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Analysis and numerical simulation of a polymerization model with aggregation and Ostwald ripening for the growth phenomenon

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Abstract In this paper we present an analytical and numerical modeling of a general polymerization process with possible lengthening by coagulation mechanism. The proposed model takes into account the 2D spatial diffusion of the monomers for the mass transfer between monomers and polymers. We investigate the well-posedness of this general polymerization model and propose an adequate numerical scheme based on a generalization of the anti-dissipative method developed in [14].

Keywords Polymerization process, hyperbolic-parabolic coupling, coagulation operator, numerical simulation, anti-diffusive method, finite volume method.

Mathematics Subject Classification (2000) MSC 58F15 · MSC 58F17 · MSC 53C35.

1 Introduction

We are interested in the polymerization process when a population of polymers is immersed in a bath of monomers with possible growth by gain or loss of monomers and possible coalescence by a coagulation mechanism. This type of models for polymer (macro-particles) and monomer mixtures is theoretically based on the standard Lifshitz-Slyozov system [25,19] which is commonly used to understand the so called Ostwald ripening phenomenon. This phenomenon refers to the mecanism of the growth of larger polymers at the expense of smaller ones due to the minimization of the interfacial surface energy of the system which governs the processes of gain and loss of monomers.

Initially, the standard Lifschitz-Slyozov system describes the dynamics of a solution of macro-particles, characterized by their size distribution function $f(t,\xi)$, $t,\xi\geq 0$, which interacts with monomers (free size particles) characterized by their concentration c(t), $t\geq 0$. This interaction is governed by kinetic coefficients named a,b and represent the rate at which monomers are added to or removed from polymers. Of course the rates a and b depend on the considered processes of precipitation/dissolution. In [25], Lifshitz and Slyozov propose the choice $a(\xi)=\xi^{1/3}$ and $b(\xi)=1$ for the assumption that mass transfer in the interaction is based on monomer diffusion. Thanks to this choice, the growth rate $V(t,\xi)=a(\xi)c(t)-b(\xi)$ vanishes at all time $t\geq 0$ which means there exists a critical size, ξ_{crit} , such that $V(t,\xi_{crit})=0$. So all polymers of size less than ξ_{crit} shrink and those of size greater than ξ_{crit}

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grow. Other choices of kinetic coefficients and their physical meaning can be found in [33].

To go beyond the classical Lifshitz-Slyozov system in order to understand the asymptotic trend of the family of self-similar solutions for the macro-particles distribution functions, other works focus on variants of this system for instance when possible coalescence (coagulation) of large polymers is taken into account. It is the case in [20] where in addition to the encounter process, the evolution equation for the volume (size) distribution function of macro-particle is coupled with a conservation of matter equation involving the monomers concentration. The author analyzes in [20] the well-posedness of his model by performing compactness properties of the solutions to approximating equations for the weak topology $L^1(0, +\infty)$. Other existence proofs exist like the one done in [6] using characteristic curves. One can refer to [25,33,6,18,14] for various modified Lifshitz-Slyozov system where coalescence of polymers is taken into account. For the parabolic correction of the Lifshitz-Slyozov model derived from the Becker-Döring model, an infinite system of ODEs when polymers have discrete sizes, see [37, 8,9,16,27].

In paper [13], the authors propose another variant derived from the Lifschitz-Slyozov standard system by assuming that monomers are subject to space diffusion. This assumption is motivated by the physical description of the sintering processes. They perform a rigorous proof of the existence and uniqueness of the polymers distribution function in the case of a free coagulation mechanism.

In this paper, we wish to understand the behavior of the Lifschitz-Slyozov system when monomers are assumed to follow a diffusion equation as in [13] and polymers are allowed to merge (coalesce) with each other as in [14]. Let us remind here that the main conjecture in [14] concerning the coagulation effect is that it allows to keep the right expected behavior of the polymers distribution function. In our study, no diffusion is taken into account for the polymers distribution function. Some extensions where a diffusion term is added to take into account fluctuations exist (see [26,30] and references therein). In our modeling, we deliberately choose a constant coagulation kernel and there is no physical motivation behind.

All these variants of the Lifshitz-Slyozov standard system are motivated by the amount of applications related to the polymerization process which is often use in industrial processes for producing metallic alloys such as stainless steel or nickel alloys used in jewelry [19,25]; in population dynamics when for instance one is interested in the synthesis of DNA stand which is made by sequences of deoxyribonucleotides or when one is interested in the mechanism of Prion diseases where the polymerization of Prion protein is a central event [32,2,3,15,23]. Recently several papers in Alzheimer disease modeling refer to such process of polymerization with aggregation (coagulation) in order to describe the ways of oligomerization and fibrillation which are considered to our knowledge as the central mechanisms of the evolution of the disease [17,34].

In our study, we denote as in [13] the size distribution function of polymers by $f(t, x, \zeta)$ with $t \geq 0, x \in \Omega \subset \mathbb{R}^2$ and $\zeta \geq 0$ the time, space and size variables respectively and by c(t, x) the concentration of monomers at time $t \geq 0$ and position x. So the considered model stands as follows:

$$\begin{cases}
\partial_t f(t, x, \xi) + \partial_{\xi} ((a(\xi)c(t, x) - 1)f(t, x, \xi)) = \lambda Q(f)(t, x, \xi), & t \ge 0, \ x \in \Omega, \ \xi \ge 0, \\
\partial_t \Big(c(t, x) + \int_0^\infty \xi f(t, x, \xi) \, \mathrm{d}\xi \Big) - \Delta_x c(t, x) = 0, & t \ge 0, \ x \in \Omega, \\
\partial_{\nu} c = \nabla c \cdot \nu = 0, & \text{on } \partial\Omega,
\end{cases}$$
(1.1)

where Ω is a smooth bounded domain, with boundary $\partial\Omega$ and $\nu(x)$ to be the outward unit normal vector at the point $x \in \partial\Omega$. The parameter λ is a scale constant parameter for the coalescence process. The dynamics of the polymers is governed by the growth rate $a(\xi)c(t,x) - b(\xi)$ where, in our case, we choose $b(\xi) = 1$.

The kinetic coefficients a and b are non negative functions and quantify the rates at which monomers are added to or removed from the polymers. Note that the precise expression of the coefficients depends on the modeling of mass transfer between monomers and polymers. In the case where mass transfer is based on monomer diffusion, [25] proposes the choice $a(\xi) = \xi^{1/3}$ and $b(\xi) = 1$. One can refer to [33] for other formulas for the kinetic coefficients. In any time, there exists a critical size ξ_{crit} such that the growth rate vanishes. So all polymers of size smaller than ξ_{crit} shrink while the larger

ones grow.

The operator Q(f) describes the encounters between polymers and is written

$$Q(f)(t, x, \xi) = \frac{1}{2} \int_0^{\xi} K(\xi - \xi', \xi') f(t, x, \xi - \xi') f(t, x, \xi') d\xi' - \int_0^{\infty} K(\xi, \xi') f(t, x, \xi) f(t, x, \xi') d\xi'$$

$$= \frac{1}{2} Q^+(f)(t, x, \xi) - f(t, x, \xi) L_f(t, x) \text{ where } L_f(t, x) = \int_0^{\infty} K(\xi, \xi') f(t, x, \xi') d\xi'.$$
(1.2)

The first term in the right hand side of the equality in (1.2) represents the gain of polymers of size ξ when one of size $\xi - \xi'$ encounters another of size ξ' smaller than ξ ($\xi' \leq \xi$) with the rate $K(\xi - \xi', \xi')$; while the second term represents the loss of polymers of size ξ when it encounters another of any size ξ' with the rate $K(\xi,\xi')$. The coagulation kernel $K(\xi_1,\xi_2)$ is a symmetric function from $[0,\infty]^2$ into \mathbb{R}_+ . It represents the rate of coalescence between particles of size ξ_1 and ξ_2 . This coagulation operator is widely used for the dynamics of cluster growth especially in most coagulationfragmentation type models. For instance in [24], the author use the Smoluchowski operator to describe coalescence and breakage for a system of particles. He analyzed the existence solution for a class of coagulation and fragmentation kernels. We mention Norris, [31], who obtains an existence result in the pure coagulation equation, by assuming that there exists a sub-linear function ϕ on $]0,\infty[$, such that $K(\xi,\xi') \leq \phi(\xi)\phi(\xi')$ and $\int_0^\infty \phi^2(\xi)f^0(x,\xi)d\xi < \infty$. He also investigates the case where $K(\xi,\xi')$ blows up as $\xi \to 0$ or $\xi' \to 0$ and the case where any local regularity conditions is assumed on K. Of course this encounter mechanism doesn't change the total mass of the polymers $\int_0^\infty \xi Q(f)(t,x,\xi)\,\mathrm{d}\xi = \int_0^\infty \xi Q(f)(t,x,\xi)\,\mathrm{d}\xi$ 0 and it decreases the number of polymers by collision $\int_0^\infty Q(f)(t,x,\xi) d\xi \leq 0$.

Here for analytical convenience we assume that the encounter rate of polymers is constant.

We assume that the problem (1.1) is endowed with the following initial condition

$$f(t = 0, x, \xi) = f^{0}(x, \xi) \ge 0,$$
 $c(t = 0, x) = c^{0}(x).$

In the following, we will refer to the continuity equation of (1.1) as $(1.1)_1$ and to the monomer diffusion equation as $(1.1)_2$. The mathematical analysis of this kind of interactions between polymers and monomers is quite intriguing in view of the classical paper of Lifshitz and Slyozov [25]. Many works discuss the existence and uniqueness results in different functional frameworks and one can refer to [7,21,22,28,29] for more details. Numerical simulations exist for this kind of interaction without space variables and one can refer to [4,5,14].

In our specific case we investigate the problem (1.1) and look to the influence of monomer spacediffusion and the encounter phenomenon on the evolution of the polymer size distribution. The aim of this paper is to analyze theoretically the well posedness and the numerical issues of (1.1). Without loss of generality, we assume

Hypothesis 11 The data satisfy

- $c^0 \in L^{\infty}(\Omega)$, $f^0 \in L^{\infty}(\Omega; L^1((0,\infty), (1+\xi) d\xi))$.

The kinetic coefficients satisfy

- b = 1,
- a is non decreasing with a(0) = 0 and $a(+\infty) = +\infty$,
- $a \in C^0([0,\infty)) \cap C^1((0,\infty))$ and for any $\xi_0 > 0$, there exists $L_a > 0$ such that $0 \le a'(\xi) \le L_a$ for any $\xi \ge \xi_0 > 0$.

One can make the obvious remark that the gain rate, $a(\xi) = \xi^{1/3}$, proposed in [25] fulfills the previous hypothesis. That is the case for the rates of the form $a(\xi) = \mathcal{O}(\sqrt{(\xi)})$ as used in [37]. Formally, by simple integration of the continuity equation $(1.1)_1$ against the size ξ , it is easy to remark that the diffusion equation can be recasted in the following simpler form

$$\partial_t c(t,x) + c(t,x) \int_0^\infty a(\xi) f(t,x,\xi) \,\mathrm{d}\xi = \Delta_x c(t,x) + \int_0^\infty f(t,x,\xi) \,\mathrm{d}\xi. \tag{1.3}$$

Integrating $(1.1)_2$ on Ω we obtain thanks to the Neumann boundary condition the following mass preservation relation

$$\frac{\mathrm{d}}{\mathrm{d}t} \left[\int_{\Omega} \int_{0}^{\infty} \xi f(t, x, \xi) \,\mathrm{d}\xi \,\mathrm{d}x + \int_{\Omega} c(t, x) \,\mathrm{d}x \right] = 0. \tag{1.4}$$

In what follows we put our analysis in (1.1) where the diffusion equation $(1.1)_2$ is replaced by (1.3) and throughout the paper we investigate the following main result

Theorem 1.1 From **Hypothesis 11** and previous chosen properties for the coagulation operator Q(f), the system (1.1) where the diffusion equation (1.1)₂ is replaced by (1.3) has a unique "mild" solution (c, f) with $c \in L^2([0, T]; H^1(\Omega)) \cap C([0, T]; L^2(\Omega))$ and $f \in L^{\infty}([0, T]; L^1(\mathbb{R}_+, (1 + \xi)d\xi))$.

Most of the technical tools used in the proof of this main result comes from [13] with appropriate modifications. So we organize the paper as follows. In Section 2 we establish the general tools related to the monomer time evolution equation and polymer continuity equation by using a slight modification of **Hypothesis 11** which consists in assuming the kinetic coefficient a to be Lipschitz continuous on $[0, \infty)$. In Section 3 we first present the analysis of the well-posedness of our system by applying a double fixed point theorem in the case where a is Lipschitz continuous on $[0, \infty)$ and we generalize the well-posedness in the conditions of hypothesis 11. Section 4 is devoted to the 2D numerical simulations of the model.

2 General tools related to polymer and monomer equations

2.1 Tools related to the monomer diffusion equation

The well-posedness of the equation (1.3) is obtained as a consequence of the following result on parabolic equations.

Proposition 2.1 Let $0 < T < \infty$. Consider non negative functions $A, B \in L^{\infty}((0,T) \times \Omega)$. If we assume that there exists $N_0 \in \mathbb{R}_+$ such that

$$0 < B(t,x) < N_0 \quad \forall (t,x) \in (0,T) \times \Omega,$$

then for all $c^0 \in L^2(\Omega)$ there exists a unique solution $c \in L^2((0,T); H^1(\Omega)) \cap C([0,T]; L^2(\Omega))$ of the parabolic equation

$$\begin{cases}
\partial_t c(t,x) + A c(t,x) - \Delta_x c(t,x) = B(t,x), & in (0,T) \times \Omega, \\
\partial_\nu c = \nabla c \cdot \nu = 0, & on (0,T) \times \partial \Omega, \\
c(t=0,x) = c^0(x), & on \overline{\Omega}.
\end{cases}$$
(2.1)

In addition, for all $0 \le t \le T < \infty$ there exists a constant C_T such that

$$\int_{\Omega} |c(t,x)|^2 dx \le C_T; \qquad \int_0^t \int_{\Omega} |\nabla_x c(s,x)|^2 dx ds \le C_T.$$

And, if $0 \le c^0 \in L^{\infty}(\Omega)$, then the solution c satisfies the maximum principle relation

$$0 \le c(t, x) \le K_T$$
 with $K_T = K_T(N_0, ||c^0||_{\infty}, T)$.

Proof The proof of Proposition 2.1 is very classical and is based on the analog of the Lax-Milgram theorem for parabolic equations. For more details see [13].

2.2 Tools related to the polymer transport equation

Here we adopt the same reasoning as in the paper [13] by neglecting the space variable which appears only as a parameter in the continuity equation. So, making abstraction to the space variable "x" and taking $\lambda = 1$, we consider the following transport equation

$$\begin{cases}
\partial_t f(t,\xi) + \partial_{\xi}(Vf)(t,\xi) = Q(f)(t,\xi), t, \xi > 0, \\
V(t,\xi) = a(\xi)c(t) - 1, & t, \xi > 0, \\
f(t=0,\xi) = f^0(\xi), & \xi > 0,
\end{cases}$$
(2.2)

such that the kinetic coefficients are required to satisfy for a given locally bounded c ($0 \le c \le K_T$) the following assumptions

- $||a'||_{\infty} \leq L_a$ and $a \in L^{\infty}(\mathbb{R})$,
- a(0) = 0,

where $M_T = La K_T$.

With these assumptions, it is straightforward to deduce that V satisfies

$$V(t,0) \le 0, \ V(t,\xi) \le M_T \xi, \ |V(t,\xi)| \le M_T (1+\xi) \text{ and } |V(t,\xi) - V(t,\xi')| \le M_T |\xi - \xi'|.$$

So we can introduce the characteristic curves associated to V

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}s} \mathscr{E}(s;t,\xi) = V(s,\mathscr{E}(s;t,\xi)), \\ \mathscr{E}(t;t,\xi) = \xi. \end{cases}$$
 (2.3)

We define the mild formulation which arises by integrating (2.2) along the characteristic curves associated to V. So, the solution of (2.2) in its mild formulation is given by

$$f(t,\xi) = f^{0}(\mathscr{E}(0;t,\xi)) \ J(0;t,\xi) + \int_{0}^{t} Q(f)(s;\mathscr{E}(s;t,\xi)) \ J(s;t,\xi) \, \mathrm{d}s$$
 (2.4)

which is obtained by using the differential equation fulfilled by $f(s, \mathcal{E}(s; t, \xi))$ and where J is the jacobian of the change of variables $\xi \mapsto \mathcal{E}(s; t, \xi)$ and is defined by

$$J(s;t,\xi) = \partial_{\xi} \mathscr{E}(s;t,\xi) = \exp\left(-\int_{-t}^{t} \partial_{\xi} V(\sigma,\mathscr{E}(\sigma;t,\xi)) d\sigma\right) \ge 0.$$

The previous assumptions on the kinetic coefficients allows to infer the following results on the characteristics and the distribution function f.

Lemma 2.1 If the previous hypothesis on the kinetic coefficients is satisfied, then

- 1. $\forall t \geq 0, \mathcal{E}(0; t, 0) \geq 0$,
- 2. $\forall t \geq 0$, $\lim_{\xi \to +\infty} \mathscr{E}(0; t, \xi) = +\infty$,
- 3. $\forall 0 \leq t \leq T < \infty$ and $\xi \geq 0$, there exists $L_T > 0$ such that $\mathscr{E}(t; 0, \xi) \leq L_T \xi$.

If f is a solution of the characteristic view point, that is to say it satisfies equation (2.4), then 4. $f^0 \ge 0$ implies $f(t,\xi) \ge 0$,

5. $f^0 \in L^1((0,\infty); (1+\xi) d\xi)$ implies that $\forall t \geq 0$, $f(t,\cdot) \in L^1((0,\infty); (1+\xi) d\xi)$ and more precisely one has

$$f \in C^{0}([0,T]; L^{1}(\mathbb{R}_{+})), \quad \int_{0}^{\infty} f(t,\xi) \, \mathrm{d}\xi \le \int_{0}^{\infty} f^{0}(\xi) \, \mathrm{d}\xi \quad and$$
$$\int_{0}^{\infty} \xi f(t,\xi) \, \mathrm{d}\xi \le e^{M_{T}T} \left(\int_{0}^{\infty} \xi f^{0}(\xi) \, \mathrm{d}\xi + M_{T}T \int_{0}^{\infty} f^{0}(\xi) \, \mathrm{d}\xi \right).$$

6. If we assume $\partial_{\xi}V(t,\xi) = c(t)\partial_{\xi}a(\xi) \geq 0 \ \forall \ \xi \geq 0 \ and \ t \in [0,T]$ then

$$f^0 \in L^1((0,\infty))$$
 implies that $f \in L^\infty((0,T); L^1(0,\infty))$ and one can deduce $||f||_{L^\infty(0,T;L^1(0,\infty))} \le ||f^0||_{L^1(0,\infty)} + ||Q||_{L^1((0,T)\times(0,\infty))}.$

Proof For the proof of Lemma 2.1 one can refers to [13, Lemma 2.1 and Proposition 2].

3 Analysis of the well-posedness of problem (1.1)

The proof of the well-posedness of the problem (1.1) is a straight adaptation of the one given in [13]. The main idea consists of performing a double fixed point strategy under the assumptions of Section 2.2. The first fixed point strategy is based on the polymers distribution function and the second one on the monomers diffusion equation.

3.1 First fixed point strategy for polymers distribution function

Let us consider a given c such that $c \in \{C^0((0,T) \times \Omega), 0 \le c(t,x) \le K_T\}$. The choice of T is specified later.

We define the application $\mathcal{F}: g \to \mathcal{F}(g)(t, x, \xi) = f(t, x, \xi)$ such that

$$\begin{cases} \partial_t f + \partial_{\xi}(Vf) + Kf = Q(g) + Kg, & \text{in } (0,T) \times \Omega, \\ f_{|t=0} = f^0, & \text{on } \overline{\Omega}, \end{cases}$$
 (3.5)

where the parameter K is chosen so that

$$Q(g) + Kg : \ge 0 \quad \text{when } g \in \left\{ f \in L^{\infty}((0,T) \times \Omega; L^{1}(\mathbb{R}_{+})); \ f \ge 0, \ \|f(t,x,\cdot)\|_{L^{1}(\mathbb{R}_{+})} \le M \right\} := \mathcal{C}_{T,\Omega}.$$

The choice of the constant K is possible and depend on the bound M. Indeed let

$$Q(g) + K g : \ge 0 \Rightarrow Q^{+}(g) - L_{g} g + K g \ge 0$$

 $\Rightarrow Q^{+}(g) + (K - L_{g})g \ge 0.$

Knowing that $Q^+(g) \ge 0$, then the implication is true if $K - L_g \ge 0$ which means $K \ge L_g \ge ||g||_{L^1(\mathbb{R}_+)}$. So we need to choose K such that $K \ge M$.

The solution of (3.5) along the characteristic curves when neglecting the space variable (which acts just as a parameter) is written as

$$\mathcal{F}(g)(t,\xi) = f^0(\mathscr{E}(0;t,\xi)) J(0;t,\xi) e^{-Kt} + \int_0^t \Big(Q(g)(s;\mathscr{E}(s;t,\xi)) + Kg(s,\mathscr{E}(s;t,\xi))\Big) J(s;t,\xi) e^{-K(t-s)} \,\mathrm{d}s.$$

Looking at the L^1 norm we get thanks to the fact that $||J||_{L^{\infty}} \leq 1$,

$$\|\mathcal{F}(g)(t,\cdot)\|_{L^{1}(\mathbb{R}_{+})} \leq \|f^{0}\|_{L^{1}(\mathbb{R}_{+})} + \int_{0}^{t} \left(\|Q(g)(s,\cdot)\|_{L^{1}(\mathbb{R}_{+})} + K\|g(s,\cdot)\|_{L^{1}(\mathbb{R}_{+})} \right) ds$$

$$\leq \|f^{0}\|_{L^{1}(\mathbb{R}_{+})} + T\|g\|_{L^{\infty}((0,T);L^{1}(\mathbb{R}_{+}))} \left(K + \frac{1}{2} \|g\|_{L^{\infty}((0,T);L^{1}(\mathbb{R}_{+}))} \right).$$

Knowing that $\mathcal{F}(g) = f$, then we can fix M such as $||f^0||_{L^1(\mathbb{R}_+)} \leq \frac{M}{2}$ and choose a small T such that $T(K+2M) \leq \frac{1}{2}$. So, one can choose $M(f^0)$ so that

$$0 \le K \le \frac{1}{2T} - 2M$$
 and $K \ge M$.

With this choice of K, one has $\mathcal{F}(g) \in \mathcal{C}_{T,\Omega}$ if $g \in \mathcal{C}_{T,\Omega}$.

Consider f_1 and f_2 defined by $f_1 =: \mathcal{F}(g_1)$ and $f_2 =: \mathcal{F}(g_2)$ two solutions of the problem (3.5) associated to $g_1, g_2 \in \mathcal{C}_{T,\Omega}$ and with the same initial condition. Following the characteristic curves, one deduces

$$\|(f_1 - f_2)(t)\|_{L^1(\mathbb{R}_+)} \le \int_0^t \left(\|(Q(g_1) - Q(g_2))(s)\|_{L^1(\mathbb{R}_+)} + K\|(g_1 - g_2)(s)\|_{L^1(\mathbb{R}_+)} \right) \mathrm{d}s, \tag{3.6}$$

since the coagulation operator satisfies, see [6, Lemma 3], the relation

$$||Q(g_1) - Q(g_2)||_{L^1(\mathbb{R}_+)} \le \frac{1}{2} \Big(||g_1||_{L^1(\mathbb{R}_+)} + ||g_2||_{L^1(\mathbb{R}_+)} \Big) ||g_1 - g_2||_{L^1(\mathbb{R}_+)}.$$

From (3.6), we get:

$$\|(f_1 - f_2)(t)\|_{L^1(\mathbb{R}_+)} \le T \Big(K + \frac{1}{2} (\|g_1\|_{L^{\infty}((0,T);L^1(\mathbb{R}_+))} + \|g_2\|_{L^{\infty}((0,T);L^1(\mathbb{R}_+))}) \Big) \|g_1 - g_2\|_{L^{\infty}((0,T);L^1(\mathbb{R}_+))}.$$

The fact that g_1 and g_2 belong to $\mathcal{C}_{T,\Omega}$ implies that

$$||(f_1 - f_2)(t)||_{L^1(\mathbb{R}_+)} \le T(K + 2M)||g_1 - g_2||_{L^{\infty}((0,T);L^1(\mathbb{R}_+))}.$$

So \mathcal{F} is a contraction and this gives the existence and uniqueness of f satisfying

$$\partial_t f + \partial_{\varepsilon}(V f) = Q(f)$$
 and $f \in L^{\infty}([0,T]; L^1(\mathbb{R}_+)).$

Here one remarks that there is a constraint on T depending implicitly on the bounds of the initial distribution function. To go further in time, the trick is to take $f(T, x, \cdot)$ as the new initial distribution function and reiterate the process on [T, 2T] then on [2T, 3T] and so on. This achieves the proof of the well-posedness for polymers continuity equation.

Remark 3.1 For initial data satisfying $\xi f^0 \in L^1(\mathbb{R}_+)$, using **Proposition 2.1** one obtains $\xi f \in L^{\infty}((0,T);L^1(\mathbb{R}_+))$ and thanks to the hypothesis on the operator Q the following relation on the variation of polymers total mass holds

$$\frac{d}{\mathrm{d}t} \left(\int_0^\infty \xi f \, \mathrm{d}\xi \right) = \int_0^\infty V f \, \mathrm{d}\xi.$$

3.2 Second fixed point strategy for monomers diffusion equation

This fixed point strategy follows exactly the same reasoning as in [13]. The analysis is based on equation (1.3) and the hypothesis 11.

Let $\mathbb{Q}_T = [0,T] \times \Omega$ for fixed T. We note $N_0 = \sup_{x \in \Omega} \int_0^\infty f_0(x,\xi) \, \mathrm{d}\xi < \infty$ and we put $K_T = \|c_0\|_{L^\infty} + N_0 T$ the constant obtained in the maximum principle (**Proposition 2.1**). For the set

$$\mathbb{E}_T = \left\{ c \in L^2(\mathbb{Q}_T) \text{ such that } 0 \le c(t, x) \le K_T \text{ and } c \in C^0(\mathbb{Q}_T) \right\},\,$$

we define the application

$$\mathscr{C}: \mathbb{E}_T \longrightarrow L^2(\mathbb{Q}_T)$$
$$\tilde{c} \longmapsto \mathscr{C}(\tilde{c}) = c,$$

with c satisfying

$$\begin{cases} \partial_t c(t,x) + c(t,x) \int_0^\infty a(\xi) f(t,x,\xi) \,\mathrm{d}\xi - \varDelta_x c(t,x) = \int_0^\infty f(t,x,\xi) \,\mathrm{d}\xi, & \text{in } (0,T) \times \varOmega, \\ \partial_\nu c = 0, & \text{on } (0,T) \times \partial \varOmega, \\ c_{|t=0} = c_{\text{init}}, & \text{on } \overline{\varOmega} \end{cases}$$

where f solves

$$\begin{cases} \partial_t f(t,x,\xi) + \partial_\xi \big((a(\xi)\tilde{c}(t,x) - 1) f(t,x,\xi) \big) = Q(f)(t,x,\xi), & \text{in } (0,T) \times \Omega \times (0,\infty), \\ f_{|t=0} = f^0, & \text{on } \overline{\Omega} \times (0,\infty). \end{cases}$$

We can state the following results on the well-posedness of the application \mathscr{C} as in Lemma 3.1 below and on the continuity of \mathscr{C} as in Proposition 3.1 below.

Lemma 3.1 The application \mathscr{C} given above is well-defined and $\mathscr{C}(\mathbb{E}_T)$ is compact in $L^2(\mathbb{Q}_T)$.

Proof The assumptions of Section 2.2 and $\tilde{c} \in \mathbb{E}_T$ allow to apply the results in Section 2.1 by using the characteristics approach with the x variable acting as a space parameter. So one obtains

$$f(t, x, \xi) = f^{0}(x, \mathcal{E}(0; t, x, \xi)) \ J(0, t, x, \xi) + \int_{0}^{t} Q(f)(s, x, \mathcal{E}(s; t, x, \xi)) \ J(s, t, x, \xi) \, \mathrm{d}s,$$

where \mathscr{E} and J are associated to \tilde{c} .

Thanks to Lemma 2.1 one has the relations

$$\sup_{x \in \Omega} \int_0^\infty f(t, x, \xi) \, \mathrm{d}\xi \le \sup_{x \in \Omega} \int_0^\infty f^0(x, \xi) \, \mathrm{d}\xi = N_0 < \infty,$$
 and

$$\sup_{x \in \Omega} \int_0^\infty \xi \ f(t, x, \xi) \, \mathrm{d}\xi \le e^{M_T T} \left(\sup_{x \in \Omega} \int_0^\infty \xi f^0(x, \xi) \, \mathrm{d}\xi + M_T T \sup_{x \in \Omega} \int_0^\infty f^0(x, \xi) \, \mathrm{d}\xi \right) < \infty.$$

Then we deduce $0 \le \int_0^\infty a(\xi) f(t, x, \xi) d\xi \in L^\infty(\mathbb{Q}_T)$ and $0 \le \int_0^\infty f(t, x, \xi) d\xi \le N_0$. So, the **Proposition 2.1** gives the well posedness of the application $\mathscr C$ with

$$c = \mathscr{C}(\tilde{c}) \in L^2([0,T]; H^1(\Omega)) \cap C([0,T]; L^2(\Omega))$$
 and fulfilling $0 \le c(t,x) \le K_T \Rightarrow \mathscr{C}(\mathbb{E}_T) \subset \mathbb{E}_T$.

Now we know that $\mathscr{C}(\tilde{c})$ is bounded in $L^2([0,T];H^1(\Omega))$ and $\partial_t c$ is also bounded in $L^2([0,T];H^{-1}(\Omega))$ so the compact embedding $H^1(\Omega) \subset L^2(\Omega)$ allows to apply J. Simon's compacity lemma [35] and to deduce the compactness of $\mathscr{C}(\mathbb{Q}_T)$ in $L^2(\mathbb{Q}_T)$.

Proposition 3.1 Let $(f_n)_{n\in\mathbb{N}}$ and f solutions of the problem with the same initial data $f(t = 0, x, \xi) = f_n(t = 0, x, \xi)$.

Let define a sequence $(\tilde{c_n})_{n\in\mathbb{N}}\in\mathbb{E}_T$ which converges toward \tilde{c} in $L^2(Q_T)$. Then \tilde{c} belongs to $\mathscr{C}(\mathbb{E}_T)$. More precisely $\mathscr{C}(\tilde{c_n})\to\mathscr{C}(\tilde{c})$ in $L^2(\mathbb{Q}_T)$ when n tends to infinity.

Proof Using to the characteristic curves, one obtains

$$\begin{cases} f_n(t,x,\xi) = f^0(x,\mathscr{E}_n(0;t,x,\xi)) \ J_n(0;t,x,\xi) + \int_0^t Q(s,x,\mathscr{E}_n(s;t,x,\xi)) \ J_n(s;t,x,\xi) \, \mathrm{d}s, \\ f(t,x,\xi) = f^0(x,\mathscr{E}(0;t,x,\xi)) \ J(0;t,x,\xi) + \int_0^t Q(s,x,\mathscr{E}(s;t,x,\xi)) \ J(s;t,x,\xi) \, \mathrm{d}s, \end{cases}$$

where

$$J_n(s;t,x,\xi) = \exp\left(-\int_s^t a'\left(\mathscr{E}_n(\sigma;t,x,\xi)\right)\tilde{c_n}(\sigma;x)\,\mathrm{d}\sigma\right)$$

and

$$J(s;t,x,\xi) = \exp\left(-\int_{s}^{t} a' \left(\mathscr{E}(\sigma;t,x,\xi)\right) \tilde{c}(\sigma;x) \,\mathrm{d}\sigma\right).$$

In what follows, we give a sketch of the proof and let the readers refer to lemma 3.2 and lemma 3.3 of [13] for more details.

The first step is to show the following convergence results in $L^2(\mathbb{Q}_T)$:

$$-\int_0^\infty a(\xi)f_n(t,x,\xi)\,\mathrm{d}\xi \longrightarrow \int_0^\infty a(\xi)f(t,x,\xi)\,\mathrm{d}\xi \text{ when } n\to\infty,$$
$$-\int_0^\infty f_n(t,x,\xi)\,\mathrm{d}\xi \longrightarrow \int_0^\infty f(t,x,\xi)\,\mathrm{d}\xi \text{ when } n\to\infty.$$

These convergence results are obtained by quantifying the difference between two characteristic curves associated to two growth rates $V_1 = a(\xi)c_1(t,x) - 1$ and $V_2 = a(\xi)c_2(t,x) - 1$ for $c_1, c_2 \in \mathbb{E}_T$. So, under the assumptions of Section 2.2 one deduces the following estimation

$$|\mathscr{E}_1 - \mathscr{E}_2|(s; t, x, \xi) \le L_T(1+\xi) \left(\int_s^t |c_1 - c_2|^2(\sigma, x) d\sigma\right)^{1/2} \ \forall \ 0 \le s, t \le T < \infty.$$
 (3.7)

On one hand:

$$\begin{split} &\int_0^\infty f_n(t,x,\xi)\,\mathrm{d}\xi - \int_0^\infty f(t,x,\xi)\,\mathrm{d}\xi \\ &= \int_0^\infty f^0(x,\mathscr{E}_n(0;t,x,\xi))J_n(0;t,x,\xi) + \int_0^t Q(s,x,\mathscr{E}_n(s;t,x,\xi))\,J_n(s;t,x,\xi)\,\mathrm{d}s\,\mathrm{d}\xi \\ &- \int_0^\infty f^0(x,\mathscr{E}(0;t,x,\xi))J(0;t,x,\xi) - \int_0^t Q(s,x,\mathscr{E}(s;t,x,\xi))\,J(s;t,x,\xi)\,\mathrm{d}s\,\mathrm{d}\xi \\ &= \int_{\mathscr{E}_n(0;t,x,0)}^\infty f^0(x,\delta)\,\mathrm{d}\delta + \int_0^t \int_{\mathscr{E}_n(s;t,x,0)}^\infty Q(s,x,\delta)\,\mathrm{d}\delta\,\mathrm{d}s - \int_{\mathscr{E}(0;t,x,0)}^\infty f^0(x,\delta)\,\mathrm{d}\delta \\ &- \int_0^t \int_{\mathscr{E}(s;t,x,0)}^\infty Q(s,x,\delta)\,\mathrm{d}\delta\,\mathrm{d}s \\ &= \left(\int_{\mathscr{E}_n(0;t,x,0)}^\infty f^0(x,\delta)\,\mathrm{d}\delta - \int_{\mathscr{E}(0;t,x,0)}^\infty f^0(x,\delta)\,\mathrm{d}\delta\right) \\ &+ \left(\int_0^t \int_{\mathscr{E}_n(s;t,x,0)}^\infty Q(s,x,\delta)\,\mathrm{d}\delta\,\mathrm{d}s - \int_0^t \int_{\mathscr{E}(s;t,x,0)}^\infty Q(s,x,\delta)\,\mathrm{d}\delta\,\mathrm{d}s\right). \end{split}$$

It follows that for all $s \in [0, T]$

$$\begin{split} &|\int_0^\infty f_n(t,x,\xi) \,\mathrm{d}\xi - \int_0^\infty f(t,x,\xi) \,\mathrm{d}\xi|(t,x) \\ &\leq |\int_{\mathscr{E}(0;t,x,0)}^{\mathscr{E}_n(0;t,x,0)} f^0(x,\delta) \,\mathrm{d}\delta| + |\int_0^t \int_{\mathscr{E}(s;t,x,0)}^{\mathscr{E}_n(s;t,x,0)} Q(s,x,\delta) \,\mathrm{d}\delta \,\mathrm{d}s| \\ &\leq \|f^0\|_{L^\infty(\mathbb{Q}_T)} |\mathscr{E}_n - \mathscr{E}|(0;t,x,0) + T\|Q\|_{L^\infty(\mathbb{Q}_T \times \mathbb{R}_+)} |\mathscr{E}_n - \mathscr{E}|(s;t,x,0). \end{split}$$

Simple integration along Ω yields

$$\|\int_0^\infty (f_n - f)(t, x, \xi) d\xi\|_{L^2(\Omega)}^2 \le 4\|f^0\|_{L^\infty(\mathbb{Q}_T)}^2 \int_{\Omega} |\mathscr{E}_n - \mathscr{E}|^2(0; t, x, 0) dx + 4T^2 \|Q\|_{L^\infty(\mathbb{Q}_T \times \mathbb{R}_+)}^2 \int_{\Omega} |\mathscr{E}_n - \mathscr{E}|^2(s; t, x, 0) dx.$$

Using the result (3.7) we obtain

$$\begin{split} &\| \int_{0}^{\infty} (f_{n} - f)(t, x, \xi) \, \mathrm{d}\xi \|_{L^{2}(\Omega)}^{2} \\ &\leq 4L_{T}^{2} \left(\int_{0}^{t} \int_{\Omega} |\tilde{c_{n}} - \tilde{c}|^{2}(\sigma, x) \, \mathrm{d}x \, \mathrm{d}\sigma \right) \|f^{0}\|_{L^{\infty}(\mathbb{Q}_{T})}^{2} + 4T^{2}L_{T}^{2} \|Q\|_{L^{\infty}(\mathbb{Q}_{T} \times \mathbb{R}_{+})}^{2} \int_{s}^{t} \int_{\Omega} |\tilde{c_{n}} - \tilde{c}|^{2}(\sigma, x) \, \mathrm{d}x \, \mathrm{d}\sigma \\ &\leq \left(4L_{T}^{2} \|f^{0}\|_{L^{\infty}(\mathbb{Q}_{T})}^{2} + 4T^{2}L_{T}^{2} \|Q\|_{L^{\infty}(\mathbb{Q}_{T} \times \mathbb{R}_{+})}^{2} \right) \int_{0}^{t} \int_{\Omega} |\tilde{c_{n}} - \tilde{c}|^{2}(\sigma, x) \, \mathrm{d}x \, \mathrm{d}\sigma, \end{split}$$

since $s \geq 0$.

On the other hand, we obtain using the characteristic curves

$$\begin{split} &|\int_{0}^{\infty}a(\xi)f_{n}(t,x,\xi)\,\mathrm{d}\xi-\int_{0}^{\infty}a(\xi)f(t,x,\xi)\,\mathrm{d}\xi|\\ &=|\int_{\mathscr{E}_{n}(0;t,x,0)}^{\infty}a\big(\mathscr{E}_{n}(t;0,x,\delta)\big)f^{0}(x,\delta)\,\mathrm{d}\delta+\int_{\mathscr{E}_{n}(s;t,x,0)}^{\infty}\int_{0}^{t}a\big(\mathscr{E}_{n}(t;s,x,\delta)\big)Q(s,x,\delta)\,\mathrm{d}s\,\mathrm{d}\delta\\ &-\int_{\mathscr{E}(0;t,x,0)}^{\infty}a\big(\mathscr{E}(t;0,x,\delta)\big)f^{0}(x,\delta)\,\mathrm{d}\delta-\int_{\mathscr{E}(s;t,x,0)}^{\infty}\int_{0}^{t}a\big(\mathscr{E}(t;s,x,\delta)\big)Q(s,x,\delta)\,\mathrm{d}s\,\mathrm{d}\delta|\\ &\leq|\int_{\mathscr{E}(0;t,x,0)}^{\mathscr{E}_{n}(0;t,x,0)}a\big(\mathscr{E}_{n}(t;0,x,\delta)\big)f^{0}(x,\delta)\,\mathrm{d}\delta|+\int_{\mathscr{E}(0;t,x,0)}^{\infty}|\big(a(\mathscr{E}_{n})-a(\mathscr{E})\big)(t;0,x,\delta)|f^{0}(x,\delta)\,\mathrm{d}\delta\\ &+|\int_{\mathscr{E}(s;t,x,0)}^{\mathscr{E}_{n}(s;t,x,0)}\int_{0}^{t}a\big(\mathscr{E}_{n}(s;t,x,\delta)\big)Q(s,x,\delta)\,\mathrm{d}s\,\mathrm{d}\delta|\\ &+\int_{\mathscr{E}(s;t,x,0)}^{\infty}\int_{0}^{t}|\big(a(\mathscr{E}_{n})-a(\mathscr{E})\big)(t;s,x,\delta)||Q(s,x,\delta)|\,\mathrm{d}s\,\mathrm{d}\delta, \end{split}$$

where $(a(\mathscr{E}_n) - a(\mathscr{E}))(t; s, x, \delta) = a(\mathscr{E}_n(t; s, x, \delta)) - a(\mathscr{E}(t; s, x, \delta)), \quad \forall t, s.$

This implies that

$$\left| \int_{0}^{\infty} a(\xi) f_{n}(t, x, \xi) \, \mathrm{d}\xi - \int_{0}^{\infty} a(\xi) f(t, x, \xi) \, \mathrm{d}\xi \right| \\
\leq L_{a} \left| \int_{\mathscr{E}(0; t, x, 0)}^{\mathscr{E}_{n}(0; t, x, 0)} \mathscr{E}_{n}(t; 0, x, \delta) f^{0}(x, \delta) \, \mathrm{d}\delta \right| + L_{a} \int_{\mathscr{E}(0; t, x, 0)}^{\infty} \left| \mathscr{E}_{n} - \mathscr{E} \right| (t; 0, x, \delta) f^{0}(x, \delta) \, \mathrm{d}\delta \\
+ L_{a} \left| \int_{\mathscr{E}(s; t, x, 0)}^{\mathscr{E}_{n}(s; t, x, 0)} \int_{0}^{t} \mathscr{E}_{n}(s; t, x, \delta) Q(s, x, \delta) \, \mathrm{d}s \, \mathrm{d}\delta \right| \\
+ L_{a} \int_{\mathscr{E}(s; t, x, 0)}^{\infty} \int_{0}^{t} \left| \mathscr{E}_{n} - \mathscr{E} \right| (t; s, x, \delta) \left| Q(s, x, \delta) \right| \, \mathrm{d}s \, \mathrm{d}\delta. \tag{3.9}$$

To continue our computation we need estimations on all terms in the right hand side of the previous relation. So we write:

$$|\mathcal{E}_{n}(t;0,x,\delta)| = |\mathcal{E}_{n}(t;0,x,\delta) - \underbrace{\mathcal{E}_{n}(t;0,x,\mathcal{E}_{n}(0;t,x,0))}_{=0}|$$

$$= |\int_{\delta}^{\mathcal{E}_{n}(0;t,x,0)} \partial_{\xi} \mathcal{E}_{n}(t;0,x,\xi) \,\mathrm{d}\xi|$$

$$= |\int_{\delta}^{\mathcal{E}_{n}(0;t,x,0)} \exp\left(-\int_{t}^{0} a'(\mathcal{E}_{n}(\sigma;t,x,\xi))\tilde{c}_{n}(\sigma,x) \,\mathrm{d}\sigma\right) \,\mathrm{d}\xi|$$

$$\leq L_{T}|\delta - \mathcal{E}_{n}(0;t,x,0)|.$$
(3.10)

The fact that $\delta \in [\min(\mathscr{E}_n, \mathscr{E}), \max(\mathscr{E}_n, \mathscr{E})]$ at the point (0; t, x, 0) implies that $|\mathscr{E}_n(t; 0, x, \delta)| \leq L_T |\mathscr{E}_n - \mathscr{E}|(0; t, x, 0)$ with $L_T = \exp(-T M_T)$. Then we deduce

$$\left| \int_{\mathscr{E}(0;t,x,0)}^{\mathscr{E}_n(0;t,x,0)} \mathscr{E}_n(t;0,x,\delta) f^0(x,\delta) \,\mathrm{d}\delta \right| \le L_T |\mathscr{E}_n - \mathscr{E}|(0;t,x,0) \int_0^\infty f^0(x,\delta) \,\mathrm{d}\delta. \tag{3.11}$$

Thanks to (3.7) we also have

$$\int_{\mathscr{E}(0;t,x,0)}^{\infty} |\mathscr{E}_n - \mathscr{E}|(t;0,x,\delta) f^0(x,\delta) \,d\delta \le L_T \left(\int_0^t |\tilde{c}_n - \tilde{c}|^2(\sigma,x) \,d\sigma \right)^{1/2} \int_0^{\infty} (1+\delta) f^0(x,\delta) \,d\delta. \quad (3.12)$$

By analogy to relation (3.10) one obtains

$$|\mathscr{E}_n(s;t,x,\delta)| \le L_T |\mathscr{E}_n - \mathscr{E}|(t;s,x,0),$$

which implies that

$$\left| \int_{\mathscr{E}(s;t,x,0)}^{\mathscr{E}_{n}(s;t,x,0)} \int_{0}^{t} \mathscr{E}_{n}(s;t,x,\delta) Q(s,x,\delta) \, \mathrm{d}s \, \mathrm{d}\delta \right| \\
\leq L_{T} \int_{0}^{t} |\mathscr{E}_{n} - \mathscr{E}|(t;s,x,0) \left(\int_{\mathscr{E}(s;t,x,0)}^{\mathscr{E}_{n}(s;t,x,0)} |Q(s,x,\delta)| \, \mathrm{d}\delta \right) \, \mathrm{d}s \\
\leq L_{T} \int_{0}^{t} |\mathscr{E}_{n} - \mathscr{E}|(t;s,x,0) \int_{0}^{\infty} |Q(s,x,\delta)| \, \mathrm{d}\delta \, \mathrm{d}s \\
\leq L_{T} \sup_{s \in [0,t]} (|\mathscr{E}_{n} - \mathscr{E}|(t;s,x,0)) \int_{0}^{\infty} \int_{0}^{t} |Q(s,x,\delta)| \, \mathrm{d}\delta \, \mathrm{d}s \\
\leq L_{T} \left(\int_{s}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma,x) \, \mathrm{d}\sigma \right)^{1/2} \|Q\|_{L^{\infty}(\mathbb{Q}_{T})}. \tag{3.13}$$

For the last term of equation (3.9) we use the following majoration

$$\int_{\mathscr{E}(s;t,x,0)}^{\infty} \int_{0}^{t} |\mathscr{E}_{n} - \mathscr{E}|(t;s,x,\delta) |Q(s,x,\delta)| \, \mathrm{d}s \, \mathrm{d}\delta \\
\leq \sup_{s \in [0,T]} |\mathscr{E}_{n} - \mathscr{E}|(t;s,x,\delta) \int_{0}^{\infty} \int_{0}^{t} |Q(s,x,\delta)| \, \mathrm{d}s \, \mathrm{d}\delta \\
\leq L_{T} \left(\int_{s}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma,x) \, \mathrm{d}\sigma \right)^{1/2} \int_{0}^{t} \int_{0}^{\infty} (1+\delta) |Q(s,x,\delta)| \, \mathrm{d}\delta \, \mathrm{d}s. \tag{3.14}$$

Combining relations (3.11)–(3.14) we deduce from (3.9):

$$\left| \int_{0}^{\infty} a(\xi) f_{n}(t, x, \xi) \, d\xi - \int_{0}^{\infty} a(\xi) f(t, x, \xi) \, d\xi \right| \\
\leq L_{a} L_{T}^{2} \left(\int_{0}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2} \|f^{0}\|_{L^{\infty}(\mathbb{R}_{+})} + L_{a} L_{T} \left(\int_{0}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2} \|f^{0}\|_{L^{\infty}(\mathbb{R}_{+}, (1+\xi) \, d\xi)} \\
+ L_{a} L_{T}^{2} \left(\int_{s}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2} \|Q\|_{L^{\infty}(\mathbb{Q}_{T})} + L_{a} L_{T} \left(\int_{s}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2} \|Q\|_{L^{\infty}(\mathbb{Q}_{T}, (1+\xi) \, d\xi)} \\
\leq L_{a} L_{T}^{2} \left(\|f^{0}\|_{L^{\infty}(\mathbb{R}_{+})} + \|Q\|_{L^{\infty}(\mathbb{Q}_{T})} \right) \left(\int_{0}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2} \\
+ L_{a} L_{T} \left(\|f^{0}\|_{L^{\infty}(\mathbb{R}_{+}, (1+\xi) \, d\xi)} + \|Q\|_{L^{\infty}(\mathbb{Q}_{T}, (1+\xi) \, d\xi)} \right) \left(\int_{s}^{t} |\tilde{c}_{n} - \tilde{c}|^{2}(\sigma, x) \, d\sigma \right)^{1/2},$$

which achieves the proof of following convergence result

$$\int_0^\infty a(\xi) f_n(t, x, \xi) \, \mathrm{d}\xi \xrightarrow[L^2(\mathbb{Q}_T)]{n \to \infty} \int_0^\infty a(\xi) f(t, x, \xi) \, \mathrm{d}\xi.$$

Right now the convergence $c_n = \mathscr{C}(\tilde{c_n})$ towards $c = \mathscr{C}(\tilde{c})$ in $L^2(\mathbb{Q}_T)$ space is obtained by an energy estimate based on the following system:

mate based on the following system:
$$\begin{cases} \partial_t c_n(t,x) + c_n(t,x) \int_0^\infty a(\xi) f_n(t,x,\xi) \,\mathrm{d}\xi - \Delta_x c_n(t,x) = \int_0^\infty f_n(t,x,\xi) \,\mathrm{d}\xi & \text{in } (0,T) \times \varOmega, \\ \partial_t c(t,x) + c(t,x) \int_0^\infty a(\xi) f(t,x,\xi) \,\mathrm{d}\xi - \Delta_x c(t,x) = \int_0^\infty f(t,x,\xi) \,\mathrm{d}\xi & \text{in } (0,T) \times \varOmega, \\ \partial_\nu c_n = 0 \,; \partial_\nu c = 0 & \text{on } (0,T) \times \partial \varOmega, \\ c_{n_1t=0} = c_{|t=0} = c_{\text{init}} & \text{on } \overline{\varOmega}, \end{cases}$$

what allows to obtain the relation

$$\frac{d}{2 dt} \int_{\Omega} (c_n - c)^2(t, x) dx + \int_{\Omega} |\nabla_x (c_n - c)|^2(t, x) dx + \int_{\Omega} (c_n - c)^2(t, x) \int_0^{\infty} a(\xi) f(t, x, \xi) d\xi dx
= -\int_{\Omega} c_n (c_n - c) \left(\int_0^{\infty} a(\xi) f_n - \int_0^{\infty} a(\xi) f \right)(t, x) dx + \int_{\Omega} (c_n - c) \left(\int_0^{\infty} f_n - \int_0^{\infty} f \right)(t, x) dx.$$

Applying the Cauchy and Young inequalities and the fact that $c_n \in \mathbb{E}_T$ one obtains that

$$\frac{d}{2 dt} \int_{\Omega} (c_n - c)^2(t, x) dx + \int_{\Omega} |\nabla_x (c_n - c)|^2(t, x) dx + \int_{\Omega} (c_n - c)^2(t, x) \int_0^{\infty} a(\xi) f(t, x, \xi) d\xi dx
\leq \int_{\Omega} (c_n - c)^2(t, x) dx + \frac{K_T^2}{2} \int_{\Omega} \left(\int_0^{\infty} a(\xi) f_n(t, x, \xi) d\xi - \int_0^{\infty} a(\xi) f(t, x, \xi) d\xi \right)^2 dx
+ \frac{1}{2} \int_{\Omega} \left(\int_0^{\infty} f_n(t, x, \xi) d\xi - \int_0^{\infty} f(t, x, \xi) d\xi \right)^2 dx.$$

The gronwall lemma yields that:

$$\int_{\Omega} (c_n - c)^2(t, x) \, \mathrm{d}x \le cte \left(\int_0^t \int_{\Omega} |\int_0^\infty a(\xi) f_n \, \mathrm{d}\xi - \int_0^\infty a(\xi) f \, \mathrm{d}\xi|^2(s, x) \, \mathrm{d}x \, \mathrm{d}s \right)$$
$$+ \int_0^t \int_{\Omega} |\int_0^\infty f_n \, \mathrm{d}\xi - \int_0^\infty f \, \mathrm{d}\xi|^2(s, x) \, \mathrm{d}x \, \mathrm{d}s \right),$$

where the constant $cte = cte(T, C_0, ||f^0||_{L^{\infty}(\mathbb{Q}_T)})$. This gives us the convergence result. So by the Schauder fixed point theorem, the application \mathscr{C} admits a fixed point $c = \mathscr{C}(c)$ satisfying the equation

$$\partial_t c(t,x) + c(t,x) \int_0^\infty a(\xi) f(t,x,\xi) \,d\xi - \Delta_x c(t,x) = \int_0^\infty f(t,x,\xi) \,d\xi.$$

The proof of the uniqueness of the solution c is obvious if one applies the same reasoning as in the proof of the continuity of \mathscr{C} . The existence and uniqueness of the couple (c, f) solution of the problem (1.1) is then proved in the case where the kinetic coefficient a is Lipschitz continuous on $[0, \infty)$.

For the general case stated in **Hypothesis 11** where the polymerization rate is singular, one remarks that the Lipschitz constant L_a is not involved in the above estimations. So we can adapt the previous proof to the particular case of a non smooth kinetic coefficient $a(\xi)$ as indicated in the hypothesis. This consideration allows to take into account the kinetic coefficients, $a(\xi) = \xi^{1/3}$, used by Lifshitz and Slyozov [25] to describe the kinetics of precipitation from supersaturated solid solutions. For the adaptation of this general case, we consider a sequence of smooth kinetic coefficients $a^n(\xi)$

which converges pointwise to $a(\xi)$. So, if (f^n, c^n) is the associated solution of the system with $a^n(\xi)$, then there exists a subsequence which converges to (f, c) associated to the kinetic coefficients $a(\xi)$. Otherwise, from the pointwise convergence of a^n , we can pass to the limit when n tends to infinity and obtain (f, c) as a weak solution with the kinetic coefficients $a(\xi)$. This method of solution extension is explained in [21] for the case of homogeneous Lifshitz-Slyozov equation. The proof of the uniqueness follows the same reasoning as in [13] (see this reference for more details). Let us give some hints for the proof of the uniqueness. From two couples of solutions $(c^{(1)}, f^{(1)})$ and $(c^{(2)}, f^{(2)})$ with the same initial data of the system $(1.1)_1$ –(1.3) we have to show that $c^{(1)} = c^{(2)}$ and $f^{(1)} = f^{(2)}$ for $a.e(t,x) \in (0,T) \times \Omega$ and $\xi > 0$. One needs to derive an L^1 estimation of the monomer concentration by introducing the approximation, $S_{\epsilon}(z) = \frac{z}{\sqrt{\epsilon + z^2}}$, for the sign function. So, $Z_{\epsilon}(z) = \int_0^z S_{\epsilon}(s) ds$ approaches |z| as ϵ tends to 0. From (1.3) we have

$$(\partial_t - \Delta_x + A^{(1)})(c^{(1)} - c^{(2)}) = B^{(1)} - B^{(2)} + (A^{(2)} - A^{(1)})c^{(2)}$$

where $A^{(i)}=\int_0^\infty a(\xi)f^{(i)}(t,x,\xi)\,d\xi$ and $B^{(i)}=\int_0^\infty f^{(i)}(t,x,\xi)\,d\xi$ $i=\{1,2\},$ we apply the composition with Z_ϵ then integrate over Ω and obtain when $\epsilon\to 0$ the following L^1 estimation

$$\int_{\Omega} |c^{(1)} - c^{(2)}|(t, x) dx \le \int_{\Omega} |c_0^{(1)} - c_0^{(2)}|(t, x) dx + \int_0^t \int_{\Omega} |B^{(1)} - B^{(2)}|(s, x) dx
+ K_T \int_0^t \int_{\Omega} |A^{(2)} - A^{(1)}|(s, x) dx.$$
(3.15)

Knowing that $c_0^{(1)} = c_0^{(2)}$, from the hypothesis of the same initial data, then the first term at the right hand side of the inequality vanishes. To prove that the two other terms vanish, one can adapt the same argument as in [21] for the problem without diffusion and coalescence. More details for this adaptation can be found in [13].

4 Numerical resolution of the equations

In this section we present a numerical scheme to simulate the modified Lifschitz-Slyosov model (1.1). The construction of the scheme gives some hints concerning stability issues. For calculating the approximate solution, we give a discretization in time, space and size of the polymers. We choose to discretize the monomers by an implicit finite difference scheme in time and space. To solve the equation of polymers, the time derivative is discretized by the finite differences method, and the length one by a finite volume scheme.

The discretization provides a set of points $(t_n)_{n=1,...,N_t}$, $N_t \in \mathbb{N}$ in the time interval $]0,T[,(\zeta_l)_{l=1,...,N_l}, N_l \in \mathbb{N}$ in the size range]0,L[, and nodes $(x_{i,j})_{i,j=1,...,N}, N \in \mathbb{N}$ of the domain Ω . For simplicity a constant discretization in length and space is used. Let Δx be the space step, $\Delta \zeta$ the length step and Δt_n the time step. We set

$$t_0 = 0$$
, $t_n = t_{n-1} + \Delta t_n$, $t_{n+\frac{1}{2}} = t_n + \frac{\Delta t_n}{2}$ for $n = 1, ..., N_t$,

$$\zeta_l = l\Delta\zeta, \quad \zeta_{l+\frac{1}{2}} = (l+\frac{1}{2})\Delta\zeta \quad \text{ for } l=1,...,N_l.$$

Let us consider the discrete cells $C_l =]\zeta_{l-1/2}, \zeta_{l+1/2}[$ centered on ζ_l . We compute an approximative solution (c, f) to the problem (1.1), denoted

$$c_{i,j}^n \simeq c(t_n, x_{i,j}), \quad f_{i,j,l}^n \simeq \frac{1}{\Delta \zeta} \int_{C_l} f(t_n, x_{i,j}, \zeta) d\zeta.$$

The scheme is based on the following time-splitting between advection and aggregation:

1. First, the homogeneous advection equation is solved:

$$\partial_t f + \partial_{\varepsilon} (V f) = 0. \tag{4.1}$$

2. Second, the solution obtained from the advection equation is used to build the aggregation operator:

$$\partial_t f = \lambda \, Q(f). \tag{4.2}$$

Scheme for the advection of macro-particles The updating of the particles distribution follows by integrating the advection equation over the finite volume cells C_l :

$$f_{i,j,l}^{n+1} = f_{i,j,l}^n - \nu^n \left(V_{i,j,l+\frac{1}{2}}^n f_{i,j,l+\frac{1}{2}}^n - V_{i,j,l-\frac{1}{2}}^n f_{i,j,l-\frac{1}{2}}^n \right), \tag{4.3}$$

with $V_{i,j,l}^n \simeq V(t_n,x_{i,j},\zeta_l)$ and $\nu^n = \frac{\Delta t_n}{\Delta \zeta}$. It remains to define the interface fluxes $f_{i,j,l+\frac{1}{2}}^n$. When investigating the large time behavior of solutions to transport equations, one faces the classical drawback of usual stable schemes: numerical diffusion, in its general sense, that is, the deterioration of profiles, the spreading of the initial data and the loss of the dependence cone. High-order schemes (such as WENO ...) are a cure, but are known to spread all the same for any initial data, in very long time. On the other hand, the anti-diffusive, limited downwind scheme of Ref [13], has the advantage of avoiding this spreading, keeping in arbitrary large time the profiles. We recall its basic principles in the case of advection with constant velocity. The idea is to take a downwind flux, under some stability constraints. The stability constraints are those that lead to a local numerical maximum principle. We adapt this idea to the present problem and refer to [14] for more details.

Let us consider the following notation:

$$m_{i,j,l+\frac{1}{2}}^n = \min \Big(f_{i,j,l}^n, f_{i,j,l+1}^n \Big), \quad M_{i,j,l+\frac{1}{2}}^n = \max \Big(f_{i,j,l}^n, f_{i,j,l+1}^n \Big).$$

$$\begin{split} -\text{ If } V^n_{i,j,l}, V^n_{i,j,l+\frac{1}{2}}, V^n_{i,j,l-\frac{1}{2}} > 0, \text{ then} \\ b^n_{i,j,l+\frac{1}{2}} &= \frac{1}{\nu^n |V^n_{i,j,l}|} (f^n_{i,j,l} - M^n_{i,j,l-\frac{1}{2}}) + M^n_{i,j,l-\frac{1}{2}}, \\ B^n_{i,j,l+\frac{1}{2}} &= \frac{1}{\nu^n |V^n_{i,j,l}|} (f^n_{i,j,l} - m^n_{i,j,l-\frac{1}{2}}) + m^n_{i,j,l-\frac{1}{2}}, \\ \\ \mathcal{B}^n_{i,j,l+\frac{1}{2}} &= \begin{cases} \min \Big(B^n_{i,j,l+\frac{1}{2}}, \frac{\nu^n m^n_{i,j,l-\frac{1}{2}} |V^n_{i,j,l-\frac{1}{2}}| + f^n_{i,j,l}}{\nu^n |V^n_{i,j,l+\frac{1}{2}}|} \Big), & \text{if } m^n_{i,j,l-\frac{1}{2}} \geq 0, \\ \\ B^n_{i,j,l+\frac{1}{2}}, & \text{otherwise.} \end{cases} \end{split}$$

– If $V_{i,j,l}^n, V_{i,j,l+\frac{1}{2}}^n, V_{i,j,l-\frac{1}{2}}^n < 0$, then:

$$\begin{split} b^n_{i,j,l+\frac{1}{2}} &= \frac{1}{\nu^n |V^n_{i,j,l}|} (f^n_{i,j,l} - M^n_{i,j,l+\frac{1}{2}}) + M^n_{i,j,l+\frac{1}{2}}, \\ B^n_{i,j,l+\frac{1}{2}} &= \frac{1}{\nu^n |V^n_{i,j,l}|} (f^n_{i,j,l} - m^n_{i,j,l+\frac{1}{2}}) + m^n_{i,j,l+\frac{1}{2}}, \\ B^n_{i,j,l+\frac{1}{2}} &= \begin{cases} \min \Big(B^n_{i,j,l-\frac{1}{2}}, \frac{\nu^n m^n_{i,j,l+\frac{1}{2}} |V^n_{i,j,l+\frac{1}{2}}| + f^n_{i,j,l}}{\nu^n |V^n_{i,j,l-\frac{1}{2}}|} \Big), & \text{if } m^n_{i,j,l+\frac{1}{2}} \geq 0, \\ B^n_{i,j,l+\frac{1}{2}}, & \text{otherwise.} \end{cases} \end{split}$$

– If the $V_{i,j,l}^n,\,V_{i,j,l+\frac{1}{2}}^n,\,V_{i,j,l-\frac{1}{2}}^n$ do not have the same sign, we set

$$b^n_{i,j,l+\frac{1}{2}} = \mathcal{B}^n_{i,j,l+\frac{1}{2}} = \begin{cases} & f^n_{i,j,l} \text{ if } V^n_{i,j,l+\frac{1}{2}} > 0, \\ \\ f^n_{i,j,l+1} \text{ if } V^n_{i,j,l+\frac{1}{2}} < 0. \end{cases}$$

$$\mu^n_{i,j,l+\frac{1}{2}} = \max(m^n_{i,j,l+\frac{1}{2}},b^n_{i,j,l+\frac{1}{2}}), \quad \mathcal{M}^n_{i,j,l+\frac{1}{2}} = \min(M^n_{i,j,l+\frac{1}{2}},\mathcal{B}^n_{i,j,l+\frac{1}{2}}).$$

The following statement clarifies the principles on which the construction of the fluxes is based.

Proposition 4.1 [14] Assume that the Courant-Friedrichs-Levy stability condition:

$$CFL = \nu^n \max_{i,j,l} (|V_{i,j,l}^n|, |V_{i,j,l+\frac{1}{2}}^n|) \le 1$$
(4.4)

holds, then $[\mu_{i,j,l+\frac{1}{2}}^n, \mathcal{M}_{i,j,l+\frac{1}{2}}^n] \neq \emptyset$, for all $l=1,..,N_l$. Moreover if

$$f_{i,j,l+\frac{1}{2}}^n \in [\mu_{i,j,l+\frac{1}{2}}^n, \mathcal{M}_{i,j,l+\frac{1}{2}}^n], \quad \forall l = 1, ..., N_l,$$

the following assertions hold:

- 1. The scheme (4.3) is consistent with (4.1).
- 2. If $\Delta \zeta$ is sufficiently small then $f_{i,j,l}^n \geq 0$ implies $f_{i,j,l}^{n+1} \geq 0$. Otherwise a restricted condition $CFL \leq \frac{1}{2}$ is requested to ensure the non-negativity.
- 3. Let us consider

$$f_{i,j,l}^{n*} = f_{i,j,l}^{n} - \nu^{n} V_{i,j,l}^{n} (f_{i,j,l+\frac{1}{2}}^{n} - f_{i,j,l-\frac{1}{2}}^{n}), \quad \forall l = 1, ..., N_{l}.$$

- $(a) \ \ \textit{If} \ V^n_{i,j,l} \geq 0, \ then \ m^n_{i,j,l-\frac{1}{2}} \leq f^{n*}_{i,j,l} \leq M^n_{i,j,l-\frac{1}{2}}.$
- (b) If $V_{i,j,l}^{n} \le 0$, then $m_{i,j,l+\frac{1}{2}}^{n} \le f_{i,j,l}^{n*} \le M_{i,j,l+\frac{1}{2}}^{n}$

The goal now consists in defining $f_{i,j,l+\frac{1}{2}}^n$ so that on the one hand, **Proposition 4.1** holds, and on the other hand the numerical diffusion is reduced as possible. To this end, we adopt a downwinding approach. When $V_{i,j,l-\frac{1}{2}}^n > 0$, $V_{i,j,l}^n > 0$ and $V_{i,j,l+\frac{1}{2}}^n > 0$, we choose the closest value to $f_{i,j,l+1}^n$ that fulfills the requirements of **Proposition 4.1**. Namely $f_{i,j,l+\frac{1}{2}}^n$ will be the solution of the following problem: Minimize $|f_{i,j,l+\frac{1}{2}}^n - f_{i,j,l+1}^n|$ under the constraint $f_{i,j,l+\frac{1}{2}}^n \in [\mu_{i,j,l+\frac{1}{2}}^n, \mathcal{M}_{i,j,l+\frac{1}{2}}^n]$.

problem: Minimize $|f_{i,j,l+\frac{1}{2}}^n - f_{i,j,l+1}^n|$ under the constraint $f_{i,j,l+\frac{1}{2}}^n \in [\mu_{i,j,l+\frac{1}{2}}^n, \mathcal{M}_{i,j,l+\frac{1}{2}}^n]$. By assuming that $V_{i,j,l-\frac{1}{2}}^n > 0$, $V_{i,j,l}^n > 0$ and $V_{i,j,l+\frac{1}{2}}^n > 0$, the minimization problem leads to the following three cases:

$$f_{i,j,l+\frac{1}{2}}^n = \begin{cases} \mu_{i,j,l+\frac{1}{2}}^n \text{ if } f_{i,j,l+1}^n \leq \mu_{i,j,l+\frac{1}{2}}^n, \\ \\ f_{i,j,l+1}^n \text{ if } \mu_{i,j,l+\frac{1}{2}}^n \leq f_{i,j,l+1}^n \leq \mathcal{M}_{i,j,l+\frac{1}{2}}^n, \\ \\ \mathcal{M}_{i,j,l+\frac{1}{2}}^n \text{ if } f_{i,j,l+1}^n \geq \mathcal{M}_{i,j,l+\frac{1}{2}}^n. \end{cases}$$

In the case of locally positive velocity, the stability constraint involves $f_{i,j,l-1}^n$ and $f_{i,j,l}^n$ that are upwind values for $f_{i,j,l-\frac{1}{2}}^n$; it justifies the name of downwind flux under upwind constraint.

Treatment of the coagulation operator How the coagulation term Q modifies the asymptotic behavior of the solutions is investigated numerically. For the Smoluchowski operator treatment, two main approaches are discussed in [36]. The first "naive" approach and the second one suggested by F. Filbert and P. Laurençot [11] are discussed in [36]. The "naive" approach preserves the solution positiveness, but is very cost in CPU time. In our case, we use the approach suggested by F. Filbert and P. Laurençot for its good performances. To this end, the treatment of the collision term thanks to the approach developed in [21] is incorporated in the time-splitting algorithm.

The starting point of the method consists in rewriting $\partial_t f = \lambda Q(f)$ as follows:

$$\zeta \partial_t f = \lambda \zeta Q(f) = -\lambda \partial_\zeta J(f), \quad \text{with } J(f)(t, x, \zeta) = \int_0^\zeta \int_{\zeta - s}^\infty s f(t, x, s) f(t, x, r) dr ds.$$

The next step relies on the approximation of the integrals that define J(f) and the necessary truncation, embodied into a parameter $0 < R < \infty$, of the infinite integration domain.

The approach designed is the "Conservative method", which consists in replacing J(f) by

$$J^R(f)(t,x,\zeta) = \int_0^\zeta \int_{\zeta-s}^{R-s} sf(t,x,s)f(t,x,r)drds, \quad \text{ for } 0 < \zeta < R < \infty.$$

Note that $J^R(f)(t, x, R) = J^R(f)(t, x, 0) = 0$. Consequently, the solution f_R of

$$\zeta \frac{\partial f_R}{\partial t} = -\lambda \frac{\partial J^R}{\partial \zeta}(f_R), \quad 0 < \zeta < R < \infty$$

satisfies the preservation of the first-order moment:

$$\int_0^R \zeta J^R(f)(t,x,\zeta)d\zeta = \int_0^R \zeta J^R(f)(0,x,\zeta)d\zeta = 0.$$

One can see [12] for a thorough analysis of the method, in particular for the convergence analysis when $R \to \infty$. The problem addressed in [12] is essentially concerned with the capture of the gelation phenomenon, that is a loss of mass in finite time, a typical feature of certain coagulation equations. Here, the situation is different and it turns out that the conservation of the first moment by the process of encounter is crucial for the accuracy of the scheme and the evaluation of the monomers concentration in the last step of the splitting. That is the reason why we work here with the conservation method.

For the discrete expression of the operator $J^{R}(f)$, it is convenient to introduce the change of variables w = s + r to obtain

$$J^{R}(f)(t,x,\zeta) = \int_{0}^{\zeta} \int_{\zeta}^{R} sf(t,x,s)f(t,x,w-s)dwds.$$

The numerical scheme is written

$$\zeta_l f_{i,j,l}^{n+1} = \zeta_l f_{i,j,l}^{n+\frac{1}{2}} - \lambda \nu^n \left(J_{i,j,l+\frac{1}{2}}^{n+\frac{1}{2}} - J_{i,j,l-\frac{1}{2}}^{n+\frac{1}{2}} \right),$$

where the numerical flux $J_{i,j,l+\frac{1}{2}}^{n+\frac{1}{2}}$ is the approximation of $J^R(f)(t_{n+\frac{1}{2}},x_{i,j},\zeta_{l+\frac{1}{2}})$.

Monomers scheme For updating the monomers concentration, an implicit finite difference scheme is used to solve equation (1.1_3) . This numerical scheme is the following:

$$\frac{c_{i,j}^{n+1} - c_{i,j}^{n}}{\Delta t_{n}} - \frac{c_{i-1,j}^{n+1} + c_{i,j-1}^{n+1} - 4c_{i,j}^{n+1} + c_{i+1,j}^{n+1} + c_{i,j+1}^{n+1}}{\Delta x^{2}} = -\sum_{l=1}^{N_{l}} \zeta_{l} \frac{f_{i,j,l}^{n+1} - f_{i,j,l}^{n}}{\Delta t_{n}} \Delta l, \quad \forall i, j = 2, ..., N-1, \forall n = 1, ..., N_{t},$$

$$c_{i,j}^{0} = c_{\text{init}}(x_{i,j}), \quad \forall i, j = 1, ..., N.$$

Boundary conditions On $\partial\Omega$, the Neumann boundary conditions are approximated by the following relationships:

- For internal nodes to boundary edges:

$$c_{1,j} = c_{2,j}, c_{N,j} = c_{N-1,j} \text{ for } j = 2, ..., N-1,$$

 $c_{i,1} = c_{i,2}, c_{i,N} = c_{i,N-1} \text{ for } i = 2, ..., N-1.$

$$(4.5)$$

- At the corner of the domain:

$$c_{1,1} = c_{2,2}, c_{N,1} = c_{N-1,2}, c_{N,N} = c_{N-1,N-1}, c_{1,N} = c_{2,N-1}.$$
 (4.6)

5 Numerical results

The geometric domain, defined by $\Omega = [0, 1]^2$, is discretized using a structured mesh with a space step size h equal to 0.02. The polymers size domain is [0, 1] with 50 subdivisions. The CFL number is set to 1.

5.1 Evolution of a mixed solution of monomers and polymers

The Coagulation coefficient λ is equal to 1. The diffusion coefficient of the monomers is equal to 0.001. The monomers are initially randomly distributed in space. The polymers are also randomly distributed is size and space. Only polymers whose size are lower than 0.2 are initially present in the domain.

The evolution of the monomer spatial distribution is illustrated by Figure 5.1. The diffusion leads to a smoothing of the density. After a while, the monomers are more concentrated at the bottom and right sides of the domain.

The mean density of polymers with size included in the intervals [0.4, 0.6] and [0.8, 1] are respectively displayed in Figures 2 and 3. The polymer density evolution exhibits at the first step a growth caused by the presence of the monomers. After a while the lack of monomers causes a depolymerization of polymers.

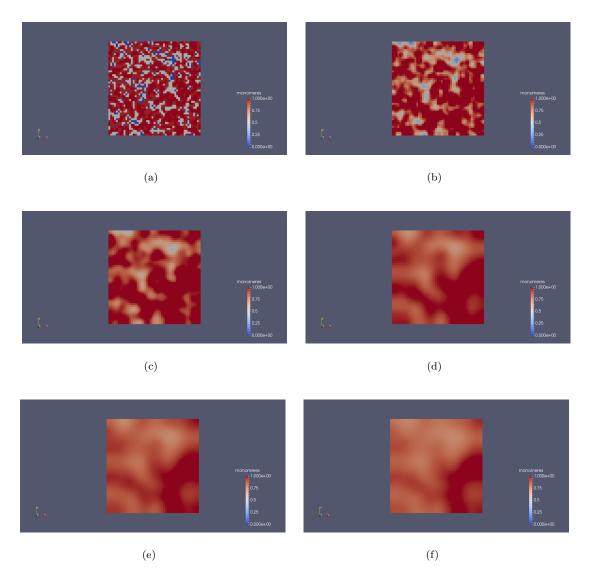


Fig. 1 Density of monomers at times 0, 0.009, 0.03, 0.14, 0.22, 0.36, from left to right and from top to bottom.

The evolution in time of the number of polymers according to their size is illustrated by Figure 4, where one can observe the growth of the polymers.

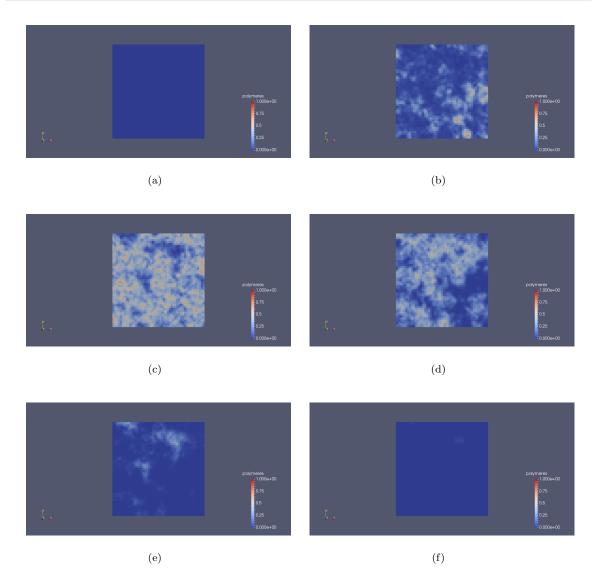


Fig. 2 Mean density of polymers with size included in the interval [0.4, 0.6] at times 0, 0.08, 0.16, 0.24, 0.36, 0.58, from left to right and from top to bottom.

The evolution of the mass of monomers and polymers is illustrated by Figure 5. One can observe first a polymerization process, followed by a depolymerization.

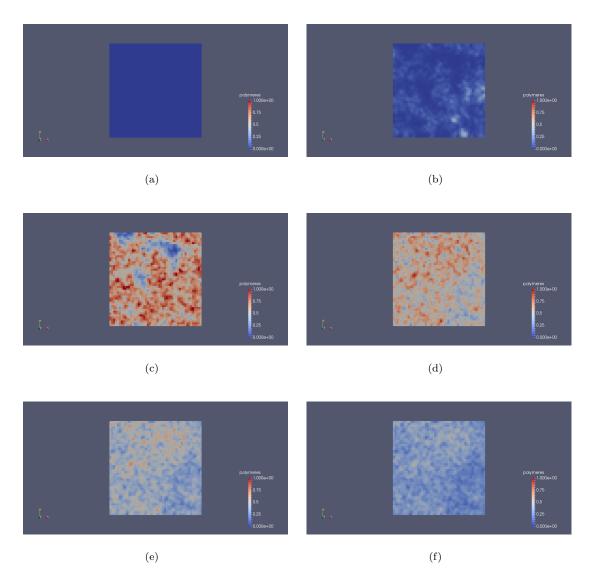


Fig. 3 Mean density of polymers with size included in the interval [0.8, 1] at times 0, 0.16, 0.36, 0.57, 0.79, 1, from left to right and from top to bottom.

5.2 Sensitivity analysis according to monomers diffusion

Figure 6 displays the evolution in time of the number of polymers; according to their size, for different values of the monomer diffusion coefficient. One can see that the growth of the number of polymers increases with the diffusion coefficient.

5.3 Sensitivity analysis according to the Coagulation coefficient

The evolution of the number of polymers, according to their size, for different values of Coagulation coefficient is displayed in Figure 7. The diffusion coefficient is set to 0.001. In this case, the polymers growth dynamic seems to be very insensitive to the caogulation coefficient change.

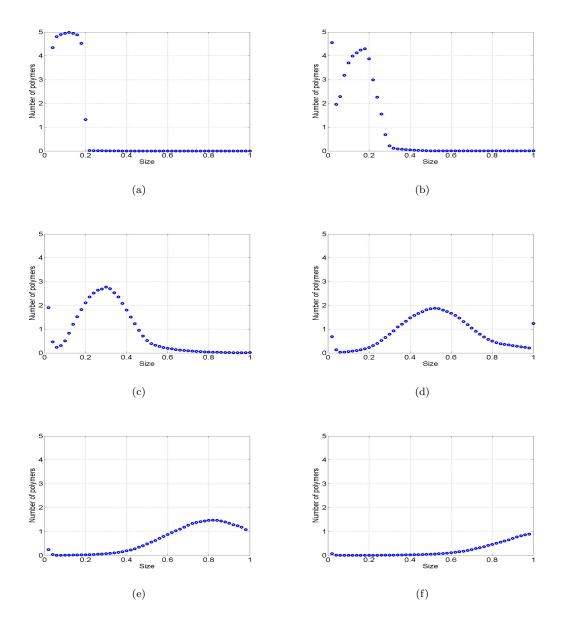


Fig. 4 Evolution of the number of polymers according to their size at times 0, 0.02, 0.1, 0.18, 0.27, 0.36, from left ro right and from top to bottom.

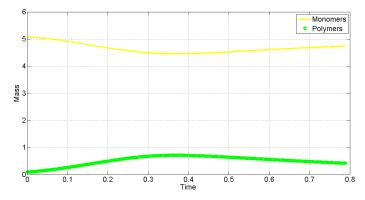


Fig. 5 Evolution in time of monomers and polymers masses.

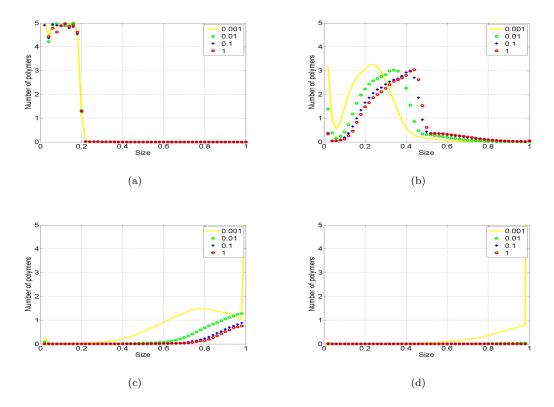


Fig. 6 Evolution of the number of polymers according to their size for different values of the diffusion coefficient 0.001, 0.01, 0.1, 1, at times 0, 0.11, 0.4, 0.53, from left to right and from top to bottom.

6 Conclusion and perspectives

We described in this study a model of polymerization where polymers are immersed in a bath of monomers. We assumed the interaction to be driven by mass transfer based on the space diffusion of monomers. We added in the model the possible lengthening of polymers when one polymer coalesces with another thanks to the Smoluchowski coagulation operator. With realistic assumptions we prove that our coupling system of hyperbolic-parabolic type is well defined and the numerical approximation based on the 2D generalization of the anti-dissipative scheme [14] is very suitable for the behavior of the solution even when the coagulation arises. Our numerical results show that monomer diffusion stimulate polymers growth. In order to go deeper in the understanding of the polymerization mechanism with others related sub-processes, we need to investigate several directions for future work. One of the interesting directions is to study the behavior of the polymerization process when in addition polymers are subject to possible coagulation and fragmentation events. In particular, coagulation and fragmentation do they regularize the asymptotic behavior of the solution toward on profile or not? An other direction not far from this previous one is to allow polymers to follow also a space diffusion equation and then investigate the well-posedness and numerical simulations of the system.

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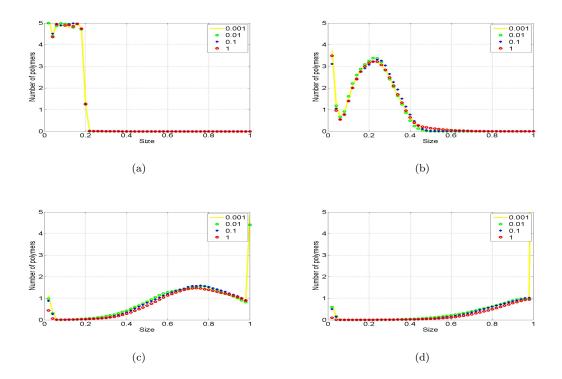


Fig. 7 Evolution of the number of polymers according to their size for different values of the coagulation coefficient 0.001, 0.01, 0.1, 1, at times 0, 0.11, 0.4, 0.53, from left to right and from top to bottom.

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