ON A SORPTION-COAGULATION EQUATION: STATEMENT, EXISTENCE AND NUMERICAL APPROXIMATION

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Abstract. This paper is devoted to the design and the mathematics of a new sorption-coagulation equation type, modeling interactions between metal ions and water-soluble polymers. We motivate a new brand model that accounts for the evolution of the configurational density of polymers and metal ions, which consists in a non-linear transport equation with a quadratic source term, the coagulation. A global in time existence result is establish and a time explicit finite volume scheme for a conservative reformulation of the problem is proposed. Then, we prove a convergence result of the sequence of numerical approximation thanks to L^1 - weak compactness arguments.

Contents

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1. Introduction

1.1. **Motivations.** A class of polymers containing metals has emerged for their potential applications in various fields, as superconducting materials, liquid crystal, and biocompatible polymers. Also, in environmental science, they can be used for instance to remove pollutant from aqueous solutions, or bacteria, fungi and algae [39]. Such polymers are called water-soluble polymers (WSP) and here we are particularly interested in their interactions with metal ions such as copper ions, lead ions, and many others.

These polymers are highly soluble macromolecules, basically composed of a repeated unit. The latter is generally a charged group, easily ionizable, which entails a high affinity of one or more metal ions with the polymers [38, 39].

One of the applications of this concept, being very promising, lies in membrane separation process. Indeed, a very high level of metal ions can be released by industrial processes in the environment. The idea is to take advantage of the polymers-ions interactions in order to extract free metal ions from an aqueous solution (water) and then filtrate the resulting solution by a membrane to separate polymers-ions from the solution, also called "washing method". The objective is to obtain water free of metal ions. Various techniques based on this method exist, and we refer to [37] and the reviews [38, 39] for a more precise description.

Nevertheless, the development of these techniques leads to some technical difficulties and gives rise to questions in order to produce an efficient method. Among these interrogations are the role of fouling effect (adhesion of polymers to the membrane), aggregation phenomenon, concentration effect, interaction with the wall of the cell (recipient) and interaction with the fluid. For recent findings, techniques and models on the subject we refer to the works in [31–36, 41] and references herein-above. Here, to go further in this direction of a better understanding of such process, we decide to propose a new model that accounts for polymer-ion and polymer-polymer interactions which would apply to particular experiments designed in laboratory to understand specifically such interactions [40].

The polymer-metal ions is the fundamental interaction to study and takes several aspects: long and short range electrostatic interactions and coordination theory; while the polymer-polymer interactions occur naturally in the solution particularly by forming coordination center, *i.e.* polymers are linked by one or more metal ions [39]. In the model developed below, we omit voluntary various phenomena, in accordance with [40], to focus on these two interactions. The point of view we chose, is a statistical or mean-field approach, so that we describe the evolution of the polymers thanks to a density function with respect to their configurations, namely the "number" of repeat unit and the "number" of bound metal ions. Then, we describe the binding process of a metal ion onto polymer (adsorption) and its elution (desorption) thank to a reversible interaction reaction (sorption process) while the polymer-polymer interaction is seen as a coagulation process.

Such approach has been used in physics for clusters formation (for instance particles of matter or droplet) and in biology for polymerization, amyloid formation. We refer to the Section 1.3 further down to get an overview of these models. For now we state in the next section the equations of the model.

1.2. **Equations.** The configuration of polymers is given by two variables. First, the size $p \in \mathbb{R}_+ := (0, +\infty)$ related to the number of functional groups or metal ions possible sites. Second, the occupied size $q \in \mathbb{R}_+$ related to the number of occupied functional groups/sites of the polymer by metal ions. Thus, the set of admissible configurations (p,q) of a given polymer is:

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

Then, we define the density function of polymers, denoted by $f(t,p,q)$, as a function of time $t \geq 0$ and configuration given by $(p,q) \in S$. The system governing the evolution of f is given by

$$\frac{\partial f}{\partial t} + \frac{\partial}{\partial q}\left(\mathcal{V} f\right) = Q(f,f), \qquad \text{on } \ \mathbb{R}_+ \times S \,, \tag{1.1}$$

where Q is the coagulation operator and $\mathcal{V}$ denotes the rate of sorption which determines the mechanism of ions transfer with a polymer (adsorption and desorption of ions), both defined below. To complete the model, we define the concentration of free metal-ions (living in the solution but not bound to polymers), denoted by $u(t)$, as a function of time $t \geq 0$, given by the constraint of metal ions conservation (bound and free), namely

$$u(t) + A\int_S q f(t,p,q)dqdp = \rho, \qquad \text{on } \ \mathbb{R}_+ \,, \tag{1.2}$$

where $\rho > 0$ is the total mass and $A > 0$ is a parameter for the dimension of the balance.

Let us now define more precisely the sorption rate $\mathcal{V}$. As a general form for $\mathcal{V}$ we consider the following chemical reactions rate

$$\mathcal{V}(u(t),p,q) = k(p,q)u(t)^\gamma - l(p,q) \,,$$

where k is the adsorption rate at which a free monomers bind to a polymer (depending on the type of interaction and the diffusion rate of the particles) and l is the desorption rate (depending on the strength of the interaction). For sake of simplicity we restrict our self to $\gamma = 1$ which is the order of the reaction. A relevant example of sorption rate would be an analogy to the Langmuir's law, namely

$$\mathcal{V}(u(t),p,q) = k_0(p-q)^\alpha u(t)^\gamma - l_0 q^\beta \,, \tag{1.3}$$

with k_0, $l_0 > 0$ parameters and α, $\beta > 0$ geometrical factor, see [42].

Next we explicit the coagulation operator Q. We introduce first the notation $C_{p,q}$ for a polymer chain with configuration $(p,q) \in S$. Then, the coagulation can be written in term of a kinetic scheme, that is for any two polymers $(p,q)\times(p',q') \in S^2$,

$$C_{p,q} + C_{p',q'} \xrightarrow{a(p,q;p',q')} C_{p+p',q+q'} \,,$$

where the coagulation rate a is defined as a nonnegative function over $S \times S$ satisfying the symmetry assumption

$$a(p,q;p',q') = a(p',q';p,q) \,. \tag{1.4}$$

Thus, Q can be decomposed by a gain term Q^+ and a depletion term Q^- that is

$$Q = Q^+ - Q^-,$$

where

$$Q^+(f,f)(p,q) = \frac{1}{2}\int_0^p \int_0^{p'} a(p',q',p-p',q-q')\,\mathbf{1}_{(0,p-p')}(q-q') \times f(p',q')f(p-p',q-q')\,dq'dp' \,, \quad (1.5)$$

$$Q^-(f,f)(p,q) = L(f)(p,q)f(p,q)\,,$$
$$\text{with} \quad L(f)(p,q) = \int_0^\infty \int_0^{p'} a(p,q,p',q')f(p',q')\,dq'dp' \,. \quad (1.6)$$

The problem (1.1)-(1.2) is completed with a boundary condition:

$$f = 0, \qquad \text{on} \;\; \partial S \,, \quad (1.7)$$

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

$$f(t=0,\cdot) = f^{in} \text{ on } \; S, \text{ and } u(t=0) = u^{in} \,. \quad (1.8)$$

1.3. **Contents of the paper and related works.** The remainder of this paper is devoted to the existence of global solutions to problem (1.1)-(1.2) and its numerical approximation.

In Section 2, we investigate the existence of solutions for any time interval with the result states by Theorem 2.2. We give a sketch of proof including the main arguments which lead to the use of two fix point theorems, one to treat the coagulation operator (1.5)-(1.6) , the second for the constraint (1.2). The technique used, implying hypotheses of regularity on the coefficients, is based on the works on Lifshitz-Slyozov (LS) equation in [6] and LS with encounters (coagulation) in [5]. Techniques also re-adapted in [22] for biological polymers. The LS equation is a size structured model for clusters (polymers or more general) formation by addition-depletion of monomers [30], while LS with encounters also take into account merging clusters . The coagulation (only size-dependent) is part of the class of coagulation-fragmentation (CF) equation, where fragmentation is the reverse operator (break-up, splitting of clusters), and it has been studied from a mathematical point of view for instance in [11, 26], also in [1, 29] for the CF equation with space diffusion, and in [3] which generalized CF equation with a kinetic approach (maybe in some sense the closest operator to the one here). In the references right before, the assumptions on the coagulation rate are relaxed, and much more general than the one use here since it authorizes unbounded rate. Nevertheless, as in [28] for LS and [27] for LS with coagulation, a possible approach to extend the result is to combine a weak stability principle to a sequence of approximation (with bounded rate or cut-off). So, the result given here, states the framework, introduces the particularity of the coagulation operator presented here, and appears to be a first step toward a generalization of the class of coefficients.

In Section 3, we propose a finite volume scheme to construct numerical solutions to this problem. The numerical scheme, which is proposed, is in the spirit of the works made in [2] and [15], where the authors propose a reformulation of the CF equation in a manner well-adapted to a finite volume scheme, namely a conservative form. Here, we write a similar conservative form, but as a cross derivative with respect to both variables. For suitable numerical scheme, we also refer to [17] for LS, to [20] for LS with encounters and to [19] for a model with space diffusion.

Then the rest of the section is devoted to the proof of the convergence result given in Theorem 3.4. It is based on L^1 weak compactness of sequences of approximations. Thus, the technique used here has the advantage to provide the basic ideas and estimations that could extend the result of Section 2 to a larger class of coefficients by weak stability principle.

2. Rescaling and existence of global solutions

2.1. **Rescaled problem.** The space of configuration S is not really convenient for computations both for the theoretical point of view and the numerical implementation. Thus, we decide to rescale the problem and operate a change of variable in the density f, introducing a physically relevant new variable $r \in (0,1)$, called ion ratio, such that for $(p,q) \in S$ we let

$$r := \frac{q}{p}\,.$$

One can see the number of polymers in an infinitesimal volume $dqdp$, center in $(p,q) \in S$ at a time $t \geq 0$, as

$$f(t,p,q)dqdp = f(t,p,rp)pdrdp\,.$$

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

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

The constant A is the normalization parameter involved in the constraint (1.2). Then, we operate a rescaling of the sorption and coagulation rate, by introducing $\tilde{\mathcal{V}}$ define over $\mathbb{R} \times \mathcal{S}$ and $\tilde{a}$ over $\mathcal{S} \times \mathcal{S}$, such that

$$\tilde{\mathcal{V}}(u,p,r) = \mathcal{V}(u,p,rp), \text{ and } \tilde{a}(p,r;p',r') = \frac{1}{A}a(p,pr;p',p'r')\,.$$

Thus, they satisfy

$$\tilde{\mathcal{V}}(u,p,r) = \tilde{k}(p,r)u - \tilde{l}(p,r)\,, \tag{2.1}$$

with $\tilde{k}(p,r) = k(p,rp)$ and $\tilde{l}(p,r) = l(p,rp)$. Also, the symmetry assumption (1.4) becomes

$$\tilde{a}(p,r;p',r') = \tilde{a}(p',r';p,r)\,. \tag{2.2}$$

A formal computation leads to the assessment

$$\partial_t \tilde{f}(t,p,r) + \frac{1}{p}\partial_r\left(\tilde{\mathcal{V}}(u(t),p,r)\tilde{f}(t,p,r)\right)\Big|_{r=q/p} = pAQ(f,f)(t,p,q)\,.$$

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

$$\tilde{Q}^+(\tilde{f},\tilde{f})(p,r) = \frac{1}{2}\int_0^p\int_0^1 \frac{p}{p-p'}\tilde{a}(p',r',p-p',r^*)\,\mathbf{1}_{(0,1)}(r^*) \times\ \tilde{f}(p',r')\tilde{f}(p-p',r^*)\,dr'dp'\,, \tag{2.3}$$

$$\tilde{Q}^-(\tilde{f},\tilde{f})(p,r) = \tilde{L}(\tilde{f})(p,r)\tilde{f}(p,r) \quad \text{with} \quad \tilde{L}(\tilde{f})(p,r) = \int_0^\infty\int_0^1 \tilde{a}(p,r;p',r')\tilde{f}(p',r')\,dr'dp'\,, \tag{2.4}$$

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

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

In the following and for the rest we drop tildes in the rescaled problem, for sake of clarity. Now, we are able to reformulate the problem which is to find the density f satisfying

$$\frac{\partial f}{\partial t} + \frac{1}{p}\frac{\partial}{\partial r}\left(\mathcal{V} f\right) = Q(f,f), \qquad \text{on } \ \mathbb{R}_+ \times \mathcal{S}\,, \tag{2.5}$$

with the constraint

$$u(t) + \iint_{\mathcal{S}} rpf(t,p,r)drdp = \rho, \qquad \text{on } \ \mathbb{R}_+\,. \tag{2.6}$$

and boundary condition (1.7) remains given by

$$f = 0, \qquad \text{on } \ \partial\mathcal{S}\,, \tag{2.7}$$

while the initial conditions is a rescaled version of (1.8):

$$f(t=0,\cdot) = f^{in} \text{ on } \mathcal{S}, \text{ and } u(t=0) = u^{in}\,. \tag{2.8}$$

2.2. **Hypotheses and result.** In order to study rigorously the problem (2.5)-(2.6), some natural and other technical assumptions are made. Namely we assume that:

H1. The initial density $f^{in} \in L^1\left(\mathcal{S}, (1+p)drdp\right)$ is nonnegative and $u^{in} \geq 0$ such that

$$\rho \coloneqq u^{in} + \iint_{\mathcal{S}} rpf^{in}(p,r)\, drdp < +\infty\,. \tag{2.9}$$

H2. The coagulation rate $a \in L^\infty(\mathcal{S}\times\mathcal{S})$ is nonnegative, satisfies (2.2) and

$$\|a\|_{L^\infty} \leq K\,. \tag{2.10}$$

H3. The rates functions $p \mapsto k(p,\cdot),\ l(p,\cdot) \in L^\infty(\mathbb{R}_+; W^{2,\infty}(0,1))$ are both nonnegatives and

$$\|k\|_{L^\infty(\mathbb{R}_+;W^{2,\infty}(0,1))} + \|l\|_{L^\infty(\mathbb{R}_+;W^{2,\infty}(0,1))} \leq K\,. \tag{2.11}$$

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

$$\|k(p,\cdot)\|_{W^{2,\infty}(0,1)} + \|l(p,\cdot)\|_{W^{2,\infty}(0,1)} \leq Kp\,. \tag{2.12}$$

H4. For all $u \geq 0$ and $p \in \mathbb{R}_+$,

$$\mathcal{V}(u,p,r=0) \geq 0, \text{ and } \mathcal{V}(u,p,r=1) \leq 0\,, \tag{2.13}$$

and

$$\partial_r \mathcal{V}(u,p,r) = \partial_r k\ u - \partial_r l \leq 0 \quad \text{a.e. } (u,p,r) \in \mathbb{R}_+ \times \mathcal{S}_P\,. \tag{2.14}$$

Here, $K > 0$ denotes a constant. Note that (2.13) ensures the characteristics remain in the set $\mathcal{S}$ and allows us to prescribe condition the boundary (2.7). In fact, it is equivalent with respect to (2.1) and (H4) to

$$k(p,0) \geq 0,\ l(p,0) = 0 \text{ and } k(p,1) = 0,\ l(p,1) \geq 0\,, \tag{2.15}$$

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

Remark 2.1. With such scaling, we note that example (1.3) 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.

Now, we are in position to give a definition of the solutions to the problem (2.5)-(2.6).

Definition 2.1 (weak solution 1)**.** Let $T > 0$ and the initial conditions f^{in} and u^{in} satisfying (H1). A weak solution to (2.5)-(2.6) on $[0, T)$ is a couple (f, u) of nonnegative functions such that

$$f \in C\left([0,T); w - L^1(\mathcal{S})\right) \cap L^\infty\left([0,T), L^1(\mathcal{S}, pdrdp)\right)\,, \tag{2.16}$$

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

$$\begin{aligned}\int_S f(t,p,r)\varphi(p,r)\,drdp - \int_S f^{in}(p,r)\varphi(p,r)\,drdp \\ = \int_0^t \int_S \frac{1}{p}\mathcal{V}(u(s),p,r)f(s,p,r)\partial_r\varphi(p,r)\,drdpds \\ + \int_0^t \int_S Q(f,f)(s,p,r)\varphi(p,r)\,drdpds\,,\end{aligned} \tag{2.17}$$

together with (2.6)

We remark here that regularity (2.16), where $C\left([0,T); w - X\right)$ means continuous from $[0,T)$ to X a Banach space with respect to the weak topology of X. Hypothesis (H1) to (H3) suffice to define (2.17). Particularly, (2.3)-(2.4) entail, as we will see later, that $Q(f,f)$ belongs to $L^\infty\left(0,T; L^1(\mathcal{S})\right)$.

We can now state the main result:

Theorem 2.2 (Global existence)**.** *Let $T > 0$. Assume that f^{in} and u^{in} satisfy (H1) and that hypotheses (H1)-(H4) are fulfilled. Then, there exists a solution (f,u) to the problem* (2.5)-(2.6) *in the sense of Definition 2.1. Moreover, the solution has the regularity*

$$f \in C\left([0,T); L^1(\mathcal{S})\right)\,,$$

with both

$$\int_S f(t,p,r)drdp \le \int_S f^{in}(p,r)\,drdp\,,$$

and

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

Proof of Theorem 2.2 relies on 2 main steps, which are similar to the ones that have been used for instance in [5] and [6] for LS equation: The first step consists in building a mild solution f for a given u to (2.5) via a fixed point theorem by virtue of contraction property of the coagulation; The second step is another fixed point in order to couple the problem to the constraint (2.6) on u.

Since the method is rather classical, we will only provide in the next section the essentials arguments useful to achieve the proof enlightening the differences between our problem and LS equation with encounter.

2.3. **Existence of solutions.**

2.3.1. *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 (2.6). A well-know approach is to construct the characteristics of the transport operator. These latter are the curves parametrized by $p \in \mathbb{R}_+$ and associated to u given, for any $(t,r) \in [0,T] \times (0,1)$, by 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 (2.11)-(2.12) and (2.15), there exists a unique solution $R_p(\cdot;t,r) \in C^1([0,T])$. We only consider the characteristic while they are defined, *i.e* $R_p(s;t,r) \in (0,1)$. We remark that (H4) ensures the characteristic remains in $(0,1)$ for any $s \geq t$ (once in the domain it cannot go out). Moreover, we define the origin time $\sigma_p(t,r) = \inf\{s \in [0,t] : 0 < R_p(s;t,r) < 1\}$. So, to these latter we associate the so-called mild-formulation which is f solution of

$$f(t,p,r) = \begin{cases} f^{in}(p,R_p(0;t,r))J_p(0;t,r) \\ \quad + \displaystyle\int_0^t Q(f,f)(s,p,R_p(s;t,r))J_p(s;t,r)\,ds\,, & \text{if } \sigma_p(t,r) = 0 \\ \displaystyle\int_{\sigma_p(t,r)}^t Q(f,f)(s,p,R_p(s;t,r))J_p(s;t,r)\,ds\,, & \text{otherwise.} \end{cases} \tag{2.18}$$

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

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

Note that, for an enough regular solution, the boundary condition (2.7) is satisfy by (2.18) since $\sigma_p(t,0) = \sigma_p(t,1) = t$.

Then, to prove Theorem 2.2 we need to link the notion of mild formulation and the one of weak solution. This is given by the following the result:

Lemma 2.3. *If $f^{in} \in L^1(\mathcal{S})$ and $Q(f,f) \in L^1((0,T)\times\mathcal{S})$ then, Then the following statements are equivalent:*

i) $f \in C([0,T],L^1(\mathcal{S}))$ and is solution in the weak sense, i.e. *satisfies* (2.17).
ii) f is a mild solution, i.e. *satisfies* (2.18).

This result is well known and comes from a change of variable and an identification process, we refer to [5, 6] for LS equation or [10] for Boltzmann equation. It is important to take care with the boundary so that we proceed as in [22] with the origin of the characteristic σ in (2.18). The monotonicity in hypothesis (2.14) is here to separate continuously the characteristics coming from 0 and 1 and hence to be able to construct the weak solution from (2.18). Thanks to this property it is now sufficient prove the existence of mild solution.

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

$$\|Q(f,f)\|_{L^1(\mathcal{S})} \leq 2K\,\|f\|^2_{L^1(\mathcal{S})}\,, \tag{2.19}$$

$$\|Q(f,f) - Q(g,g)\|_{L^1(\mathcal{S})} \leq 2K\left(\|f\|_{L^1(\mathcal{S})} + \|g\|_{L^1(\mathcal{S})}\right)\|f-g\|_{L^1(\mathcal{S})}\,. \tag{2.20}$$

These latter ensure that Q maps $L^1(\mathcal{S})$ into itself and as a Lipschitz operator on any bounded subset of $L^1(\mathcal{S})$. Finally, we remark that for any $f \in L^1(\mathcal{S})$ and

$\varphi \in L^\infty(\mathcal{S})$,

$$\iint_{\mathcal{S}} Q(f,f)(p,r)\varphi(p,r)\,drdp = \frac{1}{2}\iint_{\mathcal{S}\times\mathcal{S}} a(p,r;p',r')f(p,r)f(p',r') \times \Big[\varphi(p+p',r^{\#}) - \varphi(p,r) - \varphi(p',r')\Big]dr'dp'drdp\,. \quad (2.21)$$

with $r^{\#} = (rp+r'p')/(p+p') \in (0,1)$. It is obtained by inversion of integrals applying Fubini's theorem, then changes of variable. In particular, when $\varphi = \mathbf{1}_{\mathcal{S}}$,

$$\iint_{\mathcal{S}} Q(f,f)(p,r)\,drdp \le 0\,. \quad (2.22)$$

And, if moreover $f \in L^1(\mathcal{S}, pdrdp)$, then

$$\iint_{\mathcal{S}} pQ(f,f)(p,r)\,drdp = 0\,. \quad (2.23)$$

Now, we claim the following proposition when u belongs to

$$\mathcal{B} = \{u \in C([0,T]) : 0 \le u(t) \le \rho\}\,.$$

Proposition 2.4. *Let $T > 0$ and $\rho > 0$ with u belongs to the associated set $\mathcal{B}$.$f^{in} \in L^1(\mathcal{S},(1+p)drdp)$, then there exists a unique nonnegative mild solution,* i.e. *satisfying* (2.18)*,*

$$f \in L^\infty\left(0,T;L^1(\mathcal{S},(1+p)drdp)\right)\,.$$

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

$$\iint_{\mathcal{S}} f(t,p,r)\,drdp \le \iint_{\mathcal{S}} f^{in}(p,r)\,drdp\,, \quad (2.24)$$

and

$$\iint_{\mathcal{S}} pf(t,p,r)\,drdp = \iint_{\mathcal{S}} pf^{in}(p,r)\,drdp\,. \quad (2.25)$$

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

Step 1. Existence and uniqueness. The local existence of a unique nonnegative solution $f \in L^\infty\left(0,T';L^1(\mathcal{S})\right)$, 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 (2.18) on a bounded subset of $L^\infty\left(0,T';L^1(\mathcal{S})\right)$. To that, we follow line-to-line [5] using properties (2.19) and (2.20).

Then, the global existence, for any time $T > 0$, is obtained using estimation (2.24), indeed by a classical argument we construct a unique solution on intervals $[0,T']$, $[T',2T']$, *etc.* So, it remains to prove (2.24), which follows from the integration of (2.18), using that $f^{in} \in L^1(\mathcal{S})$ and (2.22).

Step 2. Mass conservation. It remains to prove (2.25). We have to prove that indeed $f \in L^\infty\left(0,T;L^1(\mathcal{S},pdrdp)\right)$, so that $Q(f,f)$ too. But, identity (2.21) holds only for $\varphi \in L^\infty(\mathcal{S})$ and *a priori* $pQ(f,f)$ is not integrable. We follow the proof of [5, Lemma 4] which involves a regularization procedure using $a_P(p,r;p',r') = a(p,r;p',r')\,\mathbf{1}_{(0,P)}(p)\,\mathbf{1}_{(0,P)}(p')$ in (2.18) to construct a sequence of approximation $f_P \in L^\infty\left(0,T;L^1(\mathcal{S})\right)$ and to prove that it converge strongly toward the solution f when $P \to +\infty$ with

$$\iint_{\mathcal{S}} pf_P(t,p,r) \le C(T)\,,$$

for some constant $C(T) > 0$ obtained by a Gronwall's lemma. So, we obtain that $f \in L^\infty\big(0,T;L^1(\mathcal{S},(1+p)drdp)\big)$ and that $pQ(f,f)$ is integrable. Coming back to (2.18) and integrating it against p, it yields (2.25) thanks to (2.23). □

We close this section by stating the key argument to couple the constraint (2.6) to (2.5). It is given by the additional regularity of the pseudo-moment of the mild solution given in the following corollary.

Corollary 2.5. *Under hypotheses of Proposition 2.4,*

$$M(t) := \iint_{\mathcal{S}} rpf(t,p,r)\,drdp \leq \iint_{\mathcal{S}} pf^{in}(p,r)\,drdp\,,$$

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

$$M'(t) = \iint_{\mathcal{S}} \mathcal{V}(u(t),p,r)f(t,p,r)\,drdp\,. \tag{2.26}$$

Proof. The first estimation is a direct consequence of Proposition 2.4. Then, we use the formulation (2.17) and as a test function we let $\varphi_\varepsilon(p,r) = r\xi_\varepsilon(p)$ such that $\xi_\varepsilon \in C^1_c(\mathbb{R}_+$ and $\xi_\varepsilon(p) = p$ over $(2\varepsilon, 1/2\varepsilon)$ with $supp\,\xi \subset (\varepsilon,1/\varepsilon)$, thus

$$\begin{aligned}\iint_{\mathcal{S}} rf(t,p,r)\xi_\varepsilon(p)\,drdp = \iint_{\mathcal{S}} & rf^{in}(p,r)\xi_\varepsilon(p)\,drdp \\ &+ \int_0^t \iint_{\mathcal{S}} \frac{1}{p}\mathcal{V}(u(s),p,r)f(s,p,r)\xi_\varepsilon(p)\,drdpds \\ &\qquad + \int_0^t \iint_{\mathcal{S}} rQ(f,f)(s,p,r)\xi_\varepsilon(r)\,drdpds\,,\end{aligned}$$

Since we have $f \in L^\infty\big(0,T;L^1(\mathcal{S},(1+p)drdp)\big)$, by the use of (2.12) and (2.23), with the Lebesgue theorem we pass to the limit $\varepsilon \to 0$ and we get

$$M(t) = \iint_{\mathcal{S}} rpf^{in}(p,r)\,drdp + \int_0^t \iint_{\mathcal{S}} \mathcal{V}(u(s),p,r)f(s,p,r)\,drdpds\,.$$

So, we conclude that

$$\frac{d}{dt}M(t) = \iint_{\mathcal{S}} \mathcal{V}(u(t),p,r)f(t,p,r)\,drdp\,.$$

□

We are now ready to apply the second fix point to connect u and f in the system.

2.3.2. *Fix point on u.* Again we follow [5, 6], *i.e* we let $T > 0$ and we define the map

$$\mathcal{M} : u \in C([0,T]) \mapsto \tilde{u} = \left[\rho - \iint_{\mathcal{S}} rpf(t,p,r)\,drdp\right]_+\,,$$

where $[\,\cdot\,]_+$ is the positive part and f the unique mild solution on $[0,T]$ associated to u thanks to Proposition 2.4. It follows that $\mathcal{M}$ maps $\mathcal{B}$ into itself. Moreover, using (2.26)

$$t \mapsto \rho - \iint_{\mathcal{S}} rpf(t,p,r)\,drdp \in W^{1,\infty}(0,T)\,,$$

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

$$\frac{d}{dt}\tilde{u} = \begin{cases} 0\,, & \text{if } \displaystyle\iint_{\mathcal{S}} rpf(t,p,r)\,drdp \geq \rho\,, \\ -\displaystyle\iint_{\mathcal{S}} \mathcal{V}(u(t),p,r)f(t,p,r)\,drdp\,, & \text{otherwise.} \end{cases}$$

a.e. $t \in (0,T)$, see [43, Theorem 2.1.11]. Thus, for any $u \in \mathcal{B}$ by using hypothesis on the rates (H3), it yields

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

Next, we invoke Ascoli theorem to claim that $\mathcal{M}(\mathcal{B}) \subset \mathcal{B}$ is relatively compact in $C([0,T])$. Now, a Schauder fix point theorem would achieve the proof of Theorem 2.2. It remains to prove the continuity of the map $\mathcal{M}$. 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

$$\sup_{t\in(0,T)} \left| \iint_{\mathcal{S}} rpf_n(t,p,r)\,drdp - \iint_{\mathcal{S}} rpf(t,p,r)\,drdp \right| \\ \leq \sup_{t\in(0,T)} \iint_{\mathcal{S}} p\,|f_n(t,p,r) - f(t,p,r)|\;drdp\,.$$

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

$$\iint_{\mathcal{S}} rpf(t,p,r) < \rho \quad \forall t \in [0,T]\,,$$

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

$$u(t) = \mathcal{M}(u) = \rho - \iint_{\mathcal{S}} rpf(t,p,r) \geq 0\,.$$

This achieves the proof of Theorem 2.2.

3. Numerical approximation

3.1. **A conservative truncated formulation.** The discretization of the problem (1.1)-(1.2) gives rise to three main difficulties. First, the unboundedness of the space. 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 decided to proceed as in [2] and carry out a truncation of 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 Section 1.3 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 second issue arises when we look toward conservations of 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 to provide exact conservations at the discrete level.

The departing point is the formal identity (2.21). One can take $\varphi(u,v) = u\,\mathbf{1}_{(0,p)}(u)\,\mathbf{1}_{(0,r)}(v)$ for some $(p,r)\in\mathcal{S}$ and we formally get an expression of the form

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

where the coagulation reads now

$$\begin{aligned} &C(f,f)(p,r) \\ &\quad = \int_0^p\int_0^1\int_0^{p-u}\int_0^1 ua(u,v;u',v')\,\mathbf{1}_{(0,r)}(v^{\#})f(u,v)f(u',v')\,dv'du'dvdu \\ &\qquad\qquad - \int_0^p\int_0^r uL(f)(u,v)f(u,v)\,dvdu\,, \end{aligned} \tag{3.1}$$

where $v^{\#} = (uv+u'v')/(u+u')$. Now the coagulation operator has been reformulated in a manner well adapted to a finite volume scheme (the volumes averages of f are brought out directly). It remains to truncate the problem. It can be achieved in two different ways as mentioned in [2,17], the authors discuss about conservative and non-conservative form. These two options can be derived respectively by taking $a \coloneqq a\,\mathbf{1}_{(0,P)}(u+u')$ or $a \coloneqq a\,\mathbf{1}_{(0,P)}(u)\,\mathbf{1}_{(0,P)}(u')$. The first option avoids the formation of clusters larger than P thus it will preserve the mass, while the second induces a loss of polymers due to the creation of larger clusters than P. This latter is convenient to study gelation phenomenon, see [13] for a review on coagulation. Here, we restrict ourself to the conservative form and obtain the truncated operator by taking

$$L_P(f)(u,v) = \int_0^{P-u}\int_0^1 a(u',v';u,v)f(u',v')dv'du'\,.$$

Then, replacing L by L_P in (3.1) it yields, for any $(p,r)\in\mathcal{S}_P \coloneqq (0,P)\times(0,1)$, to

$$\begin{aligned} &C_P(f,f)(p,r) \\ &\quad = \int_0^p\int_0^1\int_0^{p-u}\int_0^1 ua(u,v;u',v')\,\mathbf{1}_{(0,r)}(v^{\#})f(u,v)f(u',v')\,dv'du'dvdu \\ &\qquad\qquad - \int_0^p\int_0^r uL_P(f)(u,v)f(u,v)\,dvdu\,. \end{aligned} \tag{3.2}$$

The last main issue lies in the discretization of (1.2), *i.e.* the algebraic constraint driving u. We will not be able to properly derive an approximation of $\mathbf{1}_{(0,r)}(v^{\#})$ in the coagulation operator which would allow us to control the sign of $\rho - \int_{\mathcal{S}_P} rpf(t,p,r)\,drdp$. Once again, we reformulate this constraint obtaining an evolution equation on u by a time derivation of it. Thus the problem (1.1)-(1.2) reads now

$$p\frac{\partial f}{\partial t} + \frac{\partial}{\partial r}(\mathcal{V}f) = \frac{\partial C_P(f,f)}{\partial p\partial r}, \quad (t,p,r)\in\mathbb{R}_+\times\mathcal{S}_P\,, \tag{3.3}$$

and

$$\frac{d}{dt}u(t) = -\iint_{\mathcal{S}_P}\mathcal{V}(u(t),p,r)f(t,p,r)\;drdp, \quad t\geq 0\,. \tag{3.4}$$

The boundary condition reads now

$$f = 0, \qquad \text{on}\;\; \partial\mathcal{S}_P\,, \tag{3.5}$$

and the initial data are

$$f(t=0,\cdot) = f^{in} \text{ over } \mathcal{S}_P \text{ and } u(t=0) = u^{in}\,. \tag{3.6}$$

It is now appropriate to introduce the technical assumptions used through this section:

H1. The initial density $f^{in} \in L^1(\mathcal{S}_P)$ is nonnegative and $u^{in} \geq 0$, with

$$\rho := u^{in} + \iint_{\mathcal{S}_P} rpf^{in}(p,r)\,drdp < +\infty\,. \tag{3.7}$$

H2. The coagulation rate $a \in L^\infty(\mathcal{S}_P \times \mathcal{S}_P)$ is nonnegative and

$$\|a\|_{L^\infty} \leq K\,. \tag{3.8}$$

H3. The rate functions $p \mapsto k(p,\cdot),\ l(p,\cdot) \in L^\infty\left(0,P;W^{1,\infty}(0,1)\right)$ are nonnegatives and

$$\|k\|_{L^\infty(0,P;W^{1,\infty})} + \|l\|_{L^\infty(0,P;W^{1,\infty})} \leq K\,. \tag{3.9}$$

H4. The function $r \mapsto \mathcal{V}(u,p,r)$ is a non-increasing function:

$$\partial_r \mathcal{V}(u,p,r) = \partial_r k\ u - \partial_r l \leq 0 \quad \text{a.e. } (u,p,r) \in \mathbb{R}_+ \times \mathcal{S}_P\,. \tag{3.10}$$

Remark 3.1. We emphasize that hypotheses 2 and 3 are not so restrictive in front of the truncation, it could allow unbounded rate on the full configuration space $\mathcal{S}$ locally bounded which seems reasonable.

We are now in position to give an alternative definition to our problem (2.5)-(2.6).

Definition 3.1 (Weak solutions 2)**.** Let $T > 0$, a cut-off $P > 0$ and let f^{in} and u^{in} satisfying (3.7). A weak solution to (3.3)-(3.4) on $[0,T)$ is a couple (f,u) of nonnegative functions, such that

$$f \in C\left([0,T);L^1(\mathcal{S}_P)\right) \quad \text{and} \quad u \in C([0,T)) \tag{3.11}$$

satisfying for all $t \in [0,T)$ and $\varphi \in C^2(\mathcal{S}_P)$

$$\begin{aligned}\iint_{\mathcal{S}_P} pf(t,p,r)\varphi(p,r)\,drdp &= \iint_{\mathcal{S}_P} pf^{in}(p,r)\varphi(p,r)\,drdp \\ + \int_0^t \iint_{\mathcal{S}_P} &\left(\mathcal{V}(u(s),p,r)f(s,p,r)\frac{\partial\varphi}{\partial r}(p,r) + C_P(s,p,r)\frac{\partial\varphi}{\partial p \partial r}(s,p,r)\right) drdpds \\ - \int_0^t \int_0^1 C_P(s,P,r)\frac{\partial\varphi}{\partial r}(s,P,r)\,drds &- \int_0^t \int_0^P C_P(s,r,1)\frac{\partial\varphi}{\partial p}(s,p,1)\,dpds\,,\end{aligned} \tag{3.12}$$

with

$$u(t) = u^{in} - \int_0^t \iint_{\mathcal{S}_P} \mathcal{V}(u(s),p,r)f(s,p,r)\,dpdrds\,. \tag{3.13}$$

Remark 3.2 (Consistence of Definition 3.1)*.* First, we emphasize that weak formulation (3.12) is classically obtained after multiplying (3.3) by p, then integrating over $(0,t) \times \mathcal{S}_P$. An integration by parts with respect to the boundary conditions (3.5). Note that the two last integrals in the right hand side correspond to the remaining terms coming from the integration of the coagulation. Second, the regularity (3.11) of f together with the definition of the coagulation operator (3.2) provide that for any $t \in [0,T)$ we have $C_P(f,f) \in L^\infty((0,t)\times\mathcal{S}_P)$, $C_P(f,f)(p=P) \in L^\infty((0,t)\times(0,1))$ and $C_P(f,f)(r=1) \in L^\infty((0,t)\times(0,P))$. Third, by virtue of hypothesis (H3), for any $U>0$ we get

$$\sup_{u\in(0,U)} ||\mathcal{V}(u,\cdot)||_{L^\infty(\mathcal{S}_P)} \le ||k||_{L^\infty(\mathcal{S}_P)}U + ||l||_{L^\infty(\mathcal{S}_P)} \le K(U+1)\,.$$

Thus, $\mathcal{V} \in L^\infty([0,t)\times\mathcal{S}_P)$. This ensures that equation (3.12)-(3.13) are well defined under such regularity and hypotheses.

Remark 3.3. A solution in the sense of Definition 3.1 regular enough, with an initial datum compactly supported in $(0,P)$, is also a solution in the sense of Definition 2.1, *i.e* on the entire space $\mathcal{S}$, at least up to a time T small enough. Indeed, since Q is Lipschitz by (2.20), the speed of propagation of the support of f is finite.

Remark 3.4. In general, the definition can be relaxed by taking the solution f belongs to $C\left([0,T);w-L^1(\mathcal{S}_P,pdrdp)\right)$ which is sufficient to define the formulation (3.12). Nevertheless, we will see that the sequence of approximation is in fact equicontinuous for the strong topology of $L^1(\mathcal{S}_P)$ thus Definition 3.1 remains stronger but true.

3.2. **The numerical scheme and convergence statement.** This section is devoted to introduce an approximation of the truncated problem presented in Section 3.1. 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 $[0,T]\times\mathcal{S}_P$ on which we will approach the problem (3.3-3.4). Once the scheme is established, we present the main result, namely the convergence in a sense defined later.

Formulation (3.3) allow us to use a finite volume method for the configuration space. This is approaching the average of the solution on volume controls at discrete times t_n for $n\in\{0,\dots,N\}$ 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 $\mathcal{S}_P$. For sake of simplicity, we consider a uniform mesh of $\mathcal{S}_P$ that is given, for some large integer J and I, by $(\Lambda_{j,i})_{(j,i)\in\{0,\dots,J\}\times\{0,\dots,I\}}$ where

$$\Lambda_{j,i} = (p_{j-1/2},p_{j+1/2})\times(r_{i-1/2},r_{i+1/2}) \subset \mathcal{S}_P\,,$$

such that $(p_{j-1/2})_{j\in\{0,\dots,J+1\}}$ and $(r_{i-1/2})_{i\in\{0,\dots,I+1\}}$ 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 3.5. We believe that for a non-uniform mesh it would work, we refer for instance to [2] for a non-uniform discretization of the so-called coagulation-fragmentation equation.

The average of the solution f to (3.3) at a time t_{n+1} on a cell $\Lambda_{j,i}$ is obtain by integration of (3.3) 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 to derive 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

$$f^n_{j,i} \approx \frac{1}{|\Lambda_{j,i}|}\int_{\Lambda_{j,i}} f(t_n,p,r)\,drdp\,,$$

The integration of (3.3) lets appear two types of fluxes which need to be approached. First, the transport term that accounts for the sorption phenomenon given by the r-derivative, leads to the numerical fluxes $(F^n_{j,i-1/2})_{(j,i)\in\{0,\dots,J\}\times\{0,\dots,I+1\}}$, hopefully consistent approximation of:

$$F^n_{j,i-1/2} \simeq \frac{1}{\Delta p}\int_{t_n}^{t_{n+1}}\int_{p_{j-1/2}}^{p_{j+1/2}} \mathcal{V}(u(t),p,r_{i-1/2})f(t,p,r_{i-1/2})\,dpdt\,,$$

We will use an Euler explicit scheme in time t. Moreover, we use the so-called first order upwinding method to get

$$F^n_{j,i-1/2} = \mathcal{V}^{n+}_{j,i-1/2}f^n_{j,i-1} - \mathcal{V}^{n-}_{j,i-1/2}f^n_{j,i}\,, \tag{3.14}$$

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

$$\mathcal{V}^n_{j,i-1/2} = \mathcal{V}(u^n,p_{j-1/2},r_{i-1/2})\,,$$

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

$$F^n_{j,-1/2} = F^n_{j,I+1/2} = 0\,, \tag{3.15}$$

which is in accordance with (3.5). Then the fluxes of coagulation given by the second order derivative is also approached by an Euler explicit method in time, namely our fluxes read

$$\begin{aligned}\mathcal{C}^n_{j-1/2,i-1/2} = {} & \sum_{j'=0}^{j-1}\sum_{i'=0}^{I}\sum_{j''=0}^{(j-1)-j'}\sum_{i''=0}^{I} p_{j'}a_{j',i';j'',i''}\delta^{i-1}_{j',i';j'',i''}f^n_{j',i'}f^n_{j'',i''}(\Delta p\Delta r)^2 \\ & - \sum_{j'=0}^{j-1}\sum_{i'=0}^{i-1}\sum_{j''=0}^{J-j'}\sum_{i''=0}^{I} p_{j'}a_{j',i';j'',i''}f^n_{j',i'}f^n_{j'',i''}(\Delta p\Delta r)^2\,,\end{aligned} \tag{3.16}$$

where the discrete coagulation rate is

$$a_{j,i;j,i'} = \frac{1}{|\Lambda_{j,i}|\times|\Lambda_{j',i'}|}\int_{\Lambda_{j,i}\times\Lambda_{j',i'}} a(p,r;p',r')\,drdpdr'dp'\,, \tag{3.17}$$

and the characteristic function $\mathbf{1}_{(0,r)}(v^{\#})$ is approached by

$$\delta^{i-1}_{j',i';j'',i''} = \begin{cases}1 & \text{if } V^{\#}_{j',i';j'',i''} = \frac{r_{i+1/2}p_{j+1/2}+r_{i'+1/2}p_{j'+1/2}}{p_{j-1/2}+p_{j-1/2}} < r_{i-1/2}\\ 0 & \text{otherwise.}\end{cases} \tag{3.18}$$

Finally, we use the convention that

$$\mathcal{C}^n_{-1/2,i-1/2} = \mathcal{C}^n_{j-1/2,-1/2} = 0, \quad \forall (j,i)\,. \tag{3.19}$$

Now, we are almost ready to define the scheme. Indeed, it remains to approach the initial data (3.6) which are classically obtained, for $(j,i)\in\{0,\dots,J\}\times\{0,\dots,I\}$, by

$$f^0_{j,i} = \frac{1}{|\Lambda_{j,i}|}\int_{\Lambda_{j,i}} f^{in}(p,r)\;drdp\,. \tag{3.20}$$

and which is nothing but

$$u^0 = u^{in}\,. \tag{3.21}$$

Thus, the scheme is defined as follows.

Definition 3.2 (Numerical scheme)**.** Let us consider the discretization mentioned above and a given initial data (3.20)-(3.21). The numerical scheme gives us a sequence $(f_{j,i}^n)_{n,j,i}$ and $(u^n)_n$, for $n \in \{0,\dots,N\}$ and $(j,i) \in \{0,\dots,J\}\times\{0,\dots,I\}$, defined recursively by

$$p_j f_{j,i}^{n+1} = p_j f_{j,i}^n - \frac{\Delta t}{\Delta r}\left(F_{j,i+1/2}^n - F_{j,i-1/2}^n\right) + \frac{\Delta t}{\Delta r \Delta p} C_{j,i}^n\,, \tag{3.22}$$

and

$$u^{n+1} = u^n - \Delta t \sum_{j=0}^{J}\sum_{i=0}^{I} F_{j,i-1/2}^n\, \Delta r \Delta p\,, \tag{3.23}$$

where

$$C_{j,i}^n = \left(\mathcal{C}_{j+1/2,i+1/2}^n - \mathcal{C}_{j+1/2,i-1/2}^n\right) - \left(\mathcal{C}_{j-1/2,i+1/2}^n - \mathcal{C}_{j-1/2,i-1/2}^n\right)\,. \tag{3.24}$$

In the above definition, the coagulation is written with fluxes defined by (3.16). But, note that it can be also expressed as follows

$$\begin{aligned} C_{j,i}^n = \sum_{j'=0}^{j}\sum_{i'=0}^{I}\sum_{i''=0}^{I} p_{j'} a_{j',i';j-j',i''} f_{j',i'}^n f_{j-j',i''}^n \delta_{j',i';j-j',i''}^{i,i-1} (\Delta p \Delta r)^2 \\ - \left(\sum_{j'=0}^{J-j}\sum_{i'=0}^{I} p_{j'} a_{j,i;j',i'} f_{j',i'}^n \Delta p \Delta r\right) f_{j,i}^n\, \Delta p \Delta r\,. \end{aligned} \tag{3.25}$$

where

$$\delta_{j',i';j-j',i''}^{i,i-1} = \begin{cases} 1 & \text{if } r_{i-1/2} \le V_{j',i';j'',i''}^{\#} < r_{i-1/2} \\ 0 & \text{otherwise.} \end{cases}$$

This is obtained when reordering summation behind (3.24). Such a formulation is not only simpler to implement numerically, but also useful in several estimations in the next section. We also remark, by virtue of (3.19) and (3.24), that the coagulation satisfy

$$\sum_{j=0}^{J}\sum_{i=0}^{I} C_{j,i}^n = 0, \quad \forall n \in \{0,\dots,N\}\,, \tag{3.26}$$

which will ensure mass conservation at the discrete level.

Now the scheme is stated, we focus on its convergence. This will be achieved by a well-suited construction of sequences of approximations. For this purpose, we let $h = \max(\Delta r, \Delta p, \Delta t)$.

Definition 3.3 (Sequences of approximations)**.** Let the sequences $(f_{j,i}^n)_{n,j,i}$ and $(u^n)_n$ construct by virtue of Definition 3.2. We define the piecewise constant approximation f_h on $[0,T)\times\mathcal{S}_P$ by

$$f_h(t,p,r) = \sum_{n=0}^{N-1}\sum_{j=0}^{J}\sum_{i=0}^{I} f_{j,i}^n\, \mathbf{1}_{\Lambda_{j,i}}(p,r)\, \mathbf{1}_{[t_n,t_{n+1})}(t)\,, \tag{3.27}$$

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

$$\tilde{f}_h(t,p,r) = \sum_{n=0}^{N-1}\sum_{j=0}^{J}\sum_{i=0}^{I}\left(\frac{f_{j,i}^{n+1}-f_{j,i}^{n}}{\Delta t}(t-t_n)+f_{j,i}^{n}\right) \times \mathbf{1}_{\Lambda_{j,i}}(p,r)\,\mathbf{1}_{[t_n,t_{n+1})}(t)\,. \tag{3.28}$$

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

$$u_h(t) = \sum_{n=0}^{N-1} u^n\,\mathbf{1}_{[t_n,t_{n+1})}(t), \quad \text{on } [0,T)\,. \tag{3.29}$$

Here, we mention that under such definition both approximations satisfy at time $t=0$ the same initial condition which is given by $f_h(0,p,r) = \tilde{f}_h(0,p,r) = f_h^{in}(p,r)$ where

$$f_h^{in}(p,r) = \sum_{(j,i)\in\sigma_{J,I}} f_{j,i}^{0}\,\mathbf{1}_{\Lambda_{j,i}}(p,r), \quad \text{on } \mathcal{S}_P\,. \tag{3.30}$$

and that $u_h(0) = u^{in}$. We are now ready to state the convergence result we obtain.

Theorem 3.4 (Convergence)**.** *Let $T>0$, assume that f^{in} and u^{in} satisfy (H1), and that hypotheses (H2) to (H4) are fulfilled. Moreover, we make the stability assumption that*

$$4\frac{\Delta t}{\Delta r}||\mathcal{V}||_{L^\infty((0,U_T)\times\mathcal{S}_P)} < 1 \text{ and } 2KM^{in}(1+P)\Delta t < 1\,, \tag{3.31}$$

where

$$U_T = e^{KM^{in}T}u^{in} \text{ and } M^{in} = \int_{\mathcal{S}_p} f^{in}(p,r)\,drdp\,. \tag{3.32}$$

Then there exists a couple (f,u) solution of the problem (3.3-3.4) in the sense of Definition 3.1 such that, up to a subsequence (not relabeled)

$$f_h \underset{h\to 0}{\longrightarrow} f, \qquad w-L^1((0,T)\times\mathcal{S}_P)\,, \tag{3.33}$$

$$\tilde{f}_h \underset{h\to 0}{\longrightarrow} f, \qquad C\left([0,T];w-L^1(\mathcal{S}_P)\right)\,, \tag{3.34}$$

$$u_h \underset{h\to 0}{\longrightarrow} u, \qquad \forall t\in[0,T]\,. \tag{3.35}$$

with $\left\|f_h^{-}\tilde{f}_h\right\|_{L^\infty(0,T;L^1(\mathcal{S}_P))} \to 0$ *when* $h\to 0$.

Remark 3.6. At this stage, we emphasize that hypothesis (3.31) involved in Theorem 3.4 is classical. The first one is the so-called *Courant-Friedrich-Lax* condition (or CFL condition) which ensures a well-know convex formulation of the transport part. The second is to control the sign of the coagulation term.

For technical reasons we consider a carefully reconstruction of the coagulation term. This one involves the coagulation kernel which is approached by

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

where the $a_{j,i;j',i'}$ are given by (3.17). A classical result of piecewise approximation, since a satisfy (3.8), is

$$a_h \underset{h\to 0}{\longrightarrow} a, \quad L^1(\mathcal{S}_P).$$

Further, we mention that a_h converges towards a a.e. $\mathcal{S}_P \times \mathcal{S}_P$, which holds true up to a subsequence. Also, we will reconstruct the characteristic function (3.18), this delicate point responsible of a lack of conservation in our scheme will be discussed later, as well as the rate of sorption $\mathcal{V}$.

Remark 3.7. In the remainder of the paper most of the result will involve more extraction of sequences, so that, for sake of clarity, we use the same index even for all the sequences, even if we extract a new subsequence of the previous one.

3.3. **Estimations and weak compactness.** The aim of this section is to introduce the well-suited estimations leading to the required compactness to prove Theorem 3.4. The method used here has been extensively developed in the field of coagulation-fragmentation equations and/or 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 of all, we introduce here some useful notation which will help us lighten the next computation:

$$
\begin{aligned}
P_h(p) &= \sum_{j=0}^{J} p_j\, \mathbf{1}_{[p_{j-1/2},p_{j+1/2})}\,, & R_h(r) &= \sum_{i=0}^{I} r_i\, \mathbf{1}_{[r_{i-1/2},r_{i+1/2})}\,,\\
P_h^-(p) &= \sum_{j=0}^{J} p_{j-1/2}\, \mathbf{1}_{[p_{j-1/2},p_{j+1/2})}\,, & R_h^-(r) &= \sum_{i=0}^{I} r_{i-1/2}\, \mathbf{1}_{[r_{i-1/2},r_{i+1/2})}\,,\\
P_h^+(p) &= \sum_{j=0}^{J} p_{j+1/2}\, \mathbf{1}_{[p_{j-1/2},p_{j+1/2})}\,, & R_h^+(r) &= \sum_{i=0}^{I} r_{i+1/2}\, \mathbf{1}_{[r_{i-1/2},r_{i+1/2})}\,.
\end{aligned}
$$

and

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

Moreover, for sake of conciseness we denote

$$
\sigma \coloneqq \{0,\dots,J\} \times \{0,\dots,I\}\,,
$$

when no confusion on I and J holds. Then, as long as it does not entail any ambiguity, we use

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

Also, we denote $l=(j,i)$, $l'=(j',i')$ and $l''=(j'',i'')$. Thus, the summation notation in a compact form are

$$\sum_{j=0}^{J}\sum_{i=0}^{I}=\sum_{l\in\sigma},$$

$$\sum_{j=0}^{J}\sum_{i=0}^{I}\sum_{j'=0}^{J-j}\sum_{i'=0}^{I}=\sum_{l\in\sigma}\sum_{l'\in\sigma^*},$$

$$\sum_{j'=0}^{J}\sum_{i'=0}^{I}\sum_{j''=0}^{J-j'}\sum_{i''=0}^{I}=\sum_{l'\in\sigma}\sum_{l''\in\sigma^*}.$$

3.3.1. *Discrete estimations.* To begin, we establish some properties of the sequences constructed in Definition 3.2. We emphasize that the original continuous problem involves, a decreased of the moment of order 0 (2.22), while the p-moment of order 1 (2.23) is conserved and the total balance (1.2) 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 3.2, given by

$$M_{0,h}^n=\sum_{l\in\sigma} f_{j,i}^n\,\Delta r\Delta p, \quad \text{and} \quad M_{1,h}^n=\sum_{l\in\sigma} p_j f_{j,i}^n\,\Delta r\Delta p\,. \tag{3.36}$$

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

Proposition 3.5 (Non-negativeness, moments and conservation)**.** *Let f^{in} and u^{in} satisfying (H1), together with $(f_{j,i}^n)_{(n,j,i)\in\sigma}$ and $(u^n)_n$ construct by virtue of Definition 3.2. We assume that the stability condition* (3.31) *holds true. Then, the sequences $(f_{j,i}^n)_{(n,j,i)}$ and $(u^n)_n$ are both nonnegatives and satisfy for all $n\in\{0,\dots,N-1\}$:*

$$0\le M_{0,h}^{n+1}\le M_{0,h}^n\le M^{in}\,,$$

and $n\in\{0,\dots,N\}$

$$0\le M_{1,h}^n=M_{1,h}^0 \quad \textit{and} \quad 0\le u^n\le U_T\,,$$

where M^{in} and U_T are both given in (3.32)*. Moreover, there exist a constant $C>0$ independent on h such that for all $n\in\{0,\dots,N-1\}$ we have*

$$\sum_{(j,i)\in\sigma}|f_{j,i}^{n+1}-f_{j,i}^n|\Delta r\Delta p\le C\Delta t \quad \textit{and} \quad |u^{n+1}-u^n|\le C\Delta t\,.$$

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

$$0\le M_{0,h}^n\le M^{in}, \quad \text{and} \quad u^n\le(1+\Delta t K M^{in})^n u^0\,.$$

We easily check that it is true for $n=0$. Indeed, the nonnegativeness is given by hypothesis (H1) on f^{in} and u^{in} together with the initial approximation (3.20)-(3.21). Then, by the definitions of f_h^{in} in (3.30) and the constant M^{in} in (3.32), we get

$$M_{0,h}^0=\iint_{\mathcal{S}_P} f_h^{in}(p,r)\;drdp=M^{in}, \tag{3.37}$$

and

$$M_{1,h}^0 = \iint_{\mathcal{S}_P} P_h(p) f_h^{in}(p,r)\; drdp \leq PM^{in}. \tag{3.38}$$

The rest of the proof is separated in four steps. We start by estimate the moments, next we bound u^{n+1}, then we prove the nonnegativeness of f^{n+1} and finally we prove the last two "time" estimations of the proposition.

Step 1. Moments estimation. We first remark the sorption fluxes F^n are null at the boundary, it is (3.15), thus

$$\sum_{i=0}^{I} (F_{j,i+1/2}^n - F_{j,i-1/2}^n) = 0, \quad \forall j\,.$$

It remains to estimate the contribution of the coagulation in the moments. The first order moment is naturally conserved from the construction of our scheme, it is (3.26). These two remarks lead, by equation (3.22) giving the $f_{j,i}^{n+1}$, to the fact that

$$M_{1,h}^{n+1} = M_{1,h}^n\,.$$

Now, for the zeroth order moment, we estimate

$$\sum_{l\in\sigma} \frac{1}{p_j} C_{j,i}^n = \sum_{l\in\sigma}\sum_{l'\in\sigma^*} \frac{p_j}{p_{j+j'}} a_{j,i;j',i'} f_{j,i}^n f_{j',i'}^n\,(\Delta p \Delta r)^2 \\ - \sum_{l\in\sigma}\sum_{l'\in\sigma^*} \frac{p_{j'}}{p_j} a_{j,i;j',i'} f_{j',i'}^n f_{j,i}^n\,(\Delta p \Delta r)^2\,,$$

which is obtained from expression (3.25) after inverting and re-indexing the summation. Next, we remark that $-p_{j'}/p_j \leq -p_{j'}/p_{j+j'}$ and by nonnegativeness of $(f_{j,i}^n)_{(j,i)\in\sigma}$ and $a_{j,i,j',i'}$ together with its symmetry, we get

$$\sum_{l\in\sigma} \frac{1}{p_j} C_{j,i} \leq 0.$$

It proves the discrete zeroth order moment decreases which is the desired property.

Step 2. properties of u^{n+1}. By definition of the fluxes F^n in (3.14), the nonnegativeness of $(f_{j,i}^n)_{(j,i)}$ and hypothesis (H3) on the rate $\mathcal{V}$, we get that

$$F_{j,i-1/2}^n \leq \mathcal{V}_{j,i-1/2}^{n+} f_{j,i-1}^n \leq K u^n f_{j,i-1}^n\,.$$

which implies by the expression of u^{n+1} in (3.23) that

$$u^{n+1} \geq \left(1 - K\Delta t \sum_{l\in\sigma} f_{j,i}^n \Delta p \Delta r\right) u^n\,.$$

Finally, since we hypothesized that $M_{0,h}^n \geq 0$ is bounded by M^{in}, we get

$$u^{n+1} \geq \left(1 - KM^{in}\Delta t\right) u^n.$$

This latter entails the nonnegativeness of u^{n+1} by the stability assumption (3.31). It remains to bound u^{n+1}. Indeed, we have

$$u^{n+1} \leq u^n + \Delta t \sum_{l\in\sigma} V_{j,i-1/2}^{n-} f_{j,i} \Delta p \Delta r \leq (1 + \Delta t K M^{in}) u^n\,.$$

Step 3. Nonnegativeness 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 (3.14) and since we have $\mathcal{V}^n_{j,i-1/2} = \mathcal{V}^{n+}_{j,i-1/2} - \mathcal{V}^{n-}_{j,i-1/2}$, we get the following decomposition

$$F^n_{j,i+1/2} - F^n_{j,i-1/2} = (\mathcal{V}^n_{j,i+1/2} - \mathcal{V}^n_{j,i-1/2}) f^n_{j,i} \\ + \mathcal{V}^{n-}_{j,i+1/2}(f^n_{j,i} - f^n_{j,i+1}) + \mathcal{V}^{n+}_{j,i-1/2}(f^n_{j,i} - f^n_{j,i-1})\,. \tag{3.39}$$

Now, we denote by

$$A^n_{j,i} = \frac{1}{\Delta r}\int_{r_{i-1/2}}^{r_{i+1/2}} \left(-\frac{\partial}{\partial r}\mathcal{V}(u^n, p_{j-1/2}, r)\right) dr = \frac{\mathcal{V}^n_{j,i-1/2} - \mathcal{V}^n_{j,i+1/2}}{\Delta r}\,, \tag{3.40}$$

which is nonnegative for any $(j,i) \in \sigma$ by the monotonicity hypothesis (H4). It results from the formulation (3.39) that

$$\frac{1}{2} f^n_{j,i} - \frac{\Delta t}{\Delta r}\left(F^n_{j,i+1/2} - F^n_{j,i-1/2}\right) = \Delta t A^n_{j,i} f^n_{j,i} \\ + \frac{1}{4}\Big[\big(1 - 4\frac{\Delta t}{\Delta r}\mathcal{V}^{n-}_{j,i+1/2}\big) f^n_{j,i} + 4\frac{\Delta t}{\Delta r}\mathcal{V}^{n-}_{j,i+1/2} f^n_{j,i+1}\Big] \\ + \frac{1}{4}\Big[\big(1 - 4\frac{\Delta t}{\Delta r}\mathcal{V}^{n+}_{j,i-1/2}\big) f^n_{j,i} + 4\frac{\Delta t}{\Delta r}\mathcal{V}^{n+}_{j,i-1/2} f^n_{j,i-1}\Big], \tag{3.41}$$

Thus, the nonnegativeness of the $A^n_{j,i}$ in (3.40) and the convex combination of the nonnegative $f^n_{j,i}$, we get by the definition of the $f^{n+1}_{j,i}$ in (3.22) that

$$f^{n+1}_{j,i} \geq \left(\frac{1}{2} - \Delta t \sum_{j'=0}^{J-j}\sum_{i'=0}^{I} p_{j'} a_{j,i;j',i'} f^n_{j',i'} \Delta p \Delta r\right) f^n_{j,i}\,.$$

We conclude using hypothesis (H2) on the coagulation kernel, the stability assumption (3.31) and estimation (3.38) that

$$f^{n+1}_{j,i} \geq \frac{1}{2}\left(1 - 2KPM^{in}\Delta t\right) f^n_{j,i} \geq 0\,.$$

Step 4. Time estimation. From the definition of $f^{n+1}_{j,i}$ in (3.22), we easily obtain

$$|f^{n+1}_{j,i} - f^n_{j,i}|\Delta r \Delta p \leq \Delta t \frac{1}{p_j}|F^n_{j,i+1/2} - F^n_{j,i-1/2}|\Delta p + \Delta t\frac{1}{p_j}|C^n_{j,i}|\,.$$

On the one hand, we have from the definition of the discrete coagulation in (3.25) and hypothesis (H1) that

$$\sum_{(j,i)\in\sigma} \frac{1}{p_j}|C^n_{j,i}| \leq 2KPM^{in\,2}\,.$$

On the other hand, since for all $j \in \{0,\ldots,J\}$ we have $p_j \geq \Delta p/2$, then

$$\sum_{(j,i)\in\sigma} \frac{\Delta p}{p_j}|F^n_{j,i+1/2} - F^n_{j,i-1/2}| \leq 8M^{in} \sup_{u\in(0,U_T)} ||\mathcal{V}(u,\cdot)||_{L^\infty(\mathcal{S}_P)}\,.$$

Thus, summing the first inequality together with the two last ones we prove the required estimation. Finally, we remark that from the expression of u^{n+1} in (3.23), we have

$$u^{n+1} - u^n = \Delta t \sum_{(j,i)\in\sigma} F^n_{j,i-1/2}.$$

We have to bound the fluxes (3.14). Indeed, we have for any $(j,i)\in\sigma$ and $i\neq 0$

$$\left|F^n_{j,i-1/2}\right| \leq \sup_{u\in(0,U_T)} ||\mathcal{V}(u,\cdot)||_{L^\infty(\mathcal{S}_P)}(f^n_{j,i-1}+f^n_{j,i})\,,$$

and then summing over σ we get

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

It 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 3.6. *Under hypothesis of Proposition 3.5. Let the sequences of approximations $(f_h)_h$, $(\tilde{f}_h)_h$ and $(u_h)_h$ construct by Definition 3.3. Then, for all discretization parameter h,*

$$f_h \in L^\infty(0,T;L^1(\mathcal{S}_P)) \quad \text{and} \quad \tilde{f}_h \in C([0,T];L^1(\mathcal{S}_P))$$

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

$$\iint_{\mathcal{S}_P} f_h(t,r,p)\;drdp \leq \iint_{\mathcal{S}_P} f_h(s,r,p)\;drdp \leq M^{in}, \quad \forall t\geq s\,, \tag{3.42}$$

and

$$\iint_{\mathcal{S}_P} P_h(p) f_h(t,r,p)\;drdp = \iint_{\mathcal{S}_P} P_h(p) f^{in}_h(r,p)\;drdp, \quad \forall t\in[0,T)\,. \tag{3.43}$$

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

$$0\leq \iint_{\mathcal{S}_P} \tilde{f}_h(t,r,p)\;drdp \leq M^{in}, \quad \forall t\in[0,T]\,, \tag{3.44}$$

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

$$\left\|\tilde{f}_h(t,\cdot)-\tilde{f}_h(s,\cdot)\right\|_{L^1(\mathcal{S}_P)} \leq C|t-s|, \quad \forall s,t\in[0,T]\,. \tag{3.45}$$

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

$$\|u_h\|_{L^\infty(0,T)} \leq U_T, \quad \text{and} \quad \|u_h\|_{BV(0,T)} < CT\,. \tag{3.46}$$

Proof. The regularity and non negativeness of the sequences $(f_h)_h$ and $(u_h)_h$ readily follow from Proposition 3.5 and Definition 3.3. And for now, by the same arguments, it is clear that $\tilde{f}_h\in L^\infty(0,T;L^1(\mathcal{S}_P))$. Next, (3.42) and (3.43) follow from the properties of the discrete moment in Proposition 3.5, by a simple reformulation using the definition of f_h in 3.27. Then, for all $n\in\{0,\dots,N-1\}$ and $t\in[t_n,t_{n+1})$,

$$\frac{f^{n+1}_{j,i}-f^n_{j,i}}{\Delta t}(t-t_n)+f^n_{j,i} = \frac{(t-t_n)}{\Delta t} f^{n+1}_{j,i} + \left(1-\frac{(t-t_n)}{\Delta t}\right) f^n_{j,i}\,. \tag{3.47}$$

Thus, by definition of $\tilde{f}_h$ in 3.28, the discrete moment (3.36) and the convex combination mentioned above, we have for all $t\in[0,T]$:

$$0\leq \iint_{\mathcal{S}_P} \tilde{f}_h(t,r,p)\;drdp \leq \sup_{n\in\{0,\dots,N-1\}} \max(M^{n+1}_{0,h},M^n_{0,h}) \leq M^{in}\,.$$

and that $\tilde{f}_h$ are nonnegatives. It provides the uniform bound (3.44). Next, estimation (3.45) is against a direct consequence of Proposition 3.5 (last estimation). It provides the regularity in time of the sequence $\tilde{f}_h$. Finally, (3.46) is a consequence of Proposition 3.5 and the definition of u_h in (3.29).

□

Before coming back to the proof of Theorem 3.4, we emphasize on the fact that, as mentioned before, our scheme preserves the mass (3.43). Nevertheless, the algebraic condition (1.2), transformed into (3.4) is no more preserved at the discrete level. The following corollary is not use in the demonstration of the convergence, but only state that the lack of mass that occurs in our scheme can be control. Indeed, the deviation from the initial value is of magnitude Δr.

Corollary 3.7. *Under hypotheses of Proposition 3.5, for any $n \in \{0, \dots, N\}$ we define*

$$\rho^n := u^n + \sum_{(j,i)\in\sigma} r_i p_j f^n_{j,i},$$

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

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

Proof. We remark that summing (3.22) tested against r_i and with (3.23), we get

$$\rho^{n+1} - \rho^n = \Delta t \sum_{(j,i)\in\sigma} r_i C^n_{j,i}.$$

Then by (3.24), we obtain

$$\sum_{(j,i)\in\sigma} r_i C^n_{j,i} = \sum_{i=0}^{I} C_{J+1/2,i+1/2} \Delta r.$$

Combining these two equalities and by definition of the flux (3.16) and the bound M^{in} in (3.32), we get

$$\left|\rho^{n+1} - \rho^n\right| \leq 2KPM^{in2}\Delta r \Delta t,$$

which ends the proof. □

3.3.2. *Weak compactness.* We introduced, from the scheme established in Definition 3.2, sequences of approximations in Definition 3.3 satisfying the properties stated in Corollary 3.6 that suppose to approach the solution to our problem. An important issue in proving this result is to get the convergence, towards some functions, of these sequences in a sense that allow us to obtain an enough regular solution to (3.3)-(3.4). The answer to this issue is obtain by 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 Theorem [24], also we refer to [8, Chap. II, Theorem 22] for a probabilistic approach. Indeed, since $f^{in} \in L^1(\mathcal{S}_P)$ is nonnegative, there exists

$$\begin{gathered} \phi \in C^1([0,+\infty)) \text{ nonnegative, convex, with concave derivative,} \\ \text{with } \phi(0) = 0, \quad \phi'(0) = 0, \quad \text{and} \quad \frac{\phi(r)}{r} \underset{r\to+\infty}{\longrightarrow} +\infty\,, \end{gathered} \tag{3.48}$$

such that

$$\iint_{\mathcal{S}_P} \phi(f^{in}(p,r))\, drdp < +\infty\,. \tag{3.49}$$

Therefore, proving that (3.49) 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 3.8. *Let ϕ satisfying* (3.48) *such that* (3.49) *holds true. Then, there exists $C \geq 0$ independent on h, such that for any $t \in [0, T)$, we have*

$$\iint_{\mathcal{S}_P} \phi(f_h^{\Delta t}(t,p,r))\, drdp \leq e^{CT} \int_{\mathcal{S}_R} \phi(f^{in}(p,r))\, drdp\,. \tag{3.50}$$

and

$$\iint_{\mathcal{S}_P} \phi(\tilde{f}_h^{\Delta t}(t,p,r))\, drdp \leq e^{CT} \int_{\mathcal{S}_R} \phi(f^{in}(p,r))\, drdp\,. \tag{3.51}$$

Proof. Let us derive first (3.51) from (3.50). By the definition of $\tilde{f}_h$ in (3.28), the convex combination (3.47), and since ϕ is convex by (3.48), we have for any $t \in [0, T]$

$$\begin{aligned}\iint_{\mathcal{S}_P} \phi(\tilde{f}_h(t,p,r))\ drdp \leq \sup_{n\in\{0,\dots,N\}} \sum_{(j,i)\in\sigma} \phi(f_{j,i}^n)\Delta r \Delta p \\ \leq \sup_{t\in[0,T]} \int_{\mathcal{S}_P} \phi(f_h(t,p,r))\ drdp\end{aligned}$$

Thus, it remains to prove (3.50) to conclude. We split the computation into two parts, in order to treat first the transport part and then the coagulation.

Step 1. The transport. This first part involves the convexity of ϕ and is closely related to the estimation done in [16, Lemma 3.5]. Indeed, let us denote the intermediate value:

$$\tilde{f}_{j,i}^n = f_{j,i}^n - \frac{\Delta t}{\Delta r}(F_{j,i+1/2}^n - F_{j,i-1/2}^n)\,. \tag{3.52}$$

From the convex formulation (3.41), we easily obtain for any $(j, i) \in \sigma$ the following expression

$$\begin{aligned}\tilde{f}_{j,i}^n = (\frac{1}{2} + \Delta t A_{j,i}^n) f_{j,i}^n + \frac{1}{4}\Big[\big(1 - 4\frac{\Delta t}{\Delta r}\mathcal{V}_{j,i+1/2}^{n-}\big) f_{j,i}^n + 4\frac{\Delta t}{\Delta r}\mathcal{V}_{j,i+1/2}^{n-} f_{j,i+1}^n\Big] \\ + \frac{1}{4}\Big[\big(1 - 4\frac{\Delta t}{\Delta r}\mathcal{V}_{j,i-1/2}^{n+}\big) f_{j,i}^n + 4\frac{\Delta t}{\Delta r}\mathcal{V}_{j,i-1/2}^{n+} f_{j,i-1}^n\Big]\end{aligned} \tag{3.53}$$

with the convention $f_{j,I+1} = f_{j,-1} = 0$ and $A_{j,i}^n$ the discrete gradient defined in (3.40). Our aim is to write $\tilde{f}_{j,i}^n$ as a complete convex combination of the $f_{j,i}^n$'s together with 0. Thus, let us introduce the coefficients

$$\begin{gathered}\lambda_{j,i}^0 = \frac{1}{2} + \Delta t A_{j,i}^n, \\ \lambda_{j,i}^1 = \frac{1}{4} - \frac{\Delta t}{\Delta r}\mathcal{V}_{j,i+1/2}^{n-}\,, \quad \lambda_{j,i}^2 = \frac{\Delta t}{\Delta r}\mathcal{V}_{j,i+1/2}^{n-}\,, \\ \lambda_{j,i}^3 = \frac{1}{4} - \frac{\Delta t}{\Delta r}\mathcal{V}_{j,i-1/2}^{n+}\,, \quad \lambda_{j,i}^4 = \frac{\Delta t}{\Delta r}\mathcal{V}_{j,i-1/2}^{n+}\,,\end{gathered}$$

which are non negatives since $A_{j,i}^n \geq 0$, by monotonicity hypothesis (H4), and by stability assumption (3.31). Then, by virtue of hypothesis (H3) and since u_h satisfies the bound (3.46), we get that

$$||\partial_r \mathcal{V}(u,p,r)||_{L^\infty((0,U_T)\times\mathcal{S}_P)} = ||\partial_r k||_{L^\infty(\mathcal{S}_P)} U_T + ||\partial_r k||_{L^\infty(\mathcal{S}_P)} \leq K_T\,,$$

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

$$\tilde{\lambda}^k_{j,i} = \frac{\lambda^k_{j,i}}{1+2K_T\Delta t}, \qquad k=0,\dots,4\,.$$

From (3.53), it follows that

$$\frac{\tilde{f}^n_{j,i}}{1+2K_T\Delta t} = \tilde{\lambda}^0_{j,i} f^n_{j,i} + \tilde{\lambda}^1_{j,i} f^n_{j,i} + \tilde{\lambda}^2_{j,i} f^n_{j,i+1} + \tilde{\lambda}^3_{j,i} f^n_{j,i} + \tilde{\lambda}^4_{j,i} f^n_{j,i-1}\,.$$

It remains to remark that

$$0 \le 1 - \tilde{\lambda}^5_{j,i} = \sum_{k=0}^{4} \tilde{\lambda}^k_{j,i} = \frac{1+a^n_{j,i}\Delta t}{1+2K_T\Delta t} \le \frac{1}{2}\,,$$

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

$$\phi\left(\frac{\tilde{f}^n_{j,i}}{1+2K\Delta t}\right) \le \tilde{\lambda}^0_{j,i}\phi(f^n_{j,i}) + \tilde{\lambda}^1_{j,i}\phi(f^n_{j,i}) + \tilde{\lambda}^2_{j,i}\phi(f^n_{j,i+1}) + \tilde{\lambda}^3_{j,i}\phi(f^n_{j,i}) + \tilde{\lambda}^4_{j,i}\phi(f^n_{j,i-1})\,.$$

Then, summing over i, reordering the sum and remarking that

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

it is straight forward that

$$\sum_{(j,i)\in\sigma} \phi\left(\frac{\tilde{f}^n_{j,i}}{1+2K\Delta t}\right) \le \sum_{(j,i)\in\sigma} \phi(f^n_{j,i})\,. \tag{3.54}$$

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

$$\phi(\delta x) \le \delta^2\phi(x), \quad \forall(\delta,x)\in[1,+\infty)\times\mathbb{R}_+\,. \tag{3.55}$$

We conclude this intermediate estimation, using (3.54) and (3.55),

$$\sum_{(j,i)\in\sigma} \phi(\tilde{f}^n_{j,i}) \le (1+2K_T\Delta t)^2 \sum_{(j,i)\in\sigma} \phi(f^n_{j,i})\,. \tag{3.56}$$

Step 2. The coagulation. Now we get the first part of our estimation, it remains to take into account the coagulation. We estimate the following quantity

$$\sum_{(j,i)\in\sigma} \phi(f^{n+1}_{j,i}) - \phi(\tilde{f}^n_{j,i}) \le \sum_{(j,i)\in\sigma} (f^{n+1}_{j,i} - \tilde{f}^n_{j,i})\phi'(f^{n+1}_{j,i})\,,$$

which comes from the convexity of ϕ. By definition of the $\tilde{f}^n_{j,i}$ in (3.52) together with the expression of $f^{n+1}_{j,i}$ in (3.22)

$$\sum_{(j,i)\in\sigma} \phi(f^{n+1}_{j,i}) - \phi(\tilde{f}^n_{j,i}) \le \frac{\Delta t}{\Delta p\Delta r} \sum_{(j,i)\in\sigma} C_{j,i}\phi'(f^{n+1}_{j,i})\,. \tag{3.57}$$

Nonnegativity of f^n yields

$$C_{j,i} \le K \sum_{j'=0}^{j} \sum_{i'=0}^{I} \sum_{i''=0}^{I} p_{j'} f^n_{j',i'} f^n_{j-j',i''} \delta^{i,i-1}_{j',i';j-j',i''} (\Delta p\Delta r)^2\,.$$

then summing over j and i, we get

$$\begin{aligned}\sum_{(j,i)\in\sigma}\sum_{j'=0}^{j}\sum_{i'=0}^{I}\sum_{i''=0}^{I} p_{j'} f^n_{j',i'} f^n_{j-j',i''}\delta^{i,i-1}_{j',i';j-j',i''}\phi'(f^{n+1}_{j,i})\,(\Delta p\Delta r)^2 \\ = \sum_{(j',i')\in\sigma} p_{j'} f^n_{j',i'}\left(\sum_{(j'',i'')\in\sigma^*} f^n_{j'',i''}\phi'(f^{n+1}_{j'+j'',i^\#})\right)(\Delta p\Delta r)^2 \quad (3.58)\end{aligned}$$

where $i^\# \in \{0,\dots,I\}$ such that $\delta^{i^\#,i^\#-1}_{j',i';j'',i''}=1$. Now, we remark as in [2, Lemma 3.2] and proving for instance with the help of [29, Lemma B.1] that when ϕ fulfills (3.48), we get that

$$x\phi'(y) \le \phi(x)+\phi(y), \quad \forall (x,y)\in\mathbb{R}^2_+\,.$$

Using this property and the bound on the first moment (3.38) in (3.58), it follows

$$\begin{aligned}&\sum_{(j,i)\in\sigma} C_{j,i}\phi'(f^{n+1}_{j,i}) \\ &\le K\sum_{(j',i')\in\sigma} p_{j'} f^n_{j',i'}\left(\sum_{(j'',i'')\in\sigma}\phi(f^n_{j'',i''})+\sum_{(j'',i'')\in\sigma}\phi(f^{n+1}_{j'+j'',i^\#})\right)(\Delta p\Delta r)^2 \\ &\le KPM^{in}\left(\sum_{(j,i)\in\sigma}\phi(f^n_{j,i})+\sum_{(j,i)\in\sigma}\phi(f^{n+1}_{j,i})\right)\Delta p\Delta r\,. \quad (3.59)\end{aligned}$$

Combining both (3.56) and (3.59) with (3.57), we get

$$\begin{aligned}\sum_{(j,i)\in\sigma}\phi(f^{n+1}_{j,i}) \le (1+2K_T\Delta t)^2\sum_{(j,i)\in\sigma}\phi(f^n_{j,i}) \\ + PKM^{in}\Delta t\left(\sum_{(j,i)\in\sigma}\phi(f^n_{j,i})+\sum_{(j,i)\in\sigma}\phi(f^{n+1}_{j,i})\right).\end{aligned}$$

or in other term, when $\Delta t<1$

$$\begin{aligned}(1-PKM^{in}\Delta t)\left(\sum_{(j,i)\in\sigma}\phi(f^{n+1}_{j,i})-\sum_{(j,i)\in\sigma}\phi(f^n_{j,i})\right) \\ \le \left(4K_T(K_T+1)+2PKM^{in}\right)\Delta t\sum_{(j,i)\in\sigma}\phi(f^n_{j,i})\end{aligned}$$

Dividing by $1-PKM^{in}\Delta t \ge 1/2$ regarding the stability condition (3.31), thus it holds that for any $n\in\{0,\dots,N\}$

$$\sum_{(j,i)\in\sigma}\phi(f^n_{j,i}) \le e^{CT}\sum_{(j,i)\in\sigma}\phi(f^0_{j,i})\,,$$

where $C=8K_T(K_T+1)+4PKM^{in}$. The conclusion follows from the definition of f_h in (3.27) and f_h^{in} in (3.30) with the Jensen inequality, since

$$\phi(f^0_{j,i}) = \phi\left(\frac{1}{|\Lambda_{j,i}|}\int_{\Lambda_{j,i}} f^{in}(p,r)\,dpdr\right) \le \frac{1}{|\Lambda_{j,i}|}\int_{\Lambda_{j,i}}\phi\left(f^{in}(p,r)\right)dpdr\,.$$

It ends the proof. □

The direct consequence of Lemma 3.8 is that $(f_h)_h$ is weakly relatively compact in $L^1((0,T)\times\mathcal{S}_P)$ as a consequence of the Dunford-Pettis theorem, see [12, Theorem 4.21.2]. It proves there exists a subsequence (not relabeled) and $f \in L^1((0,T)\times\mathcal{S}_P)$ such that

$$f_h \underset{h\to 0}{\rightharpoonup} f \qquad w - L^1((0,T)\times\mathcal{S}_P).$$

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 3.1. 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 $L^1(\mathcal{S}_P)$. Then, by Corollary 3.6 we have that the sequence is equicontinuous in time for the strong topology of $L^1(\mathcal{S}_P)$, thus for the weak topology. So, applying Ascoli Theorem, there exists a subsequence of $\tilde{f}_h^{\Delta t}$ (not relabeled) converging towards a g in $C\left([0,T]; w - L^1(\mathcal{S}_P)\right)$. Next, we remark that

$$\sup_{t\in(0,T)} ||\tilde{f}_h(t,\cdot) - f_h(t,\cdot)||_{L^1(\mathcal{S}_P)} \leq C\Delta t, \tag{3.60}$$

which ensures that $g = f$. Finally, by weak convergence we get

$$||f(t,\cdot) - f(s,\cdot)||_{L^1(\mathcal{S}_P)} \leq \liminf_{h\to 0} ||\tilde{f}_h(t,\cdot) - \tilde{f}_h(s,\cdot)||_{L^1(\mathcal{S}_P)} \leq C|t-s|.$$

And this latter prove the continuity for the strong topology of $L^1(\mathcal{S}_P)$ of the limit f. This achieves the proof of the convergence (3.33)-(3.34) towards f (not yet the solution).

But, it remains to prove the convergence (3.35) of u_h before passing to the limit. Indeed, in Corollary 3.6 we have (3.46) the uniform bound, w.r.t. h, in $L^\infty(0,T)\cap BV(0,T)$, then the Helly Theorems, see [25, Theorem 36.4 and 36.5], entail that up to a subsequence (not-relabeled) 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 prove (3.35).

3.4. **Convergence of the numerical scheme.** Here we prove that the limit f and u obtained right before are solutions of the problem (3.3)-(3.4) to conclude the proof of Theorem 3.4.

3.4.1. *Reconstruction and convergence of the coagulation operator.* One of the delicate point in the proof of convergence is to give an appropriate reconstruction of the quadratic operator, the coagulation, that convergences in a relevant sense. In order to perform it, we define over $[0,T)\times\mathcal{S}_P$ the following approximation:

$$\begin{aligned} C_h(t,p,r) &= \int_{\mathcal{S}_P\times\mathcal{S}_P} \Phi^{1,h}_{p,r}(p',r';p'',r'') f_h(t,p',r') f_h(t,p'',r'')\, dr''dp''dr'dp' \\ &\quad - \int_{\mathcal{S}_P\times\mathcal{S}_P} \Phi^{2,h}_{p,r}(p',r';p'',r'') f_h(t,p',r') f_h(t,p'',r'')\, dr''dp''dr'dp'. \end{aligned}$$

where for any $(t,p,r) \in [0,T)\times\mathcal{S}_P$ and $(p',r';p'',r'') \in \mathcal{S}_P\times\mathcal{S}_P$,

$$\begin{aligned} \Phi^{1,h}_{p,r}(p',r';p'',r'') = &\ \mathbf{1}_{(0,P_h^-(p))}(p')\,\mathbf{1}_{(0,P_h^-(p)-P_h^-(p'))}(p'') \\ &\times\ \mathbf{1}_{(0,R_h^+(r))}(V_h^{\#}(p',r';p'',r''))P_h(p')a_h(p',r';p'',r''), \end{aligned}$$

and

$$\Phi^{2,h}_{p,r}(p',r';p'',r'') = \mathbf{1}_{(0,P_h^-(p))}(p')\,\mathbf{1}_{(0,P-P_h^-(p'))}(p'') \\ \times\ \mathbf{1}_{(0,R_h^-(r))}(r')P_h(p')a_h(p',r';p'',r''),$$

with

$$V_h^{\#}(p',r';p'',r'') = \frac{R_h^+(r')P_h^+(p') + R_h^+(r'')P_h^+(p'')}{P_h^-(p') + P_h^-(p')}.$$

With such definition, for all $n \in \{0,\dots,N-1\}$ 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

$$C_h(t,p,r) = C^n_{j-1/2,i-1/2}\,.$$

Now the convergence of C_h will be a consequence of the following to lemma. The first one can be find as is in [2, Lemma 3.5].

Lemma 3.9. *Let Ω be an open set of $\mathbb{R}^m$, $\kappa > 0$ and let two sequences $(v_n)_{n\in\mathbb{N}} \subset L^1(\Omega)$ and $(w_n)_{n\in\mathbb{N}} \subset L^\infty(\Omega)$. If we assume that for all $n \in \mathbb{N}$, $|w_n| \le \kappa$ and there exist $v \in L^1(\Omega)$ and $w \in L^\infty(\Omega)$ satisfying*

$$v_n \underset{n\to+\infty}{\longrightarrow} v, \quad weak - L^1(\Omega), \text{ and } w_n \underset{n\to+\infty}{\longrightarrow} w, \quad a.e. \text{ in } \Omega.$$

Then,

$$\|v_n(w_n - w)\|_{L^1(\Omega)} \underset{n\to+\infty}{\longrightarrow} 0, \text{ and } v_n w_n \underset{n\to+\infty}{\longrightarrow} vw, \quad weak - L^1(\Omega).$$

The second lemma give us some useful properties on the functions $\Phi^{i,h}_{p,r}$.

Lemma 3.10. *For $i = 1, 2$,*

$$||\Phi^{i,h}_{p,r}||_{L^\infty(\mathcal{S}_P\times\mathcal{S}_P)} \le PK, \quad \forall (p,r) \in \mathcal{S}_P,$$

and for all $(p,r) \in \mathcal{S}_P$,

$$\Phi^{1,h}_{p,r}(p',r';p'',r'') \underset{h\to 0}{\longrightarrow} \mathbf{1}_{(0,p)}(p')\,\mathbf{1}_{(0,p-p')}(p'')\,\mathbf{1}_{(0,r)}(v^{\#})p'a(p',r';p'',r''),$$
$$\Phi^{2,h}_{p,r}(p',r';p'',r'') \underset{h\to 0}{\longrightarrow} \mathbf{1}_{(0,p)}(p')\,\mathbf{1}_{(0,P-p')}(p'')\,\mathbf{1}_{(0,r)}(r')p'a(p',r';p'',r'').$$

a.e. $\mathcal{S}_P \times \mathcal{S}_P$.

Proof. The first inequality follows from hypothesis (H2). Then, we only have to check that $\mathbf{1}_{(0,R_h^+(r))}(V_h^{\#}(p',r';p'',r''))$ converge almost every where. Indeed for all $r \in (0,1)$,

$$\begin{aligned}\int_{\mathcal{S}_P\times\mathcal{S}_P} &\left|\mathbf{1}_{(0,R_h^+(r))}(V_h^{\#}) - \mathbf{1}_{(0,r)}(v^{\#})\right| dr''dp''dr'dp' \\ &\le \int_{\mathcal{S}_P\times\mathcal{S}_P} \left|\mathbf{1}_{(0,R_h^+(r))}(V_h^{\#}) - \mathbf{1}_{(0,R_h^+(r))}(v^{\#})\right| dr''dp''dr'dp' \\ &\quad + \int_{\mathcal{S}_P\times\mathcal{S}_P} \left|\mathbf{1}_{(0,R_h^+(r))}(v^{\#}) - \mathbf{1}_{(0,r)}(v^{\#})\right| dr''dp''dr'dp'\,, \end{aligned} \tag{3.61}$$

where

$$V_h^{\#}(p',r';p'',r'') = \frac{R_h^+(r')P_h^+(p') + R_h^+(r'')P_h^+(p'')}{P_h^-(p') + P_h^-(p')} \le v^{\#} = \frac{r'p' + r''p''}{p' + p''},$$

Therefore, the first integral in the right hand side of (3.61) is reduced to the measure of the set

$$A_h = \left\{(p',r',p'',r'') \in \mathcal{S}_P \times \mathcal{S}_P \ : \ V_h^{\#} \leq R_h^{+}(r) \leq v^{\#}\right\}.$$

Remarking that $V_h^{\#}$ converge everywhere to $v^{\#}$ and $R_h^{+}(r)$ towards identity, A_h converges towards $v^{\#-1}(r)$ which is a null set for the Lebesgue measure. It remains to remark that the second integral in (3.61) converges to zero too, to conclude on the $L^1(\mathcal{S}_P \times \mathcal{S}_P)$ convergence of $\mathbf{1}_{(0,R_h^+(r))}(V_h^{\#})$ to $\mathbf{1}_{(0,r)}(v^{\#})$, so the almost everywhere convergence holds true up to a subsequence (against not relabeled). $\square$

The sequence f_h do not have a sufficient regularity so, to pass to the limit, the trick is to consider the operator

$$\begin{aligned}\tilde{C}_h(t,p,r) = \int_{\mathcal{S}_P\times\mathcal{S}_P} & \Phi^{1,h}_{p,r}(p',r';p'',r'')\tilde{f}_h(t,p',r')\tilde{f}_h(t,p'',r'')\ dr''dp''dr'dp' \\ - \int_{\mathcal{S}_P\times\mathcal{S}_P} & \Phi^{2,h}_{p,r}(p',r';p'',r'')\tilde{f}_h(t,p',r')\tilde{f}_h(t,p'',r'')\ dr''dp''dr'dp'.\end{aligned}$$

Here we proceed as in [2, Section 4], applying twice Lemma 3.9 thanks to Lemma 3.10, we get

$$\tilde{C}_h \underset{h\to 0}{\longrightarrow} C_P, \quad \text{on} \ \ [0,T)\times\mathcal{S}_P\,.$$

Finally, by Lemma 3.10, Corollary 3.6 and the convergence obtained in (3.60), we have

$$\begin{aligned}&|C_h(t,p,r) - \tilde{C}_h(t,p,r)| \\ &\qquad \leq 2KP\left(\|f_h\|_{L^\infty(0,T;L^1)} + \|\tilde{f}_h\|_{L^\infty(0,T;L^1)}\right)\|f_h - \tilde{f}_h\|_{L^\infty(0,T;L^1)} \\ &\qquad\qquad \underset{h\to 0}{\longrightarrow} 0, \quad \forall (t,p,r)\in[0,T)\times\mathcal{S}_P\,.\end{aligned}$$

Thus, since $C_h = C_h - \tilde{C}_h + \tilde{C}_h$, we have

$$C_h \underset{h\to 0}{\longrightarrow} C_P, \quad \text{on} \ \ [0,T)\times\mathcal{S}_P\,.$$

Moreover, it is obvious that C_h is bounded by the bound (3.42) and Lemma 3.10, then the Lebesgue dominated convergence theorem yields

$$C_h(t,\cdot) \underset{h\to 0}{\longrightarrow} C_P(t,\cdot), \quad L^1(\mathcal{S}_P) \quad \forall t\in[0,T).$$

3.4.2. *Final stage of the proof.* The final stage of the proof is to write the discrete weak formulation of the scheme, when the equation (3.22) is multiplied by discrete test functions $\varphi_{j,i}$, and then to prove that it converges to the continuous weak formulation. Thus, let $\varphi \in C^2(\mathcal{S}_P)$ and multiply equation (3.22) by $\varphi_{j,i} = \varphi(p_{j-1/2}, r_{i-1/2})$. Then summing over (j,i) and $k = 0,\dots,n-1$ for some $n\in\{1,\dots,N\}$, we get

$$\begin{aligned}&\sum_{k=0}^{n-1}\sum_{j=0}^{J}\sum_{i=0}^{I} p_j f^{k+1}_{j,i}\varphi_{j,i}\Delta r\Delta p - \sum_{n=0}^{k-1}\sum_{j=0}^{J}\sum_{i=0}^{I} p_j f^{k}_{j,i}\varphi_{j,i}\Delta r\Delta p \\ &\qquad = -\Delta t\sum_{k=0}^{n-1}\sum_{j=0}^{J}\sum_{i=0}^{I}\left(F^k_{j,i+1/2} - F^k_{j,i-1/2}\right)\varphi_{j,i}\Delta p + \Delta t\sum_{k=0}^{n-1}\sum_{j=0}^{J}\sum_{i=0}^{I} C^k_{j,i}\varphi_{j,i}.\end{aligned}$$

Reordering the sum, and making use of the boundary conditions (3.15) and (3.19), we infer the following equation

$$X_h^n = Y_h^n + Z_h^n, \tag{3.62}$$

where

$$\begin{aligned}
X_h^n &= \sum_{j=0}^{J}\sum_{i=0}^{I} p_j f_{j,i}^n \varphi_{j,i}\Delta r\Delta p - \sum_{j=0}^{J}\sum_{i=0}^{I} p_j f_{j,i}^0 \varphi_{j,i}\Delta r\Delta p,\\
Y_h^n &= \Delta t\sum_{k=0}^{n-1}\sum_{j=0}^{J}\sum_{i=1}^{I} F_{j,i-1/2}^k(\varphi_{j,i}-\varphi_{j,i-1})\Delta p,\\
Z_h^n &= \Delta t\sum_{k=0}^{n-1}\sum_{j=1}^{J}\sum_{i=1}^{I} C_{j-1/2,i-1/2}^k\Big[(\varphi_{j-1,i-1}-\varphi_{j-1,i})-(\varphi_{j,i-1}-\varphi_{j,i})\Big]\\
&\quad + \Delta t\sum_{k=0}^{n-1}\sum_{j=1}^{J} C_{j-1/2,I+1/2}^k(\varphi_{j-1,I}-\varphi_{j,I})\\
&\quad + \Delta t\sum_{k=0}^{n-1}\sum_{i=1}^{I} C_{J+1/2,i-1/2}^n(\varphi_{J,i-1}-\varphi_{J,i}).
\end{aligned}$$

Next, we define X_h on $[0,T)$ by

$$\begin{aligned}
X_h(t) \coloneqq \iint_{\mathcal{S}_P} P_h(p) f_h(t,p,r)\varphi(P_h^-(p),R_h^-(r))\,drdp&\\
- \iint_{\mathcal{S}_P} P_h(p) f_h^{in}(p,r)\varphi(P_h^-(p),R_h^-(r))\,drdp.&
\end{aligned} \tag{3.63}$$

Then, we define Y_h by

$$Y_h(t) = Y_h^1(t) + Y_h^2(t), \tag{3.64}$$

with

$$\begin{aligned}
Y_h^1(t) = \int_0^t \iint_{\mathcal{S}_P} \mathbf{1}_{\Theta_h(t)}(s)\,\mathbf{1}_{(0,1-\Delta r)}(r)\mathcal{V}^+(u_h(s),P_h^-(p),R_h^-(r))f_h(s,p,r)&\\
\times D_h^0[\varphi](p,r)\,drdpds,&
\end{aligned}$$

and

$$\begin{aligned}
Y_h^2(t) = -\int_0^t \iint_{\mathcal{S}_P} \mathbf{1}_{\Theta_h(t)}(s)\,\mathbf{1}_{(\Delta r,1)}(r)\mathcal{V}^-(u_h(s),P_h^-(p),R_h^-(r))f_h(s,p,r)&\\
\times D_h^0[\varphi](p,r)\,drdpds,&
\end{aligned}$$

where a Taylor expansion of φ gives

$$D_h^0[\varphi](p,r) = \frac{\partial\varphi}{\partial r}((P_h^-(p),R_h^-(p))) + o(\Delta r).$$

In the same manner, we define Z_h by

$$Z_h(t) = Z_h^1(t) + Z_h^2(t) + Z_h^3(t), \tag{3.65}$$

such that

$$
\begin{aligned}
Z_h^1(t) &= \int_0^t \int_{\mathcal{S}_R} \mathbf{1}_{(0,\Theta_h(t))}(s) C_h(s,p,r) D_h^1[\varphi](p,r)\, drdpds \\
Z_h^2(t) &= \int_0^t \int_0^P \mathbf{1}_{(0,\Theta_h(t))}(s) C_h(s,p,1) D_h^2[\varphi](p,1)\, dpds \\
Z_h^3(t) &= \int_0^t \int_0^1 \mathbf{1}_{(0,\Theta_h(t))}(s) C_h(s,P,r) D_h^3[\varphi](P,r)\, drds
\end{aligned}
$$

with the expansion

$$
\begin{aligned}
D_h^1[\varphi](p,1) &= \frac{\partial^2 \varphi}{\partial p \partial r}(P_h(p), R_h(r)) + o(\Delta p) + o(\Delta r), \\
D_h^2[\varphi](P,r) &= \frac{\partial \varphi}{\partial r}(P, R_h^-(r)) + o(\Delta r), \\
D_h^3[\varphi](p,r) &= \frac{\partial \varphi}{\partial p}(P_h^-(p), 1) + o(\Delta p).
\end{aligned}
$$

It is straightforward that for any $n \in \{1, \ldots, N\}$ and $t \in [t_n, t_{n+1})$ we have

$$
X_h(t) = X_h^n, \quad Y_h(t) = Y_h^n, \quad \text{and} \quad Z_h(t) = X_h^n \,.
$$

Thus, by (3.62), it holds that for all $t \in [0, T)$

$$
X_h(t) = Y_h(t) + Z_h(t)\,. \tag{3.66}
$$

For the same reason, we get

$$
\begin{aligned}
u_h(t) = u^{in} - \int_0^t \iint_{\mathcal{S}_P} \mathbf{1}_{(0,\Theta_h(t))}(s) \Big(& \mathcal{V}^+(u_h(s), P_h^-(p), R_h^-(r)) \\
& - \mathcal{V}^-(u_h(s), P_h^-(p), R_h^-(r)) \Big) f_h(s,p,r)\, drdpds
\end{aligned} \tag{3.67}
$$

In view of (3.66) and (3.67) the conclusion readily follows. We do not detail the computations, but give to the reader some of the arguments. Indeed, to pass to the limit in (3.63), it is convenient to introduce $\tilde{X}_h$ where f_h is replaced by $\tilde{f}_h$, then the same arguments as Section 3.4.1 holds true. We write $X_h = X_h - \tilde{X}_h + \tilde{X}_h$, then it is clear that

$$
\left\| X_h - \tilde{X}_h \right\|_{L^\infty(0,T)} \to 0\,,
$$

by virtue of (3.60). Then, for all $t \in (0, T)$ we prove that $\tilde{X}_h$ converge towards the right term by Lemma 3.9. For (3.64) and (3.65) we do the same decomposition, remarking two points. On one hand, the continuity of $\mathcal{V}$ and the pointwise convergence of u_h allow us to correctly pass to the limit in the positive and negative parts of $\mathcal{V} = \mathcal{V}^+ - \mathcal{V}$. On the other hand, the time integral is treated thanks to the Lebesgue dominated convergence theorem. There is no more comments for (3.67). Proof of Theorem 3.4 is achieved.

4. Conclusion

In this work, we dealt with a new model with applications to polymers with particular affinity with metal-ions. These equations can be seen as a variation around the coagulation equation or LS equation. Nevertheless, it includes various specificities which make it an original problem. We want to mention particularly the conservations involved, the nature of the configuration space and the structure of the coagulation operator. 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. The techniques used was arguments of L^1 compactness and provide *de facto* the key ingredients to prove a weak stability principle to the continuous equation in order to prove the existence of solutions for a larger class of coefficients.

Our next objectives is now to confront our model to simulations and particularly to get a more precise idea of the long-time asymptotic behavior that remains an important issue, particularly for chemists. We believe that the link between both variables and the nature of the configurational space would lead to very particular asymptotic. Contrary to the LS model in [7, 23], here the density would concentrate to the nullclines of $\mathcal{V}$ while the coagulation operator would follow an asymptotic as in [14], for pure coagulation, *i.e.* a self-similar profile. We also refers to [9] and [18] for asymptotic behavior of similar problems. An other challenge would be to take into account the aqueous solution and/or membranes in the model: we refer to [4] and [21] for the role of the space and/or the fluid surrounding, and [39] for the role of the membrane.

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