# Study of a model with diffusion

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## 1 Introduction

The first models to appear to describe the phenomenon of phase transition, and in particular the depolymerisation of molecules, are discrete models. The main drawback of such models is that they require a number of equations that is at least equal to the number of aggregate sizes. Therefore, they are unsuitable when studying large aggregates, due to their high computational cost. A big advantage in working on oligomers is that these aggregates are made up, at most, of several hundred monomers.

Like the Becker-Döring model, most models are based on mass action laws to chemical reactions. In this thesis we will focus on the Becker-Döring model and the links with its continuous analogue, the Lifshitz-Slyozov system.

On onde hand, the Becker-Döring theory is used in cases where all particle sizes are present and interact with monomers, especially the smallest ones. On the other hand, the Lifshitz-Slyozov equations apply in cases where the evolution of the system is essentially due to exchanges between large particle sizes and monomers. In such a context, the discrete polymer size variable noted $i$ in the Becker-Döring model is treated as a continuous variable $x$. If such a Taylor development of the Becker-Döring equations in order 1 gives a Lifshitz-Slyozov system, moreover in order 2 it then gives a modified Lifshitz-Slyozov equation system, which also contains a diffusion term.

In the case of our system of interest, which is the depolymerisation of large aggregates, we consider that the number of small polymers present in the solution can be considered negligible, and physico-chemical observations indicate that the molecules depolymerises as a whole. Then, the Lifshitz-Slyozov model is a transport equation model, whose reaction rate $b$ is considered constant and negative.

Our study focuses on the transition from the classic Lifshitz-Slyozov model to the modified model.

Let $b > 0$ be the depolymarisation rate and $u_0 \in L^2([0, L])$ the initial distribution of the size of the polymers. The function $u_0$ is defined on a compact set, and by a slight abuse of notation, we still denote by $u_0$ its extention with 0 on $\mathbb{R}^+$. We recall the classical Lifschitz-Slyozov model (also called the limit model) :

$$\begin{cases} \dfrac{\partial u}{\partial t} - b\dfrac{\partial u}{\partial x} = 0 & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau] \\ \\ u(x,0) = u_0(x) & \forall x \in \mathbb{R}^+ \end{cases} \tag{1}$$

This system admits a single solution noted $u \in C^1([0,\tau], H^1(\mathbb{R}^+))$.

Let us consider the modified Lifshitz-Slyozov model, which is disturbed by a coefficient diffusion term $\epsilon > 0$.

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} - b\dfrac{\partial u_\epsilon}{\partial x} - \epsilon\dfrac{\partial^2 u_\epsilon}{\partial x^2} = 0 & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau] \\ \\ u_\epsilon(x,0) = u_0(x) & \forall x \in \mathbb{R}^+ \\ \\ f(u_\epsilon)(0,t) = 0 & \forall t \in [0,\tau] \end{cases} \tag{2}$$

This system admits a single solution noted $u_\epsilon C^1([0,\tau], H^2(\mathbb{R}^+))$.

It should be noted that for the modified Lifshitz-Slyosov system, the system is only well posed by adding a condition on the border in $x = 0$. However, most modified Lifschitz-Slyozov model in litterature, used for the study of large polymers, proposes to include non-homogeneous Dirichlet nucleation, i.e. to require that the solution be equal to a positive function in $x = 0$. As this is not suitable for the study of a depolymerization system, we propose here to compare other boundary conditions. The most intuitive condition would be to set a so-called transparent (or dynamic) condition, which is exactly the transport equation :

$$\frac{\partial u_\epsilon}{\partial t}|_{x=0} - b\frac{\partial u_\epsilon}{\partial x}|_{x=0} = 0$$

The objective of this chapter is to qualify the convergence of the disturbed model to the boundary model when the diffusion coefficient $\epsilon$ tends towards 0, and in particular to study the impact of the boundary condition in $x = 0$ on the convergence speed.

In this study, we compare the convergence of the disturbed model to the limit model according to the choice of boundary condition on $x = 0$. We complete a numerical study and then a theoretical study.

Finally, we focus on the choice of a transparent boundary condition (or equivalently named dynamical boundary condition). We solve on this new disturbed system the inverse problem consisting in reconstituting the initial condition by measuring the moments of the solution. We display the least square criterion (equivalent to the classical Tikhonov regularization), and we exhibit the Riccati equations for the infinite dimension.

## 2 Existence, unicity and convergence of solutions

In this section, we introduce more precisely the mathematical elements and functional framework of our study. We study the existence and uniqueness of a solution of the perturbed transport equation by the theory of semi-groups. This functional framework will be used in the study of the inverse problem by Riccati's theory. Finally, we study the limit of the solution of the perturbed transport equation when the parameter $\epsilon$ tends towards 0.

### 2.1 Existence and unicity : semi-groups theory

For a dynamical boundary solution on $x = 0$, the system (2) reads :

$$\begin{cases} \dfrac{\partial u_\epsilon}{\partial t} - b\dfrac{\partial u_\epsilon}{\partial x} - \epsilon\dfrac{\partial^2 u_\epsilon}{\partial x^2} = 0 & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau] \\ \\ u_\epsilon(x,0) = u_0(x) & \forall x \in \mathbb{R}^+ \\ \\ \dfrac{\partial u_\epsilon}{\partial t}|_{x=0} - b\dfrac{\partial u_\epsilon}{\partial x}|_{x=0} = 0 & \forall t \in [0,\tau] \end{cases} \tag{3}$$

In order to introduce this condition with transparent limits into the variation form, let's define the space :

$$D(A) = \big\{y \mid y = (u,m) \in H^2(\mathbb{R}^+) \times \mathbb{R},\ u(0) = m\big\}$$

And the space $V = L^2(\mathbb{R}^+) \times \mathbb{R}$ with its associated norm :

$$\|y\|_V^2 = \int_0^{+\infty} u^2 + \frac{\epsilon}{b}m^2 \tag{4}$$

We denote by $(\cdot,\cdot)_V$ the scalar product associated to this norm.
Let us define the operator $A$ such that for a solution $u$, and $m = u(0,\cdot)$, we have :

$$\forall y \in D(A) \subset V \subset \mathscr{Y},\ \begin{pmatrix} \dot{u} \\ \dot{m} \end{pmatrix} = A\begin{pmatrix} u \\ m \end{pmatrix} = \begin{pmatrix} b\partial_x u + \epsilon\partial_{xx} u \\ b\partial_x u(0) \end{pmatrix} \tag{5}$$

We introduce $a$ a bilinear form such that :

$$\forall (y_1,y_2) \in D(A),\ a(y_1,y_2) \equiv -(Ay_1,y_2)_V$$

Then for all $(y_1,y_2) \in V$, if $y_1 \in D(A)$,

$$\begin{aligned} \langle Ay_1,y_2\rangle_V &= \langle b\partial_x u_1 + \epsilon\partial_{xx}u_1, u_2\rangle_{L^2} + \frac{\epsilon}{b}b\partial_x u_1(0)m_2 \\ &= \int_0^{+\infty} b(\partial_x u_1)u_2 + \int_0^{+\infty} \epsilon(\partial_{xx}u_1)u_2 + \frac{\epsilon}{b}b\partial_x u_1(0)m_2 \\ &= \int_0^{+\infty} b(\partial_x u_1)u_2 + [\epsilon(\partial_x u_1)u_2]_0^{+\infty} - \int_0^{+\infty} \partial_x u_1\partial_x u_2 + \epsilon\partial_x u_1(0)m_2 \\ &= \int_0^{+\infty} b(\partial_x u_1)u_2 - \epsilon m_2\partial_x u_1(0) - \int_0^{+\infty} \epsilon\partial_x u_1\partial_x u_2 + \epsilon\partial_x u_1(0)m_2 \\ &= \int_0^{+\infty} b(\partial_x u_1)u_2 - \int_0^{+\infty} \epsilon\partial_x u_1\partial_x u_2. \end{aligned}$$

**Proposition 2.1**

*The operator $A : D(A) \to V$ defined by :*

$$\forall (y_1,y_2) \in D(A),\ (Ay_1,y_2)_V = \int_0^{+\infty} b(\partial_x u_1)u_2 - \int_0^{+\infty} \epsilon\partial_x u_1\partial_x u_2 \tag{6}$$

*is the generator of a $C_0$ semi group of contraction in $V$.*

$\triangleright$ In order to demonstrate this proposition we will apply the Lumer-Philipps theorem. Let us check that $A$ has the needed properties :

$(i)$ The operator A is define in the domain $D(A) \subset V$, and $D(A)$ is dense in $V$.

$(ii)$ Let us prouve that $A$ is dissipative. Let $y \in V$ :

$$\begin{aligned}(Ay,y)_V &= \int_0^{+\infty} b(\partial_x u)u - \epsilon \int_0^{+\infty} (\partial_x u)^2 \\ &= \int_0^{+\infty} \frac{b}{2}\partial_x u^2 - \epsilon \int_0^{+\infty} (\partial_x u)^2 \\ &= \frac{b}{2}[u^2]_0^{+\infty} - \epsilon \int_0^{+\infty} (\partial_x u)^2 \\ &= -\frac{b}{2}u(0)^2 - \int_0^{+\infty} \epsilon(\partial_x u)^2\end{aligned}$$

Then :

$$(Ay,y)_V = -\frac{b}{2}m^2 - \epsilon \int_0^{+\infty} (\partial_x u)^2$$

Therefore $\forall\, y \in V$, $(Ay,y)_V \leq 0$.

$(iii)$
Let $y_1 = (u_1, m_1) \in \mathscr{Y}$ and $\lambda > 0$.
We are searching a solution $y$ such that $(\lambda - A)y = y_1$.
Then for all $y_2 = (u_2, m_2) \in \mathscr{Y}$, $y$ is solution of :

$$(\lambda y - Ay, y_2)_{\mathscr{Y}} = (y_1, y_2)_{\mathscr{Y}} \tag{7}$$

Moreover :

$$\lambda(\int_0^{+\infty} uu_2 + \frac{\epsilon}{b}mm_2) - \int_0^{+\infty} b(\partial_x u)u_2 + \int_0^{+\infty} \epsilon\partial_x u\partial_x u_2 = \int_0^{+\infty} u_1u_2 + \frac{\epsilon}{b}m_1m_2$$

For all $L > 0$, we choose $u_2 \in H_0^1([0,L])$, then $m_2 = 0$, and we search $u$ solution du problème variationnel :

$$\forall u_2 \in H_0^1([0,L]),\ \lambda \int_0^L uu_2 - \int_0^L b(\partial_x u)u_2 + \int_0^L \epsilon\partial_x u\partial_x u_2 = \int_0^L u_1u_2$$

We prouve that

$$\tilde{a}(u,u_2) = \lambda \int_0^L uu_2 - \int_0^L b(\partial_x u)u_2 + \int_0^L \epsilon\partial_x u\partial_x u_2$$

is bilinear, continuous, coercive over $H_0^1$. And $L(u_2) = \int_0^L u_1u_2$ is a linear contunous function of $H_0^1$. Then, given the Lax-Milgram theorem, and for any $L > 0$ there exists a unique function $u_0$ of $H_0^1(0,L)$ that is solution.
Then for $m_2 \neq 0$, we have :

$$\lambda\frac{\epsilon}{b}mm_2 = \frac{\epsilon}{b}m_1m_2$$

That defines a unique $m$ for $\lambda \neq 0$.
then we set $y = (u_0 + m_1/\lambda, m_1/\lambda)$ gives us the unique element of $V$ such that (7) is verified.
So for every $y_1 \in V$, this equation has a unique solution.
So from $(i)$,$(ii)$ and $(ii)$, we can apply the Lumer-Phillips theorem, and $A$ is the infinitesimal generator of a semi-group $C_0$.

□

**Théorème 2.2 (*Existence and uniqueness*)**

*Let's say $\tau > 0$ and $b > 0$, is $V$ a Banach space, and the of the infinitesimal generator of the semi-group $C_0$ on $V$ defined by* (6)*. So the problem of Cauchy* (2) *has a single solution in $C^0([0,\tau], V)$ that is written :*

$$\forall s \in [0,\tau]\ \ y(s) = S(s,0)y_0$$

*where $S$ is the semi-group of evolution.*

## 2.2 Convergence study

**Convergence for the norm $L^2$**

**Proposition 2.3**

*Let band $\tau$ be positive constants. Let $u_0$ be a function of $L^2(\mathbb{R}^+)$ and $f$ be the dynamical boundary condition* (12).

*Let $u_\epsilon$ be the unique solution of the system (2). Let $u$ be the unique solution of the system (1). Then if $u(\cdot,t) \in H^2$, $u_\epsilon(\cdot,t)$ converge to $u(\cdot,t)$ in norm $L^2$ when $\epsilon$ tends to $0$.*

*In particular, for all $t \in [0,\tau]$, the inequality holds true :*

$$\|u_\epsilon(\cdot,t) - u(\cdot,t)\|_{L^2(0,L)} \leq C\,\epsilon$$

*Where $C$ depends on $\|\partial_{xx} u\|$.*

$\triangleright$ Let us define $u$ and $u_\epsilon$ the respective classical solutions de (1) and (2) associated with the initial condition $u_0 \in L^2(\mathbb{R}^+)$.

We define $\tilde{u}_\epsilon$ the function $\tilde{u}_\epsilon = u_\epsilon - u$. For $u$ belonging to $H^2(\mathbb{R}^+)$, this function is a solution of :

$$\begin{cases} \dfrac{\partial \tilde{u}_\epsilon}{\partial t} - b\dfrac{\partial \tilde{u}_\epsilon}{\partial x} - \epsilon\dfrac{\partial^2 \tilde{u}_\epsilon}{\partial x^2} = \epsilon\dfrac{\partial^2 u}{\partial x^2} & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau] \\ \tilde{u}_\epsilon(x,0) = 0 & \forall x \in \mathbb{R}^+ \\ \dfrac{\partial \tilde{u}_\epsilon}{\partial t}|_{x=0} - b\dfrac{\partial \tilde{u}_\epsilon}{\partial x}|_{x=0} = 0 & \forall t \in [0,\tau] \end{cases} \tag{8}$$

Energy Estimate

We multiply by $\tilde{u}_\epsilon$ the strong solution of the equation (8) and we integrate between $0$ and $+\infty$, and it comes :

$$\begin{aligned} \frac{1}{2}\mathrm{d}_t\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} &= \int_0^{+\infty} \tilde{u}_\epsilon \partial_t \tilde{u}_\epsilon \\ &= \int_0^{+\infty} b\tilde{u}_\epsilon \partial_x \tilde{u}_\epsilon + \int_0^{+\infty} \epsilon \tilde{u}_\epsilon \partial_{xx}\tilde{u}_\epsilon + \int_0^{+\infty} \epsilon\tilde{u}_\epsilon \partial_{xx} u \\ &= -\frac{b}{2}\tilde{u}_\epsilon(0,t)^2 - \epsilon\tilde{u}_\epsilon(0,t)\partial_x\tilde{u}_\epsilon(0,t) - \int_0^{+\infty} \epsilon(\partial_x\tilde{u}_\epsilon)^2 + \int_0^{+\infty} \epsilon\tilde{u}_\epsilon\partial_{xx}u \\ &= -\frac{b}{2}\tilde{u}_\epsilon(0,t)^2 - \frac{\epsilon}{2b}\mathrm{d}_t(\tilde{u}_\epsilon(0,t)^2) - \int_0^{+\infty} \epsilon(\partial_x\tilde{u}_\epsilon)^2 + \int_0^{+\infty} \epsilon\tilde{u}_\epsilon\partial_{xx}u \end{aligned}$$

In conclusion, $\tilde{u}_\epsilon$ checks the energy estimate :

$$\frac{1}{2}\mathrm{d}_t[\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2\mathbb{R}^+} + \frac{\epsilon}{b}(\tilde{u}_\epsilon(0,t)^2)] = -\frac{b}{2}\tilde{u}_\epsilon(0,t)^2 - \epsilon\|\partial_x\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \epsilon\langle\tilde{u}_\epsilon(\cdot,t), \partial_{xx}u(\cdot,t)\rangle_{L^2(\mathbb{R}^+)}$$

From this last equation we can deduce by Cauchy Schwartz's inequality :

$$\frac{1}{2}\mathrm{d}_t[\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \frac{\epsilon}{b}(\tilde{u}_\epsilon(0,t)^2)] \leq \epsilon\|\tilde{u}_\epsilon(\cdot,t)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,t)\|_{L^2(\mathbb{R}^+)}$$

Grönwall Inequality

We integrate this inequality between $0$ and $t$, and since $\tilde{u}_\epsilon(\cdot,0) = 0$ :

$$\frac{1}{2}\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \frac{1}{2}\frac{\epsilon}{b}\tilde{u}_\epsilon(0,t)^2 \leq \epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds$$

That is, in particular :

$$\frac{1}{2}\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} \leq \epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds$$

Grönwall's lemma is applied which statement is recalled :

**Lemme 2.4**

*Let $x : [a,b] \to \mathbb{R}$ be a continuous function which satisfies the following relation :*

$$\frac{1}{2}x(t)^2 \leq \frac{1}{2}x_0^2 + \int_a^t f(s)x(s)ds \quad t \in [a,b]$$

*where $x_0 \in \mathbb{R}$ and $f$ are nonnegative continuous in $[a,b]$ . Then the estimation*

$$|x(t)| \leq |x_0| + \int_a^t f(s)ds \quad t \in [a,b]$$

*holds.*

We set $x(t) = \|\bar{u}_\epsilon(\cdot,t)\|_{L^2}$, then $x_0 = x(0) = 0$ and $f(t) = \epsilon\|\partial_{xx}u(\cdot,t)\|_{L^2}$
In conclusion, we obtained a control of $\tilde{u}_\epsilon$ by $\epsilon$, $\forall t \in [0,\tau]$ :

$$\|u_\epsilon(\cdot,t) - u(\cdot,t)\|_{L^2(\mathbb{R}^+)} \leq \epsilon C$$

□

**Convergence on the boundary** $x = 0$

**Proposition 2.5**

*Let $b$ and $\tau$ be positive constants. Let $u_0$ be a function of $L^2(\mathbb{R}^+)$ and $f$ be the dynamical boundary condition* (12). *Let $u_\epsilon$ be the unique solution of the system* (2). *Let $u$ be the unique solution of the system* (1). *Then if $u \in H^2$, $u_\epsilon(0,t)$ converge to $u(0,t)$ in norm $L^2$ when $\epsilon$ tends to* 0.
*In particular the inequality holds true :*

$$\|u_\epsilon(0,\cdot) - u(0,\cdot)\|_{L^2([0,\tau])} \leq C\,\epsilon$$

*Where $C$ depends on $\|\partial_{xx}u(\cdot,t)\|_{L^2(\mathbb{R}^+}$.*

▷ Let's take the notations from the proposition 2.3 again :

$$\begin{aligned}\frac{1}{2}\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \frac{1}{2}\frac{\epsilon}{b}(\tilde{u}_\epsilon(0,t)^2 =& -\frac{b}{2}\int_0^t \tilde{u}_\epsilon(0,s)^2 ds - \epsilon\int_0^t \|\partial_x\tilde{u}_\epsilon(\cdot,s)\|^2_{L^2(\mathbb{R}^+)}ds \\ &+ \epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds\end{aligned}$$

Then, if we isolate the boundary term on the right of the equation we obtain :

$$\begin{aligned}0 \leq \frac{b}{2}\int_0^t \tilde{u}_\epsilon(0,s)^2 ds \leq& -\frac{1}{2}\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} - \frac{1}{2}\frac{\epsilon}{b}\tilde{u}_\epsilon(0,t)^2 \\ &- \epsilon\int_0^t \|\partial_x\tilde{u}_\epsilon(\cdot,s)\|^2_{L^2(\mathbb{R}^+)}ds \\ &+ \epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds\end{aligned}$$

Then for all $t \in [0,\tau]$ :

$$\begin{aligned}0 \leq \|\tilde{u}_\epsilon(0,\cdot)\|^2_{L^2(0,t)} \leq& \frac{1}{b}\big( -\|\tilde{u}_\epsilon(\cdot,t_2)\|^2_{L^2(\mathbb{R}^+)} - \frac{\epsilon}{b}\tilde{u}_\epsilon(0,t_2)^2 \\ &- 2\epsilon\int_0^t \|\partial_x\tilde{u}_\epsilon(\cdot,s)\|^2_{L^2(\mathbb{R}^+)}ds \\ &+ 2\epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds\big) \\ \leq& 2\frac{\epsilon}{b}\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds \\ \leq& C\epsilon^2\end{aligned}$$

□

**Remarque 2.6.** *De façon peut-être non optimale, on peut trouver une autre majoration de $|\tilde{u}_\epsilon|$ pour tout $t \in [0,\tau]$ :*

$$|u_\epsilon(0,t) - u(0,t)| \leq C\,\sqrt{\epsilon}$$

*Reprenons les notations de la proposition 2.3, et en particulier :*

$$\begin{aligned}\frac{1}{2}\frac{\epsilon}{b}\tilde{u}_\epsilon(0,t)^2 \leq &\epsilon\int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2(\mathbb{R}^+)}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds\\ \leq &\epsilon^2 C\int_0^t \|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}ds\\ \leq &\epsilon^2 C^2\end{aligned}$$

*Soit :*

$$|\tilde{u}_\epsilon(0,t)| \leq C_1\sqrt{\epsilon}$$

**Convergence for the norm $H^1(\mathbb{R}^+)$**

**Proposition 2.7**

*Let $b$ and $\tau$ be positive constants. Let $u_0$ be a function of $L^2(\mathbb{R}^+)$ and $f$ be the dynamical boundary condition* (12)*. Let $u_\epsilon$ be the unique solution of the system* (2)*. Let $u$ be the unique solution of the system* (1)*. Then if $u(\cdot,t) \in H^2$, $u_\epsilon(\cdot,t)$ converge to $u(\cdot,t)$ in norm $L^2$ when $\epsilon$ tends to* 0*.*

*In particular the inequality holds true, for any $t \in [0,\tau]$ :*

$$\int_0^t \|\partial_x u_\epsilon(\cdot,s) - \partial_x u(\cdot,s)\|^2_{L^2(\mathbb{R}^+)}\mathrm{d}s \leq \ \tau C\ \epsilon,$$

*where $C$ depends on $\|\partial_{xx}u(\cdot,t)\|_{L^2(\mathbb{R}^+)}$.*

▷ Reprenons l'égalité d'énergie :

$$\frac{1}{2}\mathrm{d}_t[\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \frac{\epsilon}{b}(\tilde{u}_\epsilon(0,t)^2)] = -\frac{b}{2}\tilde{u}_\epsilon(0,t)^2 - \epsilon\|\partial_x\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} + \epsilon\langle\tilde{u}_\epsilon(\cdot,t),\partial_{xx}u(\cdot,t)\rangle_{L^2(\mathbb{R}^+)}$$

Soit en intégrant entre 0 et $t$ :

$$\frac{1}{2}[\|\tilde{u}_\epsilon(\cdot,t)\|^2_{L^2(0,L)} + \frac{\epsilon}{b}(\tilde{u}_\epsilon(0,t)^2)] = -\int_0^t \frac{b}{2}\tilde{u}_\epsilon(0,s)^2 - \epsilon\int_0^t \|\partial_x\tilde{u}_\epsilon(\cdot,s)\|^2_{L^2(\mathbb{R}^+)} + \epsilon\int_0^t \langle\tilde{u}_\epsilon(\cdot,s),\partial_{xx}u(\cdot,s)\rangle_{L^2(\mathbb{R}^+)}$$

$$\begin{aligned}0 \leq \int_0^t \|\partial_x\tilde{u}_\epsilon(\cdot,s)\|^2_{L^2(\mathbb{R}^+)} &\leq \int_0^t |\langle\tilde{u}_\epsilon(\cdot,s),\partial_{xx}u(\cdot,s)\rangle_{L^2(\mathbb{R}^+)}|\mathrm{d}s\\ &\leq \int_0^t \|\tilde{u}_\epsilon(\cdot,s)\|_{L^2}\|\partial_{xx}u(\cdot,s)\|_{L^2(\mathbb{R}^+)}\mathrm{d}s\\ &\leq \tau C\epsilon\end{aligned}$$

□

**Convergence for the norm $H^2(\mathbb{R}^+)$**

If we suppose moreover that $u_\epsilon$ is in $H^3(\mathbb{R}^+)$, than we can derive the euqtion (2) and we obtain for $v_\epsilon = \partial_x u_\epsilon$

Let us consider the modified Lifshitz-Slyozov model, which is disturbed by a coefficient diffusion term $\epsilon > 0$.

$$\begin{cases}\dfrac{\partial v_\epsilon}{\partial t} - b\dfrac{\partial v_\epsilon}{\partial x} - \epsilon\dfrac{\partial^2 v_\epsilon}{\partial x^2} = 0 & \forall(x,t) \in \mathbb{R}^+ \times [0,\tau]\\ v_\epsilon(x,0) = \partial_x u_0(x) & \forall x \in \mathbb{R}^+\\ f(v_\epsilon)(0,t) = 0 & \forall t \in [0,\tau]\end{cases} \tag{9}$$

**Proposition 2.8**

*Let $b$ and $\tau$ be positive constants. Let $u_0$ be a function of $L^2(0,L)$ and $f$ be the dynamical boundary condition* (12)*. Let $u_\epsilon$ be the unique solution of the system* (2)*. Let $u$ be the unique solution of the system* (1)*. Then if $u(\cdot,t)$ and $u_\epsilon(\cdot,t)$ are in $H^3(\mathbb{R}^+)$, with $\partial_x u_0(0) = 0$, then the inequality holds true for any $t \in [0,\tau]$ :*

$$\int_0^t \|\partial_{xx} u_\epsilon(\cdot,s) - \partial_{xx} u(\cdot,s)\|^2_{L^2(0,L)} \mathrm{d}s \leq \; C\,\sqrt{\epsilon}$$

*Where $C$ depends on $\|\partial_{xxx} u(\cdot,t)\|_{L^2(0,L)}$.*

▷ Let $u$ be the unique solution of (1), then $v = \partial_x u$ verifies :

$$\begin{cases} \dfrac{\partial v}{\partial t} - b\dfrac{\partial v}{\partial x} = 0 & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau] \\ \\ v(x,0) = \partial_x u_0(x) & \forall x \in \mathbb{R}^+ \end{cases} \tag{10}$$

Then we consider that $u(\cdot,t) \in H^3(\mathbb{R}^+)$ so $\bar{v}_\epsilon = v_\epsilon - v$ is solution of

$$\begin{cases} \dfrac{\partial \bar{v}_\epsilon}{\partial t} - b\dfrac{\partial \bar{v}_\epsilon}{\partial x} - \epsilon\dfrac{\partial^2 \bar{v}_\epsilon}{\partial x^2} = \epsilon\dfrac{\partial^2 v}{\partial x^2} & \forall (x,t) \in \mathbb{R}^+ \times [0,\tau]; \\ \\ \bar{v}_\epsilon(x,0) = 0 & \forall x \in \mathbb{R}^+; \\ \\ \dfrac{\partial v_\epsilon}{\partial x}(0,t) = 0 & \forall t \in [0,\tau]; \end{cases} \tag{11}$$

$$\begin{aligned} \frac{1}{2}\mathrm{d}_t \|\bar{v}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} &= \int_0^{+\infty} \bar{v}_\epsilon \partial_t \bar{v}_\epsilon \;\mathrm{d}x \\ &= \int_0^{+\infty} b\bar{v}_\epsilon \partial_x \bar{v}_\epsilon \;\mathrm{d}x + \int_0^{+\infty} \epsilon\bar{v}_\epsilon \partial_{xx} \bar{v}_\epsilon \;\mathrm{d}x + \int_0^{+\infty} \epsilon\bar{v}_\epsilon \partial_{xxx} u \;\mathrm{d}x \\ &= \; -\frac{b}{2}\bar{v}_\epsilon(0,t)^2 - \epsilon\bar{v}_\epsilon(0,t)\partial_x\bar{v}_\epsilon(0,t) - \int_0^{+\infty} \epsilon(\partial_x \bar{v}_\epsilon)^2 \;\mathrm{d}x + \int_0^{+\infty} \epsilon\bar{v}_\epsilon \partial_{xxx} u \;\mathrm{d}x \\ &= \; -\frac{b}{2}\bar{v}_\epsilon(0,t)^2 - \frac{\epsilon}{b}\bar{v}_\epsilon(0,t)\partial_t\bar{v}_\epsilon(0,t) - \int_0^{+\infty} \epsilon(\partial_x \bar{v}_\epsilon)^2 \;\mathrm{d}x + \int_0^{+\infty} \epsilon\bar{v}_\epsilon \partial_{xxx} u \;\mathrm{d}x \end{aligned}$$

We integrate the previous equality between 0 and $t$

$$\frac{1}{2}\|\bar{v}_\epsilon(\cdot,t)\|^2_{L^2(\mathbb{R}^+)} = -\frac{b}{2}\int_0^t \bar{v}_\epsilon(0,s)^2 \mathrm{d}s - \frac{\epsilon}{2b}\int_0^t \partial_t \bar{v}_\epsilon(0,t)^2 \mathrm{d}s - \int_0^t \epsilon\|\partial_x \bar{v}_\epsilon\|^2_{L^2} + \int_0^t\int_0^{+\infty} \epsilon\tilde{u}_\epsilon \partial_{xxx} u \;\mathrm{d}x\mathrm{d}s.$$

Then, since $\bar{v}_\epsilon(\cdot,0) = 0$

$$\begin{aligned} \epsilon\int_0^t\int_0^{+\infty} (\partial_x \bar{v}_\epsilon)^2 &\leq \frac{\epsilon}{2b}\bar{v}_\epsilon(0,0)^2 - \int_0^\tau\int_0^{+\infty} \epsilon\bar{v}_\epsilon \partial_{xxx} u \\ &\leq \int_0^\tau \epsilon\|\bar{v}_\epsilon\|_{L^2(\mathbb{R}^+)} \|\partial_{xxx} u\|_{L^2(\mathbb{R}^+)}. \end{aligned}$$

We have already proven that $\bar{v}_\epsilon = \partial_x u_\epsilon - \partial_x u$ verifies the inequality

$$\int_0^\tau \|\partial_x u_\epsilon(\cdot,t) - \partial_x u(\cdot,t)\|^2_{L^2(0,L)} dt \leq \; \tau C\;\epsilon.$$

Therefore we can conclude the proof

$$\epsilon\int_0^t \|\bar{v}_\epsilon(\cdot,\tau)\|^2_{L^2(0,L)} \leq \;\; C\sqrt{\epsilon}.$$

□

# 3 Comparison of Boundary Condition : Numerical study

In order to qualify the convergence of the modified Lifschitz-Slyozov model to the classical Lifschitz-Slyozov model according to the limit condition imposed in $x = 0$, we study this convergence numerically by the finite element method.

## 3.1 Variationnal approach for diffrent boundary condition

Suppose $b$ a known constant, corresponding to the depolimarisation rate, and suppose $\epsilon$ >0.

Dynamical boundary condition

$$f(u)(0,t) = \frac{\partial u}{\partial t}|_{x=0} - b\frac{\partial u}{\partial x}|_{x=0} = 0 \tag{12}$$

We assume that we know a subspace $V_h \subset V$ of finite dimension, configured by $h$ and such that for any $(v, \mu) \in V$, there is an element $r_h(v, \mu) \in V_h$ checking the condition : $lim_{h\to 0}\|r_h(v, \mu) - (v, \mu)\| = 0$. Let us then consider the following problem : Find the $u_h$ function belonging to $H_h$ such that : $a(u_h, v_h) = l(v_h), \forall v_h \in V_h$.

This problem also admits a unique solution because $V_h$ is a closed subspace of $V$ and therefore the hypotheses of the Lax-Milgram theorem are also verified in $V_h$.

In addition, we discretize the time in $N_T$ equal intervals such that for $n \in [0, N_T - 1]$ and $t_n = n\delta t$ and we define the family of functions :

$$u_h^n(x) = \sum_{j=0}^{N} u(x_j, t_n)\phi_j(x)$$

## 3.2 Finite Element P1

### 3.2.1 Generalities on P1 element

First, a finite element of degree one (in dimension one) is adopted to study the different boundary condition on $x = 0$. For discretization purpose, we solve the equation on the interval $[0, L]$. The boundary condition on $x = L$ is set to zero for this numerical study. Later, we will introduce a model error and simulate the unknown condition on $x = L$ by an unknown function of time.

We discretize the interval $[0, L]$ into $N$ sub-intervals or elements $T_i = [x_i, x_{i+1}]$. The $T_i$ elements have the same length denoted by $h$. $V_h$ is then the space of continuous piece by piece affines functions on the $T_i$ segments.

Each function $v_h \in V_h$ is uniquely determined by the its values at points $x_i$ for $i = 0, 1, ..., N - 1$. Indeed, let $v_h$ be the projection of an absolute continuous function $v$ on $V_h$, then $v_h$ is uniquely defined by the value of $v$ in its summits :

$$v_h(x) = \sum_{i=0}^{N_X} v(x_i)\phi_i(x)$$

The space $V_h$ is of dimension $N$ and it is generated by the Lagrange base which is formed by the $N$ functions $\phi_i \in V_h$ denoted by :

For $i \geq 1$ :

$$\phi_i(x) = \begin{cases} 1 - \dfrac{|x - x_i|}{h} & |x - x_i| < h \\ 0 & |x - x_i| \geq h \end{cases}$$

For $i = 0$ :

$$\phi_0(x) = \begin{cases} 1 - \dfrac{|x|}{h} & 0 < x < h \\ 0 & x \geq h \end{cases}$$

For $i = N$ :

$$\phi_N(x) = \begin{cases} 1 - \dfrac{|L - x|}{h} & 0 < |L - x| < h \\ 0 & |L - x| \geq h \end{cases}$$

The following matrices are defined :

$$\begin{cases} M_{ij} = \int_0^L \phi_i(x)\phi_j(x)dx \\ D_{ij} = \int_0^L \phi_i(x)\mathrm{d}_x\phi_j(x)dx \\ K_{ij} = \int_0^L \mathrm{d}_x\phi_i(x)\mathrm{d}_x\phi_j(x)dx \end{cases}$$

And after elementary calculation we obtain :

$$M = \frac{h}{6}\begin{pmatrix} 2 & 1 & 0 & & 0 \\ 1 & 4 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & 4 & 1 \\ 0 & & & 1 & 2 \end{pmatrix}$$

$$D = 1/2\begin{pmatrix} -1 & 1 & 0 & & 0 \\ -1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 0 & 1 \\ 0 & & & -1 & 1 \end{pmatrix}$$

$$K = 1/h\begin{pmatrix} 1 & -1 & 0 & & 0 \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ 0 & & & -1 & 1 \end{pmatrix}$$

#### 3.2.2 Dynamical Boundary Condition

Let be $u_h$ the projection of the solution $u$ of (2) on $V_h$ and $v_h \in V_h$ a test vector. The coordinates of the fonction $u_h$ and $v_h$, respectively $U = (u_j)$ and $V = (v_j)$, are set on the basis of $(\phi_j, \delta_{0,j})$.

The variational formulation becomes :

$$a(v_i\phi_i, u_j\phi_j) = bv_iD_{ij}u_j - \epsilon v_iK_{ij}u_j$$

With a finite difference approximation for the time derivative, the implicit schema is written :

$$\langle v_h, \partial_t u_h\rangle_V = a(v_h, u_h)$$

And therefore, for $j > 0$ and $i > 0$ :

$$v_iM_{ij}\frac{1}{\delta t}(u_j^{n+1} - u_j^n) = bv_iD_{ij}u_j^{n+1} - \epsilon v_iK_{ij}u_j^{n+1}$$

For $j = 0$ and $(\phi_0, 1)$ :

$$v_iM_{i0}\frac{1}{\delta t}(u_0^{n+1} - u_0^n) + \frac{\epsilon}{b}v_i\delta_{i,0}(u_0^{n+1} - u_0^n) = bv_iD_{i0}u_0^{n+1} - \epsilon v_iK_{i0}u_0^{n+1}$$

In conclusion, numerically we solve :

$$U^{n+1} = (M - b\delta tD + \epsilon\delta tK + \frac{\epsilon}{b}D_0)^{-1}(M + \frac{\epsilon}{b}D_0)U^n$$

with $D_0$ :

$$D_0 = \begin{pmatrix} 1 & 0 & \\ 0 & 0 & \\ & & \ddots \end{pmatrix}$$

**Remarque 3.1.** *Different choices are possible to impose the Dirichlet condition in $x = L$. For our application, since we don't want to manage a degree of freedom, we opt for the elimination technique, i.e. the last row and the last column are deleted. Another technique, known as* ***pseudo-elimination****, is to remove the dependencies between $\phi_N$ and $\phi_{N-1}$. From a matrix point of view, this means deleting the last row and column which is replaced by a 1 on the diagonal. Thus the value $u_h(L, t_n) = u_0(L) = 0$ does not change.*

#### 3.2.3 Other bouindary conditions

In order to evaluate the interest of the dynamic (or transparent) boundary condition that we have introduced, we propose to compare its convergence with the more classical homogeneous Dirichlet and Neumann conditions

Neumann

$$f(u)(0, t) = \partial_x u(0, t) = 0$$

We first compute the variationnal formulation associated with (2) for a Neumann condition on $x = 0$. Let's define the space $D(A) = \left\{u \in H^1_R([0, L]\right\}$ and we set $V = L^2$ with the classical associated norm.

$$\begin{aligned} a(v,u) &= \int_0^L bv(\partial_x u) + \int_0^L \epsilon v \partial_{xx} u \\ &= \int_0^L bv(\partial_x u) + [v\partial_x u]_0^L - \int_0^L \epsilon \partial_x v \partial_x u \\ &= \int_0^L bv(\partial_x u) - \int_0^L \epsilon \partial_x v \partial_x u \end{aligned}$$

It can be observed that the associated bilinear form is identical with the model where the boundary condition is set as a dynamic condition. However, here the space $D(A)$ is equal to $H^!_R$ instead of $H^1_R \times \mathbb{R}$.

Then, we introduce the $u_h$ the projection of the solution $u$ on $V_h$ and $v_h \in V_h$ a test vector. The coordinates of $u_h$ and $v_h$, respectively $U$ and $V$, are set on the basis of $\phi_j$. The variational formulation becomes :

$$a(v_h, u_h) = bV^T DU - \epsilon V^T KU$$

With a finite difference approximation for the time derivative, the implicit schema is written :

$$\langle v_h, \partial_t u_h \rangle = a(v_h, u_h)$$

And therefore :

$$V^T M \frac{1}{\delta t}(U^{n+1} - U^n) = bV^T DU^{n+1} - \epsilon V^T KU^{n+1}$$

$$U^{n+1} = (M - b\delta t D + \epsilon \delta t K)^{-1} MU^n$$

Dirichlet

$$f(u)(0,t) = u(0,t) = 0$$

The condition of homogeneous Dirichlet does not appear in the variational formulation but in the space. For $b = cste$, let's define the space $D(A) = \left\{u \in H^1([0, L] \mid u(0) = 0,\ u(L) = 0\right\}$

The equation integrating mass matrix and rigidity matrix is therefore written in the same way as in the case where the boundary condition in $x = 0$ is dynamic (or transparent). However, for the resolution, we proceed by elimination method (or pseudo elimination), which amounts to adding after calculation a 0 to the first term.

#### 3.2.4 Results and comparaison

We set the space domain to $[0, L] = [0, 100]$mer. We define the notation mer for monomer which is the fundamental unit aggregating into oligomers. We set the time domain to $[0, \tau] = [0, 50]$min. The depolimarisation rate $b$ is set at 2 min$^{-1}$. The initial concentration distribution of oligomers is set as the gaussian function $u_0(x) = 0.1e^{-0.5(x-50)/5^2}$. We consider a uniform space grid $0 = x_0 < \cdots < x_{N_x} = L$, with a constant space step $h = 1/200$ and a uniform time grid with a constant time step $\delta t = 1/150$.

Then we compare for norm $L^2$ the solution in $V_h$ :

$$\begin{aligned} \|u_{1h} - u_{2h}\|^2_{L^2} &= \int_0^L (u_{1h} - u_{2h})^2 dx \\ &= \sum_{i=0}^{N}\sum_{j=0}^{N} (u_{1,i} - u_{2,i})(u_{1,j} - u_{2,j}) \int_0^L \phi_i \phi_j \\ &= (U_1 - U_2)^T M (U_1 - U_2) \end{aligned}$$

This formulation allows two solutions to be compared at a time t. To calculate the total norm, we also integrate over time.

We compare for norm $H^1$ the solution in $V_h$ :

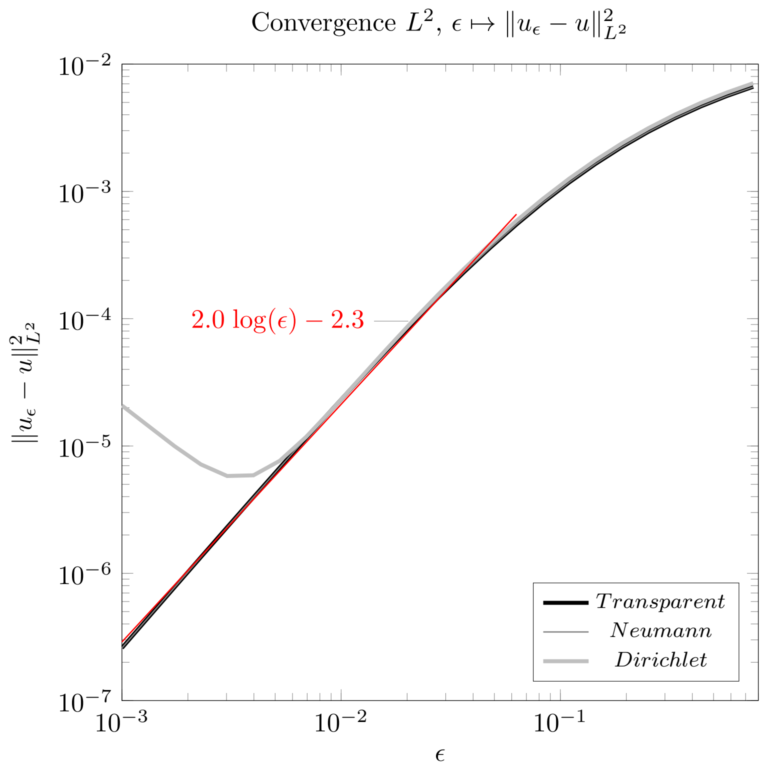


FIGURE 1 – $L^2$ norm of the distance between the solution of the equation (2) perturbed by the diffusion term $\epsilon$ and the solution of the classical Lifschitz-Slyozov equation (1).

$$\begin{aligned}
\|u_{1h} - u_{2h}\| =& \int_0^L (u_1 - u_2)^2 dx + \int_0^L \partial_x (u_1 - u_2)^2 dx \\
=& \sum_{i=0}^N \sum_{j=0}^N (u_{1,i} - u_{2,i})(u_{1,j} - u_{2,j}) \int_0^L \phi_i \phi_j + \sum_{i=0}^N \sum_{j=0}^N (u_{1,i} - u_{2,i})(u_{1,j} - u_{2,j}) \int_0^L \partial_x \phi_i \partial_x \phi_j \\
=& (U_1 - U_2)^T M (U_1 - U_2) + (U_1 - U_2)^T K (U_1 - U_2)
\end{aligned}$$

The graph below does not directly plot the $H^1$ norm but the $L^2$ norm of the derivative. We see once again that the square of the norm decreases as the square of $\epsilon$.

While the solution of the disturbed problem with a Dirichlet boundary condition does not converge, we notice that the convergence is identical for a Neumann condition and the transparent condition that we wish to impose. We therefore want to observe this convergence in $H^2$ norm for a sufficiently regular solution of the Lifschitz-Slyozov problem (the limit problem).

To do so, we need to compute the $H^1$ norm of the second derivative of the solution in $V_h$. First we have to solve the equation

$$\forall w \quad \in V_h \int_0^L w(x) v_h(x) \mathrm{d}x = - \int_0^L w'(x) u_h'(x) \mathrm{d}x.$$

So in the matricial formulation this equivalent to $\forall W$ we have $W^T M V = -W^T K U$.

$$\begin{aligned}
\|u_{1h} - u_{2h}\|^2 =& \int_0^L (u_1 - u_2)^2 dx + \int_0^L (\partial_x (u_1 - u_2))^2 dx + \int_0^L (\partial_{xx} (u_1 - u_2))^2 dx \\
=& (U_1 - U_2)^T M (U_1 - U_2) + (U_1 - U_2)^T K (U_1 - U_2) + (-M^{-1} K (U_1 - U_2))^T K (-M^{-1} K (U_1 - U_2))
\end{aligned}$$

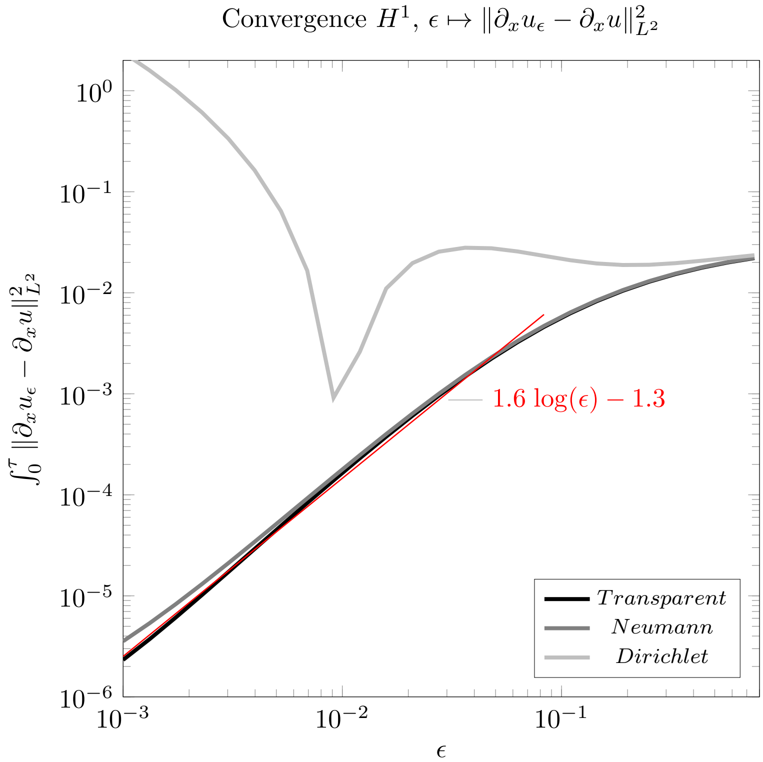


FIGURE 2 – $L^2$ norm of the distance between the derivative of the solution of the equation (2) perturbed by the diffusion term $\epsilon$ and the derivative of the solution of the classical Lifschitz-Slyozov equation (1).

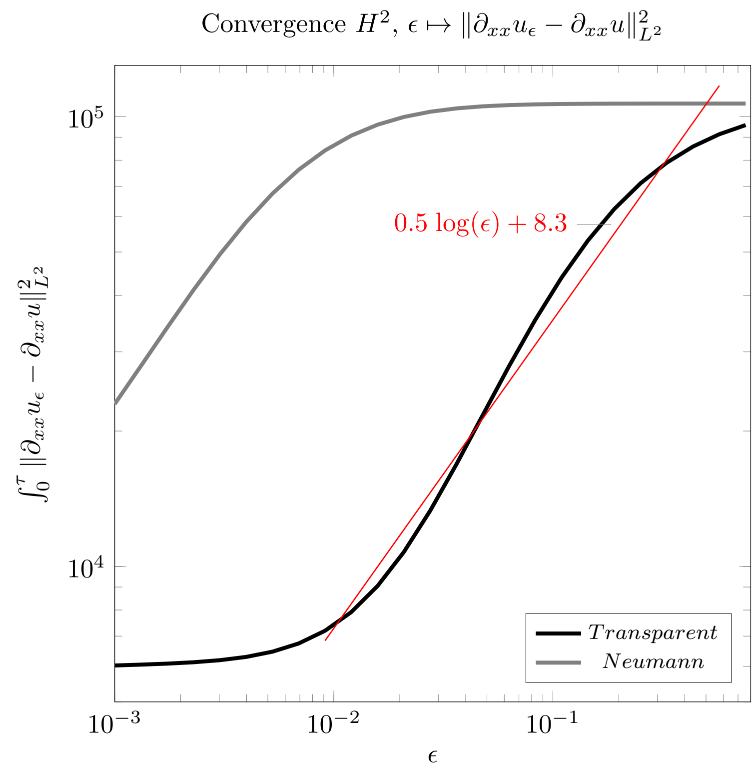


FIGURE 3 – $L^2$ norm of the distance between the second derivative of the solution of the equation (2) perturbed by the diffusion term $\epsilon$ and the second derivative of the solution of the classical Lifschitz-Slyozov equation (1). We started from a gaussian initial distribution.

# 4 Inverse problem

For the following, it is assumed that $u_0$ belongs to $L^2(0, L)$, and $f$ be the dynamical boundary condition (12). The system (2) has a unique solution denoted $u_\epsilon$ as demonstrated previously. We then introduce the mathematical measurement operator $\Psi_k$, the one that associates the initial condition $u_0$, which is of compact support $[0, L]$, to the moment of order k denoted by $\mu_k$ of the solution $u_\epsilon$ of (1) over a certain compact set $[0, \tau]$.

$$\begin{array}{cccc} \Psi_k & : & L^2([0,L]) & \to & L^2([0,\tau]) \\ & & u_0 & \mapsto & t \to \mu_k(t) = \int_0^{+\infty} x^k u_\epsilon(x,t)dx \end{array} \tag{13}$$

We set out the inverse problem : knowing the moment of order $k$ and the model, are we able to reconstruct the initial condition $u_0$ ?

The moments of the solution are linked by a recurrence formula recalled below :

**Proposition 4.1**

*Let $u_0$ be a function in $L^2(0, L)$, let $f$ be the dynamical boundary condition (12), and let $u_\epsilon$ be the solution of the system (2) associated to the initial condition $u_0$. Then the moment of $u_\epsilon$ verify the relation :*

$$\begin{cases} \dfrac{\mathrm{d}}{\mathrm{d}t}\mu_0(t) = -bu_\epsilon(0,t) - \dfrac{\epsilon}{b}\partial_t u_\epsilon(0,t) & \forall t \in [0,\tau] \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\mu_1(t) = -b\mu_0 + \epsilon u_\epsilon(0,t) & \forall t \in [0,\tau] \\ \dfrac{\mathrm{d}}{\mathrm{d}t}\mu_k(t) = -bk\mu_{k-1} + \epsilon k(k-1)\mu_{k-2} & \forall t \in [0,\tau] \end{cases} \tag{14}$$

▷ We integrate the equation (2) and we obtain the equation verified by the derivative of the moment of order 0 :

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mu_0(t) &= \int_0^{+\infty} \partial_t u_\epsilon(x,t)dx \\ &= b\int_0^{+\infty} \partial_x u_\epsilon(x,t)dx + \epsilon\int_0^{+\infty} \partial_{xx} u_\epsilon(x,t)dx \\ &= -bu_\epsilon(0,t) - \epsilon\partial_x u_\epsilon(0,t) \\ &= -bu_\epsilon(0,t) - \frac{\epsilon}{b}\partial_t u_\epsilon(0,t) \end{aligned}$$

For the moment of order $k = 1$ :

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\mu_1(t) &= \int_0^{+\infty} x\partial_t u_\epsilon(x,t)dx \\ &= b\int_0^{+\infty} x\partial_x u_\epsilon(x,t)dx + \epsilon\int_0^{+\infty} x\partial_{xx} u_\epsilon(x,t)dx \\ &= b[xu_\epsilon(x,t)]_0^{+\infty} - b\int_0^{+\infty} u_\epsilon(x,t)dx + \epsilon[x\partial_x u_\epsilon(x,t)]_0^{+\infty} - \epsilon\int_0^{+\infty} \partial_x u_\epsilon(x,t)dx \\ &= -b\mu_0 + \epsilon u_\epsilon(0,t) \end{aligned}$$

For a moment of order $k \geq 2$ :

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\mu_k(t) =& \int_0^{+\infty} x^k \partial_t u_\epsilon(x,t)dx \\
=& b\int_0^{+\infty} x^k \partial_x u_\epsilon(x,t)dx + \epsilon \int_0^{+\infty} x^k \partial_{xx} u_\epsilon(x,t)dx \\
=& -bk\int_0^{+\infty} x^{k-1} u_\epsilon(x,t)dx - \epsilon k \int_0^{+\infty} x^{k-1} \partial_x u_\epsilon(x,t)dx \\
=& -bk\int_0^{+\infty} x^{k-1} u_\epsilon(x,t)dx \\
& -\epsilon k[x^{k-1}u_\epsilon(x,t)]_0^{+\infty} + \epsilon k(k-1)\int_0^{+\infty} x^{k-2} u_\epsilon(x,t)dx \\
=& -bk\mu_{k-1} + \epsilon k(k-1)\mu_{k-2} \\
=& -bk\mu_{k-1} + \epsilon k(k-1)\mu_{k-2}
\end{aligned}
$$

□

## 4.1 Injectivity

Unlike the case of depolymerization, where the model studied is reduced to a transport equation on a compact set, we do not have an explicit formula linking the solution and its initial condition.

**Proposition 4.2**

*The operator $\Psi_0$ as (14) associated to the moment of order $0$ of a solution of the perturbed transport equation, defined from $L^2(0,L)$ to $L^2(0,\tau)$ is not injective.*

▷ Let us consider two initial condition $u_0^\alpha$ and $u_0^\beta$ tsuch that the moment of the solutions of (2) associated to those initial condition are identical. We denot $u_0 = u_0^\alpha - u_0^\beta$. Then the tequation (14) gives us :

$$
\partial_t u(0,t) + \frac{b^2}{\epsilon}u(0,t) = 0
$$

$$
\begin{cases}
u(0,t) = u_0(0)e^{-\frac{b^2}{\epsilon}t} \\
\partial_x u(0,t) = -\frac{b}{\epsilon}u_0(0)e^{-\frac{b^2}{\epsilon}t}
\end{cases}
$$

Then, if $u_0(0) = 0$, our transport diffusion equation (2) defined on $\mathbb{R}^+$ has a Neumann and Dirichlet condition on 0. We can therefore extend the solution $u$ by $u = 0$ on $[-r, 0]$, such that $u$ still verify the equation (2) on this inverval. Then by the analytic continuation theorem $u$ is null everywhere and espacially $u_0 = 0$.

In the cases where $u_0(0) \neq 0$, CLAIM : in that case the operator $\Psi_0$ is non-injective.

Let us define $H = u - u_0(0)e^{-\frac{b^2}{\epsilon}t}$. Then the function $H$ satisfy

$$
\begin{cases}
\partial_t H - b\partial_x H - \epsilon\partial_{xx} H = -\frac{b^2}{\epsilon}u_0(0)e^{-\frac{b^2}{\epsilon}t} \quad (x,t) \in \mathbb{R}^+ \times [0,+\infty) \\
H(0,t) = 0 \\
\partial_x H(0,t) = \partial_x u(0,t) = -\frac{b}{\epsilon}u_0(0)e^{-\frac{b^2}{\epsilon}t}
\end{cases}
$$

Let us denote $f(t) = \frac{b^2}{\epsilon}u_0(0)e^{-\frac{b^2}{\epsilon}t}$ Then we search for an energy inequality by multiplying this equation by $H$ and integrate between 0 and $+\infty$

$$
\mathrm{d}_t \int_0^{+\infty} \frac{1}{2}H(x,t)^2 \mathrm{d}x - b\int_0^{+\infty} H\partial_x H \mathrm{d}x - \epsilon\int_0^{+\infty} \partial_{xx} H \mathrm{d}x = -\int_0^{+\infty} f(t)H(x,t)\mathrm{d}x
$$

$$
\frac{1}{2}\|H(x,t)\|^2 - \frac{1}{2}\|H(x,0)\|^2 \leq -\int_0^t f(t)\int_0^{+\infty} H(x,t)\mathrm{d}x\ \mathrm{d}t
$$

□

## 4.2 Riccati Equation

We apply the Tikhonov regularization method to estimate the initial condition associated with evolution equation (2) observed by its moment on $\mathbb{R}^+$. We define by 5 the evolution operator $A$ defined on the space $V$ such that for $y \in V$ :

$$\begin{cases} \dot{y} = Ay \\ y(0) = \xi \end{cases} \tag{15}$$

$A$ is an unbounded operator of domain $D(A)$, generator of a continuous semi-group of contraction $(S(t))_{t\geq 0}$. $A$ is the infinitesimmal generator of a $C^0$ semi group.

The adjoint od $A$ called $A^*$ is equal to :

$$\forall y \in D(A^*) \subset \mathscr{Y}, \quad A^* \begin{pmatrix} u \\ m \end{pmatrix} = \begin{pmatrix} -b\partial_x u + \epsilon \partial_{xx} u \\ b\partial_x u(0) - \frac{b^2}{\epsilon} m \end{pmatrix} \tag{16}$$

$A^*$ is also the infinitesimmal generator of a $C^0$ semi group of contraction denoted by $(S_*(t))_{t\geq 0}$.

We define $\mathscr{Y} = L^2(0, L)$ and $\mathscr{Z} = L^2(0, \tau)$. We additionally consider to have at our disposal some measurements $z$ associated to a given trajectory $u_\epsilon$, and we denote $C$ a bounded observation operator such that :

$$C : \left| \begin{array}{l} \mathscr{Y} \to \mathscr{Z} \\ y_0 toz \end{array} \right. \tag{17}$$

Typically, we define $I$ a finite subset of $\mathbb{N}$, and $C$ is the collection of $(\Psi_k)_{k\in I}$.

We assume that the only uncertainty on the trajectory came from the initial condition. The aim is therefore to determine the trajectory that minimizes the discrepency between the observations and the measurements in the least square sense (which corresponds to the Tikhonov estimator). We therefore define the criterion to be minimized :

$$\min_{\xi \in \mathscr{Y}} \left\{ J(\xi, t) = \frac{\alpha}{2} \|\xi\|^2_{\mathscr{Y}} + \frac{\gamma}{2} \int_0^t \left( \|z(s) - Cy_{|\xi}\|^2_{\mathscr{Z}} \right) \right\} \tag{18}$$

Criterion $J$ is convex and the existence and uniqueness of the minimum and minimisers denoted by $\bar{y}$ has already been proved. The minimization of $J$ by the Lagrange multiplier method allows to obtain the dynamics of the adjoint state $q$ for all $t \in [0, \tau]$ :

$$\begin{cases} \dot{q}_\xi(s) + A^* q_\xi(s) = -C^*(z(s) - Cy_\xi(s)) \quad \in [0, t] \\ q_\xi(t) = 0 \end{cases} \tag{19}$$

Then the optimal system is the solution of a two-end problem for a given $t \in [0, \tau]$ :

$$\begin{cases} \dot{\bar{y}} = A\bar{y} \\ \dot{\bar{q}}_\xi(s) + A^* \bar{q}_\xi(s) = -C^*(z(s) - Cy_\xi(s)) \quad \in [0, t] \\ \bar{y}(0) = \gamma \bar{q}_\xi(0) \\ \bar{q}_\xi(t) = 0 \end{cases} \tag{20}$$

Another strategy may be prefered than solving the two-ends problem, which is bases on the Riccati equation :

$$\begin{cases} \dot{P} = AP + PA^* - \gamma PC^*CP \\ P(0) = P_0 \end{cases} \tag{21}$$

**Proposition 4.3**

*Let $A$ defined by (5) be the generator of strongly continuous semi-group $(S(t))_{t\geq 0}$ on $\mathscr{Y}$, let $C$ defined by (17) be a linear operator from $\mathscr{Y}$ to $\mathscr{Z}$, and let $P_0$ be a linear bounded operator on $\mathscr{Y}$. The equation (21) admits a unique solution in $C^0([0, \tau]; Sym(\mathscr{Y}))$ in the mild sense, i.e. for all $\theta \in \mathscr{Y}$ the application $t \to P(t)\theta$ is continuous and :*

$$P(t)\theta = S(t)P_0 S_*(t)\theta - \gamma \int_0^t S(t-s)C^*CP(s)S_*(t-s)\theta \mathrm{d}s$$

▷ Introduction

This proof is conducted in three parts. First we will demonstrate that the Riccati equation admits a single solution in a $r$ radius ball.

Then, in a second step, we will introduce the Hille-Yosida approximation of $A$, the bounded linear operator $A_\lambda = \lambda A(\lambda - A)^{-1}$. We introduce the solution of the Riccati equation associated with this new operator :

$$\begin{cases} \dot{P}_\lambda = A_\lambda P_\lambda + P_\lambda A_\lambda^* - \gamma P_\lambda C^* C P_\lambda \\ P_\lambda(0) = P_0 \end{cases} \tag{22}$$

We demonstrate that the solution of (22), if such a solution exists, converges on the solution of the Riccati problem (21). This intermediary allows us to build a bounded operator that converges on the expected solution.

In a third step, we therefore demonstrate by the Cauchy-Lipschitz theorem on a Banach space that there is a solution to the approximate Riccati problem.

Finally, we conclude on the existence and uniqueness of the solution of the Riccati equation.

Local existence and uniqueness

First, let's show that the riccati equation (21) admits a local solution, i.e. in a ball of radius $r > 0$.
Since $S$ is a continuous semi-group of contraction, there exists a $M \in \mathbb{R}^+$ and $\upsilon \in \mathbb{R}$ such that :

$$\|S(t)\| \leq M e^{\upsilon t} \leq M_T$$

Let us suppose that $P_0$ is bounded and let define $\tau$ in $[0, T]$ such that :

$$\begin{cases} M_T^2 \|P_0\| = M_T^2 \iota < \frac{1}{2} \\ \tau M_T^2 \gamma \|C\|^2 r^2 < \frac{1}{2} \end{cases}$$

For $\theta \in \mathscr{Y}$ and $t \in [0, \tau]$, let us define the mapping $F$ :

$$F(P)(t)\theta = S(t) P_0 S_*(t)\theta - \gamma \int_0^t S(t-s) P(s) C^* C P(s) S_*(t-s) \mathrm{d}s$$

Then :

$$\|F(P)(t)\theta\|_{\mathscr{Y}} \leq M_T^2 \|P_0\| \|\theta\|_{\mathscr{Y}} + \tau\gamma M_T^2 \|C\|^2 \|\theta\|_{\mathscr{Y}} \|P\|^2 < (\frac{1}{2} + \frac{1}{2r^2}\|P\|^2)\|\theta\|_{\mathscr{Y}}$$

Then, as long as $\|P\| \leq r$, we have for all $\theta \in \mathscr{Y}$ and $t \in [0, \tau]$ : $\|F(P)(t)\theta\|_{\mathscr{Y}} < \|\theta\|_{\mathscr{Y}}$.
We define the ball :

$$B_{r,\tau} = \left\{ P \in C^0([0,\tau]; \mathscr{Y}) | \ \|P\|_{L_\infty([0,T],\mathscr{Y})} \leq r \right\}$$

Let $P, Q$ be to operator in $B_{r,\tau}$, then we have :

$$\begin{aligned} \|F(P)(t)\theta - F(Q)(t)\theta\|_{\mathscr{Y}} &\leq \gamma M_T^2 \int_0^t \|PC^*C(Q-P)\theta + (Q-P)C^*CQ\theta\|_{\mathscr{Y}} ds \\ &\leq \tau\gamma M_T^2 r^2 \|C\|^2 \|P - Q\| \|\theta\|_{\mathscr{Y}} \\ &< \frac{1}{2}\|P - Q\| \|\theta\|_{\mathscr{Y}} \end{aligned}$$

Therefore by the contraction mapping theorem, there is a solution $P$ suchthat $P = F(P)$, ensuring the local existence of mild solution in the ball of radius $r$.

Convergence $P_\lambda \xrightarrow{\lambda \to 0} P$ in $L_\infty([0,T], \mathscr{Y})$

For $A_\lambda$ the Yoshida approximation of the operator $A$, which semi-group $(S_\lambda(t))_{t \geq 0}$ is bounded by $M_{\lambda,T} = \sup_{t \in [0,T], \ \lambda \in [0,1]}$, then we have the following properties :

$$\forall y \in \mathscr{Y} \ \ S_\lambda(t) y \xrightarrow{\lambda \to 0} S(t) \tag{23}$$

Since we have not made any assumptions about the operator $A$ in order to demonstrate the local existence of (21), this result remains valid for the operator $A_\lambda$ and (22).

Then we consider $P^n = F^n(P_0)$ and $P_\lambda^n = F_\lambda^n(P_0)$.

Then the property (23) give us the convergence : $P_\lambda^n \xrightarrow{\lambda \to 0} P^n$ in $L_\infty([0,T], \mathscr{Y})$.
Moreover the contraction mapping theorem gives us the convergence $P_\lambda^n \xrightarrow{n \to \infty} P_\lambda$ and $P^n \xrightarrow{n \to \infty} P$ in $L_\infty([0,T], \mathscr{Y})$.
Therefore, for all $\theta \in \mathscr{Y}$, for all $n \in \mathbb{N}$ :

$$\|P\theta - P_\lambda\theta\|_{\mathscr{Y}} = \|P\theta - P^n\theta\|_{\mathscr{Y}} + \|P^n\theta - P_\lambda^n\theta\|_{\mathscr{Y}} + \|P_\lambda\theta - P_\lambda^n\theta\|_{\mathscr{Y}}$$

which concludes the convergence.

Boundness of the solution $P_\lambda$

We introduce the operator $B_\lambda = A_\lambda - \frac{\gamma}{2}P_\lambda$. This operator is bounded and linear, so therefore Lipschitz. So we can apply the Cauchy-Lipischitz theorem on a Banach space to the equation :

$$\dot{(y)} = B_\lambda y$$

We denote by $S_B$ the evolution operator associated to the solution.

We verify that $P_\lambda = S_B v P_0 S_{B*}$ is the solution of (22) :

$$\dot{P}_\lambda = B_\lambda P_0 S_{B*} + S_B v P_0 B_\lambda^* = A_\lambda P_\lambda + P_\lambda A_\lambda^* - \gamma P_\lambda C^* C P_\lambda$$

This ensures that $P_\lambda \geq 0$ in the sense of $P \in \mathscr{S}^+(\mathscr{Y})$, with

$$\mathscr{S}^+(\mathscr{Y}) = \{P \in L(\mathscr{Y}) |\ P^* = P \ \ \forall u \in \mathscr{Y}\ \langle u, Pu\rangle_{\mathscr{Y}} \geq 0\}$$

Conclusion on existence and uniqueness of $P$

Let fix $T > 0$ and $m = M_T^2\|P_0\|$, then we choose $r$ and $\tau$ such that :

$$\begin{cases} M_T^2\|P_0\| = M_T^2\iota < \frac{1}{2} \\ \tau M_T^2\gamma\|C\|^2 r^2 < \frac{1}{2} \end{cases}$$

We have the local existence and uniqueness of $P$ and $P_\lambda$ and moreover :

$$0 \leq P_\lambda \leq m\mathbb{I}$$

The convergence of $P_\lambda$ to $P$ gives also :

$$0 \leq P \leq m\mathbb{I}$$

And therefore we can repeat the local existence and uniqueness argument from $P_n\tau$ and $P(\tau)$ to the time $2\tau$.

$\square$