that polymer–ion interactions are reversible binary chemical reactions, called sorptions. The direct reaction (one metal ion binds on one functional group) is called adsorption, and the reverse one (one metal ion is released by the polymer) is called desorption. Specifically, denote by \( P_{x, y} \) a polymer consisting of \( x \in \mathbb{N}^* \) functional groups, such that \( y \in \{0, \ldots, x\} \) of them hold one metal ion. We note that \( y \) is also the number of metal ions bound to the polymer. We call the couple \((x, y)\) the configuration of the polymer. Finally, we denote by \( M \) a free metal ion, free meaning that it is not bound to any polymer. The reversible chemical reaction between one free metal ion \( M \) and one polymer \( P_{x, y} \) is
where \( k_{x,y} \) is the adsorption rate at which a polymer of configuration \((x, y)\) binds one metal ion to get a new configuration \((x, y + 1)\), while \( I_{x,y+1} \) is the desorption rate at which a polymer \((x, y + 1)\) releases a metal ion to get the new configuration \((x, y)\). Both rates depend on the configuration of the polymer and inherently on the surrounding conditions (pH of the solution, temperature, etc) which are supposed to be fixed.

1.2.2. Polymer–polymer interactions. Under experimental conditions, the presence of other polymers leads to interpolymer complexes and can produce gels or precipitates, as pointed out in [40]. We include in the model the formation of interpolymer complexes through a binary coagulation process, which is the formation of a bigger polymer from two smaller ones. This (irreversible) reaction reads:

\[
P_{x,y} + P_{x',y'} \xrightarrow{a_{x,y,x',y'}} P_{x+x',y+y'},
\]

where the coagulation rate \( a_{x,y,x',y'} \) is the rate at which a polymer with configuration \((x, y)\) and another one with configuration \((x', y')\) will produce a new bigger macromolecule. The reaction preserves the number of functional groups and metal ions bound, so the new polymer has the configuration \((x + x', y + y')\).

1.3. Contents of the paper and related works

The rest of the paper is organized as follows. In section 2 we introduce our model consisting of a sorption-coagulation equation on the density function of polymers according to their configurations.

In section 3, we prove the existence of global solutions. The proof, somehow classical, is based on the work on the LS equation in [6] and LS with encounters (coagulation) in [5], also used in [25] for biological polymers. Nevertheless, our model reveals some technical difficulties, due to the boundary conditions, the conservations involved by the coagulation and the configurational space. We would like to mention here that the LS equation is a size-structured model for cluster (polymers here) formation by addition-depletion of monomers [31]. Whereas, the coagulation (only size-dependent) is part of the class of coagulation–fragmentation (CF) equations, and it has been mathematically studied in [1, 3, 12, 28, 29].

In section 4, we propose a finite volume type approximation of the problem. Our discretization is based on [2] and [16], where the authors propose a conservative reformulation of the CF equation in a manner well-adapted to a finite volume scheme (for a one-dimensional coagulation operator). Here, we adapt their method with a conservative cut-off to the two-dimensional case, and we prove the convergence of our approximation. Let us also mention an alternative in [19], where the authors introduce a general (moments) conservative finite volume scheme for multi-dimensional coagulation operators that might be used here. This scheme works well for smooth coagulation kernels defined on the half-space \( \mathbb{R}^n_+ \), but this is not the case here because of the configuration space \( S \) defined in section 2. It could be interesting to investigate how we could adapt their scheme to our case, especially since they developed it on nonuniform meshes (being CPU time-saving). For other suitable numerical schemes, we refer the reader to [18, 20, 23, 24].
In section 5, we present a numerical simulation. We discuss and interpret the long-time behaviour of the model, and we show how it might be related to the behaviour of a non-autonomous coagulation equation. Here, it would be very interesting to connect this problem to \cite{8, 22, 26} on the LS and related models or \cite{10, 15} for the coagulation equation.

2. The model

We depart from reactions (1) and (2). The experiments consist of a large number of particles (both polymers and metal ions). That is why quantities are expressed in terms of their molar or mass concentration. Consequently, we may introduce two new convenient variables, \( p = \varepsilon x \) and \( q = \varepsilon y \), for the quantity in moles of, respectively, functional groups and bound (to metal ions) functional groups, where \( \varepsilon = 1/N_a \ll 1 \) stands for the inverse of Avogadro’s number. Therefore, in the limit \( \varepsilon \to 0 \), both variables \( p \) and \( q \) can reach a continuum of values in 

\[
S := \{(p, q) \in \mathbb{R}_+^2 : 0 < q < p\},
\]

contrary to variables \( x \) and \( y \) which are natural numbers. The system governing the evolution of \( f \) is

\[
\frac{\partial f}{\partial t} + \frac{\partial}{\partial q}(\gamma f) = Q(f, f), \quad \text{on } \mathbb{R}_+ \times S,
\]

where \( Q \) is the coagulation operator, ruling the polymer–polymer interaction given by (2) and \( V \) denotes the rate of association-dissociation, or by other means the sorption rate. It determines the mechanism of ion transfer with a polymer described in reaction (1). Both \( V \) and \( Q \) are properly defined below. Equation (3) on the configurational distribution function is not sufficient to characterize all the system. To complete the model, it remains to introduce a second equation on the molar concentration of free metal ions (being in the solution but unbound to polymers). We denote this concentration \( u(t) \), as a function of time \( t \geq 0 \), and it is given by the constraint of metal ion conservation (bound and free), namely

\[
u(t) + \int_S q f(t, p, q) dq dp = \rho, \quad \text{on } \mathbb{R}_+,
\]

where \( \rho > 0 \) is a constant standing for the total quantity of metal ions in the system (bound and unbound to polymers). Indeed, as \( f(t, p, q) \Delta q \Delta p \) approaches the molar concentration of polymers with configuration \((p, q)\) in the limit of \( \Delta p \) and \( \Delta q \) small, if we multiply this quantity by \( q \) the number of occupied functional groups (= the number of metal ions bound) in moles, then we formally get the molar concentration of metal ions bound to the polymers. Thus, the integral term in (4) accounts for the molar concentration of metal ions associated with polymers and the balance equation (4) expresses the conservation of matter: both bound and free metal ions in the system.

Let us now define \( V \) and \( Q \). As a general form for \( V \) we consider the following chemical reaction rate

\[
V(u(t), p, q) = k(p, q)u(t)^\gamma - l(p, q),
\]

where \( k \) is the association rate, or adsorption, at which a free monomer binds to a polymer (depending on the type of interaction and the diffusion rate of the particles) and \( l \) is the dissociation rate, or desorption (depending on the strength of the interaction). The association rate is multiplied by \( u(t)^\gamma \), as a classical law of mass action and for the sake of simplicity we restrict ourselves to \( \gamma = 1 \) which is the order of the reaction. A relevant example of
The association-dissociation rate would be an analogy to Langmuir’s law (for the adsorption of metal ions on a surface), namely

\[ V(u(t), p, q) = k_0 (p - q) \alpha u(t) - l_0 q^\beta, \]  

(5)

with \( k_0, l_0 > 0 \) parameters and \( \alpha, \beta > 0 \) geometrical factors, see [43]. Indeed, the association rate depends on the quantity of available functional groups \( p - q \) while the dissociation rate is proportional to the quantity of metal ions bound to the polymers \( q \).

Next, we make explicit the coagulation operator \( Q \) with the coagulation rate \( a \) defined as a nonnegative function over \( S \times S \) satisfying the symmetry assumption

\[ a(p, q; p', q') = a(p', q'; p, q). \]  

(6)

This gives the rate at which two polymers with configurations \( (p, q) \) and \( (p', q') \) will coagulate. The symmetry assumption follows from the impossibility to distinguish the coagulation of \( (p, q) \) with \( (p', q') \) or the coagulation of \( (p', q') \) with \( (p, q) \) because it is the same reaction.

Then, we decompose \( Q \) in a gain term \( Q^+ \) and a depletion term \( Q^- \) that is

\[ Q = Q^+ - Q^-, \]

where

\[ Q^+(f, f)(p, q) = \frac{1}{2} \int_0^p \int_0^{p'} a(p', q', p - p', q - q') \mathbf{1}_{(0,p-\cdot)}(q - q') f(p', q') f(p - p', q - q') \, dq' \, dp', \]  

(7)

\[ Q^-(f, f)(p, q) = L(f)(p, q)f(p, q), \]

with

\[ L(f)(p, q) = \int_0^\infty \int_0^p \mathbf{a}(p, q, p', q') f(p', q') \, dq' \, dp'. \]  

(8)

The gain term \( Q^+ \) accounts for the production of polymers with configuration \( (p, q) \) thanks to the coagulation of \( (p', q') \) with \( q' < p' < p \) and \( (p - p', q - q') \) with \( 0 < q - q' < p - p' \). Likewise, the depletion term accounts for the disappearance in the system of a polymer \( (p, q) \) when coagulating with any other \( (p', q') \) for the benefit of a new polymer with configuration \( (p + p', q + q') \).

The problem (3)–(4) is completed by a Dirichlet boundary condition:

\[ f = 0, \quad \text{on } \partial S, \]  

(9)

which, of course, supposes suitable assumptions on the characteristics discussed later. Finally, we require two initial conditions:

\[ f(t = 0, \cdot) = f^{in} \quad \text{on } S, \quad \text{and} \quad u(t = 0) = u^{in}. \]  

(10)

**Remark 2.1.** We could consider a discrete version of the problem considering the concentrations of all the \( P_{x,y} \), with \( x \) and \( y \) as natural numbers. Nevertheless, this would be mathematically less tractable due to the huge number of equations involved. But, we can see the continuous model as a limit of the discrete one, through an appropriate scaling and here we have in mind the parameter \( \epsilon \). The reader can get an idea of the discrete model here and how it is linked to the continuous one, by consulting [7, 30]. In these papers, the authors derived rigorously the continuous LS equation from the Becker–Döring model, both models being close to the one presented here.
3. Rescaling and the existence of global solutions

3.1. Rescaled problem

The nature of the configurational space $S$ is awkward for computations both from the theoretical point of view and the numerical implementation. Thus, we decide to scale the problem and to perform a change of variable in the distribution $f$ with respect to a physically relevant new variable $r$. We call it the ion ratio (without dimension) and its definition is, for $(p, q) \in S$,

$$
 r := \frac{q}{p} \in (0, 1).
$$

We introduce then the new unknown $\tilde{f}$ defined, over the new configuration space $S := \mathbb{R}_+ \times (0, 1)$, by

$$
 \tilde{f}(t, p, r) = pf(t, p, rp).
$$

Then, we perform a change of variable in the association-dissociation and coagulation rates, by introducing $\tilde{V}$ defined over $\mathbb{R} \times S$ and $\tilde{\alpha}$ over $S \times S$, such that

$$
 \tilde{V}(u, p, r) = V(u(p, rp)), \quad \text{and} \quad \tilde{\alpha}(p, r; p', r') = \alpha(p, rp; p', r'p').
$$

Thus, they satisfy

$$
 \tilde{V}(u, p, r) = \tilde{k}(p, r)u - \tilde{I}(p, r), \quad (11)
$$

with $\tilde{k}(p, r) = k(p, rp)$ and $\tilde{I}(p, r) = I(p, rp)$. Also, the symmetry assumption (6) becomes

$$
 \tilde{\alpha}(p, r; p', r') = \tilde{\alpha}(p', r'; p, r). \quad (12)
$$

A formal computation leads to the equation

$$
 \partial_t \tilde{f}(t, p, r) + \frac{1}{p} \partial_r(\tilde{V}(u(t), p, r)\tilde{f}(t, p, r)) = p\tilde{Q}(\tilde{f}, \tilde{f})(t, p, q).
$$

Finally, letting $\tilde{Q} = \tilde{Q}^+ - \tilde{Q}^-$ such that

$$
 \tilde{Q}^+(\tilde{f}, \tilde{f})(p, r) = \frac{1}{2} \int_0^p \int_0^1 \frac{p}{p - p'} \alpha(p', p - p', r^*) \mathbf{1}_{(0,1)}(r^*) \times \delta(p', r') \delta(p - p', r^*) \, dr' \, dp', \quad (13)
$$

$$
 \tilde{Q}^-(\tilde{f}, \tilde{f})(p, r) = \tilde{L}(\tilde{f})(p, r) \tilde{f}(p, r)
$$

with $\tilde{L}(\tilde{f})(p, r) = \int_0^\infty \int_0^1 \tilde{\alpha}(p, r; p', r') \tilde{f}(p', r') \, dr' \, dp'$,

$$
 \tilde{Q}^-(\tilde{f}, \tilde{f})(p, r) = \tilde{L}(\tilde{f})(p, r) \tilde{f}(p, r)
$$

with $r^* = \frac{p' - r'}{p - r'}$, we get

$$
 \tilde{Q}(\tilde{f}, \tilde{f})(t, p, r) = p\tilde{Q}(\tilde{f}, \tilde{f})(t, p, rp).
$$

In the following and for the rest we drop tildes in the re-scaled problem, for clarity. Now, we can reformulate the problem: find the distribution $f$ satisfying

$$
 \frac{\partial f}{\partial t} + \frac{1}{p} \frac{\partial}{\partial r}(\tilde{V}f) = Q(f, f), \quad \text{on} \quad \mathbb{R}_+ \times S, \quad (15)
$$

with the constraint
\[ u(t) + \int_{\mathcal{S}} r p f(t, p, r) \, dr \, dp = \rho, \quad \text{on } \mathbb{R}_+ \]  

(16)

and boundary condition (9) still given by
\[ f = 0, \quad \text{on } \partial \mathcal{S}, \]  

(17)

while the initial conditions consist in a change of variables in (10) and read:
\[ f(t = 0, \cdot) = f^\text{in} \text{ on } \mathcal{S}, \text{ and } u(t = 0) = u^\text{in}. \]  

(18)

### 3.2. Hypotheses and result

The study of the problem (15)–(16) with (17) and (18) requires some hypotheses. Namely, we assume that:

**H1.** The initial distribution \( f^\text{in} \in L^1(\mathcal{S}, (1 + p) \, dp) \) is nonnegative and \( u^\text{in} \geq 0 \) such that
\[ \rho := u^\text{in} + \int_{\mathcal{S}} r p f^\text{in}(p, r) \, dr \, dp < +\infty. \]  

(19)

**H2.** The coagulation rate \( a \in L^\infty(\mathcal{S} \times \mathcal{S}) \) is nonnegative, satisfies (12) and
\[ \|a\|_{L^\infty} \leq K. \]  

(20)

**H3.** The rates functions \( p \mapsto k(p, \cdot), l(p, \cdot) \in L^\infty(\mathbb{R}_+; W^{2,\infty}(0, 1)) \) are both nonnegative and
\[ \|k\|_{L^\infty(\mathbb{R}_+; W^{2,\infty}(0, 1))} + \|l\|_{L^\infty(\mathbb{R}_+; W^{2,\infty}(0, 1))} \leq K. \]  

(21)

and for all \( p \in \mathbb{R}_+ \),
\[ \|k(p, \cdot)\|_{W^{2,\infty}(0, 1)} + \|l(p, \cdot)\|_{W^{2,\infty}(0, 1)} \leq Kp. \]  

(22)

**H4.** For all \( u \geq 0 \) and \( p \in \mathbb{R}_+ \),
\[ \mathcal{V}(u, p, r = 0) \geq 0, \text{ and } \mathcal{V}(u, p, r = 1) \leq 0, \]  

(23)

and
\[ \partial_t \mathcal{V}(u, p, r) = \partial_p k u - \partial_l l \leq 0 \quad \text{a.e. } (u, p, r) \in \mathbb{R}_+ \times \mathcal{S}. \]  

(24)

Here, \( K > 0 \) is a constant. Note that (23) ensures that the characteristics remain in the set \( \mathcal{S} \) and allows us to prescribe the boundary (17). This hypothesis is equivalent, with respect to (11) and (H4), to assuming
\[ k(p, 0) \geq 0, \quad l(p, 0) = 0 \text{ and } k(p, 1) = 0, \quad l(p, 1) \geq 0, \]  

(25)

for all \( p \in \mathbb{R}_+ \).

**Remark 3.1.** With such variables, we note that example (5) becomes
\[ \frac{1}{p} \mathcal{V}(u(t), p, r) = k_0 p^{\alpha - 1} (1 - r)^\alpha u(t) - l_0 p^{\beta - 1} r^\beta. \]  

And, hypothesis (H4) is consistent with this example while (H3) is still restrictive and would be relaxed.

Now, we are in a position to give a definition of the solutions to the problem (15)–(16).
**Definition 3.1 (weak solution 1).** Let $T > 0$ and the initial conditions $f^{in}$ and $u^{in}$ satisfy (H1). A weak solution to (15)–(16) on $[0, T)$ is a couple $(f, u)$ of nonnegative functions such that

$$f \in C([0, T); w - L^1(S)) \cap L^\infty([0, T), L^1(S, p\, dp)),$$

and $u \in C([0, T]),$ satisfying for all $t \in [0, T)$ and $\varphi \in C^1_0(\mathbb{R}_+ \times [0, 1])$

$$\int_S f(t, p, r)\varphi(p, r)\, dp - \int_S f^{in}(p, r)\varphi(p, r)\, dp = \int_0^t \int_S \frac{1}{p}V(u(s), p, r)f(s, p, r)\partial_r\varphi(p, r)\, dr\, dp\, ds$$

$$+ \int_0^t \int_S Q(f, f)(s, p, r)\varphi(p, r)\, dr\, dp\, ds,$$

(27)

together with (16).

We remark here that regularity (26), where $C([0, T); w - X)$ means continuous from $[0, T)$ to $X$ a Banach space with respect to the weak topology of $X$. Hypotheses (H1) to (H3) suffice to define (27). Particularly, (13)–(14) entail, as we will see later, that $Q(f, f)$ belongs to $L^\infty([0, T); L^1(S)).$

We can now state the main result:

**Theorem 3.2 (Global existence).** Let $T > 0.$ Assume that $f^{in}$ and $u^{in}$ satisfy (H1) and that hypotheses (H2)–(H4) are fulfilled. Then, there exists at least one solution $(f, u)$ to the problem (15)–(16) in the sense of definition 3.1. Moreover, a solution has the regularity

$$f \in C([0, T); L^1(S)),$$

with both

$$\int_S f(t, p, r)\, dp \leq \int_S f^{in}(p, r)\, dp,$$

and

$$\int_S pf(t, p, r)\, dp = \int_S pf^{in}(p, r)\, dp.$$

Proof of theorem 3.2 relies on two main steps, which are similar to the ones used for instance in [5] and [6] for the LS equation. The first step consists in the construction of a mild solution $f$ of equation (15) for a given $u.$ We achieve it through a fixed point theorem by virtue of the contraction property of the coagulation operator. The next step follows a second fixed point which associates (15) to the constraint (16) on $u.$

Since the method is rather classical, we only provide in the next section the key arguments of the proof, by highlighting the differences between our problem and the LS equation with encounters. Particularly, the treatment of the characteristics.

### 3.3. Existence of solutions

3.3.1. **The autonomous problem.** We start the analysis of the problem for a given nonnegative $u \in C([0, T])$ with $T > 0,$ i.e. we avoid the difficulty induced by the constraint (16). A well-known approach is to construct the characteristics of the transport operator. A characteristic
curve parametrized by \( p \in \mathbb{R}_+ \) and associated to a given \( u \), which arrived in \( r \in (0, 1) \) at time \( t \in [0, T] \), is the solution of

\[
\frac{d}{ds} R_p(s; t, r) = \frac{1}{p} \mathcal{V}(u(s), p, R_p(s; t, r)) \quad \text{on } [0, T]
\]

\( R_p(t; t, r) = r. \)

According to (21)–(22) and (25), there exists a unique solution \( R_p(\cdot; t, r) \) that is continuously differentiable on a time interval such that the solution is defined, i.e. \( R_p(s; t, r) \in (0, 1) \). We would first remark that (H4) ensures that the characteristics remain in \((0, 1)\) for any \( s \geq t \). Moreover, we define the origin time \( \sigma_p(t, r) = \inf \{ s \in [0, t] : 0 < R_p(s; t, r) < 1 \} \). Now, from the characteristics curves we construct the so-called mild-formulation which is a solution of

\[
f(t, p, r) = \begin{cases} 
  f^\text{in}(p, R_p(0; t, r)) J_p(0; t, r) 
  + \int_0^t Q(f, f)(s, p, R_p(s; t, r)) J_p(s; t, r) \, ds, & \text{if } \sigma_p(t, r) = 0 \\
  \int_{\sigma_p(t, r)}^t Q(f, f)(s, p, R_p(s; t, r)) J_p(s; t, r) \, ds, & \text{otherwise.}
\end{cases}
\]

(28)

for all \( t \in [0, T] \) and a.e. \((p, r) \in \mathcal{S}\) and

\[
J_p(s; t, r) := \frac{\partial R_p(s; t, r)}{\partial r} = \exp \left( - \int_s^t \frac{1}{p} (\partial_r \mathcal{V})(\sigma, p, R_p(\sigma; t, r)) \, d\sigma \right).
\]

Note that, for regular enough solutions, the boundary condition (17) is satisfied by (28) since \( \sigma_p(t, 0) = \sigma_p(t, 1) = t \).

Then, to prove theorem 3.2 we need to recover the notion of a weak solution from that of a mild solution. The following result states the equivalence of both notions:

**Lemma 3.3.** If \( f^\text{in} \in L^1(\mathcal{S}) \) and \( Q(f, f) \) \( \in L^1((0, T) \times \mathcal{S}) \), then the following statements are equivalents:

(i) \( f \in C([0, T], L^1(\mathcal{S})) \) and is a solution in the weak sense, i.e. satisfies (27).

(ii) \( f \) is a mild solution, i.e. satisfies (28).

This result is well known and comes from a change of variable and an identification process, we refer to [5, 6] for the LS equation or [11] for the Boltzmann equation. The only sensitive point remains in the treatment of the origin time \( \sigma_p \) and to this end we should proceed as in [25]. The monotony hypothesis (24) is crucial to separate continuously the characteristics coming from 0 and 1 to construct the weak solution from (28). Now, with the help of this lemma, it suffices to prove the existence of a mild solution.

Before claiming the existence of a mild solution for a given \( u \), let us introduce some *a priori* properties of the coagulation operator. Namely, for any \( f \) and \( g \) both belonging to \( L^1(\mathcal{S}) \), we have

\[
\|Q(f, f)\|_{L^1(\mathcal{S})} \leq 2K \|f\|_{L^1(\mathcal{S})}^2,
\]

(29)

\[
\|Q(f, f) - Q(g, g)\|_{L^1(\mathcal{S})} \leq 2K(\|f\|_{L^1(\mathcal{S})} + \|g\|_{L^1(\mathcal{S})}) \|f - g\|_{L^1(\mathcal{S})},
\]

(30)

These two estimates ensure that \( f \mapsto Q(f, f) \) maps \( L^1(\mathcal{S}) \) into itself and is Lipschitz on any bounded subset of \( L^1(\mathcal{S}) \). Finally, we would remark that for any \( f \in L^1(\mathcal{S}) \) and \( \varphi \in L^\infty(\mathcal{S}) \), it holds

Note that, for regular enough solutions, the boundary condition (17) is satisfied by (28) since \( \sigma_p(t, 0) = \sigma_p(t, 1) = t \).

Then, to prove theorem 3.2 we need to recover the notion of a weak solution from that of a mild solution. The following result states the equivalence of both notions:

**Lemma 3.3.** If \( f^\text{in} \in L^1(\mathcal{S}) \) and \( Q(f, f) \) \( \in L^1((0, T) \times \mathcal{S}) \), then the following statements are equivalents:

(i) \( f \in C([0, T], L^1(\mathcal{S})) \) and is a solution in the weak sense, i.e. satisfies (27).

(ii) \( f \) is a mild solution, i.e. satisfies (28).

This result is well known and comes from a change of variable and an identification process, we refer to [5, 6] for the LS equation or [11] for the Boltzmann equation. The only sensitive point remains in the treatment of the origin time \( \sigma_p \) and to this end we should proceed as in [25]. The monotony hypothesis (24) is crucial to separate continuously the characteristics coming from 0 and 1 to construct the weak solution from (28). Now, with the help of this lemma, it suffices to prove the existence of a mild solution.

Before claiming the existence of a mild solution for a given \( u \), let us introduce some *a priori* properties of the coagulation operator. Namely, for any \( f \) and \( g \) both belonging to \( L^1(\mathcal{S}) \), we have

\[
\|Q(f, f)\|_{L^1(\mathcal{S})} \leq 2K \|f\|_{L^1(\mathcal{S})}^2,
\]

(29)

\[
\|Q(f, f) - Q(g, g)\|_{L^1(\mathcal{S})} \leq 2K(\|f\|_{L^1(\mathcal{S})} + \|g\|_{L^1(\mathcal{S})}) \|f - g\|_{L^1(\mathcal{S})},
\]

(30)

These two estimates ensure that \( f \mapsto Q(f, f) \) maps \( L^1(\mathcal{S}) \) into itself and is Lipschitz on any bounded subset of \( L^1(\mathcal{S}) \). Finally, we would remark that for any \( f \in L^1(\mathcal{S}) \) and \( \varphi \in L^\infty(\mathcal{S}) \), it holds
\[
\int \int_{S} Q(f, f)(p, r) \varphi(p, r) \, dr \, dp = \frac{1}{2} \int \int_{S \times S} a(p, r; p', r') f(p, r) f(p', r') \\
\times [\varphi(p + p', r^*) - \varphi(p, r) - \varphi(p', r^*)] \, dr' \, dp' \, dr \, dp. \quad (31)
\]

with \( r^* = (rp + rp')/(p + p') \in (0, 1) \), which is called weak formulation of the coagulation operator, see [10, 14, 29]. We obtain this identity by inversion of integrals applying Fubini’s theorem, then changes of variable. In particular, when \( \varphi = 1_{S} \),

\[
\int \int_{S} Q(f, f)(p, r) \, dr \, dp \leq 0. \quad (32)
\]

Moreover, if \( f \in L^{1}(S, p \, dp) \), then

\[
\int \int_{S} p Q(f, f)(p, r) \, dr \, dp = 0. \quad (33)
\]

Now, for a given \( \rho > 0 \), we define the set:

\[
B = \{ u \in C([0, T]) : 0 \leq u(t) \leq \rho \},
\]

and we are ready to claim the next proposition.

**Proposition 3.4.** Let \( T > 0 \) and \( \rho > 0 \) with \( u \) belonging to the associated set \( B \). If \( f^{m} \in L^{1}(S, (1 + p) \, dp) \), then there exists a unique nonnegative mild solution, i.e. satisfying (28), with

\[
f \in L^{\infty}(0, T; L^{1}(S, (1 + p) \, dp)).
\]

Moreover, for all \( t \in (0, T) \) we have

\[
\int \int_{S} f(t, p, r) \, dr \, dp \leq \int \int_{S} f^{m}(p, r) \, dr \, dp, \quad (34)
\]

and

\[
\int \int_{S} pf(t, p, r) \, dr \, dp = \int \int_{S} pf^{m}(p, r) \, dr \, dp. \quad (35)
\]

**Proof.** Here we only give a sketch of the proof.

**Step 1. Existence and uniqueness.** The local existence of a unique nonnegative solution \( f \in L^{\infty}(0, T'; L^{1}(S)) \), for some \( T' > 0 \) small enough, readily follows from the Banach fixed-point theorem applied to the operator that maps \( f \) to the right-hand side of (28) on a bounded subset of \( L^{1}(0, T'; L^{1}(S)) \). To do so, we follow line-to-line [5] using properties (29) and (30).

Then, the global existence, for any time \( T > 0 \), is obtained using estimate (34), indeed by a classical argument we construct a unique solution on intervals \([0, T'] \), \([T', 2T']\), etc. So, it remains to prove (34), which directly follows from the integration of (28), using that \( f^{m} \in L^{1}(S) \) and (32).

**Step 2. Mass conservation.** It remains to prove (35) which needs \( f \) to belong to \( L^{\infty}(0, T; L^{1}(S, p \, dp)) \) and \( Q(f, f) \) too. But, identity (31) holds only for \( \varphi \in L^{\infty}(S) \) and a priori \( p \varphi \) is not integrable. We can follow [5, lemma 4] which involves a regularization procedure using \( a_{\rho}(p, r; p', r') = a(p, r; p', r') \mathbf{1}_{(0, p)}(p) \mathbf{1}_{(0, p)}(p') \) in (28) and construct a sequence of approximation \( f_{\rho} \in L^{\infty}(0, T; L^{1}(S)) \). Then, computing the \( L^{1} \) norm of \( f - f_{\rho} \) with the mild formulation yields to the strong convergence of \( f_{\rho} \) toward the solution \( f \) in \( L^{\infty}(0, T; L^{1}(S)) \) when \( \rho \rightarrow +\infty \), since \( a_{\rho} \rightarrow a \) a.e. \( S \times S \). Finally, because \( a_{\rho} \) has a compact support, \( p f_{\rho} \) is integrable and from (H2) we get the uniform bound (in \( P \)):
for some constant \( C(T) > 0 \) obtained by a Gronwall’s lemma on the mild formulation. We get \( f \in L^\infty(0,T;L^1(S,(1+p)drdp)) \) and \( pQ(f,f) \) is integrable. We conclude by coming back to (28) and integrating it against \( p \), which yields (35) thanks to (33).

\[ \square \]

**Remark 3.2.** The fact \( a \) is bounded in the estimation used in the proof above was a key ingredient. Indeed, without this, the control of the mass could break down, this is known as gelation phenomena. Nevertheless, the condition could be relaxed, generally up to a sub-linear coagulation kernel, see for instance [14].

We end this section by stating an additional regularity on the pseudo-moment of the mild solution, the key argument to couple the constraint (16) to (15).

**Corollary 3.5.** Under hypotheses of proposition 3.4,

\[ M(t) := \int_S rpf(t,p,r) \, drdp \leq \int_S pf^{in}(p,r) \, drdp, \]

and \( M \in W^{1,\infty}(0,T) \) with

\[ M'(t) = \int_S \mathcal{V}(u(t),p,r)f(t,p,r) \, drdp. \]

\[ (36) \]

**Proof.** The first estimate is a direct consequence of proposition 3.4. Then, we use the formulation (27) and for the test function we let \( \varphi \equiv \rho \xi \) such that \( \xi \geq \rho \), \( \xi \in C^1(\bar{R}_+\times S) \) and \( \xi(p) = p \) over \((2\varepsilon,1/2\varepsilon)\) with \( \text{supp } \xi \subseteq (\varepsilon,1/\varepsilon) \), thus

\[ \int_S r \xi(t,p,r) \, drdp = \int_S r^{	ext{in}}(p,r) \xi(t,p,r) \, drdp \]

\[ + \int_0^t \int_S r \mathcal{V}(u(s),p,r)f(s,p,r) \xi(t,p,r) \, drdp \, ds \]

\[ + \int_0^t \int_S rQ(f,f)(s,p,r) \xi(t,p,r) \, drdp \, ds. \]

Since we have \( f \in L^\infty(0,T;L^1(S,(1+p)drdp)) \), by the use of (22) and (33), with the Lebesgue theorem we pass to the limit \( \varepsilon \to 0 \) and we get

\[ M(t) = \int_S rpf^{in}(p,r) \, drdp + \int_0^t \int_S \mathcal{V}(u(s),p,r)f(s,p,r) \, drdp \, ds. \]

So, we conclude that

\[ \frac{d}{dt} M(t) = \int_S \mathcal{V}(u(t),p,r)f(t,p,r) \, drdp. \]

\[ \square \]

We are now ready to apply the second fixed-point to connect \( u \) and \( f \) in the system.

3.3.2. **Fixed-point on \( u \).** Again we follow \([5,6]\), i.e. we let \( T > 0 \) and we define the map

\[ \mathcal{M} : u \in B \mapsto \tilde{u} = \left[ p - \int_S rpf(t,p,r) \, drdp \right]_+. \]
where $[\cdot]_+$ is the positive part and $f_\mu$ the unique mild solution on $[0, T]$ associated to $u$ thanks to proposition 3.4. It follows that $M$ maps $\mathcal{B}$ into itself. Moreover, using \eqref{eq:36}

$$t \mapsto \rho - \int_S \rho f_\mu(t, p, r) \, dr dp \in W^{1,\infty}(0, T),$$

then, since $[\cdot]_+$ is Lipschitz, it holds that $\tilde{u} \in W^{1,\infty}(0, T)$ with

$$\frac{d}{dt} \tilde{u} = \begin{cases} 0, & \text{if } \int_S \rho f_\mu(t, p, r) \, dr dp \geq \rho, \\
\int_S \nabla(u(t), p, r)f_\mu(t, p, r) \, dr dp, & \text{otherwise.} \end{cases}$$

a.e. $t \in (0, T)$, see \cite[theorem 2.1.11]{45}. Thus, for any $u \in \mathcal{B}$ by using hypothesis on the rates (H3), it yields

$$\left\| \frac{d}{dt} \tilde{u} \right\|_{L^\infty(0, T)} \leq K(\rho + 1) \| f^\infty \|_{L^\infty(S)}.$$

Next, we invoke the Ascoli theorem to claim that $M(\mathcal{B}) \subset \mathcal{B}$ is relatively compact in $C([0, T])$. Now, a Schauder fixed-point theorem would achieve the proof of theorem 3.2. It remains to prove the continuity of the map $M$. Let $(u_n)_n$ be a sequence of $\mathcal{B}$ converging to $u$ for the uniform norm. We need to prove that

$$\lim_{n \to +\infty} \| \tilde{u}_n - \tilde{u} \|_{L^\infty(0, T)} = 0,$$

which is done by estimating

$$\sup_{t \in (0, T)} \left| \int_S \rho f_\mu(t, p, r) \, dr dp - \int_S \rho f_\mu(t, p, r) \, dr dp \right| \leq \sup_{t \in (0, T)} \int_S |f_\mu(t, p, r) - f_\mu(t, p, r)| \, dr dp.$$

Indeed, the right-hand side of this inequality goes to zero following line-to-line the proof of \cite[lemmas 5 and 6]{5} to conclude on the one hand the continuity and on the other hand that, in fact,

$$\int_S \rho f_\mu(t, p, r) < \rho \quad \forall t \in [0, T],$$

to drop $[\cdot]_+$. Thus, there exists $u \in \mathcal{B}$ such that

$$u(t) = M(u) = \rho - \int_S \rho f_\mu(t, p, r) \geq 0.$$ 

The proof of theorem 3.2 is achieved.

4. Numerical approximation

4.1. A conservative truncated formulation

The discretization of the problem \eqref{eq:3}–\eqref{eq:4} gives rise to three main difficulties. First, the space is not bounded. Indeed, one of the two variables has been reduced to the interval $(0, 1)$, with a physical meaning, but the $p$-variable can reach any size in $\mathbb{R}_+$. Thus, we decide to proceed as in \cite{2}, we truncate the problem considering a ‘maximal reachable size’, or cut-off, $P > 0$. The
link between both problems, truncated and full, when $P \to +\infty$ is not taken in consideration here. The reader can refer to step 2 in the proof of proposition 3.4 to get some hints related to this topic. The purpose is to provide a converging numerical approximation of a truncated problem for a fixed $P$. The next issue arises when we look at conservations in the system. In [2], the authors propose a reformulation of the coagulation operator into a divergence form. We are inspired by this method and adapt it to our problem. Indeed, this formulation appears natural for finite volume scheme and has the advantage of providing exact conservations at the discrete level.

The starting point is the weak formulation of $Q$, see (31). One can take $\varphi(u, v) = u_{1,0,p}(u)1_{0,r,f}(v)$ for some $(p, r) \in \mathcal{S}$ and we formally get an expression of the form

$$\frac{\partial C}{\partial \rho \partial r} = pQ(f, f)$$

where the coagulation reads now

$$C(f, f) (p, r) = \int_0^p \int_0^{u_0} \int_0^{v_0} \int_0^{v_0} u_{a}(u, v; u', v')1_{0,0}(v) f(u, v)f(u', v') \, dv' \, du' \, du
- \int_0^p \int_0^{v_0} u_{L}(f)(u, v)f(u, v) \, dv, \quad \text{(37)}$$

where $v^\# = (uv + u'v')(u + u')$. Now the coagulation operator has been reformulated so that it might be discretized by finite volume quite easily. It remains to truncate the problem. It can be achieved in two different ways as mentioned in [2, 18], where the authors discuss conservative and non-conservative forms. These two options can be derived respectively by taking $a := a_{1,0,p}(u + u')$ or $a := a_{1,0,p}(u)1_{0,0}(u')$. The first option avoids the formation of clusters larger than $P$, it preserves the mass, while the second induces a loss of polymers due to the creation of larger polymers than $P$. This latter is convenient for studying gelation phenomena, see [14] for a review on coagulation. Here, we restrict ourselves to the conservative form and obtain the truncated operator by taking

$$L_{p}(f)(u, v) = \int_0^p \int_0^{v_0} a(u', v'; u, v)f(u', v') \, dv' \, du'.$$

Then, replacing $L$ by $L_{p}$ in (37) it yields, for any $(p, r) \in \mathcal{S}_{p} := (0, P) \times (0, 1)$, to

$$C_{p}(f, f) (p, r) = \int_0^p \int_0^{v_0} \int_0^{v_0} u_{a}(u, v; u', v')1_{0,0}(v) f(u, v)f(u', v') \, dv' \, du' \, du
- \int_0^p \int_0^{v_0} u_{L_{p}}(f)(u, v)f(u, v) \, dv, \quad \text{(38)}$$

The last main issue lies in the discretization of (4), i.e. the algebraic constraint driving $u$. We cannot properly derive an approximation of $1_{0,r,f}(v^\#)$ in the coagulation operator which would allow us to control the sign of $\rho - \int_{\mathcal{S}} \eta f(t, p, r) \, drdp$. Once again, we reformulate this constraint obtaining an evolution equation on $u$ by a time derivation of it. Thus, problem (3)–(4) now reads

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}(Vf) = \frac{\partial C_{p}(f, f)}{\partial \rho \partial r}, \quad (t, p, r) \in \mathbb{R}_+ \times \mathcal{S}_p, \quad \text{(39)}$$
and
\[
\frac{d}{dt} u(t) = - \int_S \int_S V(u(t), p, r) f(t, p, r) \, dr \, dp, \quad t \geq 0. \tag{40}
\]
The boundary condition now reads
\[
f = 0, \quad \text{on } \partial S_p, \tag{41}
\]
and the initial data are
\[
f(t = 0, \cdot) = f^{in} \text{ over } S_p \text{ and } u(t = 0) = u^{in}. \tag{42}
\]
We now introduce the technical assumptions used through this section:

**H1'.** The initial distribution \(f^{in} \in L^1(S_p)\) is nonnegative with \(\partial f^{in} \in L^1(S_p)\) and \(u^{in} \geq 0\), with
\[
\rho := u^{in} + \int_S \int_S rf^{in}(p, r) \, dr \, dp < +\infty. \tag{43}
\]

**H2'.** The coagulation rate \(a \in L^\infty(S_p \times S_p)\) is nonnegative and
\[
\|a\|_{L^\infty} \leq K. \tag{44}
\]

**H3'.** The rate functions \(p \mapsto k(p, \cdot), l(p, \cdot) \in L^\infty(0, P; W^2,\infty(0, 1))\) are nonnegative and for all \(p \in (0, P)\)
\[
\|k(p, \cdot)\|_{W^{2,\infty}} + \|l(0, \cdot)\|_{W^{2,\infty}} \leq Kp. \tag{45}
\]

**H4'.** The function \(r \mapsto V(u, p, r)\) is a non-increasing function:
\[
\partial_r V(u, p, r) = \partial_r k u - \partial_r l \leq 0 \quad \text{a.e. } (u, p, r) \in \mathbb{R}_+ \times S_p. \tag{46}
\]

**Remark 4.1.** We emphasize that hypotheses H2' and H3' are not so restrictive in front of the truncation, and could allow a locally bounded rate on the full configuration space \(S\).

We are now in a position to give an alternative definition to our problem (15)–(16).

**Definition 4.1 (Weak solutions 2).** Let \(T > 0\), a cut-off \(P > 0\) and let \(f^{in}\) and \(u^{in}\) satisfy (H1'). A weak solution to (39)–(40) on \([0, T)\) is a couple \((f, u)\) of nonnegative functions, such that
\[
f \in C([0, T); L^1(S_p)) \text{ and } u \in C([0, T)) \tag{47}
\]
satisfying for all \(t \in [0, T)\) and \(\varphi \in C^2(S_p)\)
\[
\int_S \int_S pf(t, p, r) \varphi(p, r) \, dr \, dp = \int_S \int_S pf^{in}(p, r) \varphi(p, r) \, dr \, dp \\
+ \int_0^t \int_S \left( V(u(s), p, r) f(s, p, r) \frac{\partial \varphi}{\partial r}(p, r) + C_p(s, p, r) \frac{\partial \varphi}{\partial dr}(s, p, r) \right) \, dr \, ds \\
- \int_0^t \int_0^r C_p(s, P, r) \frac{\partial \varphi}{\partial r}(s, p, r) \, dr \, ds - \int_0^t \int_0^p C_p(s, r, 1) \frac{\partial \varphi}{\partial p}(s, p, 1) \, dp \, ds, \tag{48}
\]
with
\[
u(t) = u^{in} - \int_0^t \int_S V(u(s), p, r) f(s, p, r) \, dr \, dp \, ds. \tag{49}
\]
Remark 4.2 (Consistence of definition 4.1) First, we emphasize that weak formulation (48) is classically obtained after multiplying (39) by \( p \), then integrating over \( (0, t) \times S_p \). An integration with parts with respect to the boundary conditions (41). Note that the last two integrals in the right-hand side correspond to the remaining terms coming from the integration of the coagulation. Next, the regularity (47) of \( f \) together with the definition of the coagulation operator (38) provide that for any \( u \in (0, t) \times S_p \), we have
\[
\sup_{u(t) \in (0, t)} \| \nabla u \|_{L^\infty(S_p)} \leq \| k \|_{L^\infty(S_p)} U + \| l \|_{L^\infty(S_p)} \leq KP(U + 1).
\]
Thus, \( V \in L^\infty((0, t) \times S_p) \). We ensure, under such regularity and hypotheses, that equations (48)–(49) are well defined.

Remark 4.3. A solution in the sense of definition 4.1 being regular enough, with an initial datum compactly supported in \((0, P)\), is also a solution in the sense of definition 3.1, i.e. on the entire space \( S \), at least up to a time \( T \) small enough. Indeed, since \( Q \) is Lipschitz by (30), the speed of propagation of the support of \( f \) is finite.

Remark 4.4. In general, the definition can be relaxed by taking the solution \( f \) in \( C((0, T); w - L^1(S_p, pdrdp)) \) which is sufficient to define the formulation (48). Nevertheless, we will see that the sequence of approximation is in fact equicontinuous for the strong topology of \( L^1(S_p) \), thus, definition 4.1 remains stronger, but true.

4.2. The numerical scheme and convergence statement

This section is devoted to introducing an approximation of the truncated problem presented in section 4.1. Thus in the remainder of this section, both the truncation parameter \( P > 0 \) and the time parameter \( T > 0 \) are fixed. Our aim is to provide a discretization of \([0, T] \times S_p\) on which we will approach the problem (39)–(40). Once the scheme is established, we present the main result, namely the convergence in a sense defined later.

Formulation (39) allows us to use a finite volume method for the configuration space. We approach the average of the solution on volume controls at discrete times \( t_n \) for \( \{n \in \mathbb{N} \} \) such that
\[
t_n = n \Delta t \quad \text{with} \quad \Delta t = T/N \quad \text{and} \quad N \in \mathbb{N}^*.
\]
We turn now to the discretization of the configuration space \( S_p \). For the sake of simplicity, we consider a uniform mesh of \( S_p \) that is given, for some large integer \( J \) and \( I \), by \((A_{j,i})_{i<j} \in (0, J + 1) \times (0, I + 1)\) where
\[
A_{j,i} = (p_{j-1/2}, p_{j+1/2}) \times (r_{i-1/2}, r_{i+1/2}) \subset S_p,
\]
such that \((p_{j-1/2}) \in [0, J + 1] \) and \((r_{i-1/2}) \in [0, I + 1] \) are given by
\[
p_{j-1/2} = j \Delta p \quad \text{and} \quad r_{i-1/2} = i \Delta r,
\]
with \( \Delta p = P/(J + 1) < 1 \) and \( \Delta r = 1/(I + 1) \).

Remark 4.5. We believe that a non-uniform mesh would work too, we refer for instance to [2, 19] for a non-uniform discretization of the so-called coagulation–fragmentation equation.
The average of the solution \( f \) to (39) at a time \( t_{n+1} \) on a cell \( \Lambda_{j,i} \) is obtained by integration of (39) over \([t_n, t_{n+1}) \times \Lambda_{j,i}\) and dividing by the volume of the cell \( |\Lambda_{j,i}| = \Delta p \Delta r \). We aim at deriving an induction, in order to obtain an approximation of this average at time \( t_{n+1} \), knowing the approximation at time \( t_n \) given by

\[
f_{j,i}^n \approx \frac{1}{|\Lambda_{j,i}|} \int_{t_n} f(t_n, p, r) \, dr \, dp.
\]

The integration of (39) emphasizes two types of fluxes which need to be approximated. First, the transport term that accounts for the association-dissociation phenomenon given by the \( r \)-derivative, leads to the numerical fluxes \( F_{j,i}^n \) given by (50), consistent approximation of:

\[
F_{j,i}^n \approx \frac{1}{\Delta p} \int_{t_n} \int_{p_{n-1/2}}^{p_{n+1/2}} \mathcal{V}(u(t), p, n) f(t, p, n) \, dr \, dp.
\]

We will use a Euler explicit scheme in time \( t \). Moreover, we use the so-called first order upwind method to get

\[
F_{j,i}^n = \mathcal{V}_{j,i}^{n+1/2} f_{j,i}^{n+1} - \mathcal{V}_{j,i}^{n-1/2} f_{j,i}^{n},
\]

where the velocity at the interface, in function of \( u^n \approx u(t_n) \), is given by

\[
\mathcal{V}_{j,i}^{n+1/2} = \mathcal{V}(u^n, p_j - 1/2, n - 1/2),
\]

and using the notation \( x^+ = \max(x, 0) \) and \( x^- = \max(-x, 0) \) for any \( x \in \mathbb{R} \). The boundary is conventionally taken, for any \( j \in \{0, \ldots, J\} \), by

\[
F_{j,0}^n = F_{J,j}^n = 0,
\]

which agrees with (41) and is consistent with the approximation (50). Then, the fluxes of coagulation given by the second order derivative are also approached by a Euler explicit method in time, namely our fluxes read

\[
C_{j-1/2,i-1/2}^n = \sum_{j'=0}^{j-1} \sum_{r'=0}^{r-1} \int_{p_j - 1/2}^{p_j + 1/2} \int_{p_r - 1/2}^{p_r + 1/2} p_{j'} a_{j',j; r',r} \delta_{j,j'}^{r,r} f_{j',j}^{n+1/2} f_{j',j'}^{n+1/2} (\Delta p \Delta r)^2 \, dp \, dr - \sum_{j'=0}^{j-1} \sum_{r'=0}^{r-1} \int_{p_j - 1/2}^{p_j + 1/2} \int_{p_r - 1/2}^{p_r + 1/2} p_{j'} a_{j',j; r',r} \delta_{j,j'}^{r,r} f_{j',j}^{n-1/2} f_{j',j'}^{n-1/2} (\Delta p \Delta r)^2,
\]

where the discrete coagulation rate is

\[
a_{j,i;j',i'} = \frac{1}{|\Lambda_{j,i}| \times |\Lambda_{j',i'}|} \int_{\Lambda_{j,i} \times \Lambda_{j',i'}} a(p, r; p', r') \, dp \, dr \, dp' \, dr',
\]

and the characteristic function \( \mathbf{1}_{(0,\rho)}(\nu^\#) \) is approximated by

\[
\delta_{j,j',r,r'}^{r-1/2} = \begin{cases} 
1 & \text{if } \nu^\#_{j,j',r,r'} = \frac{p_{j+1/2} f_{j+1/2} + p_{j+1/2} f_{j+1/2}}{p_{j+1/2} + p_{j+1/2}} < r_{j+1/2} \\
0 & \text{otherwise.}
\end{cases}
\]

Finally, we use the convention that

\[
C_{-1/2,i-1/2}^n = C_{j-1/2,i-1/2}^n = 0, \quad \forall (j, i),
\]
which is consistent with the fact that $C_p(t, 0, r) = C_p(t, p, 0) = 0$ by definition of $C_p$ in (38).

Now, we are almost ready to define the scheme. Indeed, it remains to approximate the initial data $(42)$ which are classically obtained, for $(j, i) \in \{0, \ldots, J\} \times \{0, \ldots, I\}$, by

$$f_{j, i}^0 = \frac{1}{|\Lambda_{j, i}|} \int_{\Lambda_{j, i}} f^{\text{in}}(p, r) \, dp,$$

and we fix

$$u^0 = u^{\text{in}}.$$

Thus, the scheme is defined as follows.

**Definition 4.2 (Numerical scheme).** Let us consider the discretization mentioned above and a given initial data $(57)$–(58). The numerical scheme gives us a sequence $(f^n_{j, i})_{n, j, i}$ and $(u^n)_n$, for $n \in \{0, \ldots, N\}$ and $(j, i) \in \{0, \ldots, J\} \times \{0, \ldots, I\}$, defined recursively by

$$p_j f_{j, i}^{n+1} = p_j f_{j, i}^n - \frac{\Delta t}{\Delta r} (F^n_{j+1/2} - F^n_{j-1/2}) + \frac{\Delta t}{\Delta r} \Delta p C^n_{j, i},$$

and

$$u^{n+1} = u^n - \Delta t \sum_{j=0}^{J} \sum_{i=0}^{I} F^n_{j, i} \Delta r \Delta p.$$

where

$$C^n_{j, i} = (C^n_{j+1/2, i+1/2} - C^n_{j+1/2, i-1/2}) - (C^n_{j-1/2, i+1/2} - C^n_{j-1/2, i-1/2}).$$

In the above definition, the coagulation is written with fluxes defined by (53). But, it can be also expressed as follows

$$C^n_{j, i} = \sum_{j'=0}^{J} \sum_{i'=0}^{I} \sum_{j''=0}^{J} \sum_{i''=0}^{I} p_{j'} a_{j', j''} f_{j', i'} f_{j'', i''} \delta_{j', j''} (\Delta p \Delta r)^2,$$

where

$$\delta_{j', j''} = \begin{cases} 1 & \text{if } r_{j''} \leq V_{j', j''} < r_{j''+1/2} \\ 0 & \text{otherwise.} \end{cases}$$

This expression is obtained when reordering the summation behind (61). Such a formulation is not only simpler to implement numerically but also useful to obtain several estimates in the next section. We also remark, by virtue of (56) and (61), that the coagulation satisfies

$$\sum_{j=0}^{J} \sum_{i=0}^{I} C^n_{j, i} = 0, \quad \forall n \in \{0, \ldots, N\},$$

which ensures mass conservation at the discrete level.

Now the scheme is stated, we focus on the convergence. This will be achieved by a suitable construction of sequences of approximations. For this purpose, we let $h = \max(\Delta r, \Delta p, \Delta t)$.
Definition 4.3 (Sequences of approximations). Let the sequences \((f^n_{j,i})_{n,j,i}\) and \((u^n)_{n}\) be constructed by virtue of definition 4.2. We define the piecewise constant approximation \(f_h\) on \([0,T)\times S_p\) by

\[
f_h(t, p, r) = \sum_{n=0}^{N-1} \sum_{j=0}^{J} \sum_{i=0}^{I} f^n_{j,i} 1_{A_j}(p, r) 1_{[n, n+1)}(t),
\]

and then the piecewise linear (in time) approximation \(\tilde{f}_h\)

\[
\tilde{f}_h(t, p, r) = \sum_{n=0}^{N-1} \sum_{j=0}^{J} \sum_{i=0}^{I} \left( \frac{f^n_{j,i+1} - f^n_{j,i}}{\Delta t} (t - t_n) + f^n_{j,i} \right) \times 1_{A_j}(p, r) 1_{[n, n+1)}(t).
\]

Moreover, we define the piecewise approximation of \(u\) on \([0, T)\)

\[
u_h(t) = \sum_{n=0}^{N-1} u^n 1_{[n, n+1)}(t), \quad \text{on } [0, T).
\]

Here, we mention that under such a definition both approximations satisfy at time \(t = 0\) the same initial condition that is given by

\[
\left( \begin{array}{c}
fp \\
rp \\
1
\end{array} \right) = \left( \begin{array}{c}
0 \\
f_{0} \\
0
\end{array} \right) \text{ on } S_p,
\]

and that \(u_0(0) = u^0\). We are now ready to state the convergence result we obtain.

Theorem 4.4 (Convergence). Let \(T > 0\), assume that \(f^m\) and \(u^m\) satisfy \((H1')\), and that hypotheses \((H2')\) to \((H4')\) are fulfilled. Moreover, we make the stability assumption that

\[
4 \frac{\Delta t}{\Delta x} \| \mathcal{V} \|_{L^{\infty}(0,T) \times S_p} < 1 \text{ and } 2KM^m(1 + P)\Delta t < 1,
\]

where

\[
K = e^{KM^m}u^m \text{ and } M^m = \int_{S_p} f^m(p, r) \, dp.
\]

Then there exists a couple \((f, u)\) solution to the problem \((39)-(40)\) in the sense of definition 4.1 such that, up to a subsequence (not relabelled)

\[
f_h \rightharpoonup_{h \to 0} f, \quad \text{ and } \quad w \in L^1([0,T) \times S_p),
\]

\[
\tilde{f}_h \rightharpoonup_{h \to 0} f, \quad \text{ and } \quad C([0,T]; w \in L^1(S_p)),
\]

\[
u_h \rightharpoonup_{h \to 0} u, \quad \forall t \in [0,T].
\]

Remark 4.6. At this stage, we emphasize that hypothesis \((68)\) in theorem 4.4 is classical. The first one is the so-called Courant–Friedrich–Lax condition (or CFL condition) which
ensures a well-known convex formulation of the transport part. The second is to control the sign of the coagulation term.

For technical reasons, we consider a careful reconstruction of the coagulation term. This one involves the coagulation kernel that is approached by

$$a_h(p, r; p', r') = \sum_{j=0}^{J} \sum_{i=0}^{I} \sum_{j'=0}^{J} \sum_{i'=0}^{I} a_{j, i, j', i'} 1_{\mathcal{H}_j}(p, r) 1_{\mathcal{H}_{j'}}(p', r').$$

where the $a_{j, i, j', i'}$ are given by (54). Since $a$ satisfies (44), a classical result of piecewise approximation is

$$a_h \rightarrow a, \quad L^1(S_0).$$

Further, we mention that $a_h$ converges towards $a$ a.e. $S_0 \times S_0$, which holds true up to a subsequence. Also, we will reconstruct the characteristic function (55), this delicate point, responsible for a lack of conservation in our scheme, will be discussed later, as well as the rate $V$.

**Remark 4.7.** In the remainder of the paper, most of the results will involve more extraction of sequences, so that, for the sake of clarity, we use the same index for all the subsequences we extract.

### 4.3. Estimations and weak compactness

The aim of this section is to introduce the well-suited estimates leading to the required compactness to prove theorem 4.4. The method used here has been extensively developed in the field of coagulation–fragmentation equations and/or the LS equation and their derivatives, see section 1.3 for more details. Briefly, here we proceed in two steps. We provide some discrete properties of the scheme. Then, we establish compactness results on both $f_h$ and $\tilde{f}_h$ and we treat $u_h$ by classical results on sequences of bounded variation functions.

First, we introduce here some useful notations that will help us shed light on the following computations:

$$P_h(p) = \sum_{j=0}^{J} p_j 1_{[\rho_{j-1/2}; \rho_{j+1/2})}, \quad R_h(r) = \sum_{i=0}^{I} r_i 1_{[\rho_{i-1/2}; \rho_{i+1/2})},$$

$$P_h^\pm(p) = \sum_{j=0}^{J} p_j 1_{[\rho_{j-1/2}; \rho_{j+1/2})}, \quad R_h^\pm(r) = \sum_{i=0}^{I} r_i 1_{[\rho_{i-1/2}; \rho_{i+1/2})},$$

and

$$\Theta_\Delta(t) = \sum_{n=0}^{N-1} t_n 1_{(t_n, t_{n+1}]}(t).$$

Moreover, for the sake of conciseness we denote $\sigma := \{0, \ldots, J\} \times \{0, \ldots, I\}$, when no confusion on $I$ and $J$ holds. Then, as long as it does not entail any ambiguity, we use

$$\sigma^* = \{0, \ldots, J-j\} \times \{0, \ldots, I\} \text{ if indexed on } (j', i'),$$

$$\sigma^{**} = \{0, \ldots, J-j'\} \times \{0, \ldots, I\} \text{ if indexed on } (j'', i'').$$

Also, we denote $l = (j, i)$, $l' = (j', i')$ and $l'' = (j'', i'')$. Thus, the summation notation in a compact form is
4.3.1. Discrete estimations. To begin, we establish some properties of the sequences constructed in definition 4.2. We emphasize that the original continuous problem involves a decrease of the moment of order 0 (32), while the p-moment of order 1 (33) is conserved and the total balance (4) remains constant. This latter will be discussed later while the two other remain true at the discrete level and will be part of the next proposition. To that, we introduce the discrete moments of the sequences defined in definition (4.2), given by

\[ M^n_{0,h} = \sum_{i \in \sigma} f^n_{i,j} \Delta r \Delta p, \quad \text{and} \quad M^n_{1,h} = \sum_{i \in \sigma} p f^n_{i,j} \Delta r \Delta p. \]  

So, the next proposition establishes the basic properties of our scheme and particularly of these moments.

**Proposition 4.5 (Nonnegativeness, moments and conservation).** Let \( f^{in} \) and \( u^{in} \) satisfy (H1'), together with \( (f^n_{i,j}, u^n_{i,j})_{i,j \in \sigma} \) and \( (u^n)_{h} \) construct by virtue of definition 4.2. We assume that the stability condition (68) holds true. Then, the sequences \( (f^n_{i,j})_{i,j} \) and \( (u^n)_{h} \) are both nonnegative and satisfy for all \( n \in \{0, \ldots, N-1\} \):

\[ 0 \leq M^n_{0,h} \leq M^n_{1,h} \leq M^{in}, \]

and \( n \in \{0, \ldots, N\} \)

\[ 0 \leq M^n_{1,h} = M^n_{1,h} \quad \text{and} \quad 0 \leq u^n \leq U_T, \]

where \( M^{in} \) and \( U_T \) are both given in (69). Moreover, there exists a constant \( C > 0 \) independent on \( h \) such that for all \( n \in \{0, \ldots, N-1\} \) we have

\[ \sum_{i \in \sigma} |f^n_{i,j} - f^{n+1}_{i,j}| \Delta r \Delta p \leq C \Delta t \quad \text{and} \quad |u^{n+1} - u^n| \leq C \Delta t. \]

**Proof.** We prove this proposition by induction. We suppose that \( (f^n_{i,j})_{i,j} \) is a nonnegative sequence and \( u^{n} \) a nonnegative datum, both given for some \( n \in \{0, \ldots, N-1\} \) satisfying

\[ 0 \leq M^n_{0,h} \leq M^{in}, \quad \text{and} \quad u^n \leq (1 + \Delta t K M^{in}) u^{n-1}. \]

We easily check it for \( n = 0 \). Indeed, the nonnegativity is given by hypothesis (H1) on \( f^{in} \) and \( u^{in} \) together with the initial approximation (57)–(58). Then, by the definitions of \( f^{in}_{h} \) in (67) and the constant \( M^{in} \) in (69), we get

\[ M^n_{0,h} = \int_{S_p} f^{in}_{h}(p, r) \, dr \, dp = M^{in}, \]  

(74)

and

\[ M^n_{1,h} = \int_{S_p} P_{h}(p) f^{in}_{h}(p, r) \, dr \, dp \leq PM^{in}. \]  

(75)
The rest of the proof is separated into four steps. We start by estimating the moments, next we bound \( u_{n+1} \), then we prove the nonnegativity of \( f_{n+1} \) and finally we prove the last two ‘time’ estimations of the proposition.

**Step 1. Moments estimation.** We first remark that the fluxes \( F_n \) are null at the boundary by (52), thus
\[
\sum_{j=0}^{l} (F_{j+1/2}^n - F_{j-1/2}^n) = 0, \quad \forall j.
\]
It remains to estimate the contribution of the coagulation in the moments. Next, we remark that the first order moment is naturally conserved from the construction of our scheme by (63). These two remarks lead, by equation (59) giving the \( f_{ji}^n \), to the fact that
\[
M_{1,h}^n = M_{1,h}^0.
\]

Now, for the zeroth order moment. We remark that \( p_j/p_{j+1} - 1 \leq 0 \) and by nonnegativity of \( (f_{ji}^n)_{i,j} \), together with its symmetry, we get
\[
\sum_{i \in \sigma} \frac{1}{p_j} C_{j,i} = \sum_{i \in \sigma} \sum_{f \in \sigma^f} \frac{p_j}{p_{j'}} a_{j,i,f'} f_{ji}^n f_{j'i'}^n (\Delta p \Delta r)^2
\begin{align*}
&- \sum_{i \in \sigma} \sum_{f \in \sigma^f} a_{j,i,f'} f_{ji}^n f_{j'i'}^n (\Delta p \Delta r)^2 \leq 0,
\end{align*}
where the equality is obtained from expression (62) after inverting and re-indexing the summation. It proves that the discrete zeroth order moment decreased, which is the desired property.

**Step 2. Properties of \( u_{n+1} \).** By definition of the fluxes \( F_n \) in (51), the nonnegativity of \( (f_{ji}^n)_{i,j} \) and hypothesis (H3') on the rate \( V \), we get that
\[
F_{j,1/2}^n - F_{j,1/2}^{n-1} \leq V_{j,1/2}^n f_{j,1}^n \leq Ku^n f_{j,1}^n f_{j,1}^n.
\]
which implies by the expression of \( u_{n+1} \) in (60) and since we assumed that \( M_{0,h}^n \geq 0 \) is bounded by \( M^0 \), we get
\[
u_n^{u+1} \geq (1 - K \Delta t \sum_{i \in \sigma} f_{ji}^n \Delta p \Delta r) u_n \geq (1 - K M^0 \Delta t) u_n.
\]
This latter entails the nonnegativeness of \( u_{n+1} \) by the stability assumption (68). It remains to prove that \( u_{n+1} \) is bounded. Indeed, we have
\[
u_n^{u+1} \leq u_n + \Delta t \sum_{i \in \sigma} V_{j,1/2}^n f_{ji}^n \Delta p \Delta r \leq (1 + \Delta t K M^0) u_n.
\]

**Step 3. Nonnegativity of \( f_{n+1} \).** We prove this result by studying separately the transport part and the coagulation part. On the one hand, using the definition of the fluxes \( F_n \) in (51) and since we have \( V_{j,1/2}^n = V_{j,1/2}^n - V_{j,1/2}^n \), we get the following decomposition
\[
F_{j,1/2}^n = F_{j,1/2}^n + (V_{j,1/2}^n - V_{j,1/2}^n) f_{ji}^n
\begin{align*}
&+ V_{j,1/2}^n (f_{ji}^n - f_{ji}^{n+1}) + V_{j,1/2}^n (f_{ji}^n - f_{ji}^{n-1}).
\end{align*}
(76)
Now, we denote by

$$A_{j,i}^n = \frac{1}{\Delta r} \int_{\rho_{j,i}^{n-1/2}}^{\rho_{j,i}^{n+1/2}} \left( -\frac{\partial}{\partial r} \mathcal{V}(u^m, p_{j,i-1/2}, r) \right) dr = \frac{\mathcal{V}_{j,i-1/2}^{n} - \mathcal{V}_{j,i+1/2}^{n}}{\Delta r},$$

(77)

which is nonnegative for any \((j,i) \in \sigma\) by the monotonicity hypothesis \((H4')\). It results from the formulation (76) that

$$\frac{1}{2} f_{j,i}^n - \frac{\Delta t}{\Delta r} (F_{j,i+1/2}^n - F_{j,i-1/2}^n) = \Delta t A_{j,i}^n f_{j,i}^n$$

$$+ \frac{1}{4} \left[ 1 - 4 \frac{\Delta t}{\Delta r} \mathcal{V}_{j,i+1/2}^{n-1} \right] f_{j,i}^n + \frac{4 \Delta t}{\Delta r} \mathcal{V}_{j,i+1/2}^{n} f_{j,i+1}^n$$

$$+ \frac{1}{4} \left[ 1 - 4 \frac{\Delta t}{\Delta r} \mathcal{V}_{j,i-1/2}^{n+1} \right] f_{j,i}^n + \frac{4 \Delta t}{\Delta r} \mathcal{V}_{j,i-1/2}^{n} f_{j,i-1}^n.$$ 

(78)

Thus, from the nonnegativity of the \(A_{j,i}^n\) in (77) and the convex combination of the nonnegative \(f_{j,i}^n\) we get

$$\frac{1}{2} f_{j,i}^n - \frac{\Delta t}{\Delta r} (F_{j,i+1/2}^n - F_{j,i-1/2}^n) \geq 0.$$

(79)

Thanks to the definition of \(f_{j,i}^{n+1}\) in (59), and using (79) we obtain

$$f_{j,i}^{n+1} \geq \frac{1}{2} f_{j,i}^n + \frac{\Delta t}{\Delta r \Delta p} \frac{1}{p_j} C_{j,i}^n.$$

Note, in the definition of \(C_{j,i}^n\) we keep only the negative term to get the following estimate

$$f_{j,i}^{n+1} \geq \left( \frac{1}{2} - \Delta t \sum_{j' < j} \sum_{r=0}^{l} a_{j,i,j',r} f_{j',i}^n \Delta p \Delta r \right) f_{j,i}^n \geq \frac{1}{2} \left( 1 - 2K \Delta M^{m} \right) f_{j,i}^n \geq 0.$$

wherein the two last inequalities we used the hypothesis \((H2')\) on the coagulation kernel, the stability assumption (68) and (74).

**Step 4. Time estimation.** From the definition of \(f_{j,i}^{n+1}\) in (59), we easily obtain

$$|f_{j,i}^{n+1} - f_{j,i}^n| \Delta r \Delta p \leq \Delta t \frac{|F_{j,i+1/2}^n - F_{j,i-1/2}^n|}{p_j \Delta r} \Delta p \Delta r + \Delta t \frac{1}{p_j} |C_{j,i}^n|.$$

On the one hand, we have from the definition of the discrete coagulation in (62) and hypothesis \((H1')\) that

$$\sum_{(j,i) \in \sigma} \frac{1}{p_j} |C_{j,i}^n| \Delta r \Delta p \leq 2K M^{m/2}.$$

(80)

On the other hand, thanks to the \(r\)-derivative of \(f^m\) and both hypotheses \((H2'–H3')\) we obtain a classical BV estimation in the \(r\) variable. Indeed, for some constant \(C(T,f^m,K) > 0\) independent on \(n\),

$$\sum_{j=0}^{l} \sum_{i=0}^{l-1} \frac{|f_{j,i+1}^n - f_{j,i}^n|}{p_j \Delta r} \Delta r \Delta p \leq C.$$
Thus, by (76) up to change of the constant $C > 0$, we obtain

$$
\sum_{(j,i) \in \sigma} \frac{|F_{j,i}^n - F_{j,i}^{n-1/2}|}{p_j \Delta r} \Delta r \Delta p \leq C.
$$

(81)

Thus, by (80) and (81), we prove the first required time estimate. Finally, we remark that from the expression of $u^{n+1}$ in (60) we have to find a bound on the fluxes (51). Indeed, we have for any $(j,i) \in \sigma$ and $i \neq 0$

$$
|F_{j,i}^{n-1/2}| \leq \sup_{u \in (0,U_T)} \|\nabla u(\cdot, \cdot)\|_{L^\infty(S_p)} (f_{j,i}^n + f_{j,i}^n),
$$

and then summing over $\sigma$ we get

$$
|u^{n+1} - u^n| \leq 2 \sup_{u \in (0,U_T)} \|\nabla u(\cdot, \cdot)\|_{L^\infty(S_p)} M \Delta t.
$$

This ends the proof.

This proposition establishes the main properties of our scheme, we now derive a corollary that transposes these properties to the sequences of approximations.

**Corollary 4.6.** Under hypothesis of proposition 4.5. Let the sequences of approximations $(f_h)_h$, $(\tilde{f}_h)_h$ and $(u_h)_h$ construct by definition 4.3. Then, for all discretization parameter $h$, $f_h \in L^\infty(0,T;L^1(S_p))$ and $\tilde{f}_h \in C([0,T];L^1(S_p))$

together with $u_h \in L^\infty(0,T)$. Moreover, we have for the sequence $(f_h)_h$ the uniform estimate

$$
\int \int_{S_p} f_h(t,r,p) \, dr \, dp \leq \int \int_{S_p} f_h(s,r,p) \, dr \, dp \leq M^n, \quad \forall t \geq s,
$$

(82)

and

$$
\int \int_{S_p} P(a(p)f_h(t,r,p) \, dr \, dp = \int \int_{S_p} P(a(p)f_h^{in}(r,p) \, dr \, dp, \quad \forall t \in [0,T].
$$

(83)

For the sequence $(\tilde{f}_h)_h$, we have

$$
0 \leq \int \int_{S_p} \tilde{f}_h(t,r,p) \, dr \, dp \leq M^n, \quad \forall t \in [0,T],
$$

(84)

and there exists a constant $C > 0$ independent on $h$ such that

$$
\left\|\tilde{f}_h(t, \cdot) - \tilde{f}_h(s, \cdot)\right\|_{L^\infty(S_p)} \leq C|t - s|, \quad \forall s,t \in [0,T].
$$

(85)

Finally, the sequence $(u_h)_h$ satisfies the uniform bound

$$
\|u_h\|_{L^\infty(0,T)} \leq U_T, \quad \text{and} \quad \|u_h\|_{BV(0,T)} < C T.
$$

(86)

**Proof.** The regularity and nonnegativity of the sequences $(f_h)_h$ and $(u_h)_h$ follow from proposition 4.5 and definition 4.3. And, by the same arguments, it is clear that $\tilde{f}_h \in L^\infty(0,T;L^1(S_p))$. Next, (82) and (83) follow from the properties of the discrete moment in proposition 4.5, by a simple reformulation using the definition of $f_h$ in (64). Then, for all $n \in \{0, \ldots, N-1\}$ and $t \in [t_n, t_{n+1}].$
\[
\frac{f_{j,i}^{n+1} - f_{j,i}^n}{\Delta t} = (t - t_n) f_{j,i}^n + \left(1 - \frac{(t - t_n)}{\Delta t}\right)f_{j,i}^n.
\] (87)

Thus, by definition of \( \tilde{f}_h \) in (65), the discrete moment (73) and the convex combination mentioned above, we have for all \( t \in [0, T] \):

\[
0 \leq \int \int S(r, t, P) \, dr \, dp \leq \sup_{n \in [0,\ldots,N-1]} \max(M_{0,h}^{n+1}, M_{0,h}^n) \leq M^\text{in}.
\]

and that \( \tilde{f}_h \) are nonnegative. This provides the uniform bound (84). Next, estimate (85) is again a direct consequence of proposition 4.5 (last estimation). It provides the regularity in time of the sequence \( \tilde{f}_h \). Finally, (86) is a consequence of proposition 4.5 and the definition of \( u_h \) in (66).

\[\square\]

**Remark 4.8.** Before coming back to the proof of theorem 4.4, we emphasize the fact that, as mentioned before, our scheme preserves the mass (83). Nevertheless, the algebraic condition (4), transformed into (40) is no more preserved at the discrete level. The following corollary is not used in the demonstration of the convergence, but only states that the lack of mass occurring in our scheme is controlled. Indeed, the deviation from the initial value is of magnitude \( \Delta r \).

**Corollary 4.7.** Under hypotheses of proposition 4.5, for any \( n \in \{0, \ldots, N\} \) we define

\[
\rho^n := u^n + \sum_{(j,i) \in \sigma} r_i \rho_j \rho_{j,i},
\]

then we have for some constant \( C = C(M^\text{in}, K) \geq 0 \) that

\[
|\rho^n - \rho^0| \leq CT \Delta r.
\]

**Proof.** We remark that summing (59) tested against \( r_i \) and with (60), we get

\[
\rho^{n+1} - \rho^n = \Delta t \sum_{(j,i) \in \sigma} r_i C_{j,i}^n.
\]

Then by (61), we obtain

\[
\sum_{(j,i) \in \sigma} r_i C_{j,i}^n = \sum_{i=0}^{l} C_{i+1/2,j+1/2}^\Delta \Delta r.
\]

Combining these two equalities and by definition of the flux (53) and the bound \( M^\text{in} \) in (69), we get

\[
|\rho^{n+1} - \rho^n| \leq 2KP M^{m^2} \Delta r \Delta t,
\]

which ends the proof.

\[\square\]

**4.3.2. Weak compactness.** We introduced, from the scheme established in definition 4.2, a sequence of approximations in definition 4.3 satisfying the properties stated in corollary 4.6. An important issue is to prove the convergence of this sequence, in a sense that allows us to obtain enough regular solutions to (39)–(40). The answer resides in an argument of compactness. In this section, we provide the necessary compactness estimates to pass to the limit.
The first estimate will follow from a refined version of the De La Vallée-Poussin lemma [4], also we refer to [9, chapter II, theorem 22] for a probabilistic approach. Indeed, since $f^m \in L^1(S_\rho)$ is nonnegative, there exists

$$\phi \in C^1([0, +\infty))$$

nonnegative, convex, with concave derivative,

with $\phi(0) = 0$, $\phi'(0) = 0$, and $\frac{\phi(r)}{r} \to +\infty$ as $r \to +\infty$.

such that

$$\int_S \int_{S_\rho} \phi(f^m(p, r)) \, dp \, dr < +\infty.$$  \hfill (89)

Therefore, proving that (89) can be propagated in time, uniformly according to $h$, will give us the uniform integrability of the sequences $f_h$ and $\tilde{f}_h$.

**Lemma 4.8.** Let $\phi$ satisfy (88) such that (89) holds true. Then, there exists $C \geq 0$ independent on $h$, such that for any $t \in [0, T)$, we have

$$\int_S \int_{S_\rho} \phi(f_h(t, p, r)) \, dp \, dr \leq e^{CT} \int_S \phi(f^m(p, r)) \, dp.$$  \hfill (90)

and

$$\int_S \int_{S_\rho} \phi(\tilde{f}_h(t, p, r)) \, dp \, dr \leq e^{CT} \int_S \phi(f^m(p, r)) \, dp.$$  \hfill (91)

**Proof.** Let us derive first (91) from (90). By the definition of $\tilde{f}_h$ in (65), the convex combination (87), and since $\phi$ is convex by (88), we have for any $t \in [0, T]

$$\int_S \int_{S_\rho} \phi(f_h(t, p, r)) \, dp \, dr \leq \sup_{n \in \{0, \ldots, N\}} \sum_{(j, i) \in \sigma} \phi(f^n_{ji}) \Delta r \Delta p$$

$$\leq \sup_{t \in [0, T]} \int_S \phi(f_h(t, p, r)) \, dp.$$  \hfill (92)

Thus, it remains to prove (90) to conclude. We split the computation into two parts, to treat first the transport part and then the coagulation.

**Step 1. The transport.** This first part involves the convexity of $\phi$ and is closely related to the estimation done in [17, lemma 3.5]. Indeed, let us denote the intermediate value:

$$\tilde{f}^n_{ji} = f^n_{ji} - \frac{\Delta t}{\Delta r}(f^n_{ji+1/2} - F^n_{ji-1/2}).$$  \hfill (93)

From the convex formulation (78), we easily obtain for any $(j, i) \in \sigma$ the following expression

$$\tilde{f}^n_{ji} = \left(\frac{1}{2} + \Delta t A^n_{ji}\right) f^n_{ji} + \frac{1}{4}\left[\left(1 - 4 \frac{\Delta t}{\Delta r} \gamma^n_{j+1/2}\right) f^n_{ji} + 4 \frac{\Delta t}{\Delta r} \gamma^n_{j+1/2} f^n_{ji+1}\right]$$

$$+ \frac{1}{4}\left[\left(1 - 4 \frac{\Delta t}{\Delta r} \gamma^n_{j-i+1/2}\right) f^n_{ji} + 4 \frac{\Delta t}{\Delta r} \gamma^n_{j-i+1/2} f^n_{ji-1}\right]$$  \hfill (94)

with the convention $f_{j,i+1} = f_{j,-1} = 0$ and $A^n_{ji}$ the discrete gradient defined in (77). Our aim is to write $\tilde{f}^n_{ji}$ as a complete convex combination of the $f^n_{ji}$ together with 0. Thus, let us introduce the coefficients
\[ \lambda_{j,i}^0 = \frac{1}{2} + \Delta t A^0_{j,i}, \]
\[ \lambda_{j,i}^1 = \frac{1}{4} - \frac{\Delta t}{\Delta r} \nu^0_{j,i+1/2}, \]
\[ \lambda_{j,i}^2 = \frac{1}{4} - \frac{\Delta t}{\Delta r} \nu^0_{j,i+1/2}, \]
\[ \lambda_{j,i}^3 = \frac{1}{4} - \frac{\Delta t}{\Delta r} \nu^0_{j,i-1/2}, \]
\[ \lambda_{j,i}^4 = \frac{1}{4} - \frac{\Delta t}{\Delta r} \nu^0_{j,i-1/2}, \]

which are nonnegatives since \( A^0_{j,i} \geq 0 \), by monotonicity hypothesis (H4), and by stability assumption (68). Then, by virtue of hypothesis (H3) and since \( u_h \) satisfies the bound (86), we get that

\[ \| \partial_r \nu(u, p, r) \|_{L^\infty((0,T) \times \mathbb{R}_+)} = \| \partial_k k \|_{L^\infty(\mathbb{R}_+)} U_T + \| \partial_k k \|_{L^\infty(\mathbb{R}_+)} \leq K_T, \]

where \( K_T = K(U_T + 1) \). Thus, we renormalized the coefficients as follows

\[ \tilde{\lambda}_{j,i}^k = \frac{\lambda_{j,i}^k}{1 + 2K_T \Delta t}, \quad k = 0, \ldots, 4. \]

From (93), it follows that

\[ \frac{\int_{j,i} f_{j,i}^n}{1 + 2K_T \Delta t} = \tilde{\lambda}_{j,i}^0 f_{j,i}^0 + \tilde{\lambda}_{j,i}^1 f_{j,i}^1 + \tilde{\lambda}_{j,i}^2 f_{j,i}^2 + \tilde{\lambda}_{j,i}^3 f_{j,i}^3 + \tilde{\lambda}_{j,i}^4 f_{j,i}^4. \]

It remains to remark that

\[ 0 \leq 1 - \tilde{\lambda}_{j,i}^5 = \sum_{k=0}^{4} \tilde{\lambda}_{j,i}^k = \frac{1 + A^0_{j,i} \Delta t}{1 + 2K_T \Delta t} \leq \frac{1}{2}, \]

and we obtain by convexity of \( \phi \) and \( \phi(0) = 0 \)

\[ \phi \left( \frac{\int_{j,i} f_{j,i}^n}{1 + 2K \Delta t} \right) \leq \tilde{\lambda}_{j,i}^0 \phi(f_{j,i}^0) + \tilde{\lambda}_{j,i}^1 \phi(f_{j,i}^1) + \tilde{\lambda}_{j,i}^2 \phi(f_{j,i}^2) + \tilde{\lambda}_{j,i}^3 \phi(f_{j,i}^3) + \tilde{\lambda}_{j,i}^4 \phi(f_{j,i}^4). \]

Then, summing over \( i \), reordering the sum and remarking that

\[ \tilde{\lambda}_{j,i}^0 + \tilde{\lambda}_{j,i}^1 + \tilde{\lambda}_{j,i}^2 + \tilde{\lambda}_{j,i}^3 + \tilde{\lambda}_{j,i}^4 = \frac{1}{1 + 2K_T \Delta t}, \]

it is straightforward that

\[ \sum_{(j,i) \in \sigma} \phi \left( \frac{\int_{j,i} f_{j,i}^n}{1 + 2K \Delta t} \right) \leq \sum_{(j,i) \in \sigma} \phi(f_{j,i}^n). \] (94)

Finally, using that the derivative of \( \phi \) is concave, we have \( \phi'(\delta y) \leq \phi'(y) \) for \( (\delta, y) \in [1, +\infty) \times \mathbb{R}_+ \) and thus integrating over \( (0, x) \) this latter, we get that

\[ \phi(\delta x) \leq \delta^2 \phi(x), \quad \forall (\delta, x) \in [1, +\infty) \times \mathbb{R}_+. \] (95)
We conclude this intermediate estimate, using (94) and (95),
\[
\sum_{(j,i) \in \sigma} \phi(f^n_{j,i}) \leq (1 + 2\mathcal{K}_T \Delta t)^2 \sum_{(j,i) \in \sigma} \phi(f^n_{j,i}).
\] (96)

**Step 2. The coagulation.** Now we have the first part of our estimation, it remains to take into account the coagulation. We estimate the following quantity
\[
\sum_{(j,i) \in \sigma} \phi(f^{n+1}_{j,i}) - \phi(f^n_{j,i}) \leq \sum_{(j,i) \in \sigma} (f^{n+1}_{j,i} - f^n_{j,i}) \phi'(f^{n+1}_{j,i}),
\]
which comes from the convexity of \( \phi \). By definition of the \( \tilde{f}_{j,i} \) in (92) together with the expression of \( f^{n+1}_{j,i} \) in (59)
\[
\sum_{(j,i) \in \sigma} \phi(f^{n+1}_{j,i}) - \phi(f^n_{j,i}) \leq \Delta t \sum_{(j,i) \in \sigma} C_{j,i} \phi'(f^{n+1}_{j,i}).
\] (97)

Nonnegativity of \( f^n \) yields
\[
C_{j,i} \leq K \sum_{J=0}^{j} \sum_{I=0}^{I} \sum_{J'=0}^{j} \sum_{I'=0}^{I} p_{J,J'} f^n_{J',I'} f^n_{J,I'} K_{J',J-I} \phi'(f^n_{J',I'}) (\Delta p \Delta r)^2.
\]
then summing over \( j \) and \( i \), we get
\[
\sum_{(j,i) \in \sigma} \sum_{J=0}^{j} \sum_{I=0}^{I} \sum_{J'=0}^{j} \sum_{I'=0}^{I} p_{J,J'} f^n_{J',I'} f^n_{J,I'} K_{J',J-I} \phi'(f^n_{J',I'}) (\Delta p \Delta r)^2 = \sum_{(J,J') \in \sigma} p_{J,J'} \phi'(f^n_{J,J'}) \left( \sum_{(J',I') \in \sigma} f^n_{J',I'} (\Delta p \Delta r)^2 \right) (98)
\]
where \( i^* \in \{0, \ldots, I\} \) such that \( \delta_{J,J',I,I'} = 1 \). Now, we remark as in [2, lemma 3.2] and proving for instance with the help of [29, lemma B.1] that when \( \phi \) fulfills (88), we get that
\[
x \phi'(y) \ll \phi(x) + \phi(y), \quad \forall (x,y) \in \mathbb{R}_+^2.
\]
Using this property and the bound on the first moment (75) in (98), it follows
\[
\sum_{(j,i) \in \sigma} C_{j,i} \phi'(f^{n+1}_{j,i}) \leq K \sum_{(J,J') \in \sigma} p_{J,J'} \phi'(f^n_{J,J'}) \left( \sum_{(J',I') \in \sigma} f^n_{J',I'} (\Delta p \Delta r)^2 \right) (99)
\]
Combining both (96) and (99) with (97), we get
\[
\sum_{(j,i) \in \sigma} \phi(f_{j,i}^{n+1}) \leq (1 + 2K_T \Delta t)^2 \sum_{(j,i) \in \sigma} \phi(f_{j,i}^n)
\]
\[+ PKM_{\text{in}} \Delta t \left( \sum_{(j,i) \in \sigma} \phi(f_{j,i}^n) + \sum_{(j,i) \in \sigma} \phi(f_{j,i}^{n+1}) \right), \]

or in other terms, when \( \Delta t < 1 \)

\[
(1 - PKM_{\text{in}} \Delta t) \left( \sum_{(j,i) \in \sigma} \phi(f_{j,i}^{n+1}) - \sum_{(j,i) \in \sigma} \phi(f_{j,i}^n) \right) \leq (4K_T(K_T + 1) + 2PKM_{\text{in}}) \Delta t \sum_{(j,i) \in \sigma} \phi(f_{j,i}^n).
\]

Dividing by \( 1 - PKM_{\text{in}} \Delta t \geq 1/2 \) regarding the stability condition (68), thus it holds that for any \( n \in \{0, \ldots, N\} \)

\[
\sum_{(j,i) \in \sigma} \phi(f_{j,i}^n) \leq e^{\Delta T} \sum_{(j,i) \in \sigma} \phi(f_{j,i}^0),
\]

where \( C = 8K_T(K_T + 1) + 4PKM_{\text{in}} \). The conclusion follows from the definition of \( f_h \) in (64) and \( f_{\text{in}} \) in (67) with the Jensen inequality since

\[
\phi(f_{j,i}^0) = \phi \left( \frac{1}{|\Lambda_{j,i}|} \int_{\Lambda_{j,i}} f_{\text{in}}(p, r) \, dp \, dr \right) \leq \frac{1}{|\Lambda_{j,i}|} \int_{\Lambda_{j,i}} \phi(f_{\text{in}}(p, r)) \, dp \, dr.
\]

This ends the proof. \( \square \)

The direct consequence of lemma 4.8 is that \( (f_h)_h \) is weakly relatively compact in \( L^1((0, T) \times \mathcal{S}_0) \) as a consequence of the Dunford–Pettis theorem, see [13, theorem 4.21.2]. It proves there exists a subsequence (not relabelled) and \( f \in L^1((0, T) \times \mathcal{S}_0) \) such that

\[
f_h \rightharpoonup f \quad w - L^1((0, T) \times \mathcal{S}_0).
\]

At this stage, the convergence is too weak to be able to pass to the limit, particularly in the quadratic term, and to get the final regularity of \( f \) in definition 4.1. To this end, we will use the piecewise linear in time approximation. Against invoking the Dunford–Pettis theorem, for all \( t \in [0, T] \) we have that \( \tilde{f}_h(t, \cdot) \) belongs to a relatively compact subset of \( L^1(\mathcal{S}_0) \). Then, by corollary 4.6 we have that the sequence is equicontinuous in time for the strong topology of \( L^1(\mathcal{S}_0) \), thus for the weak topology. So, applying the Ascoli theorem, there exists a subsequence of \( \tilde{f}_h^{\Delta t} \) (not relabelled) converging towards a \( g \) in \( C([0, T]; w - L^1(\mathcal{S}_0)) \). Next, we remark that

\[
\sup_{t \in (0, T)} \| \tilde{f}_h(t, \cdot) - f_h(t, \cdot) \|_{L^1(\mathcal{S}_0)} \leq C \Delta t,
\]

which ensures that \( g = f \). Finally, by weak convergence we get

\[
\| f(t, \cdot) - f(s, \cdot) \|_{L^1(\mathcal{S}_0)} \leq \lim_{h \to 0} \inf \| \tilde{f}_h(t, \cdot) - \tilde{f}_h(s, \cdot) \|_{L^1(\mathcal{S}_0)} \leq C |t - s|.
\]

And this latter proves the continuity for the strong topology of \( L^1(\mathcal{S}_0) \) of the limit \( f \). This achieves the proof of the convergence (70)–(71) towards \( f \) (not yet the solution).
But, it remains to prove the convergence (72) of \( u_h \) before passing to the limit. Indeed, in corollary 4.6 we have (86) the uniform bound, w.r.t. \( h \), in \( L^\infty(0, T) \cap BV(0, T) \), then the Helly theorems, see [27, theorems 36.4 and 36.5], entail that up to a subsequence (not-relabelled) there exist \( u \in BV(0, T) \) such that the sequence \( (u_h(t))_h \) converges towards \( u(t) \) for every \( t \in [0, T] \). This proves (72).

### 4.4. Convergence of the numerical scheme

Here we prove that the limit \( f \) and \( u \) obtained right before are solutions of the problem (39)–(40) to conclude the proof of Theorem (4.4).

#### 4.4.1. Reconstruction and convergence of the coagulation operator

A delicate point in the proof of convergence is to give an appropriate reconstruction of the quadratic operator, the coagulation, so that it converges in a relevant sense. In order to perform it, we define over \((t, p, r) \in [0, T] \times S_p \times S_r\) the following approximation:

\[
C_{p, h}(t, p, r) = \int_{S_p \times S_r} \Phi_{p, h}^1(p', r'; p''', r'''') f_h(t, p', r') f_h(t, p'', r'') \, dr' dr'' dp' - \int_{S_p \times S_r} \Phi_{p, h}^2(p', r'; p''', r'''') f_h(t, p', r') f_h(t, p'', r'') \, dr' dr'' dp',
\]

where for any \((t, p, r) \in [0, T] \times S_p \times S_r\) and \((p', r'; p''', r'''') \in S_p \times S_r\),

\[
\Phi_{p, h}^1(p', r'; p''', r'''') = \mathbb{1}_{(0, P^h_0)(p')} \mathbb{1}_{(0, P^h_0)(p''')} P_h^h(p'') a_h(p', r'; p''', r''''),
\]

and

\[
\Phi_{p, h}^2(p', r'; p''', r'''') = \mathbb{1}_{(0, P^h_0)(p')} \mathbb{1}_{(0, P^h_0)(p''')} P_h^h(p'') a_h(p', r'; p''', r''''),
\]

with

\[
V_{p, h}^h(p', r'; p''', r'''') = \frac{R_h^h(r')(P_h^h(p') + P_h^h(p''))}{P_h^h(p')}.
\]

With such a definition, for all \( n \in \{0, \ldots, N - 1\} \) and \((j, i) \in \sigma\), it is straightforward that for any \((t, p, r) \in [t_n, t_{n+1}] \times \Lambda_{j,i}\) we have

\[
C_h(t, p, r) = C_{p, h}^{j-1/2, i-1/2}.
\]

Now the convergence of \( C_h \) will be a consequence of the following to lemma. The first one can be found as in [2, lemma 3.5].

**Lemma 4.9.** Let \( \Omega \) be an open set of \( \mathbb{R}^n \), \( \kappa > 0 \) and let two sequences \((v_n)_n \subset L^1(\Omega)\) and \((w_n)_n \subset L^\infty(\Omega)\). If we assume that for all \( n \in \mathbb{N} \), \( |w_n| \leq \kappa \) and there exist \( v \in L^1(\Omega) \) and \( w \in L^\infty(\Omega) \) satisfying

\[
v_n \rightharpoonup v, \quad \text{weak} - L^1(\Omega), \quad \text{and} \quad w_n \rightharpoonup w, \quad \text{a.e. in} \ \Omega.
\]
Then,
\[ \|v_n(w_n - w)\|_{L^1(\Omega)} \longrightarrow 0, \quad \text{and} \quad v_nw_n \longrightarrow vw, \quad \text{weak} - L^1(\Omega). \]

The second lemma gives us some useful properties on the functions \( \Phi_{\mu,r}^{i,h} \).

**Lemma 4.10.** For \( i = 1, 2 \),
\[ \|\Phi_{\mu,r}^{i,h}\|_{L^\infty(S_p \times S_p)} \leq PK, \quad \forall (p, r) \in S_p, \]
and for all \( (p, r) \in S_p \),
\[
\Phi_{\mu,r}^{1,h}(p', r'; p'', r'') \xrightarrow{h \to 0} 1_{(0,p')(p'')(r')}(v^\#)p' a(p', r'; p'', r''),
\]
\[
\Phi_{\mu,r}^{2,h}(p', r'; p'', r'') \xrightarrow{h \to 0} 1_{(0,p')(p'')(r')}(v^\#)p' a(p', r'; p'', r'').
\]
a.e. \( S_p \times S_p \).

**Proof.** The first inequality follows from hypothesis (H2'). Then, we only have to check that \( 1_{(0,R_r^i(r))(V^\#_h,p',r',p'',r'')} \) converge almost everywhere. Indeed, for all \( r \in (0,1) \),
\[
\int_{S_p \times S_p} |1_{(0,R_r^i(r))(V^\#_h)} - 1_{(0,r)(v^\#)}|dr''dp''dr'dp' = \int_{S_p \times S_p} |1_{(0,R_r^i(r))(V^\#_h)} - 1_{(0,r)(v^\#)}|dr''dp''dr'dp' + \int_{S_p \times S_p} |1_{(0,R_r^i(r))(v^\#)} - 1_{(0,r)(v^\#)}|dr''dp''dr'dp', \tag{101}
\]
where
\[ V^\#_h(p', r'; p'', r'') = \frac{R^i_h(r')P^i_h(p') + R^i_h(r'')P^i_h(p'')} {P^i_h(p')} \leq v^\# = \frac{r'p' + r''p''} {p' + p''}. \]

Therefore, the first integral on the right-hand side of (101) is reduced to the measure of the set
\[ A^i_h = \{(p', r', p'', r'') \in S_p \times S_p : V^\#_h < R^i_h(r) \leq v^\# \}. \]

Remarking that \( V^\#_h \) converge everywhere to \( v^\# \) and \( R^i_h(r) \) towards identity, \( A^i_h \) converges towards \( v^\#^{-1}(r) \) which is a null set for the Lebesgue measure. It remains to note that the second integral in (101) converges to zero too, and conclude that \( 1_{(0,R_r^i(r))(V^\#_h)} \) converges toward \( 1_{(0,r)(v^\#)} \) in \( L^1(S_p \times S_p) \). Thus, we have the convergence almost everywhere on \( S_p \times S_p \), up to a subsequence (against not relabled). \[
\square
\]

The sequence \( f^i_h \) do not have a sufficient regularity so, to pass to the limit, the trick is to consider the operator
\[
\tilde{C}_{p,h}(t,p,r) = \int_{S_p \times S_p} \Phi_{p,h}^{1,h}(p', r'; p'', r'') f^i_h(t,p',r') f^i_h(t,p'',r'') dp''dr''dr'dp',
\]
\[
- \int_{S_p \times S_p} \Phi_{p,h}^{2,h}(p', r'; p'', r'') f^i_h(t,p',r') f^i_h(t,p'',r'') dp''dr''dr'dp'.
\]
Here we proceed as in [2, section 4], applying twice lemma 4.9 thanks to lemma 4.10, we get
Finally, by lemma 4.10, corollary 4.6 and the convergence obtained in (100), we have
\[ |\tilde{C}_{p,h}(t,p,r) - \tilde{C}_{p,h}(t,p,r)| \leq 2KP(\|f_h\|_{L^\infty(0,T,L^1)} + \|\tilde{f}_h\|_{L^\infty(0,T,L^1)}) \|f_h - \tilde{f}_h\|_{L^\infty(0,T,L^1)} \xrightarrow[h \to 0]{} 0, \quad \forall (t,p,r) \in [0,T) \times \mathcal{S}_p. \]

Thus, since \( C_{p,h} = C_{p,h} - \tilde{C}_{p,h} + \tilde{C}_{p,h} \), we have
\[ C_{p,h} \xrightarrow[h \to 0]{} C_p, \quad \text{on } [0,T) \times \mathcal{S}_p. \]

Moreover, it is obvious that \( C_{p,h} \) is bounded since we have (82) and lemma 4.10, then the Lebesgue dominated convergence theorem yields
\[ C_{p,h}(t,\cdot) \xrightarrow[h \to 0]{} C_p(t,\cdot), \quad L^1(\mathcal{S}_p) \quad \forall t \in [0,T). \]

**4.4.2. Final stage of the proof.** The final stage of the proof is to write the discrete weak formulation of the scheme, when the equation (59) is multiplied by discrete test functions \( \varphi_{j,i} \), and then to prove that it converges to the continuous weak formulation. Thus, let \( \varphi \in \mathcal{C}^2(\mathcal{S}_p) \) and multiply equation (59) by \( \varphi_{j,i} = \varphi(p_{j-1/2}, r_{i-1/2}) \). Then summing over \((j,i)\) and \(k = 0, \ldots, n - 1\) for some \( n \in \{1, \ldots, N\} \), we get
\[
\sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} p_j f^k_{j,i} \varphi_{j,i} \Delta r \Delta p - \sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} p_j f^k_{j,i} \varphi_{j,i} \Delta r \Delta p
= -\Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} (F^k_{j,i+1/2} - F^k_{j-1/2,i}) \varphi_{j,i} \Delta p + \Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} C^k_{j,i} \varphi_{j,i,\cdot}.
\]

Reordering the sums, and making use of the boundary conditions (52) and (56), we infer the following equation
\[
X^n_h = Y^n_h + Z^n_h, \quad (102)
\]
where
\[
X^n_h = \sum_{j=0}^{J} \sum_{i=0}^{I} p_j f^0_{j,i} \varphi_{j,i} \Delta r \Delta p - \sum_{j=0}^{J} \sum_{i=0}^{I} p_j f^0_{j,i} \varphi_{j,i} \Delta r \Delta p,
\]
\[
Y^n_h = \Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} F^k_{j,i+1/2} (\varphi_{j,i} - \varphi_{j,i-1}) \Delta p,
\]
\[
Z^n_h = \Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} \sum_{i=0}^{I} C^k_{j-1/2,i-1/2} (\varphi_{j-1,i-1} - \varphi_{j-1,i}) - (\varphi_{j,i-1} - \varphi_{j,i})] + \Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} C^k_{j+1/2,i+1/2} (\varphi_{j+1,i+1} - \varphi_{j+1,i}) + \Delta t \sum_{k=0}^{n-1} \sum_{j=0}^{J} C^n_{j+1/2,i+1/2} (\varphi_{j+1,i} - \varphi_{j,i}).
\]
Next, we define \( X_h \) on \([0, T)\) by
\[
X_h(t) := \int \int_S P_h(p)f_h(t, p, r) \varphi(P_h(p), R_h(r)) \, dp \, dr - \int \int_S P_h(p)f_h^\infty(p, r) \varphi(P_h(p), R_h(r)) \, dp \, dr.
\] (103)

Then, we define \( Y_h \) by
\[
Y_h(t) = Y_h^1(t) + Y_h^2(t),
\] (104)
with
\[
Y_h^1(t) = \int_0^t \int_S 1_{\Theta_h(t)}(s) \delta h(s) \varphi(P_h(p), R_h(r)) \, dp \, dr \, ds,
\]
and
\[
Y_h^2(t) = -\int_0^t \int_S 1_{\Theta_h(t)}(s) \delta h(s) \varphi(P_h(p), R_h(r)) \, dp \, dr \, ds,
\]
where a Taylor expansion of \( \varphi \) gives
\[
D^{[\varphi]}(p, r) = \frac{\partial \varphi}{\partial r}(P_h(p), R_h(r)) + o(\Delta r).
\]
In the same manner, we define \( Z_h \) by
\[
Z_h(t) = Z_h^1(t) + Z_h^2(t) + Z_h^3(t),
\] (105)
such that
\[
Z_h^1(t) = \int_0^t \int_S 1_{\Theta^1_h(t)}(s) \epsilon h(s) \varphi(P_h(p), R_h(r)) \, dp \, dr \, ds
\]
\[
Z_h^2(t) = \int_0^t \int_S 1_{\Theta^2_h(t)}(s) \epsilon h(s, 1) \varphi(P_h(p), R_h(r)) \, dp \, dr \, ds
\]
\[
Z_h^3(t) = \int_0^t \int_S 1_{\Theta^3_h(t)}(s) \epsilon h(s, P, r) \varphi(P_h(p), R_h(r)) \, dp \, dr \, ds
\]
with the expansion
\[
D^{[\varphi]}(p, r) = \frac{\partial^2 \varphi}{\partial p^2}(P_h(p), R_h(r)) + o(\Delta p) + o(\Delta r),
\]
\[
D^{[\varphi]}(P, r) = \frac{\partial \varphi}{\partial r}(P_h(p), R_h(r)) + o(\Delta r),
\]
\[
D^{[\varphi]}(P, r) = \frac{\partial \varphi}{\partial p}(P_h(p), 1) + o(\Delta p).
\]
It is straightforward that for any \( n \in \{1, \ldots, N\} \) and \( t \in [t_n, t_{n+1}) \) we have
\[
X_h(t) = X_h^n, \quad Y_h(t) = Y_h^n, \quad \text{and} \quad Z_h(t) = Z_h^n.
\]
Thus, by (102), it holds that for all \( t \in [0, T) \)
\[ X_h(t) = Y_h(t) + Z_h(t). \]  
(106)

For the same reason, we get

\[ u_h(t) = u^{in} - \int_0^t \int_{S_p} 1_{(0,0.01)}(s)(V^+(u_h(s), P_h(p), R_h(r))) \]
\[ - V^-(u_h(s), P_h(p), R_h(r))) f_h(s, p, r) \, dr \, dp. \]  
(107)

In view of (106) and (107) the conclusion readily follows. Indeed, to pass to the limit in (103), it is convenient to introduce \( \tilde{X}_h \) where \( f_h \) is replaced by \( \tilde{f}_h \), then the same arguments as section 4.4.1 hold true. We write \( \tilde{X}_h = X_h - \tilde{X}_h + \tilde{X}_h \), then it is clear that

\[ \|X_h - \tilde{X}_h\|_{L^\infty(0,T)} \to 0, \]

by virtue of (100). Then, for all \( t \in (0, T) \) we prove that \( \tilde{X}_h \) converge towards the right term by lemma 4.9. For (104) and (105) we do the same decomposition, noting two points. On one hand, the continuity of \( V \) and the pointwise convergence of \( u_h \) allow us to pass correctly to the limit in the positive and negative parts of \( V = V^+ - V^- \). On the other hand, the time integral is treated thanks to the Lebesgue dominated convergence theorem. Equation (107) is treated by the same arguments. Proof of theorem 4.4 is achieved.

5. Numerical illustration and long-time behaviour

In this section, we choose to illustrate our numerical scheme by simulating a particular example that depicts the asymptotic behaviour of the solution. The simulation of this example seeks to show the typical behaviour of the long-time solution for a wide class of coefficients.

5.1. The numerical examples

Let us first introduce the coefficients and initial conditions we choose for the simulation. We let \( u^{in} = 0.9, P = 1 \) and for all \( (p, r) \in (0, P) \times (0, 1) \)

\[ f^{in}(p, r) = m \cdot \exp\left(-\frac{1}{2} \cdot \frac{(\log(p) + 2)^2}{2 \cdot 0.4^2} - \frac{(r - 0.2)^2}{2 \cdot 0.05^2}\right) \]

with \( m \) is a normalization constant such that

\[ \int_0^P \int_0^1 r pf^{in}(p, r) \, dr \, dp = 0.1. \]

We note in \( r = 0 \) and \( 1 \) this function is close to zero, so numerically we require that it vanishes. In this case, \( \rho = 1 \) since

\[ u^{in} + \int_0^P \int_0^1 r pf^{in}(p, r) \, dr \, dp = \rho. \]

Then, we used the association-dissociation and the coagulation rates

\[ V(u, p, r) = 4p(1 - r)u - r, \quad \text{and} \quad a(p, r, p', r') = 1. \]

In figures 1 and 2, we present the results obtained with the numerical scheme introduced in section 4. The first picture of figure 1 is the initial condition. Then, in the second and third, we see that polymers are capturing metal ions since for each \( p \) the distribution shifts towards greater \( r \). This is confirmed by figure 3, where the concentration \( u \) at the same time
is decreasing. In the last picture of figure 1, the biggest polymers appear since the tail of the distribution moves to the right. Finally, in figure 2, the distribution seems to be well concentrated onto a curve while the mass moves towards the biggest polymers (right). At this stage, the concentration of metal ions seems to reach a steady state, see figure 3, and the coagulation is predominant.

5.2. Long-time behaviour

In the case where the association-dissociation rate has a unique 0, for fixed \( u(t) > 0 \) and \( p > 0 \), there exists a unique number denoted by \( r(p) \) such that

\[
\chi(u(t), p, r(p)) = 0,
\]

then, the distribution function \( f \) concentrates towards the curve \( p \mapsto r(p) \). From a chemical point of view, this curve represents the instantaneous quantity of metal ions at equilibrium with a polymer of size \( p \). It rests on the hypothesis that each size of polymers (under fixed
conditions) gets a unique preferential ratio of metal ions \( r \). The case where \( V \) has more than one zero would be more complex.

Then, if \( u(t) \) converges to a constant \( u^\infty \) when \( t \to +\infty \) this curve is given by \( r_\infty(p) \). In the numerical example we gave, this curve is

\[
r_\infty(p) = \frac{4p}{4pu^\infty + 1}.
\]

Moreover if we take \( u^\infty \simeq u(T = 5) \) this curve fits well with what we see in figure 2. This hypothesis would mean that each size \( p \) of polymers has a preferential ratio \( r \) of metal ions for given conditions of temperature, pH, etc. It would remain to prove that experimentally. If not, and if \( V \) has more than one nullcline, the behaviour would be different and probably dependent on the initial conditions.

Thus, if we had to conjecture on the long-time behaviour of the solution, we would say it behaves like

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**Figure 2.** Evolution of the configurational distribution of polymers after a while. Each snapshot represents the solution at different times from left to right and up to down with \( t = 1, 2, 3.5, 5 \) where \( p \) is in the x-axis and \( r \) in the y-axis and the greyscale colour varies from white to black when \( f(t, p, r) \) varies from 0 to 350. The simulation was performed with the condition described in section 5 on a regular grid 100 \times 100, i.e. \( \Delta p = \Delta r = 0.01 \) and a time step \( \Delta t = 1.25 \times 10^{-4} \).
where \( g \) satisfies an equation (defined later) and \( r_t(p, r) \) is the solution of \( \mathcal{V}(u(t, p, r(t))) = 0 \), uniquely defined for all \( p > 0 \) and \( t \geq 0 \). It gives the instantaneous equilibrium of the association-dissociation reactions. Now, if we plug \( g(t, p)\delta_{\delta_p}(r) \) (which is a measure) in the weak formulation, we formally get, when taking a test function \( \phi \),

\[
\int_{0}^{\infty} g(t, p)\psi(p) \, dp - \int_{0}^{\infty} g^{in}(p)\psi(p) \, dp = \int_{0}^{t} \int_{0}^{\infty} Q(g, g)(s, p)\psi(p) \, dp \, ds, \tag{108}
\]

with

\[
\int_{0}^{\infty} Q(g, g)(t, p)\psi(p) \, dp = \frac{1}{2} \int_{0}^{\infty} \int_{0}^{\infty} b(t; p, p')g(t, p)g(t, p') \times [\psi(p + p') - \psi(p) - \psi(p')] \, dp' \, dp. \tag{109}
\]

where \( b(t; p, p') = a(p, n(p); p', n(p')) \). The operator \( Q \) in (109) is exactly the weak formulation of the classical coagulation operator, see for instance \([29]\) among others, with a non-autonomous coagulation rate. To our knowledge, the non-autonomous coagulation equation has received little attention up to now, except in \([32]\).
Thus \( g \) would satisfy a non-autonomous coagulation equation (108). But in the case where \( u(t) \) reach a steady state, 
\[ b(t; p, p') \rightarrow b_{\infty}(p, p') = a(p, r_{\infty}(p); p', r_{\infty}(p')). \]
A non-autonomous coagulation equation might behave asymptotically like an autonomous coagulation equation with coefficient \( b_{\infty} \). The long-time behaviour of an autonomous coagulation equation reveals self-similarity, see for instance [21]. Here, the interpretation we propose from numerical simulations is a propagation, probably with a self-similar profile, of the distribution over the curve \( p \mapsto r_{\infty}(p) \). Analysis of this problem would be a full work on its own. So we leave it for now.

Nevertheless, such behaviour would be taken into account in the experimental procedures. Indeed, the choice of the size distribution could be crucial in the efficacy of the process, but they need to diminish the effect of the coagulation to avoid its interference with the membrane, for instance [40, 41].

6. Conclusion

In this paper, we dealt with a new model with applications to water-polymers gaining a particular affinity for metal ions. This equation can be seen as a variation on the coagulation equation or the LS equation. Nevertheless, it includes various specific features (conservations involved, the nature of the configuration space and the structure of the coagulation operator) that make an original problem itself. We established a first result of existence for a large class of initial data. Then, we established a finite volume scheme, and we proved a convergence result of the sequence of approximations. This numerical scheme is used to illustrate the long-time behaviour of the solution.

There are several possible extensions of this work. In the first section, the class of coefficient should be relaxed, and maybe the monotonicity. It would be possible to use a similar \( L^1 \)–weak stability principle as is done for the convergence of the numerical scheme, using regularization of the coefficients. Of course, the question of uniqueness is still open here. Concerning the numerical scheme. It would be interesting to develop a new approach, capturing in a better manner the concentration on the curve. Finally, It remains to demonstrate the question of the long-time behaviour rigorously.

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