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École des Ponts ParisTech

THÈSE DE DOCTORAT
de l'École des Ponts ParisTech

Cross-diffusion systems in moving-boundary domains

École doctorale MSTIC

Discipline : Mathématiques

Thèse préparée au CERMICS, équipe Inria MATHERIALS

Thèse soutenue le 15 décembre 2023, par

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À mes parents

Résumé

Titre français : Systèmes à diffusion croisée dans des domaines à frontière mobile.

Cette thèse traite de l'analyse, de la stabilisation et de l'approximation numérique de systèmes d'EDP à diffusion croisée dans des domaines à frontière mobile. Elle est motivée par la modélisation d'un processus de dépôt vapeur pour la synthèse de couches minces. Le travail original est divisé en trois parties.

Un premier travail concerne la stabilisation d'un système à diffusion croisée dans un domaine unidimensionnel en expansion : considérant que l'on peut contrôler les données au bord du système, nous construisons via la méthode de backstepping des lois de rétroaction qui stabilisent exponentiellement et même en temps fini les états stationnaires du système.

Nous étudions dans un second travail le même système couplé à des termes de Cahn-Hilliard dans un domaine fixe en dimension inférieure ou égale à 3. Nous obtenons des résultats sur les minimiseurs de l'énergie de Ginzburg-Landau dégénérée associée et utilisons la méthode d'entropie pour étudier la dynamique en temps long quand la diffusion domine. Nous introduisons un schéma volumes finis semi-implicite qui préserve la structure du système continu et présentons des résultats numériques en dimensions 1 et 2.

Un troisième travail est dédié à une extension du modèle unidimensionnel précédent, où nous couplons deux systèmes à diffusion croisée via une interface mobile et une loi d'échange linéaire de type Butler-Volmer. Nous étudions les propriétés formelles du modèle, en particulier sa structure entropique variationnelle et ses états stationnaires. Nous introduisons ensuite un schéma volumes finis où le maillage est localement modifié pour suivre l'interface. Nous donnons des éléments d'analyse du schéma et illustrons numériquement la dynamique.

Mots clefs : équations aux dérivées partielles paraboliques ; diffusion croisée ; stabilisation ; analyse numérique ; volumes finis ; analyse non linéaire ; modélisation.

Abstract

English title : Cross-diffusion systems in moving-boundary domains.

This thesis deals with the analysis, stabilization and numerical approximation of cross-diffusion systems of PDEs in domains with moving boundaries. It is motivated by the modeling of a vapor deposition process for thin film synthesis. The original work is divided into three parts.

The first part focuses on the stabilization of a cross-diffusion system in an expanding one-dimensional domain. Assuming that we can control the boundary data, we construct feedback laws using the backstepping method that stabilize exponentially and even in finite time the steady states of the system.

In the second part of the work, we study the same system coupled with Cahn-Hilliard terms in a fixed domain in dimension less than 3. We obtain results concerning the minimizers of the associated degenerate Ginzburg-Landau energy and use the entropy method to study the long-time dynamics when diffusion dominates. We introduce a semi-implicit finite volume scheme that preserves the structure of the continuous system and present numerical results in dimensions 1 and 2.

The third part is dedicated to an extension of the previous one-dimensional model, where we couple two cross-diffusion systems through a moving interface and a linear exchange law of Butler-Volmer type. We study the formal properties of the model, including its variational entropy structure and steady states. We then introduce a finite volume scheme where the mesh is locally modified to follow the interface. We provide elements of analysis for the scheme and numerically illustrate the dynamics.

Keywords : parabolic partial differential equations ; cross-diffusion ; stabilization ; numerical analysis ; finite volume ; nonlinear analysis ; modelling.

List of Contributions

Published papers

JC1 Jean Cauvin-Vila, Virginie Ehrlacher, Amaury Hayat. Boundary stabilization of one-dimensional cross-diffusion systems in a moving domain: Linearized system, *Journal of Differential Equations*, 350, p. 251–307, 2023. https://doi.org/10.1016/j.jde.2022.12.021

JC2 Clément Cancès, Jean Cauvin-Vila, Claire Chainais-Hillairet, Virginie Ehrlacher. Structure preserving finite volume approximation of cross-diffusion systems coupled by a free interface, *Finite Volume for Complex Applications X - Volume 1, Elliptic and Parabolic Problems*, p. 205-213, 2023. https://doi.org/10.1007/978-3-031-40864-9_15

Preprints

JC3 Jean Cauvin-Vila, Virginie Ehrlacher, Greta Marino, Jan-Frederik Pietschmann. Stationary solutions and large-time asymptotics to a cross-diffusion Cahn-Hilliard system, 2023. https://doi.org/10.48550/arXiv.2307.05985

In preparation

JC4 Clément Cancès, Jean Cauvin-Vila, Claire Chainais-Hillairet, Virginie Ehrlacher. Cross-diffusion systems coupled by a free interface.

Codes

Some works are supplemented with numerical simulations provided by original code written in the Julia language.

- The code used in JC2 can be consulted at https://doi.org/10.5281/zenodo.8214626.
- The code used in JC3 can be consulted at https://doi.org/10.5281/zenodo.8117581.

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Je suis heureux que tu aies dirigé ma thèse, Virginie. Merci de m'avoir fait confiance et proposé un très beau sujet alors que j'étais dans une période d'angoisse et de doute. Il me semble que je vais bien mieux aujourd'hui, et je pense que tu y es pour beaucoup. D'abord parce qu'à tes côtés j'ai appris à faire des maths plutôt qu'à les apprendre. Lors des premiers mois de la thèse, j'étais obsédé par mon ignorance, par mes lacunes. Je m'attendais à ce que, peu à peu, tu me distribues le savoir qui les comblerait. Or tu n'avais bien entendu pas les réponses à toutes mes questions, d'ailleurs je pense que toutes ne te paraissaient pas passionnantes mais tu m'encourageais toujours à me renseigner si cela m'intéressait. Je dois dire qu'au début, cela m'a un peu déçu, je n'avais pas encore déconstruit la figure du professeur-maître, loin de là. Alors j'ai lu à toute vitesse des chapitres de livre, des notes de cours, des articles de recherche des années 70. Je me targuais d'être un grand collectionneur de fichiers pdf soigneusement annotés, surlignés. J'ai fait quasiment toutes les semaines l'inventaire des cours de M2 parisiens susceptibles de m'intéresser, me suis inscrit à toutes les listes de diffusion possibles et imaginables, consulté frénétiquement les sites d'annonces de colloques et d'écoles d'été pour ne rien manquer. Et puis je me suis rendu compte que tout ça ne faisait pas beaucoup avancer ma recherche. Que d'ailleurs, ça ne me faisait pas beaucoup avancer, moi, non plus, puisque j'avais tendance à oublier, ou à mal assimiler ce que je lisais et entendais. Et je me suis mis à étudier comment, toi, tu t'y prenais. Ce qui m'a frappé d'abord, c'est la grande diversité des sujets de mathématiques que tu abordais. Je me suis dit qu'il fallait beaucoup de courage et d'humilité pour procéder ainsi, pour s'ouvrir toujours à de nouvelles questions et méthodes au lieu de camper un rôle d'expert dans une chasse gardée. Ces deux qualités, je les voyais en action dans nos réunions de travail : le courage de s'attaquer frontalement aux problèmes, aux calculs ardus, directement au tableau, sans se soucier des erreurs, des hésitations, des remarques des collègues, des corrections en direct. L'humilité, essentielle : je crois que je ne t'ai jamais entendue affirmer quelque chose sans prendre la peine de le vérifier avec moi. Quand tu as des intuitions, tu laisses toujours une place au doute. À l'inverse, la parole des autres est toujours présumée juste tant qu'on ne l'a pas infirmée. J'ai trouvé cela remarquable et c'est ce dont j'ai essayé de m'inspirer pour mener mes recherches. Petit à petit, je me suis senti plus à l'aise et, je crois, plus heureux.

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J'ai passé la majeure partie de mon temps de thèse au Cermics, à l'École des Ponts. Ancien élève, j'appréhendais de passer trois années supplémentaires sur un campus qu'il me semblait déjà trop bien connaître. Or je m'y suis senti très bien. Il règne, parmi les jeunes chercheurs du laboratoire, une très bonne ambiance qui tient principalement, à mon avis, en l'absence totale de compétition entre les membres. C'en était enfin fini : on s'aide, partage, s'encourage et on est motivé par la réussite des autres. On y travaille naturellement en équipe. Je sais que, par tempérament, je n'étais pas le plus investi dans la vie du laboratoire. Je tiens toutefois à assurer à mes camarades que j'étais bien heureux que cette vie existe : avoir des relations sociales au laboratoire, même ténues, a été

essentiel pour moi après la période pandémique, sans quoi je n'aurais probablement pas terminé cette thèse. Je crois même avoir noué, incidemment, quelques relations durables. Je remercie tous mes collègues qui ont joué le jeu et contribué à cette ambiance. Je remercie particulièrement ici Isabelle et Stéphanie dont le travail nous offre des conditions exceptionnelles. Je n'oublie pas non plus le plaisir que j'ai pris à me rendre occasionnellement à l'Inria où je fus toujours bien accueilli, et j'en profite pour saluer le soutien formidable et la bonne humeur constante de Julien.

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Prologue for non-mathematicians

Before delving into the topics of my thesis, I would like to provide a personal perspective on my activities. I seize this opportunity to answer a question I have been asked many times by non-mathematicians during the course of my thesis: " What is it exactly that you do ?". I have never been able to give a satisfying answer in a casual conversation, so I hope this prologue can make it a little clearer. I apologise in advance to anyone who may find this section overly simplistic, as I am merely sharing the narrative that has guided me thus far.

At the core of my activity lies the concept of a *mathematical model*. I believe most people are already familiar with it, since mathematical modelling is extensively used in the educational system, even from a very young age. The process typically begins with a *problem*, such as the one I found by searching "elementary math problem" online: "*Camille has some money. They compute that, to buy 4 books, they are 5.5€ short. Knowing that each book costs 14.5€, how much money does Camille have ?*" Presented in this manner, the answer may not appear immediately, so we need to engage in some problem-solving and first construct a mathematical model. The *unknown* of the problem is the amount of money that Camille possesses and we denote it by the *variable* x (in euros). The problem provides us with an *equation* that x must satisfy, which is

$$x + 5.5 = 4 \times c_b,$$

where $c_b = 14.5$ denotes the price of a book in euros and is a *constant* of the problem. We have used all the available information, therefore modelling is over and we would like now to *solve* the model, that is, to compute the value of the unknown x. The solution is

$$x = 4 \times c_b - 5.5 = 62.5.$$

The problem is fully solved. What makes the previous problem an elementary one ?

i) No modelling choice has to be made: the unknown is clearly identified, the equation follows immediately from the statement of the problem, there does not seem to be an alternative model.

ii) The model has a unique solution. We say that the problem is *well-posed*.

iii) The unique solution is explicitly computable in a few elementary operations.

In interesting problems, point iii) is almost never matched, and this makes point ii) much more important: if one cannot compute directly the solution, one should at least

be able to prove that there exists a (unique) one. Schematically, the work of the applied mathematician can be divided into three components which can first be considered distinctly, although it quickly becomes clear that they are intimately related:

Modelling. Translating the problem into a mathematical model. Requires a good understanding of the problem and, when applicable, the collaboration of specialists from another field: physics, chemistry, biology, economy, social science *etc.*

Analysis. Proving properties of the model. Is the model well-posed ? Does it at least have a solution (the very definition of a mathematical solution is itself a challenge) ? Since we cannot give an explicit formula for the solution, can we give some *qualitative information* about it ? Example: in the previous problem, imagine we were not able to compute x, we would at least have liked to prove that a unique solution exists and that it should be a nonnegative number (since it is an amount of money).

Computing. Calculating an *approximation* of a solution, using an *algorithm* that is generally executed on a computer. When the problem arises from natural sciences, we speak of *numerical simulations* because the real-world phenomenon is simulated on the computer.

The reader may be confused that it is the job of a mathematician to translate a problem into a model, and not the job of, for example, a physicist. Indeed the task is sometimes very similar. However, from my experience, there seems to be a slightly different motivation. On the one hand, the physicist is primarily interested in natural phenomena, and the mathematical modelling is a convenient tool to study them. The *predictions* of the model should be compared, when possible, with *experiments*, to evaluate the quality of the model. When experiments are not available, they are replaced by numerical simulations and the outcome of the simulations is itself valuable to the physicist.

On the other hand, the model is a central object for the mathematician. It is not of primary importance that the model matches exactly the experiments, because the model is interesting *in itself*, and many mathematicians use the expression *toy model* to highlight it. To the mathematician, it is somehow more important that the model is simple enough so that the analysis can be carried out, a theory can be developed and results can be obtained. The independent development of the resulting theory is essential in mathematics. When the mathematicians do the modelling, they are already concerned about the analysis step that comes afterwards and this influences heavily the modelling choices. To a mathematician, the quality of a model is demonstrated in the analysis: the point is to prove that the model enjoys some of the desired structural properties. Numerical simulations are used to illustrate these properties.

In this thesis, we are motivated by problems of physico-chemical nature arising from materials science (see Section 1.1). However, as always in mathematics, the scope of the results is broader, because problems arising from different fields may share similar characteristics that may be translated into common mathematical features in the model. The main phenomenon under study is *diffusion*. The models we are considering are of *deterministic* nature, as opposed to *random* models. They are also *macroscopic*, which means that the unknown are typically functions $f(t, x)$ that depend on the continuous time t and space point x (think of the temperature for example). The equations we are looking at are either of *differential* type, which means that f should be related to some of its *derivatives*, or of *variational* type, meaning that f should optimize some numerical criterion $E(f)$. Most of the time, the two interpretations co-exist.

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Chapter 1

General introduction

This thesis addresses some questions related to the modelling, analysis, stabilization and numerical approximation of systems of Partial Differential Equations (PDEs) of cross-diffusion type, posed in moving-boundary domains. The original research work of the thesis is distributed in Chapters 2, 3 and 4, which are self-contained and can be read independently from each other.
The purpose of this introductory chapter is to present some background material and to emphasise the unity of the thesis. It is meant to progressively guide the reader through the stakes of the thesis and related fields. It is a deliberate choice not to give a formal exposition of the topics and I try as much as possible to convey the main ideas without going into all the technical details. The reader interested in a more complete presentation may consult the references that are given throughout the text or refer to the following chapters, where priority is given to full mathematical rigour.

In Section 1.1, I give a short introduction to thin film deposition techniques and explain how it motivates the mathematical problems addressed in the manuscript. We retain three essential features of the problem: multicomponent diffusion phenomena for which I give an introduction to the theory of cross-diffusion systems in Section 1.2; domains of moving-boundary type, for which I discuss some related mathematical aspects in Section 1.3; control and optimization, for which I present some ideas of stabilization in Section 1.4. Finally, I detail our contributions in Section 1.5 and mention some perspectives in Section 1.6.

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1.1 Motivation from thin film deposition

Let me begin with a definition taken from the Wikipedia page for "Thin film":

A thin film is a layer of material ranging from fractions of a nanometer (monolayer) to several micrometers in thickness (see Figure 1.1). The controlled synthesis of materials as thin films (a process referred to as deposition) is a fundamental step in many applications. [...] Advances in thin film deposition techniques during the 20th century have enabled a wide range of technological breakthroughs in areas such as magnetic recording media, electronic semiconductor devices, integrated passive devices, LEDs, optical coatings (such as antireflective coatings), hard coatings on cutting tools, and for both energy generation (e.g. thin-film solar cells) and storage (thin-film batteries). [...] In addition to their applied interest, thin films play an important role in the development and study of materials with new and unique properties. Examples include multiferroic materials, and superlattices that allow the study of quantum phenomena.

This is more than enough to convince an applied mathematician to model, analyze, control and simulate thin film deposition techniques. We have a particular interest for applications to thin film solar cells fabrication, and our work can somehow be seen as the continuation of the Ph.D thesis of Athmane Bakhta [23], which focused more specifically on mathematical models for photovoltaic devices. The reader interested in the physics of solar cells may consult the introduction therein, the Ph.D thesis [166] or the monograph [231].

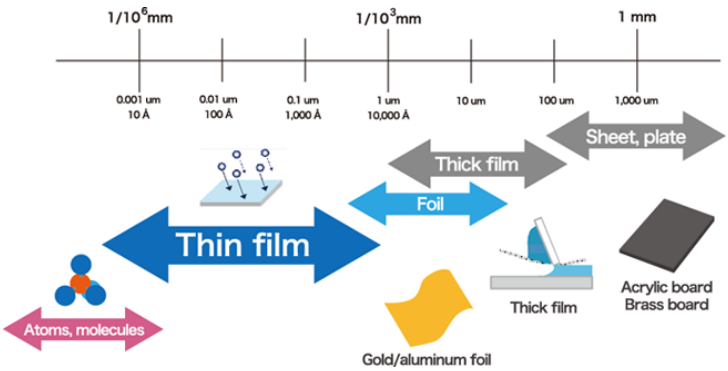

Figure 1.1: Different scales of materials. [1]

Let me now write a few words about deposition techniques, using mainly the introductory book [196]. Generically, all thin film deposition methods require vacuum or some sort of reduced-pressure environment. They fall into two broad categories, depending on whether the process is primarily chemical or physical. Physical deposition uses mechanical, electromechanical or thermodynamic means to produce a thin film of solid. An everyday example is the formation of frost. *Evaporation* and *sputtering* are two of the most important physical deposition methods. Their common objective is to controllably transfer atoms from a source to a substrate where film formation and growth proceed atomistically. In evaporation, atoms are removed from the source by thermal means (see Figure 1.2), wheras in sputtering they are dislodged from solid target (source) through impacts of gaseous ions. Most of these method can be classified as Physical Vapor Deposition (PVD) and I refer to the monograph [184] on this topic. On the other hand, in chemical deposition, a fluid precursor undergoes a chemical change at a solid surface, leaving a solid layer. An everyday example is the formation of soot on a cool object when it is placed inside a flame. The process is further categorized by the phase of the precursor. More information on chemical deposition can be found in [207].

A subset of thin-film deposition processes is focused on the so-called *epitaxial growth* of materials, the deposition of crystalline thin films that grow following the crystalline structure of the substrate. The term epitaxy comes from the Greek roots epi, meaning "above", and taxis, meaning "an ordered manner". It can be translated as "arranging upon". The term homoepitaxy refers to the specific case in which a film of the same material is grown on a crystalline substrate. This technology is used, for instance, to grow a film which is more pure than the substrate, has a lower density of defects, and to fabricate layers having different doping levels. Heteroepitaxy refers to the case in which the film being deposited is different from the substrate.

In this thesis, we *do not* distinguish specifically between the different deposition techniques, but rather build "simple" mathematical models that, hopefully, capture some of the main common phenomena.

[1] https://www.susumu.co.jp/usa/tech/know_how_02.php

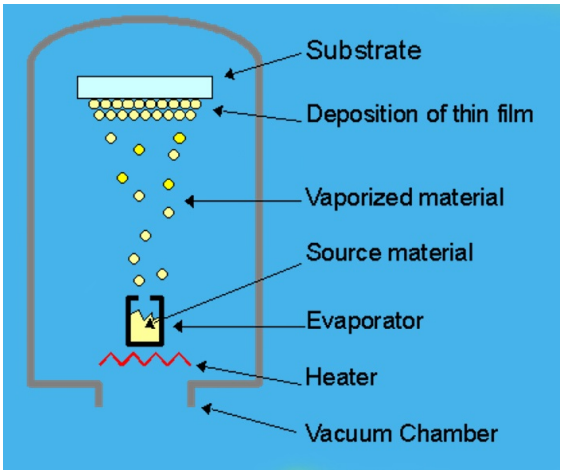

Figure 1.2: A schematic diagram of a deposition device.[2]

1.1.1 In the mathematical community

Roughly speaking, I can identify two communities of mathematicians who work on problems related to thin films or thin layers, depending on whether they rather address static or dynamical problems.

- On the one hand, the community of calculus of variations has a historical connection with mechanics and materials science, as demonstrated in the short review [27] (see also the conference report [175]). A topic of particular interest in the recent years is epitaxial growth of thin-films [73, 74, 134, 143, 31, 103, 97, 104]. These works are primarily concerned with static problems: the main object of study is some energy functional of the system and the associated equilibrium configurations depending on various scale and physical parameters.

- On the other hand, thin-film deposition can be addressed from the point of view of evolution equations. In some situations, these equations can be interpreted as gradient flows of some energy, hence the link with the community of calculus of variations. The resulting equations can be of different types: partial differential equations set in a fixed domain, but exhibiting an implicit free boundary behaviour, as is the case for the porous medium equation [227]; PDEs set in moving-boundary domains [209]; geometric evolution equations [14].

Naturally, the previous separation is somehow artificial and many researchers contribute actively to both fields. This thesis is clearly oriented towards the dynamical aspects of the process, although some results from Chapter 3 are concerned with the energy functional itself.

[2] https://www.scientificworldinfo.com/2022/02/brief-history-of-thin-film-deposition.html

1.1.2 A first one-dimensional deposition model

Let me fix the ideas by presenting the one-dimensional model introduced by Athmane Bakhta and Virginie Ehrlacher in [24], which serves as a basis for all the developments in this thesis. The model describes a PVD process, which can be simply described as follows: a wafer is introduced in a hot chamber where chemical elements are injected under gaseous form. As the latter deposit on the substrate, a heterogeneous solid layer grows upon it. Because of the high temperature conditions, diffusion occurs in the bulk until the wafer is taken out and the system is frozen.

In this model, the solid layer is composed of $n+1$ different chemical species and occupies a domain of the form $(0, e(t)) \subset \mathbb{R}_+$, where $e(t) > 0$ denotes the thickness of the film. The resulting non-cylindrical domain is denoted by

$$U_e := \bigcup_{t \in \mathbb{R}_+^*} \{t\} \times (0, e(t)).$$

For all $i = 0, \dots, n$, let $F_i \in L^1_{\mathrm{loc}}(\mathbb{R}_+^*)$ be a non-negative function so that $F_i(t)$ represents the flux of atoms of species i absorbed at the surface of the thin layer at time t. The evolution of the thickness of the film is determined by the fluxes $(F_i)_{i=0,\dots,n}$ and reads as

$$e(t) = e_0 + \int_0^t \sum_{i=0}^n F_i(s) ds, \ t > 0. \tag{1.1.1}$$

where $e_0 > 0$ denotes the initial thickness of the film. The local volume fractions of the different species $u_0(t,x), \dots, u_n(t,x)$ are expected to satisfy the constraints

$$u_i(t,x) \geq 0 \text{ and } \sum_{j=0}^n u_j(t,x) = 1, \ i = 0, \dots, n, \ t > 0, \ x \in (0, e(t)), \tag{1.1.2}$$

These constraints allow one to equivalently express u_0 as $1 - \sum_{i=1}^n u_i$. As a consequence, the whole system can be equivalently rewritten using the unknown vector $u := (u_1, \dots, u_n)^T$. More precisely, denoting by F the vector-valued function $(F_1, \dots, F_n)^T$, the cross-diffusion system in the solid layer reads:

$$\begin{cases} \partial_t u - \partial_x (A(u) \partial_x u) = 0, & (t,x) \in U_e, \\ (A(u)\partial_x u)(t,0) = 0, & t \in \mathbb{R}_+^*, \\ (A(u)\partial_x u)(t, e(t)) + e'(t) u(t, e(t)) = F(t), & t \in \mathbb{R}_+^*, \\ u(0,x) = u^0(x), & x \in (0, e_0), \end{cases} \tag{1.1.3}$$

for some matrix-valued mapping $A : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ which is called the *diffusion matrix* of the system and some initial condition u^0 compatible with the requirements (1.1.2). The boundary conditions express that the system is isolated at $x = 0$ but that there is an incoming (vector-valued) flux $F(t)$ at $x = e(t)$ where the extra term $e'(t)u(t, e(t))$ accounts for the growth of the layer.

This model already exhibits the mathematical features we will be interested in all along in this thesis: first, the description of the strongly coupled diffusion of the constituents in the layer leads to a cross-diffusion system, that is, a nonlinear parabolic system of partial differential equations. I give an overview of such systems in Section 1.2. Second, the equations have to be written in a moving-boundary domain since the layer is growing with time and, in Section 1.3, I present some mathematical approaches to such problems. Finally, if one is to optimize the process, it is natural to consider the gaseous fluxes $(F_0, \dots, F_n)$ injected during the PVD process as *boundary control variables*. I present in Section 1.4 some ideas of stabilization, focusing on the backstepping method for PDEs.

1.2 Cross-diffusion systems

This section is an introduction to the theory of cross-diffusion systems. My main references are the introduction in the thesis [23], the book chapter [155, Chapter 4] and the paper [156], I refer to them for further details. I also used some material from a recent mini-course given by Ansgar Jüngel in Konstanz, Germany.

1.2.1 Abstract systems

Let $n \in \mathbb{N} \setminus \{0, 1\}$ be the number of components of the system, $d \in \mathbb{N}^*$ be the spatial dimension, $\Omega \subset \mathbb{R}^d$ be a smooth bounded domain and $0 < T \leq +\infty$ be a time horizon. The variable of interest is the vector-valued function $u(t, x) = (u_1(t, x), \dots, u_n(t, x))^T$. Cross-diffusion systems are second-order parabolic quasilinear systems of PDEs of the form

$$\partial_t u_i - \operatorname{div}\left(\sum_{j=1}^{n} A_{ij}(u)\nabla u_j\right) = 0,\ (t, x) \in (0, T) \times \Omega,\ i = 1, \dots, n,$$

where the $A_{ij}(u)$ are the diffusion coefficients. This can be conveniently recast in compact form as

$$\partial_t u - \operatorname{div}(A(u)\nabla u) = 0,\ (t, x) \in (0, T) \times \Omega. \tag{1.2.1a}$$

The system is supplemented with an initial condition

$$u(0, x) = u^0(x),\ x \in \Omega, \tag{1.2.1b}$$

boundary conditions over $\partial\Omega$, such as no-flux boundary conditions

$$(A(u)\nabla u) \cdot \nu = 0,\ x \in \partial\Omega, \tag{1.2.1c}$$

where $\nu = (\nu_1, \dots, \nu_n)^T$ is the exterior unit normal vector to Ω, and possibly with the constraints (the constraint on the sum is usually referred to as *volume filling*)

$$u_i(t, x) \geq 0,\ i = 1, \dots, n,\ \text{and}\ \sum_{j=1}^{n} u_j(t, x) = 1,\ (t, x) \in (0, T) \times \Omega. \tag{1.2.2}$$

The mapping $A : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ is the diffusion matrix and it should enjoy a minimal parabolicity assumption, namely the *normal ellipticity* condition on the spectrum of $A(u)$

$$\sigma(A(u)) \subset \{z \in \mathbb{C} \mid Re(z) > 0\}, \tag{1.2.3}$$

for any u belonging to (a subset of) $\mathbb{R}^n$. This structural condition was identified long ago by Herbert Amann [11, 12, 13] to be sufficient for *local-in-time well-posedness* of systems of the form (1.2.1) (the theory applies to more general systems). The theory of Amann also provides sufficient conditions for the extension of this local solution up to T, namely a global control in the Sobolev space $W^{1,p}$ with $p > d$, but estimates in this high-regularity space are very difficult to obtain in dimension higher than two.

Global existence of weak solutions is difficult to prove in general for systems of the form (1.2.1), because of the lack of *a priori* estimates. Indeed, no maximum principle is in general available for systems of equations, and in addition the diffusion matrix may not be symmetric and its symmetric part may not be positive definite (classical ellipticity-parabolicity condition). In fact, cross-diffusion systems under the mere assumption (1.2.3) do not enjoy the regularity theory of parabolic scalar equations and some counter-examples were given: it was proven in [221] that there exist Hölder continuous solutions to certain parabolic systems with bounded coefficients which develop singularities in finite time. Therefore, a global-in-time theory of existence can only be constructed if one reduces the considered class of systems by adding some more structure to the equations. This will be done in Section 1.2.3.

1.2.2 Some important examples

Many applications in physics, chemistry and biology can be modelled by reaction-diffusion systems with cross-diffusion, describing the evolution of the densities of concentration of a multicomponent system. I focus in this section on three important instances arising from different applications. For convenience, I restrict the presentation to the case $n = 2$ of two species, but the systems can be defined for an arbitrary number of components. The first system below is described because of its historical importance in the literature, but is not addressed in the thesis. In contrast, the size-exclusion diffusion matrix plays a role in all the following chapters and the Stefan-Maxwell system is studied in Chapter 4.

The SKT system

The possibly most famous cross-diffusion system was introduced by Nanako Shigesada, Kohkichi Kawasaki and Ei Teramoto in 1979 [216] to model the evolution of segregating populations. The diffusion matrix reads

$$A_{\mathrm{SKT}}(u_1, u_2) = \begin{pmatrix} a_{10} + 2a_{11}u_1 + a_{12}u_2 & a_{12}u_1 \\ a_{21}u_2 & a_{20} + a_{21}u_1 + 2a_{22}u_2 \end{pmatrix}, \tag{1.2.4}$$

for nonnegative parameters $a_{ij} \geq 0$. The system is supplemented by reaction terms of *Lotka-Volterra* type

$$f_i(u_1, u_2) = (b_{i0} - b_{i1}u_1 - b_{i2}u_2)u_i, \ i = 1, 2,$$

but the main difficulties arise from the cross-diffusion coupling. The solutions are expected to be nonnegative but not necessarily bounded: the system is not of volume-filling type.

A size-exclusion system

Diffusion phenomena on a crystalline lattice can be modelled by stochastic hopping particle models on a discrete grid [217, 53]. *Size-exclusion* effects are modelled by assuming that the jump probabilities between two neighboring sites do not only depend on the type of atom, but also on the level of occupation of the site. Choosing an appropriate diffusion scaling and letting the space and time steps go to zero, one can formally derive from the discrete hopping model a macroscopic model on the *volume fraction variables* $u_0, \ldots, u_n$ (see a derivation in [24, Appendix 7.1] and generalizations in [233, Appendix A]). The size-exclusion effects lead to the volume-filling constraint

$$\sum_{i=0}^{n} u_i = 1, \tag{1.2.5}$$

thus one only needs n evolution equations on $u_1, \ldots, u_n$ while u_0 is determined from $u_0 = 1 - \sum_{i=1}^{n} u_i$. The system obtained in the limit is of cross-diffusion type, with diffusion matrix given by ($n = 2$)

$$A_{\mathrm{SE}}(u_1, u_2) = \begin{pmatrix} k_{10} + (k_{12} - k_{10})u_2 & (k_{10} - k_{12})u_1 \\ (k_{20} - k_{12})u_2 & k_{20} + (k_{21} - k_{20})u_1 \end{pmatrix}, \tag{1.2.6}$$

for positive cross-diffusion coefficients $k_{ij} > 0$.

The Stefan-Maxwell system

The Stefan-Maxwell equations describe diffusive transport phenomena into gas mixtures [168]. We consider a three components mixture with volume fractions u_0, u_1, u_2 which should be nonnegative and satisfy the volume-filling constraint (1.2.5). The cross-diffusion matrix is given by

$$A_{\mathrm{SM}}(u_1, u_2) = \frac{1}{a(u_1, u_2)} \begin{pmatrix} k_{20} + (k_{12} - k_{20})u_1 & (k_{12} - k_{10})u_1 \\ (k_{12} - k_{20})u_2 & k_{10} + (k_{12} - k_{10})u_2 \end{pmatrix}, \tag{1.2.7}$$

with $k_{ij} > 0$ and $a(u_1, u_2) = k_{10}k_{20}(1 - u_1 - u_2) + k_{12}(k_{10}u_1 + k_{20}u_2)$. Note that the latter is very similar to (1.2.6). In fact, it can be verified that the two models are strongly related via

$$A_{\mathrm{SM}} = A_{\mathrm{SE}}^{-1}.$$

1.2.3 Entropy, gradient flow, variational structure

Before presenting in details what it means for me that a cross-diffusion system has an entropy structure, let me say some words about the notion of *gradient flow*. Generally, the gradient flow of some functional $\mathcal{H} : \mathcal{X} \to \mathbb{R}$ is the evolution equation defined as

$$\partial_t u = -\text{grad } \mathcal{H}_{|u},$$

provided one can give a meaning to the generalized gradient operator above. When $\mathcal{X}$ is a Hilbert space, this is simply the Euclidean gradient. A typical application in the field of partial differential equations is the following: the space is $\mathcal{X} = L^2(\mathbb{R}^d;\mathbb{R})$ for $d \geq 1$, the functional is the Dirichlet energy $\mathcal{H}(u) = \frac{1}{2}\int_{\mathbb{R}^d} |\nabla u(x)|^2 \, dx$ if $u \in H^1(\mathbb{R}^d)$ and $\mathcal{H}(u) = +\infty$ otherwise. It follows from integration by parts that the associated gradient flow is the heat equation

$$\partial_t u = -\nabla_{L^2}\mathcal{H}(u) = \Delta u.$$

Note that the gradient with respect to the L^2 scalar product is often denoted by $\frac{\delta \mathcal{H}}{\delta u}$ in the literature. The definition of the gradient operator is easily extended when $\mathcal{X}$ is a manifold equipped with a Riemannian metric, in which case the gradient of $\mathcal{H}$ does not exist anymore in $\mathcal{X}$ but in the local tangent space. The concept of gradient flow can even be generalized to metric spaces, a particularly celebrated application being the set of probability measures endowed with the Wasserstein metric and its connections with optimal transportation theory, which provides in particular a new interpretation of the heat equation as a gradient flow. There are many excellent and complementary references on this topic [15, 100, 205, 212, 229].

In contrast, as far as we are concerned, *gradient flow structure* is simply a synonym of *entropy structure* or *variational structure* in the following sense

$$\partial_t u - \text{div}\left(M(u)\nabla\frac{\delta\mathcal{H}}{\delta u}\right) = 0, \tag{1.2.8}$$

where

$$\mathcal{H}(u) = \int_\Omega h(u) \, dx \tag{1.2.9}$$

is the *entropy* or *free energy* functional of the system and $h(u)$ the associated density. In this context, $M(u) \in \mathbb{R}^{n\times n}$ is referred to as the *mobility matrix* and is required to be *positive semidefinite* (its symmetric part). The gradient flow interpretation of this type of equation with respect to the Wasserstein metric, originally in the scalar case with linear mobility $M(u) = \alpha u$, $\alpha \in \mathbb{R}_+$, goes back to the work of Felix Otto and collaborators [154, 197] and has produced an important literature since then, see for example [201, 99, 113, 67, 178, 186, 187, 236]. We refer to the introduction in [24] concerning the applications of this theory to well-posedness for cross-diffusion systems.

Although all the models studied in this thesis share the structure (1.2.8), we *do not* use any tool from abstract gradient flow theory or mass transportation. The reason is that this theory has so far turned out to be limited in proving global existence in the

case of systems ($n \geq 2$). However, the *a priori* estimates that stem from the formulation (1.2.8) are fundamental to us. Let me compute, integrating by parts and neglecting the boundary terms,

$$\begin{aligned} \frac{d}{dt}\mathcal{H}(u) &= \int_\Omega \partial_t u^T \frac{\delta \mathcal{H}}{\delta u}\, dx = \int_\Omega \frac{\delta \mathcal{H}}{\delta u}^T \operatorname{div}\left(M(u)\nabla \frac{\delta \mathcal{H}}{\delta u}\right)\, dx \\ &= -\int_\Omega \nabla \frac{\delta \mathcal{H}}{\delta u} : M(u)\nabla \frac{\delta \mathcal{H}}{\delta u}\, dx \leq 0, \end{aligned} \tag{1.2.10}$$

where the sign follows from the positive semidefiniteness of M. We say that $\mathcal{H}$ is a *Lyapunov functional* of the evolution. The relation (1.2.10) is called the *dissipation equality* (resp. inequality) and is at the core of the global existence theory presented in the next section.

Let me now clarify the link between (1.2.8) and cross-diffusion systems of the form (1.2.1a). First note that it follows from (1.2.9) that $\frac{\delta \mathcal{H}}{\delta u} = Dh(u) \in \mathbb{R}^n$, so that, given any strictly convex entropy density h, any cross-diffusion system (1.2.1a) can be rewritten under the variational form (1.2.8), provided one defines the mobility matrix as

$$M(u) = A(u)(D^2 h(u))^{-1} \tag{1.2.11}$$

Then the dissipation estimates (1.2.10) can be rewritten

$$\frac{d}{dt}\mathcal{H}(u) = -\int_\Omega \nabla Dh(u) : M(u)\nabla Dh(u)\, dx = -\int_\Omega \nabla u : D^2 h(u) A(u) \nabla u\, dx \leq 0. \tag{1.2.12}$$

Therefore, a cross-diffusion system (characterized by its diffusion matrix A) is said to have an entropy structure if there exists a strictly convex entropy density h such that the mobility matrix given by (1.2.11) (or equivalently the matrix $D^2h(u)A(u)$) is positive semidefinite. When does a given cross-diffusion system enjoy such a structure ? This can be partially mathematically addressed, looking for necessary and sufficient algebraic conditions on the diffusion matrix A, as done in [82]. On the other hand, the intuition of the right entropy functional to consider usually follows from physical considerations about the model at hand. In particular, it should be of no surprise when modelling diffusion that the Boltzmann entropy density plays a major role. Let me define a variant of the latter as

$$h_{\mathrm{B}}(u) = \sum_{i=1}^n u_i \left(\log u_i - 1\right), \ u \in \mathbb{R}_+^n. \tag{1.2.13}$$

In this context, the gradient of the entropy density is simply a log variable

$$Dh_B(u) = \log(u), \ u \in (\mathbb{R}_+^*)^n, \tag{1.2.14}$$

and note that the chain rule $\nabla Dh(u) = D^2h(u)\nabla u$ used in (1.2.12) relies in this case on the scalar chain rule (I will come back to this in Section 1.2.6)

$$\nabla \log f = \frac{\nabla f}{f}, \ f > 0. \tag{1.2.15}$$

Additional terms may be added to model various effects, for example of electrical or chemical nature. In this context, the variable $Dh(u) = \frac{\delta \mathcal{H}}{\delta u}$ can often be interpreted as a chemical potential. In fact, when modelling dissipative systems, it is tempting to go the other way around, defining first the functional $\mathcal{H}$ and the dissipation mechanisms M, then deducing the resulting system of PDEs. The advantage of this *variational modelling* is that it automatically produces models that are *thermodynamically consistent*, which is another synonym to refer to the underlying variational structure. We refer to the lecture notes [205] for a modelling approach. We point out that the concept of variational structure can be extended in various directions, in particular to cross-diffusion systems with reaction terms in the bulk [186, 187] or on the interface [142].

The three prototype cross-diffusion systems presented in Section 1.2.2 have an entropy structure related to an entropy of the form (1.2.13). For the SKT diffusion matrix (1.2.4), one can consider a variant of the Boltzmann entropy density defined by

$$h_{\mathrm{skt}}(u_1, u_2) = a_{21} u_1 (\log u_1 - 1) + a_{12} u_2 (\log u_2 - 1).$$

Assuming $u_1, u_2 > 0$, then $\partial_{u_1} h_{\mathrm{skt}} = a_{21} \log u_1$, $\partial_{u_2} h_{\mathrm{skt}} = a_{12} \log u_2$ and one can compute that

$$\begin{aligned} \frac{d}{dt} \int_\Omega h_{\mathrm{skt}}(u_1, u_2)\, dx &= -\int_\Omega a_{21}(a_{10} + 2a_{11}u_1) \frac{|\nabla u_1|^2}{u_1}\, dx \\ &- \int_\Omega a_{12}(a_{20} + 2a_{22}u_2) \frac{|\nabla u_2|^2}{u_2}\, dx - a_{21}a_{12} \int_\Omega \frac{|u_1 \nabla u_2 + u_2 \nabla u_1|^2}{u_1 u_2}\, dx \le 0, \end{aligned}$$

so h_{skt} indeed defines a Lyapunov functional for the SKT system. In the case of the volume-filling systems (1.2.6) and (1.2.7), the Boltzmann entropy is modified into

$$h_{\mathrm{B}}^{\mathrm{vf}}(u) = \sum_{i=1}^{n} u_i \left(\log u_i - 1\right) + (1 - \rho_u) \left(\log(1 - \rho_u) - 1\right), \tag{1.2.16}$$

where $\rho_u = \sum_{i=1}^n u_i$, so that $1 - \rho_u$ accounts for the eliminated species u_0. Then similar computations show that $\int_\Omega h_{\mathrm{B}}^{\mathrm{vf}}(u)\, dx$ is indeed a Lyapunov functional for both systems (see Chapter 4).

1.2.4 Global existence theory

The general way to show the existence of global weak solutions to cross-diffusion systems of the form (1.2.1) enjoying an entropy structure is by *approximation-compactness*. The first step is to collect as many *a priori* estimates as possible on potential solutions, relying crucially on the entropy structure. Then one needs to derive an approximation procedure of the system that, on the one hand, preserves enough of the structure to save the *a priori* estimates and, on the other hand, simplifies sufficiently the system so that the existence of an approximating solution can be shown. Finally, one wants to pass to the limit in the approximation, building on the estimates at hand to obtain compactness of the sequence of approximations.

The dissipation relation (1.2.12) provides the first estimate $\mathcal{H}(u(t)) \leq \mathcal{H}(u^0)$. This is generally not enough since gradient estimates are usually needed to achieve compactness of Aubin-Lions type [83]. Thus, more assumptions on the mobility matrix M are needed. The second challenge is to ensure nonnegativity and even boundedness of the solution u in the case when one expects to satisfy the volume-filling constraint in (1.2.2). The *boundedness-by-entropy* principle, introduced as such in [156] building on previous works [76, 77, 53, 159, 160], addresses these two challenges. The main assumption is the following (it can be generalized):

(H) There exists a nonnegative convex function $h \in C^2(\mathcal{D})$, where $\mathcal{D} \subset (0,1)^n$, such that its gradient $Dh : \mathcal{D} \to \mathbb{R}^n$ is invertible and such that there exist $m_1, \ldots, m_n > 0$ such that for any $z = (z_1, \ldots, z_n)^T \in \mathbb{R}^n, u = (u_1, \ldots, u_n)^T \in \mathcal{D}$,

$$z^T D^2 h(u) A(u) z \geq \sum_{i=1}^{n} u_i^{2(m_i-1)} z_i^2. \tag{1.2.17}$$

This assumption builds on the entropy structure introduced in the previous section, requiring in addition

- the coercivity condition (1.2.17). Note that the latter is not uniform in u and may degenerate as u_i goes to 0 in the case where $m_i > 1$ (some terms on the right-hand side may become arbitrarily close to 0). It follows from this condition and the entropy dissipation inequality (1.2.12) that

$$\frac{d}{dt}\mathcal{H}(u) + \int_\Omega \sum_{i=1}^{n} u_i^{2(m_i-1)} |\nabla u_i|^2 \, dx \leq 0, \tag{1.2.18}$$

  which provides a L^2 control on $\nabla u_i^{m_i}$ for any $i = 1, \ldots, n$. Note that in the light of the relation

$$\nabla u \sim u^{1-m} \, \nabla u^m, \tag{1.2.19}$$

  one also needs to control the terms $u_i^{1-m_i}$ to recover estimates on ∇u_i. Yet in some situations, the estimates on $\nabla u_i^{m_i}$ provide enough compactness [83];

- the invertibility of Dh from a *bounded* subset to $\mathbb{R}^n$. This property enables to work with the *entropy variable* $w = Dh(u)$ for which the system reads

$$\partial_t u(w) - \operatorname{div}\left(B(w)\nabla w\right), \; B(w) = M(u(w)), \tag{1.2.20}$$

  and then to transform back to the variable $u(w) = Dh^{-1}(w) \in \mathcal{D}$, ensuring automatically uniform bounds on u and compensating for the lack of a maximum principle.

I state an existence theorem.

Theorem 1 (Global existence, special case of Theorem 2 in [156]). *Let assumption (H) holds. Assume in addition that $A \in C^0(\mathcal{D};\mathbb{R}^{n\times n})$ and that there exists $a^* > 0$ such that for all $u \in \mathcal{D}$ and $i,j = 1,\dots,n$ for which $m_j > 1$ in (H), it holds that, $|A_{ij}(u)| \le a^*|u_j|^{m_i-1}$. Let $u^0 \in L^1(\Omega;\mathbb{R}^n)$ be such that $u^0(x) \in \overline{\mathcal{D}}$ for $x \in \Omega$. Then there exists a bounded weak solution u to (1.2.1) satisfying $u(t,x) \in \overline{\mathcal{D}}$ for $(t,x) \in \mathbb{R}_+^* \times \Omega$. More precisely, u is said to be a weak solution to (1.2.1) if, for all $T > 0$,*

i) $u \in L^2((0,T);H^1(\Omega;\mathbb{R}^n))$, $\partial_t u \in L^2((0,T);H^1(\Omega,\mathbb{R}^n)')$,

ii) for any $\phi \in L^2((0,T);H^1(\Omega,\mathbb{R}^n))$,

$$\int_0^T \langle \partial_t u, \phi\rangle dt + \int_0^T \int_\Omega \nabla\phi : A(u)\nabla u \; dx \; dt = 0,$$

iii) $u(t=0) = u^0$ *is satisfied in* $L^2(\Omega;\mathbb{R}^n)$.

The proof is techically involved but essentially follows the following steps:

- *Approximation:* the system under the form (1.2.20) is approximated by replacing the time derivative by its Euler implicit discretization to avoid time regularity issues and deal only with elliptic equations. A regularizing term of the form $\varepsilon((-\Delta)^m + I)$ is added in the system, where $I \in \mathbb{R}^{n\times n}$ stands for the identity matrix.
- *Existence for the approximating system:* follows from *fixed point* arguments, using a discrete version of the entropy dissipation inequality (1.2.12) for the approximate system.
- *Passing to the limit:* the limit when the time discretization parameter $\tau > 0$ and the regularization $\varepsilon > 0$ go to 0 is performed thanks to the compactness obtained from the discrete entropy dissipation inequality, applying a discrete version of the Aubin-Lions lemma [83, 193, 16].

Theorem 1 is particularly adapted to volume-filling systems. Indeed, note that the gradient of the volume-filling Boltzmann entropy (1.2.16) is given by

$$Dh_{\mathrm{B}}^{\mathrm{vf}}(u) = \log \frac{u}{1-\rho_u}$$

which, in contrast to (1.2.14), can be inverted from the bounded domain

$$\mathcal{D} = \{(u_1,\dots,u_n) \in (0,1)^n, \; \sum_{i=1}^n u_i < 1\},$$

as, for any $w \in \mathbb{R}^n$,

$$u = (Dh_{\mathrm{B}}^{\mathrm{vf}})^{-1}(w) = \left(\frac{e^{w_i}}{1+\sum_{j=1}^n e^{w_j}}\right)_{i=1,\dots,n},$$

which answers the first requirement in (H). In fact, it can be shown that for these two systems, (H) is satisfied with $m_i = \frac{1}{2}$, see [24, Lemma 1] for the size-exclusion system and [160, Lemma 2.4] for the Stefan-Maxwell system. On the other hand, while the computations performed for the SKT system show that it satisfies (1.2.18) with $m_i = \frac{1}{2}$ or $m_i = 1$ on any subset $\mathcal{D} \subset (0, \infty)^n$, the Boltzmann entropy h_{B} can only be inverted if one considers the unbounded set $\mathcal{D} = (0, \infty)^n$, and therefore the system is not covered by Theorem 1. The proof can be adapted by regularizing the entropy density and diffusion matrix to show the existence of nonnegative global weak solutions but without upper bounds, see [156, Theorem 4]. A deeper discussion on the applicability of the boundedness-by-entropy method and several generalizations of Theorems 1 can be found in the original paper [156]. Since the introduction of the method, several works have been concerned with broadening its scope [233, 102, 147], finding novel entropy structures or dealing with more degenerate forms of (1.2.17).

Finally, let me mention that in some cases, one can take advantage of the Laplace structure

$$\operatorname{div}\left(A(u)\nabla u\right)_i = \Delta(u_i p_i(u)), \ i = 1, \ldots, n. \tag{1.2.21}$$

This allows for additional L^2 estimates on u, using the so-called *duality method* [206]. Note that, in the light of (1.2.19), this is particularly useful in cases when one has no L^∞ bounds on u, so for systems which are not volume-filling. The SKT system (1.2.4) enjoys the structure (1.2.21) and this was exploited in several works addressing generalizations where the entropies are not of the log form (1.2.13), see [109, 110, 176].

1.2.5 Long-time behaviour

Once the global-in-time existence of weak solutions is established, a question of particular relevance is their long-time behaviour. The question arises naturally from the gradient flow interpretation (1.2.8) and the dissipation relation (1.2.12), which suggest that solutions should converge to minimizers of $\mathcal{H}$ as time goes to infinity. In some situations, one expects the minimizer to be unique and globally stable, as it is the case for linear diffusion. However, it may happen that the cross-diffusion terms give rise to instability and produce *patterns*, a situation reminiscent of the *Turing instability* in reaction-diffusion systems. In fact, this latter behaviour is precisely the reason why cross-diffusion terms were first introduced in the SKT model in 1979 [216].

As long as one is only interested in the stability of equilibria, *linear stability analysis* can often be used. However, this technique does not give any qualitative indication on the dynamics starting from an arbitrary initial condition, and furthermore, even locally, it is difficult to obtain constructive rates of convergence in general. From the end of the last century and up to now, nonlinear methods have been developed to overcome these restrictions. They are usually gathered under the name of *entropy methods* and go back at least to the work of Dominique Bakry and Michel Emery [26]. In some situations, these methods yield exponential decay rates of convergence towards a steady state. Given u

and v two solutions to (1.2.1), the relative entropy of u with respect to v is defined as

$$\mathcal{H}(u|v) = \int_\Omega (h(u) - h(v) - Dh(v)^T(u-v))\ dx. \tag{1.2.22}$$

Note that a formal Taylor expansion of h around v gives

$$\mathcal{H}(u|v) \underset{u\approx v}{\sim} \frac{1}{2}\int_\Omega (u-v)^T D^2h(v)(u-v)\ dx,$$

which suggests a nonlinear generalization of the L^2 norm usually preferred in linear problems and which corresponds to $h(u) = \sum_{i=1}^n u_i^2$. I present the method in the simple case when the cross-diffusion system (1.2.1) has a unique *constant* steady state u^∞. Then the entropy dissipation (1.2.18) is unchanged when one differentiates $\mathcal{H}(u|u^\infty)$:

$$\frac{d}{dt}\mathcal{H}(u|u^\infty) \le -\int_\Omega \sum_{i=1}^n u_i^{2(m_i-1)}|\nabla u_i|^2\ dx = -\int_\Omega \sum_{i=1}^n |\nabla u_i^{m_i}|^2\ dx. \tag{1.2.23}$$

Assume that the dissipation term can be estimated from below: there exists $\lambda > 0$ such that

$$\int_\Omega \sum_{i=1}^n |\nabla u_i^{m_i}|^2\ dx \ge \lambda\mathcal{H}(u|u^\infty). \tag{1.2.24}$$

Then it follows from (1.2.23) and the Gronwall lemma that $\mathcal{H}(u|u^\infty)$ decreases exponentially fast with rate λ:

$$\mathcal{H}(u(t)|u^\infty) \le \mathcal{H}(u^0|u^\infty)e^{-\lambda t}, \quad t > 0.$$

If in addition the quantity $\mathcal{H}(u|u^\infty)$ controls some norm of $u-u^\infty$, one obtains exponential convergence for this norm.

In some situations, a classical functional inequality enables to obtain the estimate (1.2.24). A basic example is given by the linear heat equation in which case (1.2.23) holds with $h(u) = \sum_{i=1}^n u_i^2$ and $m_i = 1$. Then (1.2.24) is a Poincaré inequality. In our three cases of application, we have seen before that the entropy structure is related to entropies of log type leading to coercivity estimates (1.2.18) with exponent $m_i = \frac{1}{2}$. In this situation, the relative entropy reads

$$\mathcal{H}_{\mathrm{B}}(u|u^\infty) = \int_\Omega \sum_{i=1}^n u_i \log\frac{u_i}{u_i^\infty}\ dx,$$

and estimate (1.2.24) follows from the *logarithmic Sobolev inequality* [108, Lemma 1]. Furthermore, it follows from the Csizar-Kullback inequality [226] that $\mathcal{H}_{\mathrm{B}}(u|u^\infty)$ controls $\|u-u^\infty\|_{L^1}$, ensuring the exponential convergence to equilibrium in L^1.

For some entropies of power type, one can derive nonlinear versions (with respect to $\mathcal{H}$) of (1.2.24) using Beckner inequalities that interpolate between Poincaré and log-Sobolev

inequalities [30, 71] and conclude to algebraic decay. Nevertheless, the original entropy method was also meant as a technique to *produce* new functional inequalities adapted to the problem. The key idea was to differentiate once again (1.2.23) with respect to time and to try to estimate $\frac{d^2}{dt}\mathcal{H}(u|u^\infty)$ with respect to the dissipation term. I refer to [155, Chapter 2] and the papers [183, 17, 66] for an introduction to this method in the context of PDEs.

1.2.6 Structure preserving approximation

We now discuss the numerical approximation of cross-diffusion systems with entropy structure. It is a natural physical requirement for a discretization method to preserve as much as possible of the structure of the continuous problem such as conservation laws, nonnegativity or dissipation. In addition, such properties can be mathematically useful, since they enable to "transfer" the mathematical analysis to the discrete level. A method that preserves the dissipation of an energy (resp. entropy) is sometimes called "energy-stable" (resp. "entropy-stable") but the more general concept of "structure-preserving" approximation is gaining ground. Following the success of the entropy method, there has been considerable effort in order to preserve at the discrete level the entropy structure of scalar parabolic equations [35, 70, 63] and parabolic systems [60, 62, 61, 65, 164, 162, 101, 161, 64, 146, 157].

We focus on the finite volume method, a classical discretization method to approximate conservation laws, see a pedagogical introduction in [128] (see also the more general discretisation framework for diffusion problems [114, 115]). The general principle of the method is to approximate the system (1.2.1) after integration on a control volume K:

$$\int_K \partial_t u \, dx - \int_{\partial K} (A(u)\nabla u) \cdot \nu_K \, d\sigma = 0. \tag{1.2.25}$$

Let me first introduce a discretization of the domain and some notations. An admissible mesh of Ω is a triplet $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ where $\mathcal{T}$ is a collection of cells, $\mathcal{E}$ is a collection of faces and $(x_K)_{K\in\mathcal{T}}$ is the collection of the centers of the cells, such that the following conditions are fulfilled:

(i) Each control volume (or cell) $K \in \mathcal{T}$ is non-empty, open, polyhedral and convex. We assume that

$$K \cap L = \emptyset \text{ if } K, L \in \mathcal{T} \text{ with } K \neq L, \qquad \text{while } \bigcup_{K\in\mathcal{T}} \overline{K} = \overline{\Omega}.$$

(ii) Each face $\sigma \in \mathcal{E}$ is closed and is contained in a hyperplane of $\mathbb{R}^d$, with positive $(d-1)$-dimensional Hausdorff (or Lebesgue) measure denoted by $m_\sigma = \mathcal{H}^{d-1}(\sigma) > 0$. We assume that $\mathcal{H}^{d-1}(\sigma \cap \sigma') = 0$ for $\sigma, \sigma' \in \mathcal{E}$ unless $\sigma = \sigma'$. For all $K \in \mathcal{T}$, we assume that there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K = \bigcup_{\sigma\in\mathcal{E}_K} \sigma$. Moreover, we suppose that $\bigcup_{K\in\mathcal{T}} \mathcal{E}_K = \mathcal{E}$. Given two distinct control volumes $K, L \in \mathcal{T}$, the intersection $\overline{K} \cap \overline{L}$ either reduces to a single face $\sigma \in \mathcal{E}$ denoted by $K|L$, or its $(d-1)$-dimensional Hausdorff measure is 0.

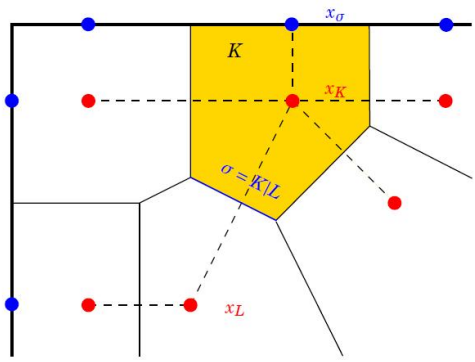

Figure 1.3: An orthogonal mesh.

(iii) The cell-centers $(x_K)_{K\in\mathcal{T}}$ satisfy $x_K \in K$, and are such that, if $K, L \in \mathcal{T}$ share a face $K|L$, then the vector $x_L - x_K$ is orthogonal to $K|L$.

We denote by m_K the d-dimensional Lebesgue measure of the control volume K. The set of the faces is partitioned into two subsets: the set $\mathcal{E}_{\text{int}}$ of the interior faces defined by

$$\mathcal{E}_{\text{int}} = \{\sigma \in \mathcal{E} \mid \sigma = K|L \text{ for some } K, L \in \mathcal{T}\},$$

and the set $\mathcal{E}_{\text{ext}} = \mathcal{E} \setminus \mathcal{E}_{\text{int}}$ of the exterior faces defined by $\mathcal{E}_{\text{ext}} = \{\sigma \in \mathcal{E} \mid \sigma \subset \partial\Omega\}$. For a given control volume $K \in \mathcal{T}$, we also define $\mathcal{E}_{K,\text{int}} = \mathcal{E}_K \cap \mathcal{E}_{\text{int}}$ (respectively $\mathcal{E}_{K,\text{ext}} = \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}$) the set of its faces that belong to $\mathcal{E}_{\text{int}}$ (respectively $\mathcal{E}_{\text{ext}}$). For such a face $\sigma \in \mathcal{E}_{K,\text{int}}$, thanks to the property ii) above, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. Given $\sigma \in \mathcal{E}$, we let

$$d_\sigma := \begin{cases} |x_K - x_L| & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ |x_K - x_\sigma| & \text{if } \sigma \in \mathcal{E}_{K,\text{ext}}, \end{cases} \qquad \text{and} \qquad \tau_\sigma = \frac{m_\sigma}{d_\sigma}.$$

We use boldface notations for any mesh-indexed quantity, typically for elements of $\mathbb{R}^{|\mathcal{T}|}$, $\mathbb{R}^{|\mathcal{E}|}$, $(\mathbb{R}^{|\mathcal{T}|})^n$ and $(\mathbb{R}^{|\mathcal{E}|})^n$. Given any discrete scalar field $\boldsymbol{v} = (v_K)_{K\in\mathcal{T}} \in \mathbb{R}^{|\mathcal{T}|}$, we define for all cell $K \in \mathcal{T}$ and interface $\sigma \in \mathcal{E}_K$ the mirror value $v_{K\sigma}$ of v_K across σ by setting:

$$v_{K\sigma} = \begin{cases} v_L & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ v_K & \text{if } \sigma \in \mathcal{E}_{\text{ext}}. \end{cases}$$

We also define the oriented jumps of $\boldsymbol{v}$ across any edge by

$$D_{K\sigma}\boldsymbol{v} = v_{K\sigma} - v_K, \ \forall K \in \mathcal{T}, \ \forall \sigma \in \mathcal{E}_K.$$

It can be checked that the following discrete integration by parts formula holds, for any $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^{|\mathcal{T}|}$:

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_\mathcal{K}} D_{K\sigma}\boldsymbol{w}.v_K = -\sum_{\sigma\in\mathcal{E}_{\text{int}}} D_{K\sigma}\boldsymbol{w}.D_{K\sigma}\boldsymbol{v},$$

where the expression on the right-hand side does not depend on the chosen cell K such that $\sigma \in \mathcal{E}_K$. Concerning the time discretization of $(0, T)$, we consider a mesh parameter Δt defined such that $N_T \Delta t = T$ with $N_T \in \mathbb{N}^*$.

Let me now address the scheme. We restrict ourselves to the Euler implicit method for the time discretization. Then (1.2.25) is approximated as, for $p = 1, \ldots, N_T$,

$$\frac{m_K}{\Delta t}\left(u_K^p - u_K^{p-1}\right) + \sum_{\sigma \in \mathcal{E}_{K,\mathrm{int}}} F_\sigma^p = 0,$$

where $\sum_{\sigma \in \mathcal{E}_{K,\mathrm{int}}} F_{K\sigma}^p$ is an approximation of the boundary integral in (1.2.25). We only consider two-point formulas, meaning that, for an edge $\sigma = K|L$, F_σ only depends on the discrete values in the cells K and L (see a discussion about this choice in [127]). Thanks to the orthogonality condition (iii) on the mesh, the term $\nabla u \cdot \nu$ can be consistently approximated by $\frac{1}{d_\sigma} D_{K\sigma}\boldsymbol{u}$. It remains to approximate $A(u)$ on the boundary, and thus to define the edge values $(\boldsymbol{u}_\sigma)_{\sigma \in \mathcal{E}}$. One natural choice would be to define them as arithmetic means of u_K and $u_{K\sigma}$. However, in many cases, this choice does not preserve the entropy structure in the sense that it does not allow to write the chain rule

$$A(u_\sigma) D_{K\sigma}\boldsymbol{u} = M(u_\sigma) D_{K\sigma} Dh(\boldsymbol{u}), \ K \in \mathcal{T}, \ \sigma \in \mathcal{E}_K,$$

so that the dissipation inequality (1.2.12) does not hold at the discrete level. As an example, let me focus again on the case of the Boltzmann entropy (1.2.13). Then we have seen that the entropy variable is a log variable and the chain rule (1.2.15) suggests to define the edge value as a *logarithmic mean* [62]

$$u_\sigma = \frac{D_{K\sigma}\boldsymbol{u}}{D_{K\sigma}\log \boldsymbol{u}} \tag{1.2.26}$$

to obtain a *discrete dissipation inequality*. The availability of the latter allows to more or less imitate the analysis of Section 1.2.4 to prove convergence (up to a subsequence) of a solution to the scheme towards a global weak solution of the system, using tools from discrete functional analysis [163] (see also [96, 129, 34, 16]). The asymptotic behaviour of the scheme can be studied if discrete versions of functional inequalities of the form (1.2.24) are available [70]. These techniques can be gathered under the name of *discrete entropy methods* and their range of applications goes beyond numerical analysis and up to the study of the long-time behaviour of Markov chains, see [155, Chapter 5].

1.2.7 Further topics

Derivation

The issue of the derivation of a given cross-diffusion system is of major importance to the modelling. From the analysis perspective, a rigorous derivation can also provide new approximation schemes that may lead to new results or new proofs on the given system [111]. The derivation can follow from phenomenological arguments using thermodynamics [38], hydrodynamic limits from kinetic models [42, 40], random walks on lattices [53, 233], stochastic differential equations of interacting particles [51, 135, 81, 75, 111] *etc.* Rigorous derivation is usually a very challenging problem.

Uniqueness and weak-strong uniqueness

Uniqueness of weak solutions is mainly an open question and the methods that have been used so far seem to be restricted to very specific cases. We refer to [23, Section 1.4], [155, Section 4.7] and the paper [80] for a presentation of these methods and their applications. On the other hand, many recent works have been concerned with proving *weak-strong uniqueness* (or weak-strong stability) [81, 32, 158, 147, 150, 172]. Weak-strong uniqueness means that, whenever a strong solution exists (usually only locally in time), any weak solution with the same initial data coincides with it. In particular, uniqueness of the strong solution implies uniqueness of the weak solution. Since it is usually easier to prove uniqueness in the class of strong solution, the weak-strong uniqueness principle somehow establishes an equivalence between the existence of a strong solution and uniqueness in the class of weak solutions.

The idea to prove such a result is again based on the relative entropy method where the relative entropy is defined by (1.2.22) (in some situations, linear energy estimates are enough [32]). Instead of comparing a weak solution to a stationary one as in Section 1.2.5, one considers a weak solution u, a strong solution v starting from the same initial condition and differentiate $\mathcal{H}(u|v)$. The goal is to prove an inequality of the form

$$\frac{d}{dt}\mathcal{H}(u|v) \leq C(v) \int_\Omega \mathcal{H}(u|v)\ dx,$$

where $C(v) > 0$ depends on some strong norms of v. Then again, it follows from Gronwall lemma that $\mathcal{H}(u(t)|v(t)) = 0$ for any $t \geq 0$ and therefore that $u = v$.

Regularity

The solutions obtained in Section 1.2.4 are weak, typically L^2 in time and H^1 in space. We have seen that in some situations one can prove that they are bounded. On the other hand, for systems with a Laplace structure (1.2.21), the duality method may provide more integrability on u. However, the global existence of classical or even strong solutions is still mainly open in general. Some results can be obtained in specific settings: low space dimension, perturbative setting from diagonal diffusion leading to restrictions on the cross-diffusion coefficients, initial data close to equilibrium *etc*, see for example [53, 32]. Let me also mention the partial Hölder regularity result [48].

1.3 Moving interfaces

In this section, I present some problems where one has to deal with moving interfaces. These problems arise in many applications such as materials science, phase transition, fluid-structure interactions, image processing, differential geometry and many more. Section 1.3.1 is concerned with *sharp interface* models: I start by introducing a one-dimensional Stefan model which is closely related to the model of Bakhta and Ehrlacher presented in 1.1.2 and the work presented in Chapters 2 and 4. In order to reach higher

space dimension, I introduce some material about curvature-driven interface evolutions and discuss briefly the different approaches to tackle them. Then in Section 1.3.2, I present in more details the phase-field approach which leads to diffuse interface models such as the Allen-Cahn and Cahn-Hilliard equations. This section motivates the work of Chapter 3. Section 1.3.3 is an introduction to the different variants of the one-species Cahn-Hilliard equation, which is useful reading before addressing the multispecies cross-diffusion-Cahn-Hilliard model in Chapter 3.

I have been much inspired by the review [138]. Much more information can be found in the monograph [209] and [14, Chapter 1] about sharp-interface models and geometric evolutions, in [117] about the phase-field method and in particular its numerical aspects and in [195] and [190] about the Cahn-Hilliard equation.

1.3.1 Sharp interfaces and geometric evolutions

Moving interface models of sharp type are better considered starting from a historical example of paramount importance, namely the *Stefan problem*. The model describes a material undergoing a phase change such as the melting of ice in water. While the heat equation has to be solved in both phases, the *Stefan condition* relates the dynamics of the interface to the interface temperature, thus coupling the two phases.
Let me describe the simple one-dimensional one-phase model: I consider a block of ice occupying the domain $(0, e(t))$. The variable u is the temperature of the ice which satisfies the heat equation. A fixed temperature is imposed on the left boundary while the interface temperature is required to be at melting point. The problem is supplemented with an initial condition, leading to

$$\begin{cases} \partial_t u - \partial^2_{xx} u = 0, & t > 0,\ x \in (0, e(t)), \\ u(t, 0) = 1, & t > 0, \\ u(t, e(t)) = 0, & t > 0, \\ e(0) = e_0, & \\ u(x, 0) = 0, & x \in (0, e_0). \end{cases}$$

Such a model would normally be closed if the domain was fixed, but here the evolution of the interface $t \to e(t)$ is an additional unknown which requires an additional condition. The Stefan condition reads

$$e'(t) = -\frac{\partial}{\partial x} u(t, e(t)).$$

The simplicity of this problem comes from its one-dimensional nature: the equation on the interface is simply an ordinary differential equation and there is no geometric difficulty. On the other hand, it has the advantage of coupling the interface displacement with the physical situation away from the surface in a *non-local* way. The sharp interface models considered in Chapters 2 and Chapters 4 are of one-dimensional nature and share similarities with the Stefan problem.

In dimension $d \geq 2$, moving interfaces problems require the introduction of new mathematical tools. In the simplest case, the interface evolution does not depend on the

situation away from the interface but only on its own *local* geometry. The equations that describe such a motion are called *surface* or *geometric evolution equations*. In many cases, these motions are *curvature-driven*, the most prominent example being the *mean curvature flow*. Let me introduce the latter with a variational approach. I consider a smooth, compact, oriented hypersurface Γ in $\mathbb{R}^d$ without boundary. The simplest surface energy of such a hypersurface is proportional to its surface area. I hence consider the area functional

$$E(\Gamma) := \mathcal{H}^{d-1}(\Gamma) \tag{1.3.1}$$

where $\mathcal{H}^{d-1}$ is the $(d-1)$-dimensional surface measure. The goal now is to make Γ evolve in such a way that the surface area decreases most rapidly. Roughly speaking, this will be achieved by flowing Γ in the direction of the negative "gradient" of E. In order to define the gradient, we first of all need to determine the first variation (the "derivative") of the area functional. To compute a directional derivative of E, we embed Γ in a one-parameter family of surfaces. This will be achieved with the help of a smooth vector field $\zeta : \mathbb{R}^d \to \mathbb{R}^d$. We define

$$\Gamma_t := \{x + t\zeta(x) \mid x \in \Gamma\},\ t \in \mathbb{R},$$

and a classical computation gives (see the appendix in [106])

$$\frac{d}{dt} E(\Gamma_t)_{|t=0} = -\int_\Gamma HV d\mathcal{H}^{d-1}. \tag{1.3.2}$$

Here H is the mean curvature of Γ defined as the sum of the principal curvatures, $V = \zeta \cdot \nu$ is the normal velocity of the evolving surface $(\Gamma_t)_{t\in\mathbb{R}}$ at $t = 0$ and by $d\mathcal{H}^{d-1}$ I denote integration with respect to the $(d-1)$-dimensional surface measure. On Γ, I have chosen a normal vector field ν and I here take the sign convention that the surface has positive mean curvature if it is curved in the direction of the normal. The formula (1.3.2) shows that the surface area decreases if the surface moves in the direction of the mean curvature vector $H\nu$, and in addition that the L^2-gradient of E is given by $-H$. Therefore, the L^2 gradient flow of E is given by the mean curvature flow

$$V = H, \tag{1.3.3}$$

which completely determines the evolution of the surface. One drawback of the mean curvature flow is that it does not preserve the volume enclosed by the surface, while in some applications volume conservation is required from physical arguments. A natural way to fix the volume is to consider normal velocities V with zero mean. Indeed, the following identity can be shown (see again [106])

$$\frac{d}{dt}\mathrm{vol}(\Gamma_t) = \int_{\Gamma_t} V d\mathcal{H}^{d-1},$$

where ν is now chosen as the outer unit normal to the set enclosed by the hypersurface. In consequence, the mean curvature flow can be modified into its volume-preserving version

$$V = H - \frac{1}{|\Omega|}\int_\Omega H d\mathcal{H}^{d-1}.$$

A more physical volume-preserving flow that decreases the area energy is given by the *surface diffusion flow*, which is obtained as the gradient flow of the area energy (1.3.1) for the H^{-1} inner product. It requires the introduction of the surface Laplacian Δ_Γ on Γ and reads as

$$V = -\Delta_\Gamma H. \tag{1.3.4}$$

The main difficulty in the theoretical and numerical analysis of geometric evolution equations is that typically the topology of the surface changes along the evolution in dimension $d \geq 3$. This prevents the use of a classical description of the surface, since the involved parametrizations would develop singularities and break down in finite time. In consequence, weak descriptions of the solution have to be implemented and several approaches have been proposed in the literature. Ken Brakke [47] used tools from geometric measure theory to build *varifold solutions*. Fred Almgren, Jean E. Taylor and Lihe Wang [10] and Stephan Luckhaus and Thomas Sturzenhecker [180] independently came up with a variational approach based on a time-discretization of the gradient flow formulation and an approximation of the L^2 distance, constructing a solution usually referred to as the *flat flow*. The level-set method and its relations with the theory of viscosity solutions was initially developed by Yun-Gang Chen, Yoshikazu Giga and Shun'ichi Goto [84] and Lawrence C. Evans and Joel Spruck [126], see also the monograph [141]. We finally mention the phase-field approach which goes back at least to [9] and where the main idea is to replace sharp interfaces by diffuse interfaces, that is, to replace characteristic functions of sets $\xi : \Omega \to \{0, 1\}$ by smooth functions ξ_ε rapidly changing between two pure states. I give an introduction to the phase-field method in the next section because it provides the framework to understand the relationship between Chapter 3 and the rest of the thesis.

From the computational point of view, these different representations of the interface give rise to different numerical methods which all have their own advantages and drawbacks. I refer to [106] for a review of these methods.

I finish this section with some instances of problems that combine the difficulties of geometric evolutions together with physical effects of non-local type. Let Γ be a compact hypersurface in $\mathbb{R}^d$ which separates an open domain $\Omega \subset \mathbb{R}^d$ into two open sets Ω_- and Ω_+. The *Mullins-Sekerka* problem (which I think is also called the *Hele-Shaw* problem) is meant to describe the evolution of the spatial distribution of two phases driven by the reduction of interfacial area and limited by diffusion. It is given by

$$\begin{cases} -\Delta u = 0, & x \in \Omega_-(t) \cup \Omega_+(t), \\ V = -[\![\nabla u]\!] \cdot \nu, & x \in \Gamma_t, \\ u = H, & x \in \Gamma_t, \\ \nabla u \cdot \nu = 0, & x \in \partial\Omega, \end{cases}$$

where $[\![\cdot]\!]$ denotes the jump of a quantity across the interface Γ. This evolution preserves the volume of both phases and decreases $E(\Gamma_t)$. We refer to [138, Section 2.5] for a derivation of the problem as a H^{-1} gradient flow of (1.3.5). The Mullins-Sekerka problem

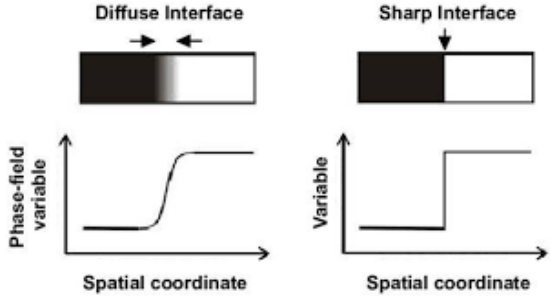

Figure 1.4: Sharp and diffuse interfaces[3]

is related to the *classical Stefan problem* in arbitrary dimension, given by

$$\begin{cases} \partial_t u = d_i \Delta u, & x \in \Omega_i(t),\ i \in \{-,+\}, \\ V = -[\![d\nabla u]\!] \cdot \nu, & x \in \Gamma_t, \\ u = 0, & x \in \Gamma_t, \\ \nabla u \cdot \nu = 0, & x \in \partial\Omega. \end{cases}$$

These problems are in general very difficult to address and I refer to [209] for analytical tools and applications to different problems of this type.

1.3.2 Diffuse interfaces via the phase-field approach

The main idea of the phase field approach is to replace sharp interfaces by diffuse interfaces (Figure 1.4), that is, to replace characteristic functions of sets by smooth functions u_ε rapidly changing between two pure states in an interfacial region whose thickness depends on the small parameter $\varepsilon > 0$. Note that, although I present the method as a way to approximate sharp models, diffuse interfaces can in fact be more physical in some situations. Let me consider the Ginzburg-Landau energy

$$E_\varepsilon(u) := \int_\Omega \left(\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon}\Psi(u) \right) dx, \tag{1.3.5}$$

where $\Psi : \mathbb{R} \to \mathbb{R}_+$ is a double-well potential having two global minima with value zero at ± 1 i.e. such that $\Psi(\pm 1) = 0$ and $\Psi > 0$ in $(-1, 1)$. A common choice is the quartic potential

$$\Psi(u) = (u^2 - 1)^2. \tag{1.3.6}$$

The term $\frac{1}{\varepsilon}\Psi(u)$ in (1.3.5) penalizes values that differ from the two minima, while the term $\frac{\varepsilon}{2}|\nabla u|^2$ penalizes oscillations. A famous result due to Luciano Modica and Stefano Mortola links (1.3.5) to the area energy (1.3.1): up to a constant factor, E_ε $\Gamma-$converges to E as $\varepsilon \to 0$. This means that, under appropriate assumptions, the minimizers and extremal values of E_ε converge to those of a multiple of E. We do not make the statement

[3] https://personal.ems.psu.edu/~fkd/courses/EGEE520/2019Deliverables/phase.pdf

more precise and refer to the original result [191] and to the book [45] for an introduction to $\Gamma-$convergence and its applications. In the light of this result and of the gradient flow interpretation of the mean-curvature and surface diffusion flows with respect to E, it is natural to approximate these flows by gradient flows of E_ε with respect to the respective associated metrics. Therefore, mirroring the approach of the previous section, we first compute the first variation of E_ε, obtaining, for $u \in H^1(\Omega)$,

$$\frac{\delta E_\varepsilon}{\delta u}(u)(v) := \frac{d}{dt} E_\varepsilon(u+tv)_{|t=0} = \int_\Omega \left(\varepsilon \nabla u \cdot \nabla v + \frac{1}{\varepsilon}\Psi'(u)v \right) \, dx,$$

where the derivative of the potential (1.3.6) reads

$$\Psi'(u) = -u + u^3.$$

Choosing the L^2 inner product, we obtain the *Allen-Cahn equation*

$$\begin{cases} \partial_t u = \varepsilon \Delta u - \dfrac{1}{\varepsilon}\Psi'(u), \ t > 0, \ x \in \Omega. \\ \nabla u \cdot \nu = 0, \ t > 0, \ x \in \partial\Omega. \end{cases} \tag{1.3.7}$$

The H^{-1} inner product provides instead the *Cahn-Hilliard equation*

$$\begin{cases} \partial_t u = \Delta \left(-\varepsilon \Delta u + \dfrac{1}{\varepsilon}\Psi'(u) \right), \ t > 0, \ x \in \Omega. \\ \nabla u \cdot \nu = \nabla \Delta u \cdot \nu = 0, \ t > 0, \ x \in \partial\Omega. \end{cases} \tag{1.3.8}$$

The Allen-Cahn equation is a parabolic equation of order 2, which does not conserve the mass. On the other hand, the Cahn-Hilliard equation is a mass-conserving parabolic equation of order 4. Both equations decrease the Ginzburg-Landau energy (1.3.5): if u is a solution to (1.3.7) or (1.3.8) then

$$\frac{d}{dt} E_\varepsilon(u(t)) \leq 0.$$

I refer to [133] for a more thorough presentation of the gradient flow interpretation of these equations.

Relating the gradient flows of E_ε to the gradient flows of E is usually referred to as a *sharp interface limit*. The goal is to show that, up to a time scaling related to ε, the family of solutions $(u_\varepsilon)_{\varepsilon>0}$ obtained from the phase-field model converges, as $\varepsilon \to 0$, to a set characteristic function $u_0 : \Omega \to \{-1, +1\}$ and that in addition, the boundary between the sets $\{u_0 = -1\}$ and $\{u_0 = 1\}$ evolves following a geometric law similar to (1.3.3) or (1.3.4). There are essentially two approaches to sharp interface limits: one approach assumes that a smooth local solution to the limiting surface evolution equation exists and uses *matched asymptotic expansion* to construct a local solution to the phase-field equation which converges to the surface evolution. This approach can be only formal or made rigorous. The other approach is *global* in time and depends on the chosen weak

formulation for the limiting surface evolution. Besides, let me point out that there have been attempts to build an abstract theory of evolutionary $\Gamma-$convergence [211, 215, 46].

As expected from the previous derivation, it has be shown by many different methods that the sharp interface limit of the Allen-Cahn problem (1.3.7) is the mean curvature flow [50, 79, 125, 151, 105]. On the other hand, the sharp-interface limit of the Cahn-Hilliard equation (1.3.8) *is not* the surface diffusion flow (1.3.4) but the previously introduced *Mullins-Sekerka* problem [204, 8, 222, 173]. To derive the surface diffusion flow, I need to introduce a variant of the Cahn-Hilliard equation (1.3.6)-(1.3.8) where the quartic potential is replaced by a logarithmic one and a degenerate mobility is introduced. This model is introduced and studied in the next section where available results about its sharp-interface limit are also discussed.

1.3.3 More about the Cahn-Hilliard equation

The Cahn-Hilliard equation as a physical model goes back to [58], long before the connection with geometric evolutions, and was initially developed to describe patterns formation in the phase separation of a two-component system where $0 \leq u(t,x) \leq 1$ represents the concentration (mass or volume fraction) of one of the two components while the other one is described by $1-u$. A general form of the Cahn-Hilliard equation is given by

$$\begin{cases} \partial_t u = \operatorname{div}\left(m(u)\nabla(F'(u) - \varepsilon^2\Delta u)\right), \ t>0, \ x\in\Omega. \\ \nabla u\cdot\nu = m(u)\nabla(F'(u)-\varepsilon^2\Delta u)\cdot\nu = 0, \ t>0, \ x\in\partial\Omega, \\ u(0,x) = u_0(x), \ x\in\Omega, \end{cases} \tag{1.3.9}$$

allowing for different form of double-well potentials $F(u)$ and mobility coefficient $m(u) \geq 0$. It is common to introduce the *chemical potential* variable

$$\mu = F'(u) - \varepsilon^2\Delta u.$$

Then testing (1.3.9) against μ and integrating over Ω gives, on the left hand-side,

$$\int_\Omega \partial_t u\mu = \frac{d}{dt}\left(\int_\Omega F(u) + \frac{\varepsilon^2}{2}|\nabla u|^2\, dx\right),$$

and one the right-hand side, using integration by parts,

$$\int_\Omega \operatorname{div}\left(m(u)\nabla\mu\right)\mu = -\int_\Omega m(u)|\nabla\mu|^2,$$

so that the Lyapunov estimate reads

$$\frac{d}{dt}\left(\int_\Omega F(u) + \frac{\varepsilon^2}{2}|\nabla u|^2\right) = -\int_\Omega m(u)|\nabla\mu|^2 \leq 0.$$

This is of course reminiscent of the gradient flow derivation from the Ginzburg-Landau energy. In fact, the Cahn-Hilliard equation with a general mobility can also be interpreted as a gradient flow of (1.3.5) for a suitable weighted H^{-1} inner-product, see [223].

The Cahn-Hilliard equation (1.3.8) derived in the previous section corresponds to the case of constant mobility $m(u) = 1$ and F given by the quartic polynomial potential (1.3.6), except for a different time-scaling $t \to \varepsilon t$ and the change of variable $u = u - (1-u) = 2u - 1$ which explains why the previous potential had minima at ± 1 whereas now F has two zero-minima at 0 and 1. The different versions co-exist in the literature and are all equivalent, except when performing the sharp-interface limit when the time-scaling is important. The constant mobility and quartic potential case is well-understood analytically: I already mentioned some results relating the sharp-interface limit to the mean curvature flow [50, 79, 125, 151, 105]. Global existence and uniqueness of strong solutions for H^2 initial data and in space dimension $d \leq 3$ was first addressed in [122]. Then the well-posedness of global weak solutions for L^2 initial data and $d \leq 3$ was proved in [194, Part 2]. Many more works have been devoted to regularity issues and long-time asymptotics and I refer to [190, Chapter 3] and the references therein. However, due to the lack of maximum principle for fourth order equations, the solutions need not to remain bounded in the interval of interest $(0, 1)$ (or $(-1, 1)$, depending on the convention), even if the initial data lies in this interval, which is physically irrelevant and motivates some changes in the model.

An important physical variant of the Cahn-Hilliard equation corresponds to the case where the potential $F(u)$ is of logarithmic type

$$F(u) = \frac{\Theta}{2}\left(u \log u + (1-u)\log(1-u)\right) + \alpha u(1-u), \tag{1.3.10}$$

for given constants $\Theta, \alpha > 0$. This choice follows from thermodynamic considerations where Θ is the fixed temperature and is associated to an entropy contribution. This potential is singular at $u = 0$ and $u = 1$ and is therefore associated to the concentration-dependent mobility

$$m(u) = u(1-u) \tag{1.3.11}$$

which degenerates at $u = 0$ and $u = 1$ and hopefully prevents the solution from escaping the interval $(0, 1)$. The Cahn-Hilliard equation (1.3.9) associated to the potential (1.3.10) and mobility (1.3.11) reads

$$\begin{cases} \partial_t u = \operatorname{div}\left(m(u)\nabla(\frac{\Theta}{2}\log\left(\frac{u}{1-u}\right) + \alpha(1-2u) - \varepsilon^2\Delta u)\right), \ t > 0, \ x \in \Omega. \\ \nabla u \cdot \nu = m(u)\left(\frac{\Theta}{2u(1-u)}\nabla u - 2\alpha\nabla u - \varepsilon^2\nabla\Delta u\right)\cdot\nu = 0, \ t > 0, \ x \in \partial\Omega, \\ u(0,x) = u_0(x), \ x \in \Omega. \end{cases} \tag{1.3.12}$$

The derivation of the latter is physically justified and (1.3.8) can in turn be obtained as a suitable aproximation of the degenerate Cahn-Hilliard equation. We point out that another nonsmooth potential, the *double obstacle potential* is frequently studied and is obtained from (1.3.10) in the the so-called *deep quench limit* $\frac{\Theta}{\alpha} \ll 1$, see [36].

Problem (1.3.12) is now of *degenerate parabolic* type, which significantly complicates the analysis and, in fact, very few analytical results are known for this equation. A

global existence result has been proved in [120] where, in particular, the solution remains bounded in the interval of interest. To my knowledge, no more analytical result is available in the exact setting (1.3.12). A global existence result has been proved more recently in the case of more general degenerate mobility matrices but with a smooth potential [98]. The long-time behaviour of (1.3.9) with the logarithmic potential (1.3.10) is investigated in the case of a mobility of constant type in [1] and of non-constant but not degenerate type in [213, 214]. Let me now discuss the sharp interface limit results for (1.3.12): in [57], the authors used formal asymptotics to show, after a time scaling $t \to \varepsilon^2 t$ in (1.3.12), the convergence to surface diffusion in two regimes: on the one hand, the deep-quench limit and associated double obstacle potential and on the other hand, the small temperature regime $\Theta = O(\varepsilon^\alpha)$, where $\alpha > 0$ is associated to the logarithmic potential (1.3.10). In addition, in a recent work [174], the authors used formal asymptotics to show that, in the case of degenerate mobility and smooth quartic potential, the limiting model is not governed by pure surface diffusion but admits a non-local contribution. To my knowledge, none of these results has been made rigorous yet.

1.4 Stabilization

A *control system* is a dynamical system on which one can act by using suitable *controls*. Control theory is historically closely related to automatics and engineering, although it is clear that applications are ubiquitous. The theory is usually divided between three subfields that correspond to three different goals, namely

- *Controllability.* The goal is to "move" the control system from a given state to another. In this case, the controls are time-dependent functions defined *a priori* for a given initial state. The system is said to be in *open loop*.

- *Optimal control.* The goal is to choose the optimal trajectory between two states with respect to a given criterion to be minimized along the path.

- *Stabilization.* The goal is to stabilize a given unstable equilibrium of the uncontrolled system. In this case, the controls are functions of the state itself (and possibly of time), one calls them *feedback laws*. The system is said to be in *closed loop*.

The significant advantage of stabilization over controllability is its robusteness with respect to various errors and uncertainties. On the other hand, it requires the observability of (part of) the state, which is not always granted in applications. On the mathematical level, well-posedness for closed-loop systems is in general more involved than for open-loop systems because of the state-dependence of the controls. When the system at hand is a (system of) partial differential equation(s), one distinguishes between *internal control*, acting in the interior of the domain and appearing in the equation itself, and *boundary control*, appearing in the boundary conditions. In many physical systems, boundary control is more realistic to achieve.

This section is not an introduction to control theory or even to boundary stabilization theory, for which I refer the reader to the monograph [85] (mostly in finite dimension). My main goal is to introduce a specific boundary stabilization method, the *backstepping method*, introduced in Section 1.4.2, mostly after [170]. To this aim, I first need to introduce some basic material about stabilization in Section 1.4.1. Jean-Michel Coron and Hoai-Minh Nguyen applied the backstepping method to stabilize in finite time the heat equation with variable coefficients in [92], which strongly inspired our work in Chapter 2. I present their approach and results in Section 1.4.3.

1.4.1 Basic notions

For the sake of clarity, I introduce some notions in finite dimension and discuss the extensions to infinite dimension at the end of the section. I first consider the dynamical system given by

$$\dot{x} = X(x) \tag{1.4.1}$$

where, to simplify, I assume that $X \in C^0(\Omega \subset \mathbb{R}^n; \mathbb{R}^n)$ so that at least one maximal solution to (1.4.1) exists when starting from some initial condition in Ω (Cauchy-Peano theorem). We also assume that $\bar{x} \in \Omega$ is an equilibrium of (1.4.1), that is $X(\bar{x}) = 0$. I give a definition of asymptotic stability, which is stated as a characterization in [85, Theorem 10.8].

Definition 1 (Asymptotic stability)**.** *One says that $\bar{x}$ is* locally asymptotically stable *for* (1.4.1) *if*

i) $\bar{x}$ is a stable point *for* (1.4.1)*, i.e., for every $\varepsilon > 0$, there exists $\eta > 0$ such that*

$$(\dot{x} = X(x) \text{ and } |x(0) - \bar{x}| < \eta) \implies (|x(t) - \bar{x}| < \varepsilon, \forall t \geq 0).$$

ii) $\bar{x}$ is an attractor *for* (1.4.1)*, i.e., there exists $\rho > 0$ such that*

$$(\dot{x} = X(x) \text{ and } |x(0) - \bar{x}| < \rho) \implies (\lim_{t \to +\infty} x(t) = \bar{x}).$$

If $\Omega = \mathbb{R}^n$ and property ii) holds for any $\rho > 0$, $\bar{x}$ is said to be globally *asymptotically stable for* (1.4.1)*.*

Here are some facts:

- For the linear system $\dot{x} = Ax$, local and global stability are equivalent. 0 is asymptotically stable for the system if and only if every eigenvalue of A has a strictly negative real part.
- *Linear test*: assume that the vector field in (1.4.1) belongs to $C^1(\Omega; \mathbb{R}^n)$. If every eigenvalue of $X'(\bar{x})$ has a stricly negative real part, then $\bar{x}$ is asymptotically stable for $\dot{x} = X(x)$. If one eigenvalue has strictly positive real part, then it is not.

The linear test does not characterize the local asymptotic stability of nonlinear systems but provides an important sufficient (resp. necessary) condition.

Let me now consider the abstract control system

$$\dot{x} = f(x, u), \tag{1.4.2}$$

with state $x \in \mathbb{R}^n$, control $u \in \mathbb{R}^m$ and f of class C^1 in a neighborhood of $(0,0) \in \mathbb{R}^n \times \mathbb{R}^m$ such that $f(0,0) = 0$.

Definition 2 (Asymptotic stabilization)**.** *The control system* (1.4.2) *is locally (resp. globally) asymptotically stabilizable by means of continuous stationary feedback laws if there exists* $u \in C^0(\mathbb{R}^n; \mathbb{R}^m)$ *satisfying* $u(0) = 0$ *such that* $0 \in \mathbb{R}^n$ *is a locally (resp. globally) asymptotically stable point for the closed-loop system*

$$\dot{x} = f(x, u(x)).$$

Here are some more facts:

- Pole-shifting theorem: Assume that the linear control system $\dot{x} = Ax + Bu$ is controllable. Given arbitrary values $\lambda_1, \ldots, \lambda_n$, there exists $K \in \mathbb{R}^{m \times m}$ such that the eigenvalues of $A + BK$ are exactly $\lambda_1, \ldots, \lambda_n$. In particular, any controllable linear system if asymptotically stabilizable by means of a continuous stationary feedback law of the form $x \to Kx$.

- It follows from the pole-shifting theorem combined with the linear test that, if the linearized version of (1.4.2) around $(0,0)$ given by

  $$\dot{x} = \partial_x f(0,0)x + \partial_u f(0,0)u$$

  is controllable, then there exists $K \in \mathbb{R}^{m \times n}$ such that $0 \in \mathbb{R}^n$ is locally asymptotically stable for the closed-loop system $\dot{x} = f(x, Kx)$.

The conclusions of the pole-shifting theorem are very strong and the main assumption is the controllability of a given autonomous linear system of the form $\dot{x} = Ax + Bu$. For this type of system, there exists a simple necessary and sufficient condition for controllability, the *Kalman condition*, which is purely algebraic on the matrices A and B. Thus in this case, the theory essentially reduces to linear algebra.

Nevertheless, there are situations when the linear test fails, and when it is not clear whether a given nonlinear control system is stabilizable or not. Moreover, the pole-shifting theorem cannot be efficiently generalized to infinite dimension even in the linear case. Hence the need to develop different methods and in particular methods that are specifically adapted to the nonlinear structure. One of the most natural and robust one is the approach based on *Lyapunov functionals*. Besides, it has been shown that, unlike the linear situation, not any controllable nonlinear system is asymptotically stabilizable by means of continuous stationary feedback laws, even in the analytic case. To overcome this, researchers have been mainly considering two other classes of feedbacks: *discontinuous*

feedbacks and *time-varying feedbacks*. I refer to [85, Chapter 11] on this topic. Many methods to derive feedback laws can be found in [85, Chapter 12].

In infinite dimension, a control system can still be stated under the form (1.4.2), but the state space to which x belongs is now an infinite-dimensional Banach space. The first difficulty arises from the well-posedness of the dynamical system, since the Cauchy-Lipschitz and Cauchy-Peano theorems cannot be used in general for PDEs applications where the involved operators are unbounded, and well-posedness depends on the definition of solution at hand. Second, since topologies are not equivalent in infinite dimension, many different choices can be made in the definition of asymptotic stability, depending on the situation [91]. On the one hand, an abstract framework can still be provided using *semigroup theory* and tools from functional analysis. On the other hand, it seems reasonable to rather describe general ideas and heuristics rather than stating general theorems, and then to try to apply these ideas to various specific problems. It is in this spirit that I present the backstepping method for PDEs in the next section.

1.4.2 The backstepping method

The backstepping method emerged at the end of the 1980s to address finite-dimensional systems having a particular "cascade" structure, which reads as

$$\begin{cases} \dot{x_1} = f_1(x_1, x_2), \\ \dot{x_2} = u, \end{cases} \tag{1.4.3}$$

where the state is $x = (x_1, x_2)^T \in \mathbb{R}^{n_1+n_2}$ with $(x_1, x_2) \in \mathbb{R}^{n_1} \times \mathbb{R}^{n_2}$ and the control is $u \in \mathbb{R}^{n_2}$. The key theorem of finite-dimensional backstepping is stated below. A proof and references can be found in [85].

Theorem 2 (Theorem 12.24 of [85])**.** *Assume that $f_1 \in C^1(\mathbb{R}^{n_1} \times \mathbb{R}^{n_2}; \mathbb{R}^{n_1})$ and that the control system*

$$\dot{x_1} = f_1(x_1, v),$$

where the state is $x_1 \in \mathbb{R}^{n_1}$ and the control is $v \in \mathbb{R}^{n_2}$, can be globally asymptotically stabilized by means of a stationary feedback law of class C^1. Then the control system (1.4.3) can be globally asymptotically stabilized by means of a continuous stationary feedback law.

Miroslav Krstic, Andrey Smyshlyaev and collaborators initiated in the 2000s an effort to extend the backstepping method to PDEs in the context of boundary control. Their intuition was that the cascade structure (1.4.3) is similar to a boundary control problem where the instability arises from the interior equation and the effect of the control has to be propagated through the dynamics. In a nutshell, the idea of the backstepping method is to transform the original unstable system into a stable *target system*, where the form of the change of variables is specifically adapted to the cascade or triangular structure of the original system and the transformation can be inverted. Let me introduce the method in the context of PDEs through an example taken from [170, Section 4.1], which

serves as the basis for further developments in this thesis. We consider the domain $(0,1)$ and the boundary problem

$$\begin{cases} \partial_t u(t,x) = \partial^2_{xx} u(t,x) + \lambda u(t,x), \quad t>0,\ x\in(0,1), \\ \quad u(t,0) = 0,\ t>0, \\ \quad u(t,1) = U,\ t>0, \end{cases} \tag{1.4.4}$$

where $\lambda \in \mathbb{R}$ and U is the boundary control. In the case $U \equiv 0$ and for λ sufficiently large, the system is unstable because of the destabilizing term λu. It is therefore natural to consider as a target the stable system

$$\begin{cases} \partial_t w(t,x) = \partial^2_{xx} w(t,x), \quad t>0,\ x\in(0,1), \\ \quad w(t,0) = 0,\ t>0, \\ \quad w(t,1) = 0,\ t>0. \end{cases} \tag{1.4.5}$$

The exponential stability of the latter simply follows from the Poincaré inequality

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2} = -\|\nabla w(t)\|^2_{L^2} \le -\|w(t)\|^2_{L^2},$$

from which one obtains

$$\|w(t)\|_{L^2} \le e^{-t}\|w(0)\|_{L^2}. \tag{1.4.6}$$

The target variable w is obtained via the Volterra integral transformation

$$w(t,x) = u(t,x) - \int_0^x k_\lambda(x,y)u(t,y)\ dy, \tag{1.4.7}$$

where k_λ is the *backstepping kernel* which will be defined later. One remarks that the triangular structure appears in the transformation since integration runs only up to the local variable x and not up to the boundary $x=1$. The method imposes the choice of the feedback law: inserting $w(t,1)=0$ in (1.4.7) gives

$$u(t,1) = \int_0^1 k_\lambda(1,y)u(t,y)dy. \tag{1.4.8}$$

Remark that the feedback law (1.4.8) requires the observation of the full state u. The main advantage of transformation (1.4.7) is that it is always invertible in $L^2(0,1)$ provided k_λ is itself in $L^2(D)$ where $D := \{(x,y)\in(0,1)^2,\ y\le x\}$. The inverse of the transformation has the form

$$u(t,x) = w(t,x) + \int_0^x l_\lambda(x,y)w(t,y)\ dy, \tag{1.4.9}$$

where l_λ is defined as

$$l_\lambda(x,y) = -k_{-\lambda}(x,y). \tag{1.4.10}$$

This guarantees that the L^2 stability of the target system can be translated into the stability of the original system, and moreover that stability rates are quantitatively related

through estimates on the kernels k_λ and l_λ. More precisely, it follows successively from (1.4.9), (1.4.6) and (1.4.7) that, for any $t > 0$,

$$\begin{aligned}\|u(t)\|_{L^2(0,1)} &\leq (1 + \|l_\lambda\|_{L^2(D)})\|w(t)\|_{L^2(0,1)} \leq (1 + \|l_\lambda\|_{L^2(D)})\|w(0)\|_{L^2(0,1)}\ e^{-t} \\ &\leq (1 + \|l_\lambda\|_{L^2(D)})(1 + \|k_\lambda\|_{L^2(D)})\|u^0\|_{L^2(0,1)}\ e^{-t}.\end{aligned} \tag{1.4.11}$$

Therefore, the boundary stabilization problem has been reduced to proving the existence of (and possibly constructing) a kernel k_λ that transforms the original PDE into the target one. Inserting (1.4.7) into the PDE satisfied by w in (1.4.5) and performing formal manipulations, one obtains that k_λ must satisfy

$$\begin{cases} \partial^2_{xx} k_\lambda - \partial^2_{yy} k_\lambda = \lambda k_\lambda,\ (x,y) \in D, \\ \qquad k_\lambda(x,0) = 0,\ x \in (0,1), \\ \qquad k_\lambda(x,x) = -\dfrac{\lambda}{2} x,\ x \in (0,1). \end{cases} \tag{1.4.12}$$

This is the *kernel problem*. Interestingly, although we started from the boundary control of a parabolic equation of heat type, we end up with a hyperbolic problem of wave type. Note also that the triangle $D = \{(x,y) \in (0,1)^2, y \leq x\}$ can be interpreted as a moving domain if the equation is thought of as a wave equation where x is interpreted as time and the space variable y evolves in $(0,x)$. It turns out that (1.4.12) is well-posed and admits a smooth solution for any $\lambda \in \mathbb{R}$. The solution can even be exlicitly constructed, using a fixed point approach and special functions, see [170, Section 4.3-4.4]. This solves the boundary stabilization problem, provided one can prove well-posedness for the controlled problem (1.4.4) with the boundary feedback $U(u) = \int_0^1 k_\lambda(1,y)u(t,y)\,dy$ where k_λ solves (1.4.12). Note that the non-local boundary condition is not so standard.

We have achieved exponential stabilization of (1.4.4) with decay rate 1. It is easily seen that, considering instead of (1.4.5) a target equation of the form $\partial_t w = \partial^2_{xx} w - \sigma w$, then the exact same reasoning would lead to kernels $k_{\lambda,\sigma}$, $l_{\lambda,\sigma}$ such that (1.4.4) is stabilized with decay rate at least σ, for any $\sigma > 0$. This is called *rapid stabilization*. Note however that the constant in the stability estimates (1.4.11) are expected to be increasing with respect to λ and σ and may become huge, thus limiting in practice the interest of rapid stabilization. It is therefore important to have a good understanding of the behaviour of this constant with respect to λ, σ, and this topic is addressed in the next section.

1.4.3 Quantitative kernel estimates and finite time stabilization

I describe here part of the work published in [92]. The authors are interested in the finite-time stabilization of the heat equation in one dimension with space-varying coefficients and Dirichlet boundary conditions, using the backstepping method described in the previous section. The system to be stabilized is given by

$$\begin{cases} \partial_t u(t,x) = \partial_x(a(x)\partial_x u(t,x)) + c(x)u(t,x),\ x \in (0,1), \\ \quad u(t,0) = 0, \quad u(t,1) = U(t). \end{cases} \tag{1.4.13}$$

They assume that $a \in H^2(0,1)$, $c \in H^1(0,1)$, that a is uniformly elliptic and they prove the following theorem.

Theorem 3 (Theorem 1 of [92]). *Let $T > 0$. There exists a piecewise constant functional $\mathcal{K} : [0,T) \to \left(L^2(0,1)\right)'$ such that, for every $u_0 \in L^2(0,1)$, if $u \in C^0([0,T); L^2(0,1))$ is the solution of (1.4.13) with $U(t)$ defined by*

$$U(t) := \mathcal{K}(t)u(t,\cdot),$$

then

$$\begin{aligned} u(t,\cdot) &\to 0 \text{ in } L^2(0,1) \text{ as } t \to T^-, \\ U(t) &\to 0 \text{ as } t \to T^-. \end{aligned}$$

The operator $\mathcal{K}(t)$ is constructed by backstepping and reads, similarly to (1.4.8), for $v \in L^2(0,1)$,

$$\mathcal{K}(t)v = \int_0^1 k_n(1,y)v(y)\, dy,$$

for $t_n \leq t < t_{n+1}$. The sequence of times $(t_n)_{n\in\mathbb{N}}$ is such that $t_0 = 0$, $t_n \to T^-$ and the sequence of kernels $(k_n)_{n\in\mathbb{N}}$ corresponds to positive damping coefficients $(\lambda_n)_{n\in\mathbb{N}}$ in the sense that, for $n \in \mathbb{N}$, the kernel k_n is defined such that, for any $t_n \leq t < t_{n+1}$, w defined by

$$w(t,x) = u(t,x) - \int_0^1 k_n(x,y)u(t,y)\, dy, \;\; x \in (0,1) \tag{1.4.14}$$

satisfies the target equation

$$\partial_t w(t,x) - \partial_x(a(x)\partial_x w(t,x)) + \lambda_n w(t,x) = 0, \;\; x \in (0,1). \tag{1.4.15}$$

It follows from (1.4.13)-(1.4.14) that w satisfies as well

$$w(t,1) = 0, \text{ and } w(t,0) = 0. \tag{1.4.16}$$

Combining (1.4.15) and (1.4.16), one can derive, for $t_n \leq t < t_{n+1}$,

$$\|w(t,\cdot)\|_{L^2} \leq e^{-\lambda_n(t-t_n)}\|w(t_n^+,\cdot)\|_{L^2}.$$

The kernel problem solved by k_n is given by

$$\begin{cases} \partial_x(a(x)\partial_x k_n(x,y)) - \partial_y(a(y)\partial_y k_n(x,y)) - [\lambda_n + c(y)]k_n(x,y) = 0, \;\; (x,y) \in D, \\ \qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad k_n(x,0) = 0, \;\; x \in (0,1), \\ 2a(x)(\partial_x k_n(x,y) + \partial_y k_n(x,y)) + a'(x)k_n(x,x) + [\lambda_n + c(x)] = 0, \quad x \in (0,1). \end{cases} \tag{1.4.17}$$

Leaving aside the variable coefficients, everything is similar to the reasoning of the previous section except that the authors have chosen to stabilize more and more rapidly the system using time-varying feedbacks (piecewise constant in time). Their analysis is however rather different, because the kernel problem (1.4.17) is not anymore explicitly

solvable and requires a weak approach to address coefficients with low regularity. In doing so, the authors are able to derive the estimates [92, Corollaries 1 and 2]

$$\|k_n\|_{H^1(D)} \leq e^{c\sqrt{\lambda_n}}, \text{ and } \|l_n\|_{H^1(D)} \leq C\lambda_n,$$

where the inverse kernel l_n is related to k_n thanks to (1.4.10) and $C > 0$ is a constant that depends only on the functions a and c. These estimates are crucial to show Theorem 3. Some additional assumptions on the sequences $(t_n)_{\mathbb{N}}$ and $(\lambda_n)_{\mathbb{N}}$ are needed, see [92, Proposition 1]. For example, the sequences $t_n = T - \frac{1}{n^2}$ and $\lambda_n = n^8$ match these assumptions.

1.5 Contributions of the thesis

The original work of this thesis is divided into three chapters. Chapter 2 is taken from the published paper [68], together with Virginie Ehrlacher and Amaury Hayat. Chapter 3 is taken from the submitted work [69] in collaboration with Virginie Ehrlacher, Greta Marino and Jan-Frederik Pietschmann. Chapter 4 is an extended version of the work [59], together with Clément Cancès, Claire Chainais-Hillairet and Virginie Ehrlacher.

1.5.1 Contributions from Chapter 2

In this chapter, we are concerned with the boundary stabilization of system (1.1.3). The main motivation of the authors of [24] for the study of such a system was to control the gaseous fluxes $(F_0, \dots, F_n)$ injected during the deposition process in order to reach target composition profiles. The global existence of weak solutions in the open-loop case (F depends only on time) was shown by adapting the *boundedness-by-entropy method*, presented in Section 1.2.4, to their moving-boundary case. The authors also proved long-time asymptotics of the volume fraction profiles in the case of constant external fluxes. However, the corresponding asymptotic profiles appeared to be stable with only a very poor convergence rate and whether one could use a better flux control F to improve their stability remained an open question that provided the motivation for our work. We refer to Section 2.2 for a complete presentation of their results.

We address the stabilization of the linearized version of (1.1.3) around uniform equilibrium states (precisely defined in Sections 2.2.2, 2.2.3, 2.3.1). The linearized system reads

$$\begin{cases} \partial_t \delta u - A(\overline{u})\partial_{xx}^2 \delta u = 0, & (t,x) \in U_{\overline{e}}, \\ A(\overline{u})\partial_x \delta u(t, \overline{e}(t)) + \overline{v}\delta u(t, \overline{e}(t)) = \delta\psi(t), & t \in \mathbb{R}_+^*, \\ A(\overline{u})\partial_x \delta u(t,0) = 0, & t \in \mathbb{R}_+^*, \\ \delta u(0,x) = \delta u^0(x), & x \in (0, \overline{e}_0), \end{cases} \tag{1.5.1}$$

where $\delta u \in \mathbb{R}^n$ is the state, $\delta\psi \in \mathbb{R}^n$ is the control vector, $\overline{v} > 0$ and $\overline{e}(t) = \overline{e}_0 + \overline{v}t$. Our result is valid under appropriate assumptions on the cross-diffusion matrix A which build on the usual entropy structure conditions to address the nonlinear problem (see

Theorem 1), together with an additional symmetry assumption on the *mobility matrix* (1.2.11) of the system at the state considered. In particular, the size-exclusion cross-diffusion matrix (1.2.6) satisfies these conditions around any such state. We show that we can obtain stabilization in arbitrary small finite time of the linearized system, with a feedback control derived using the backstepping technique inspired from the method described in Section 1.4.3.

Very few works addressed control questions on cross-diffusion systems [182, 220] and our work is, up to my knowledge, the first one to address the feedback stabilization of such systems. Although our result concerns the linearized system (1.5.1), it paves the way to the local stabilization of the nonlinear system (see the perspectives in Section 1.6). From the backstepping perspective, we extend the method described in Section 1.4.3 to a moving-boundary situation. New difficulties arise from the moving-boundary, in particular the backstepping transform (1.4.7) has to depend on time and one has to make sure that this does not jeopardize the exponential stability (resp. the finite time stability). Indeed, when applying the transformation backward to obtain the exponential stability of the original system, the cost of the estimate depends on the norm of the backstepping transform and of the norm of its inverse, which depend themselves on time (see (1.4.11)). If this norm goes to infinity exponentially fast, it could be that the original system is not exponentially stable, let alone finite-time stable, even though the target system is. We nevertheless show that this is not an obstruction to the stabilisation of (1.5.1)

Our contributions can be summarized as follows:

- We show that the entropy structure together with the symmetry assumption on the mobility matrix allow to diagonalize $A(\overline{u})$, reducing the stabilization of (1.5.1) to the stabilization of the scalar problem

$$\begin{cases} \partial_t \zeta_\lambda^\sigma - \sigma \partial_{xx}^2 \zeta_\lambda^\sigma = 0, & (t,x) \in U_{\overline{e}}, \\ \sigma \partial_x \zeta_\lambda^\sigma(t, \overline{e}(t)) + \overline{v} \zeta_\lambda^\sigma(t, \overline{e}(t)) = \delta \psi_\lambda^\sigma(t), & t \in \mathbb{R}_+^*, \\ \sigma \partial_x \zeta_\lambda^\sigma(t, 0) = 0, & t \in \mathbb{R}_+^*. \end{cases} \tag{1.5.2}$$

  The scalar target system is naturally given by

$$\begin{cases} \partial_t g_\lambda^\sigma - \sigma \partial_{xx}^2 g_\lambda^\sigma + \lambda g_\lambda^\sigma = 0, & (t,x) \in U_{\overline{e}}, \\ \sigma \partial_x g_\lambda^\sigma(t, \overline{e}(t)) + \overline{v} g_\lambda^\sigma(t, \overline{e}(t)) = 0, & t \in \mathbb{R}_+^*, \\ \sigma \partial_x g_\lambda^\sigma(t, 0) = 0, & t \in \mathbb{R}_+^*. \end{cases}$$

  This reduction is crucial for us. We comment on the difficulties encountered in the fully coupled case and present the vector-valued kernel problem in the conclusions of Chapter 2.

- We formally derive the time-dependent scalar kernel problem (2.6.9) and we remark that it admits solutions with separate variables that allow to recover the classical kernel problem (1.4.12) set in a moving domain, see (2.6.11). In a sense, this

means that the Volterra backstepping transform is "compatible" with the moving boundary. The scalar feedback law is given by

$$\delta\psi_\lambda^\sigma(t) := \sigma k_\lambda^\sigma(\overline{e}(t),\overline{e}(t))\zeta_\lambda^\sigma(t,\overline{e}(t)) + \int_0^{\overline{e}(t)} \left[\sigma\partial_x k_\lambda(\overline{e}(t),y) + \overline{v}k_\lambda(\overline{e}(t),y)\right]\zeta_\lambda^\sigma(t,y)dy.$$

The well-posedness of the backstepping transformation is then rigorously verified in a L^2 regularity setting in the results of Section 2.4.5.

- We prove well-posedness and quantitative estimates for the scalar kernel problem (see Proposition 3). The estimates read, for any $x \in (0,\overline{e}(t))$,

$$\int_0^x \left(|k_\lambda^\sigma(x,y)|^2 + |\nabla k_\lambda^\sigma(x,y)|^2\right)\, dy \le Ce^{c\overline{e}(t)\sqrt{\lambda/\sigma}}, \tag{1.5.3}$$

$$\int_0^x \left(|l_\lambda^\sigma(x,y)|^2 + |\nabla l_\lambda^\sigma(x,y)|^2\right)\, dy \le C\left(\frac{\lambda}{\sigma}\right)^4 e^{c\overline{e}(t)}.$$

  This allows to conclude to the rapid stabilization of (1.5.2) (Corollary 1) and therefore of the coupled problem (1.5.1) (Theorem 5).

- Finally, we use the estimates (1.5.3)-(1.5.1) to adapt the strategy described in Section 1.4.3 to obtain stabilization in arbitrary finite time (Theorem 6). The key point is that the constant in the stability estimate is of the form $Ce^{c\sqrt{\lambda}}$, which can always be "beaten" by the decay term $e^{-\lambda t}$ when $\lambda \gg 1$.

1.5.2 Contributions from Chapter 3

Before detailing the contributions of this chapter, I need to present the model introduced in [118]. The latter describes the evolution of a multicomponent mixture where cross-diffusion effects between the different species are taken into account, and where only one species does separate from the others. The mixture occupies an open, smooth and bounded domain $\Omega \subset \mathbb{R}^d$ with $d = 1,2,3$ and is composed of $n+1$ species whose volume fractions are denoted by u_i, $i = 0,\dots,n$. Setting $u = (u_0,\dots,u_n)$, the dynamics of the system is governed by the free energy functional

$$E(u) := \int_\Omega \left[\sum_{i=0}^n (u_i \ln u_i - u_i + 1) + \frac{\varepsilon}{2}|\nabla u_0|^2 + \beta u_0(1-u_0)\right] dx, \tag{1.5.4}$$

where ε and β are positive constants. This is a multispecies generalization of the Ginzburg-Landau energy (1.3.5) with logarithmic potential (1.3.10). Denoting by $\mu = \frac{\delta E}{\delta u} \in \mathbb{R}^{n+1}$ the chemical potential, the corresponding evolution system formally reads as

$$\partial_t u = \operatorname{div}\left(M(u)\nabla\mu\right) \quad \text{in } \Omega \times (0,+\infty), \tag{1.5.5}$$

where $M : \mathbb{R}^{n+1} \to \mathbb{R}^{(n+1)\times(n+1)}$ is a degenerate mobility matrix, see (3.1.3) and Section 3.1.2 for a complete presentation of the model. The mobility matrix is in fact

associated to the size exclusion diffusion matrix (1.2.6), already studied in the previous chapter. As expected, due to their interpretation as volume fractions, the quantities u_i must satisfy, for a.e. $x \in \Omega,\ t \in (0, +\infty)$,

$$0 \leq u_i(t,x) \leq 1 \quad \text{for all } i = 0, \dots, n \quad \text{and} \quad \sum_{i=0}^{n} u_i(t,x) = 1. \tag{1.5.6}$$

The evolution system is supplemented with no-flux boundary conditions as well as initial conditions that are consistent with the constraints. The main result from [118] is the existence of a solution to a suitable weak formulation of this problem.

The aim of our work is the study of the multispecies degenerate Ginzburg-Landau energy (1.5.4) and its relation to the system of cross-diffusion Cahn-Hilliard equations (1.5.5). First, we study some solutions to the stationary problem

$$0 = \operatorname{div}(M(u)\nabla\mu) \qquad \text{in } \Omega. \tag{1.5.7}$$

In general, the analysis of this system of coupled, degenerate elliptic equations is by no means straightforward. In this work, motivated by the gradient flow structure of the time-dependent system highlighted above, we focus our study on the set of local minimizers of the energy functional (1.5.4). The latter are natural candidates for solutions to (1.5.7) for one expects that solutions of the time-dependent system should converge in the long time limit to one of these local minimizers. We acknowledge here that other stationary solutions may exist, but stress on the fact that local energy minimizers are of particular physical relevance for the present system. When the parameters are chosen such that the energy functional is strictly convex, the unique minimizer is constant and we show that solutions to the evolution problem (3.1.2) converge to it exponentially fast.
In the non-convex case, the dynamics is much more complex and we study it using a finite volume scheme that preserves the structure of the continuous time-dependent system. The simulations demonstrate the capability of the scheme and allow to explore the dynamics for arbitrary parameter regimes.

More precisely, our work makes the following contributions

- Proving existence and uniform lower and upper bounds for the local minimizers of (1.5.4) in the $L^\infty(\Omega)^{n+1}$ topology. We emphasise that the latter, in contrast to the results of [118], requires a construction which has to preserve not only the constraints but also the mass of the competitor (candidate for lower energy in the contradiction argument), which significantly complicates the argument.

- Gaining regularity of the minimizers from the Euler-Lagrange system, we show that they qualify as classical solutions to the stationary system (1.5.7). We also show that the Euler-Lagrange equation for the void species decouples, revealing a strong link with the single-species energy.

- We study the convexity properties of (1.5.4) and are able to give explicit quantitative bounds. In a particular parameters regime, we show that the minimizers

are constant and that solutions to the dynamical system converge exponentially fast to them, for arbitrary initial data with finite energy. We give explicit rates of convergence.

- We introduce a two-point finite volume scheme that approximates the evolution problem (1.5.5), preserving the constraints (1.5.6). The discrete free energy is shown to be nonincreasing, using the logarithmic chain rule (1.2.26) and adapting the convex-concave splitting of [118] to the discrete case (this is well-known for Cahn-Hilliard approximation, see [130]). We provide numerical simulations to illustrate the behaviour of the scheme and to investigate the variety of stationary solutions in the long-time limit, see Section 3.5.

1.5.3 Contributions from Chapter 4

In this chapter, we propose and study an extension of the model (1.1.3). In the latter, the absorbed fluxes $F(t)$ were assumed to be explicitly known, which is not realistic since the values of these fluxes depend on the interaction between the gaseous and solid phases in the hot chamber. A more realistic model thus necessary has to account for the evolution of the gaseous phase and for how the deposition occurs at the interface between the two phases. We propose a first model in this direction. For the sake of simplicity, we only consider here an isolated system (no incoming fluxes in the hot chamber) in order to mainly focus on the moving-interface coupling.

Let me present the model and refer to Section 4.2 for more details. Let $\Omega = (0,1)$ be the physical domain containing both the solid and gaseous phases. For all $t \geq 0$, let $e(t) \in [0,1]$ denote the position at time t of the interface between the two phases. More precisely, at time t, the solid phase occupies the domain $(0, e(t))$ and the gaseous phase occupies the domain $(e(t), 1)$. We adopt the convention that if $e(t) = 0$ (respectively $e(t) = 1$), then the domain is entirely composed of a gaseous (respectively solid) phase. We denote by $Q := \mathbb{R}_+ \times \Omega$ the time-space domain of the problem.

We consider n different chemical species represented by their densities of molar concentration. More precisely, for all $i \in \{1, \dots, n\}$, $u_i(t,x)$ represents the density of molar concentration of species i at time $t \geq 0$ and point $x \in \Omega$ and we set $u(t,x) := (u_i(t,x))_{i \in \{1,\dots,n\}}$. Volume-filling constraints are satisfied, i.e. for almost all $(t,x) \in Q$, the vector $u(t,x)$ is expected to belong to the set

$$\mathcal{A} := \left\{ (u_1, \dots, u_n) \in \mathbb{R}_+^n, \ \sum_{i=1}^n u_i = 1 \right\}.$$

We assume that initial conditions for the model are given such that, at time $t = 0$,

$$e(0) = e^0 \text{ and } c(0,x) = c^0(x), \tag{1.5.8a}$$

for some $e^0 \in \Omega$ and $c^0 \in L^\infty(\Omega; \mathcal{A})$. Now, for almost all $(t,x) \in Q$ and all $i \in \{1, \dots, n\}$, we denote by $J_i(t,x) \in \mathbb{R}$ the molar flux of species i at time t and point $x \in \Omega$, and set

$J(t,x) := (J_1(t,x), \dots, J_n(t,x))^T$. The local conservation of matter inside the solid and gaseous phase respectively reads as

$$\partial_t c + \partial_x J = 0, \text{ a.e. in } Q. \tag{1.5.8b}$$

Let us also denote by

$$Q_s := \{(t,x) \in Q,\ x \in (0, e(t))\} \quad \text{and} \quad Q_g := \{(t,x) \in Q,\ x \in (e(t), 1)\},$$

the time-space domains associated to the solid and gaseous phases respectively. Cross-diffusion phenomena are modelled by a diffusion matrix-valued mapping $A_s : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ (resp. $A_g : \mathbb{R}^n \to \mathbb{R}^{n\times n}$) in the solid (resp. gaseous) phase, as

$$\begin{aligned} J &= -A_s(c)\partial_x c, \text{ a.e. in } Q_s, \\ J &= -A_g(c)\partial_x c, \text{ a.e. in } Q_g. \end{aligned} \tag{1.5.8c}$$

We require that the diffusion matrix mappings A_s and A_g satisfy some assumptions related to the entropy structure (H) defined in Section 1.2.4 and made precise in Section 4.2.2. On the boundary of the full domain Ω, zero-flux boundary conditions are imposed, i.e.

$$J(t,0) = J(t,1) = 0, \text{ for a.a. } t \geq 0. \tag{1.5.8d}$$

In addition, we assume that J and c are regular enough in order to define their trace on the boundary of Q_s and Q_g respectively. More precisely, for all $t \geq 0$ such that $e(t) \in (0,1)$, we assume that we can define for all $i \in \{1, \dots, n\}$,

$$\begin{aligned} J_i^s(t) &:= J_i(t, e(t)^-),\ J_i^g(t) := J_i(t, e(t)^+), \\ u_i^s(t) &:= u_i(t, e(t)^-),\ u_i^g(t) := u_i(t, e(t)^+), \end{aligned} \tag{1.5.8e}$$

and set $u^s(t) := (u_i^s(t))_{i\in\{1,\dots,n\}}$, $u^g(t) := (u_i^g(t))_{i\in\{1,\dots,n\}}$, $J^s(t) := (J_i^s(t))_{i\in\{1,\dots,n\}}$, $J^g(t) := (J_i^g(t))_{i\in\{1,\dots,n\}}$. To complete the definition of the model, we use a flux vector $F(t) = (F_i(t))_{i\in\{1,\dots,n\}}$ which accounts for phase transition mechanisms located at the vicinity of the moving interface between the solid and gaseous phases. We focus in this work on interface fluxes of Butler-Volmer type. More precisely, we introduce some constant reference chemical potentials $\mu^{*,s} := (\mu_i^{*,s})_{i\in\{1,\dots,n\}}, \mu^{*,g} := (\mu_i^{*,g})_{i\in\{1,\dots,n\}} \in \mathbb{R}^n$ and define the constants

$$\beta_i^* := \exp\left([\![\mu_i^*]\!]\right), \quad [\![\mu_i^*]\!] := \mu_i^{*,g} - \mu_i^{*,s} \quad \forall i \in \{1, \dots, n\}. \tag{1.5.8f}$$

Then, the vector $F(t)$ is defined for all $t \geq 0$ such that $e(t) \in (0,1)$ by

$$F_i(t) = \frac{1}{\sqrt{\beta_i^*}} u_i^g(t) - \sqrt{\beta_i^*} u_i^s(t),\ \forall i \in \{1, \dots, n\}. \tag{1.5.8g}$$

and by $F_i(t) = 0$ for all $i \in \{1, \dots, n\}$ for all $t \geq 0$ such that $e(t) = 0$ or $e(t) = 1$.

Then, the evolution of the location of the interface is defined, just as in (1.1.1), for almost all $t \geq 0$,

$$e'(t) = \sum_{i=1}^{n} F_i(t). \tag{1.5.8h}$$

Notice that, if there exists $t_0 \geq 0$ such that $e(t_0) = 0$ (respectively $e(t_0) = 1$), then $e(t) = 0$ (respectively $e(t) = 1$) for all $t \geq t_0$, and the system boils down to a simple cross-diffusion systems with no-flux boundary conditions on the boundary of the whole domain Ω and diffusion matrix given by A_g (respectively A_s). As long as $e(t) \in (0, 1)$, we impose the following boundary conditions across the moving interface

$$-J^s(t) + e'(t)u^s(t) = -J^g(t) + e'(t)u^g(t) = F(t). \tag{1.5.8i}$$

Our work makes the following contributions:

- We introduce a new moving-interface cross-diffusion system (1.5.8) and highlight its variational entropy structure. The latter implies the thermodynamics consistency of the model and lays the foundations for a rigorous mathematical analysis. The stationary states are identified (Proposition 6) and insights are given concerning the long-time behaviour.
- A finite-volume scheme is introduced to approximate the system. In contrast to the scheme designed in [72], we do not rescale the system to a fixed domain but rather discretize the moving-interface following a moving-mesh approach. Thus the main novelty lies in the numerical treatment of the moving interface
- We prove the existence of at least one discrete solution to the scheme at each time step and that this solution preserves the full structure of the continuous system (Proposition 7). In particular, updating the interface and the mesh preserves the decay of the entropy at the discrete level. The proofs require some more technicalities with respect to the situation of a fixed domain.
- Numerical results illustrate the properties of the model and the good behaviour of the scheme. These results also support conjectures concerning the long-time behaviour.

1.6 Perspectives

I list some research perspectives that are either in the direct continuation of the works presented in the thesis or longer-term objectives.

1.6.1 Short term

- Continuation of Chapter 2: it is natural to study the stabilization of the full nonlinear system (1.1.3). We may first consider the particular affine diffusion matrix (1.2.6). The strategy is to use the backstepping transform previously derived to

stabilize the linearized system. Applying this transformation to the nonlinear system, one recovers the stable linear target system up to some nonlinear residuals. The goal is then to estimate these residuals to show that the target system remains stable under appropriate smallness assumptions on the nonlinearities (leading to a *local* stabilization result). We expect to use intensively the previously derived kernel estimates. Although this strategy is usually successful in the backstepping literature, it is not perfectly clear that it can be direcly adapted to the moving-boundary case.
Another objective is to obtain numerical results that illustrate the stabilization of the linearized and nonlinear systems.

- Continuation of Chapter 3: following the phase-field method presented in Section 1.3.2, an interesting perspective is the formal derivation of a sharp-interface model obtained from (1.5.4)-(1.5.5) in the regime $\beta = \frac{1}{\varepsilon}$ and $\varepsilon \to 0$. First, we may study a Γ-convergence result for the multi-species energy. Then for the evolution system, we may adapt arguments from the asymptotic expansion performed in [57].

- Continuation of Chapter 4: a natural question is to prove the convergence of the finite volume scheme presented here to some weak solution of the model (1.5.8), which would yield in particular the existence of a weak solution to the model (see a definition in Section 4.6). The study of the long-time behaviour of such weak solutions is also on the scientific agenda. In particular, proving the conjecture inspired by the numerical results shown in Section 4.5 that the solutions converge exponentially fast with respect to time to some stationary state of the model is an interesting perspective.

1.6.2 Longer term

- As a prolongation of Chapters 2 and 4, we may consider the coupled model (1.5.8) with non-zero boundary conditions on the right-hand side and study the well-posedness, stabilization and approximation of the resulting system. The model would be more realistic than (1.1.3) to describe deposition because it would take into account the gas dynamics. We expect the stabilization of such a model to be difficult for the relationship between the state and control variables is very non-local.

- A particularly exciting long-term goal is to address higher dimensional models integrating geometric evolution and cross-diffusion, following the variational modelling approach of [205]. We expect that the sharp-interface limit of system (1.5.4)-(1.5.5) may provide an instance of such models.

- During the course of my thesis, I had the opportunity to visit Ansgar Jüngel at TU Vienna and to launch a collaboration. The idea is to study cross-diffusion systems that do not satisfy the normal ellipticity assumption (1.2.3) and thus for which even the local theory of Amann does not apply. Such systems possess a

mixed hyperbolic-parabolic structure which raises new analytical and numerical difficulties [116]. In particular, discontinuous solutions are expected [144, 33] and we are interested in the propagation of these fronts in a multi-species context.

Chapter 2

Boundary stabilization of cross-diffusion systems in a one-dimensional moving-boundary domain

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2.1 Introduction

Cross-diffusion systems naturally arise in diffusion models of multispecies mixtures in a wide variety of applications: tumor growth, population dynamics, materials science etc., see for example Chapter 4 of [155] for an introduction to these systems. Let $n \geq 1$ so that the number of species in the system of interest is $n+1$, $d \in \mathbb{N}^*$ the spatial dimension and $\Omega \subset \mathbb{R}^d$ the bounded spatial domain occupied by the mixture. Such a cross-diffusion system then models the evolution of $u_i(t,x)$ for all $0 \leq i \leq n$, where $u_i(t,x)$ denotes the local concentration or volume fraction of the ith species in the mixture at a time $t > 0$ and point $x \in \Omega$. Setting $\widetilde{u} := (u_0, \cdots, u_n)^T$, a typical cross-diffusion system reads as follows (together with appropriate initial and boundary conditions):

$$\partial_t \widetilde{u} - \mathrm{div}_x \left(\widetilde{A}(\widetilde{u}) \nabla_x \widetilde{u} \right) = 0 \quad \text{for } (t,x) \in \mathbb{R}_+^* \times \Omega, \tag{2.1.1}$$

for some matrix-valued mapping $\widetilde{A} : \mathbb{R}^{n+1} \to \mathbb{R}^{(n+1)\times(n+1)}$. Significant advances in the understanding of the mathematical structure of these systems have been achieved in the last ten years. Indeed, it has been understood in the seminal works [53, 159, 160, 156] that many of these systems have an *entropy structure*, which enables to obtain appropriate estimates in order to prove the existence of weak solutions to systems of the form (2.1.1).

These systems arise in particular in materials science, in order to model atomic diffusion within solids. Indeed, hydrodynamic limits of some stochastic lattice hopping models [210] read as cross-diffusion systems of the form (2.1.1). Our work here is mainly based on the study initiated in [24], where the authors considered a one-dimensional cross-diffusion system defined in a moving boundary domain in order to model a Physical Vapor Deposition process (PVD) used for the fabrication of thin film layers in the photovoltaic industry. The process can be described as follows: a wafer is introduced in a hot chamber where chemical elements are injected under gaseous form. As the latter deposit on the substrate, a heterogeneous solid layer grows upon it. Because of the high temperature conditions, diffusion occurs in the bulk until the wafer is taken out and the system is frozen.

In this model, the solid layer is composed of $n+1$ different chemical species and occupies a domain of the form $(0, e(t)) \subset \mathbb{R}_+$, where $e(t) > 0$ denotes the thickness of the film. For all $0 \leq i \leq n$, let $\phi_i \in L^1_{\mathrm{loc}}(\mathbb{R}_+^*)$ be a non-negative function so that $\phi_i(t)$ represents the flux of atoms of species i absorbed at the surface of the film layer at time t. The evolution of the thickness of the film is determined by the fluxes $(\phi_i)_{0\leq i\leq n}$ and reads as:

$$e(t) = e_0 + \int_0^t \sum_{i=0}^n \phi_i(s) ds, \tag{2.1.2}$$

where $e_0 > 0$ denotes the initial thickness of the film. The local volume fractions of the different species $u_0(t,x), \ldots, u_n(t,x)$ are naturally expected to satisfy the following constraints:

$$u_i(t,x) \geq 0, \ i = 0, \ldots, n, \ \text{and} \ \sum_{j=0}^n u_j(t,x) = 1. \tag{2.1.3}$$

These constraints (2.1.3) allows one to equivalently express u_0 as $1-\sum_{i=1}^n u_i$. As a consequence, the whole system can be equivalently rewritten using the unknown vector $u := (u_1,\dots,u_n)^T$. More precisely, denoting by φ the vector-valued function $(\phi_1,\dots,\phi_n)^T$, the cross-diffusion system in the solid layer reads:

$$\begin{cases} \partial_t u - \partial_x(A(u)\partial_x u) = 0, & \text{for } (t,x) \in \bigcup_{t\in\mathbb{R}_+^*} \{t\}\times(0,e(t)) =: U_e, \\ (A(u)\partial_x u)(t,0) = 0, & \text{for } t\in\mathbb{R}_+^*, \\ (A(u)\partial_x u)(t,e(t)) + e'(t)u(t,e(t)) = \varphi(t), & \text{for } t\in\mathbb{R}_+^*, \\ u(0,x) = u^0(x), & x\in(0,e_0), \end{cases} \tag{2.1.4}$$

for some matrix-valued mapping $A:\mathbb{R}^n\to\mathbb{R}^{n\times n}$ which is called the *diffusion matrix* of the system, and some initial condition $u^0\in L^\infty((0,e_0),\mathcal{D})$ where the set of constraints $\mathcal{D}$ is defined below in (2.2.1). The boundary conditions express that the system is isolated at $x=0$ but that there is an incoming (vector-valued) flux $\varphi(t)$ at $x=e(t)$ where the extra term $e'(t)u(t,e(t))$ accounts for the growth of the layer.

The main motivation of the authors of [24] for the study of such a system was ultimately to be able to control the gaseous fluxes $(\phi_0,\dots,\phi_n)$ injected during the PVD process in order to reach target composition profiles. The global existence of weak solutions to system (2.1.4) was shown by adapting the *boundedness-by-entropy method* [156]. The authors also proved existence of solutions to an optimization problem related to the control of the fluxes and long-time asymptotics of the volume fraction profiles in the case of constant external fluxes (i.e. when the system is in open-loop). However, it is not clear whether the corresponding asymptotic profiles are exponentially stable in open-loop, and whether one could use a better flux control φ to improve their stability remains an open question. The main difficulty lies in the expansion of the domain with time and the coupling between $u(t)$ and $e(t)$. When the domain is fixed, results concerning the exponential convergence to equilibrium of solutions to (2.1.1) were already proven for several diffusion matrices A (see [77, 159, 233, 7]) and in particular recently for the PVD cross-diffusion matrix [147].

This work is concerned with the stabilization of the linearized version of (2.1.4) around uniform equilibrium states (precisely defined in Sections 2.2.2, 2.2.3, 2.3.1), under appropriate assumptions on the cross-diffusion matrix A. These assumptions build on the usual entropy structure conditions stated in [156, 24] to address the nonlinear problem, together with an additional symmetry assumption on the *mobility matrix* of the system at the state considered. In particular, the PVD model in [24] satisfies these conditions around any such state. In this paper, we show that we can obtain finite-time stabilization of the linearized system, with a feedback control derived using the backstepping technique inspired from [92].

First introduced in [55, 167, 225] for finite dimensional systems, the backstepping approach was later used and adapted for PDE in [86, 28, 37, 218, 170]. It consists in transforming the original system, hard to stabilize, into a simpler target system, using an

isomorphism. The main difficulty is then to show the existence of such an isomorphism. The usual backstepping approach for PDE, presented in [170], searches for isomorphisms under the form of a Volterra transform of the second kind (see (2.4.3)), which are conveniently always invertible, among other advantages. Some attempts to introduce a generalized backstepping approach which does not necessarily rely on Volterra transforms have also been introduced in [90, 87, 137, 234, 235, 136, 88]. The Volterra approach has been used in many areas and for many systems in the last decades including parabolic equations (see for instance [21, 92, 123]), hyperbolic system (see for instance [169, 228, 19, 148, 18, 94, 149, 89, 93]), etc. However, no result exists on diffusion system of the form (2.1.4) where the domain extends with time (in a way that is not compensated in the dynamics). The reason is that this situation brings new difficulties, in particular the backstepping transform has to depend on time and one has to make sure that this does not jeopardize the exponential stability (resp. the finite time stability). Indeed, when applying the transformation backward to obtain the exponential stability of the original system, the cost of the estimate depends on the norm of the backstepping transform and of the norm of its inverse, which depends itself on time (see (2.4.18)). If this norm goes to infinity exponentially fast, it could be that the original system is not exponentially stable, let alone finite-time stable, even though the target system is. One can still note [152, 153] where the authors also consider a backstepping approach applied to a parabolic equation in a time-dependent domain. However, their situation is different thanks to their dynamics, and in both cases they do not consider the norm of the inverse of the backstepping transform. Concerning parabolic equations with time-dependent coefficients, one can also note the work by Smyshlyaev and Krstic [219] which considers a heat equation with a time-dependent reactivity and the work by Kerschbaum and Deutscher [165] where the authors consider the exponential stability of a system of parabolic equations with a diagonal diffusion and a time-dependent reactivity. In both cases the difficulty lies in the existence of a time-dependent kernel for the transform and is dealt by converting the kernel equations into an integral equation, using fixed point and successive approximations. We do not use such a method here as we aim for a more generic method that could be applied to more complicated systems and steady-states, and that can allow estimates such as (2.4.22) that are so crucial to reach finite time stabilization.

The outline of the paper is the following: we first recall the main mathematical properties of the moving boundary cross-diffusion system introduced in [24] in Section 2.2 and present the linearized version of this system we focus on in this work. Our main theoretical results are gathered in Section 2.3. The description of the backstepping transformation we consider here is given in Section 2.4. Proofs of our results are gathered in Section 2.5. Additional details and some technical calculations are added in the Appendices.

2.2 Preliminaries

The aim of this section is to recall the main mathematical properties of the system studied in [24] and to introduce the linearized version of this system we focus on in this work. In Section 2.2.1, we recall the assumptions needed on the diffusion matrix A for the associated cross-diffusion system to have an entropy structure and state the additional assumptions required by the stabilization analysis presented in this work. Mathematical properties of system (2.1.2)-(2.1.4) are discussed in Section 2.2.2. Finally, the linearized version of system (2.1.2)-(2.1.4) which we will focus on in this article is introduced in Section 2.2.3.

Notations: Let us first introduce some useful notation. For any continuous non-decreasing positive function $\widetilde{e} : \mathbb{R}_+ \to \mathbb{R}_+^*$ and any $T > 0$, we define the sets $U_{\widetilde{e}} := \cup_{t\in\mathbb{R}_+^*}\{t\} \times (0, \widetilde{e}(t))$ and $U_{\widetilde{e}}^T := \cup_{t\in(0,T)}\{t\} \times (0, \widetilde{e}(t))$, the time-space moving domains we consider in this paper. For any $0 < T \leq +\infty$, any $1 \leq p, q \leq \infty$, any $k \in \mathbb{Z}$, we denote by $\left[L^p((0,T), W^{k,q})\right]_{\tilde{e}}$ the set of measurable functions f from $U_{\tilde{e}}^T$ to $\mathbb{R}$ such that respectively: if $p < \infty$

$$\left(\int_0^T \|f(t)\|^p_{W^{k,q}(0,\tilde{e}(t))} dt\right)^{1/p} < \infty,$$

and if $p = \infty$,

$$\sup_{0\leq t\leq T} \|f(t)\|_{W^{k,q}(0,\tilde{e}(t))} < \infty.$$

These quantities define norms, naturally denoted by $\|\cdot\|_{\left[L^p((0,T),W^{k,q})\right]_{\tilde{e}}}$, which in turn induce a Banach structure. We generalize this notation for functions defined in more general time intervals (t_1, t_2) for $0 \leq t_1 \leq t_2 \leq T$. The sets $\left[L^p_{\text{loc}}((0,T), W^{k,q})\right]_{\tilde{e}}$ are defined similarly. The space $\left[\mathcal{C}^0((0,T), L^p)\right]_{\tilde{e}}$ is defined as the set of functions $f : U_{\widetilde{e}}^T \to \mathbb{R}$ such that the function $(0,T) \times (0,1) \ni (t,x) \mapsto f(t, x\widetilde{e}(t))$ belongs to $\mathcal{C}^0((0,T); L^p(0,1))$.

2.2.1 Entropic structure of the nonlinear system

We detail in this section the assumptions needed on the diffusion matrix A to get existence of a weak solution to the nonlinear cross-diffusion system (2.1.2)-(2.1.4) and introduce some additional notations. These assumptions coincide with the requirements highlighted in [156, 24] for system (2.1.2))-(2.1.4) to have an entropy structure. We refer to [156, 110] for more details about the entropy structure of cross-diffusion systems, and to [82] for a discussion about necessary and sufficient conditions for a cross-diffusion system to admit such a structure.

Let $\mathcal{D} \subset \mathbb{R}^n$ be defined by

$$\mathcal{D} := \left\{(u_1, \cdots, u_n) \in (\mathbb{R}_+^*)^n, \quad \sum_{i=1}^n u_i < 1\right\} \subset (0,1)^n. \tag{2.2.1}$$

Note that a solution u to (2.1.2)-(2.1.4) satisfies the constraints (2.1.3) if and only if $u(t,x) \in \overline{\mathcal{D}}$, for all $t \in \mathbb{R}_+^*$ and all $x \in (0, e(t))$. Note also that, in view of (2.1.3),

the strict inequalities in (2.2.1) imply that the $n+1$ volume fractions are positive. The following set of assumptions on the diffusion matrix A allows guaranteeing that the corresponding cross-diffusion system enjoys a favorable entropy structure.

Assumptions:

(H0) $A \in \mathcal{C}^0(\overline{\mathcal{D}}, \mathbb{R}^{n\times n})$;

(H1) there exists a bounded from below strictly convex function $h \in \mathcal{C}^0(\overline{\mathcal{D}})$ such that $h \in \mathcal{C}^2(\mathcal{D}, \mathbb{R})$, such that its derivative $Dh : \mathcal{D} \to \mathbb{R}^n$ is invertible in $\mathbb{R}^n$ and such that (the symmetric part of) the matrix $D^2h(u)A(u)$ is positive semi-definite for all $u \in \mathcal{D}$;

(H2) moreover, there exists $\alpha > 0$, and for all $1 \leq i \leq n$, there exists $1 \geq m_i > 0$, such that for all $z = (z_1, \cdots, z_n)^T \in \mathbb{R}^n$ and $u = (u_1, \cdots, u_n)^T \in \mathcal{D}$,

$$z^T D^2h(u)A(u)z \geq \alpha \sum_{i=1}^{n} u_i^{2m_i-2} z_i^2.$$

The interested reader may consult [156, 24, 53], let us briefly comment on these assumptions here. A function h such that (H1) and (H2) hold is called an *entropy density* of the cross-diffusion system. The associated *entropy functional* $\mathcal{E}$ is then defined by

$$\mathcal{E} : \left\{ \begin{array}{ccc} L^\infty(\Omega; \overline{\mathcal{D}}) & \longrightarrow & \mathbb{R} \\ u & \longmapsto & \mathcal{E}(u) := \int_\Omega h(u(x))\, dx, \end{array} \right.$$

and for all $u \in L^\infty(\Omega; \overline{\mathcal{D}})$, we identify the differential $D\mathcal{E}(u)$ with its Euclidean gradient in L^2, which is equal to the function $Dh(u)$.

The first equation of system (2.1.4) can then be formally rewritten under the following form:

$$\partial_t u - \operatorname{div}_x \left(M(u)\nabla_x D\mathcal{E}(u)\right) = 0, \qquad \text{for } (t,x) \in U_e = \bigcup_{t\in\mathbb{R}_+^*} \{t\} \times (0, e(t)), \tag{2.2.2}$$

where $M : \mathcal{D} \to \mathbb{R}^{n\times n}$ is the so-called *mobility matrix* of the system and is defined for all $u \in \mathcal{D}$ by

$$M(u) := A(u)(D^2h(u))^{-1}. \tag{2.2.3}$$

From formulation (2.2.2) and under assumption (H1), one can check that $\mathcal{E}$ is a Lyapunov functional of the system, which justifies the term "entropy functional". The fact that Dh is invertible allows one to work with the so-called entropy variables $w := Dh(u)$ and to automatically get a solution $u \in \mathcal{D}$ compatible with the constraints. Finally, under assumption (H2), (the symmetric part of) the mobility matrix $M(u)$ is even positive definite, so that the formulation (2.2.2) is even coercive and one can derive gradient estimates. In physical applications, this entropy structure has a thermodynamic interpretation and in particular the entropy variables w are strongly linked to the notion of chemical potential (see Appendix A in [156]).

Remark 1. *One particular example of diffusion matrix A is studied in [24] for the PVD model used in photovoltaics applications. This diffusion matrix is defined as follows: for all $u := (u_i)_{1\le i\le n} \in \mathbb{R}^n$, $A(u) = (A_{ij}(u))_{1\le i,j\le n} \in \mathbb{R}^{n\times n}$ where*

$$\begin{cases} \forall 1 \le i \le n,\ A_{ii}(u) = \displaystyle\sum_{1\le j\ne i\le n} (K_{ij} - K_{i0})u_j + K_{i0}, \\ \forall 1 \le i \ne j \le n,\ A_{ij}(u) = -(K_{ij} - K_{i0})u_i. \end{cases} \tag{2.2.4}$$

where, for all $0 \le i \ne j \le n$, the positive real numbers K_{ij} satisfy $K_{ij} = K_{ji} > 0$ and represent the cross-diffusion coefficients of atoms of type i with atoms of type j. Note that $A(u)$ is not *a symmetric matrix in general. It is proved in [24] that the diffusion matrix defined by (2.2.4) satisfies assumptions (H0)-(H1)-(H2), with $m_i = \frac{1}{2}$ for all $1 \le i \le n$ and with the function h being defined as the classical Boltzmann entropy density:*

$$h : \begin{cases} \overline{\mathcal{D}} & \longrightarrow & \mathbb{R} \\ u := (u_i)_{1\le i\le n} & \longmapsto & h(u) = \sum\limits_{i=1}^{n} u_i \log u_i + (1-\rho_u)\log(1-\rho_u), \end{cases} \tag{2.2.5}$$

where for all $u = (u_i)_{1\le i\le n} \in \mathbb{R}^n$, $\rho_u := \sum_{i=1}^n u_i$. Furthermore, the mobility matrix associated to (2.2.4) and (2.2.5) is given for $u \in \mathcal{D}$ as $M(u) = (M_{ij}(u))_{1\le i,j\le n}$, where:

$$\begin{cases} \forall 1 \le i \le n,\ M_{ii}(u) = \displaystyle\sum_{1\le j\ne i\le n} K_{ij}u_iu_j + K_{i0}u_i(1-\rho_u), \\ \forall 1 \le i \ne j \le n,\ M_{ij}(u) = -K_{ij}u_iu_j. \end{cases}$$

Note that $M(u)$ is always a symmetric matrix.

2.2.2 Main mathematical properties of the nonlinear model

The aim of this section is to recall the main mathematical properties of the nonlinear model (2.1.2)-(2.1.4) and highlight the open questions on the control and stabilization of this system that are of interest here.

It was proved in [24] that there exists at least one weak solution to system (2.1.2)-(2.1.4) satisfying the constraints (2.1.3) in the following sense:

Theorem 4 (Theorem 2 of [24])**.** *Assume A satisfies assumptions (H0)-(H1)-(H2) and let $h : \overline{\mathcal{D}} \to \mathbb{R}$ be the associated function so that (H1) and (H2) are satisfied. Let us assume that $u^0 \in L^\infty((0,e_0);\mathcal{D})$ satisfies $w^0 := (Dh)(u^0) \in L^\infty((0,e_0);\mathbb{R}^n)$. Let us also assume that $(\phi_0,\cdots,\phi_n) \in L^\infty_{\text{loc}}(\mathbb{R}^*_+;\mathbb{R}^{n+1}_+)$. Then, there exists a weak solution u with initial condition u^0 to (2.1.2)-(2.1.4) such that for almost all $(t,x) \in U_e$, $u(t,x) \in \overline{\mathcal{D}}$, and*

$$u \in \left[L^2_{\text{loc}}(\mathbb{R}^*_+;H^1)^n\right]_e \quad \text{and} \quad \partial_t u \in \left[L^2_{\text{loc}}(\mathbb{R}^*_+;(H^1)')^n\right]_e.$$

In the case when the fluxes $(\phi_i)_{0\le i\le n}$ are constant in time, it is legitimate to wonder if the volume fraction profiles $(u_i)_{0\le i\le n}$ will converge to some constant profiles, and if yes, at which rate. The following result was proved in [24] under the assumption that the entropy density h of the system is given by (2.2.5).

Proposition 1 (Proposition 1 of [24]). *Let us assume that the assumptions of Theorem 4 hold together with the following ones:*

(T1) for all $0 \leq i \leq n$, there exists $\overline{\phi}_i > 0$ so that $\phi_i(t) = \overline{\phi}_i$, for all $t \in \mathbb{R}_+$;

(T2) the entropy density h can be chosen so that for all $u \in \overline{\mathcal{D}}$, $h(u)$ is defined by (2.2.5).

Let us define

$$\overline{v} := \sum_{i=0}^{n} \overline{\phi}_i, \tag{2.2.6}$$

and for all $0 \leq i \leq n$,

$$\overline{u}_i := \frac{\overline{\phi}_i}{\overline{v}} \tag{2.2.7}$$

so that $\overline{u} := (\overline{u}_i)_{1 \leq i \leq n} \in \mathcal{D}$. Then, there exists a constant $C > 0$ such that for almost all $t \geq 0$,

$$\forall 1 \leq i \leq n, \quad \frac{1}{\overline{e}(t)} \|u_i(t,\cdot) - \overline{u}_i\|_{L^1(0,\overline{e}(t))} \leq \frac{C}{\sqrt{t+1}},$$

and

$$\frac{1}{\overline{e}(t)} \left\| \left(1 - \rho_{u(t,\cdot)}\right) - \overline{u}_0 \right\|_{L^1(0,\overline{e}(t))} \leq \frac{C}{\sqrt{t+1}},$$

where $\overline{e}(t)$ is the thickness at time t of the layer, given by

$$\overline{e}(t) = \overline{e}_0 + \int_0^t \sum_{i=0}^{n} \phi_i(s)\, ds = \overline{e}_0 + t\overline{v}, \tag{2.2.8}$$

for some value of the initial thickness of the layer $\overline{e}_0 > 0$.

Let us make a few comments about this result.

- In this specific case, the thickness of the boundary layer $\overline{e}(t)$ grows linearly with constant speed $\overline{v}$.
- Proposition 1 does not state that the quantity $\|u_i(t,\cdot) - \overline{u}_i\|_{L^1(0,\overline{e}(t))}$ goes to 0 as t goes to infinity, it only enables to guarantee the existence of a constant $C > 0$ such that

  $$\forall t > 0, \quad \|u_i(t,\cdot) - \overline{u}_i\|_{L^1(0,\overline{e}(t))} \leq C\sqrt{t}.$$

  Proposition 1 still states that the *rescaled* volume fraction profiles converge to constants in the long-time limit. More precisely, denoting by $v(t,y) := u(t,\overline{e}(t)y)$ for all $t > 0$ and $y \in (0,1)$ and by v_i the ith component of v for $1 \leq i \leq n$, it holds that

  $$\forall 1 \leq i \leq n, \quad \|v_i(t,\cdot) - \overline{u}_i\|_{L^1(0,1)} = \frac{1}{\overline{e}(t)} \|u_i(t,\cdot) - \overline{u}_i\|_{L^1(0,\overline{e}(t))} \leq \frac{C}{\sqrt{t+1}}. \tag{2.2.9}$$

- In the case of constant fluxes $(\overline{\phi}_i)_{0\leq i\leq n}$, i.e. when the thickness of the film at all time $t > 0$ is equal to $\overline{e}(t)$, and when the initial condition u^0 is equal to $\overline{u}$, it can be easily checked that the function u defined by $u(t,x) = \overline{u}$ for all $t > 0$ and $x \in (0, \overline{e}(t))$ is a solution to system (2.1.2)-(2.1.4). Therefore, we use the denomination "target state of (2.1.4)" to refer to a couple $(\overline{u}, \mathbb{R}_+ \ni t \mapsto \overline{e}(t))$.

The preceding remarks provided the main source of motivation for this work about the stabilization of system (2.1.2)-(2.1.4). Assuming that the initial condition u^0 at time $t = 0$ is chosen as a small perturbation of $\overline{u}$, of the form $u^0 = \overline{u} + \delta u^0$, and that the initial thickness of the film e_0 at time $t = 0$ is a small perturbation of the initial thickness $\overline{e}_0$, i.e. $e_0 = \overline{e}_0 + \delta e_0$, does there exist a set of feedback fluxes $(\phi_i)_{0\leq i\leq n}$ such that for a time t large enough, the volume fraction profiles $u(t)$ and thickness of the system $e(t)$ converge to $\overline{u}$ and $\overline{e}(t)$ in a stronger norm than the average L^1 norm used in (2.2.9) ? In other words, can the system be stabilized around the target state $(\overline{u}, \overline{e})$ and at which rate ? Can exponential stability or finite-time stability be achieved, i.e. can the system be stabilized at a rate much better than the one provided by the strategy which would consist in keeping the fluxes ϕ_i constant and equal to $\overline{\phi_i}$ as considered in Proposition 1 ?

This work can be seen as an important first step in this direction. Indeed, we provide answers on the stabilization of a *linearized* version of the system (2.1.2)-(2.1.4). From this result, we expect to be able to obtain the *local* stabilization of the original nonlinear system in a future work.

2.2.3 Linearized system and control variables

The aim of this section is to introduce the linearized system which is the main focus of this paper, together with an appropriate change of control variables that enables to decouple the control analysis of the volume fractions and the thickness of the domain.

Recall that we consider small perturbations $(\delta u^0, \delta e_0)$ at $t = 0$ around the initial condition $\overline{u}$ given by (2.2.7) and initial thickness $\overline{e}_0$. Assuming that the imposed fluxes on the system are of the form $\phi_i(t) = \overline{\phi}_i + \delta\phi_i(t)$ for all $0 \leq i \leq n$ and $t > 0$, we wish to investigate the linearized dynamic of $(\delta u(t,\cdot), \delta e(t))$ which can be seen as first-order corrections of $(u(t,\cdot) - \overline{u}, e(t) - \overline{e}(t))$, where $\overline{e}$ is given by (2.2.8). Recall also the notation (2.2.6) for the growth speed of the layer $\overline{e}$.

Then, the first order correction of the thickness reads, for all $t \geq 0$:

$$\delta e(t) = \int_0^t \sum_{i=0}^n \delta\phi_i(s)ds + \delta e_0, \qquad \text{and} \qquad \delta e'(t) = \sum_{i=0}^n \delta\phi_i(t). \tag{2.2.10}$$

In addition, the first-order corrections of the system (2.1.4) around the target state $(\overline{u}, \overline{e})$ yields the following system, the solution of which is δu, for given δu^0, $\delta\varphi :=$

$(\delta\phi_1, \cdots, \delta\phi_n)^T$ and $\delta\phi_0$:

$$\begin{cases} \partial_t \delta u - A(\overline{u})\partial^2_{xx}\delta u = 0, & \text{for } (t,x) \in U_{\overline{e}}, \\ A(\overline{u})\partial_x \delta u(t,\overline{e}(t)) + \overline{v}\delta u(t,\overline{e}(t)) = \delta\psi(t), & \text{for } t \in \mathbb{R}^*_+, \\ A(\overline{u})\partial_x \delta u(t,0) = 0, & \text{for } t \in \mathbb{R}^*_+, \\ \delta u(0,x) = \delta u^0(x), & \text{for } x \in (0,\overline{e}_0). \end{cases} \tag{2.2.11}$$

where for any $t \geq 0$,

$$\delta\psi(t) := \delta\varphi(t) - \delta e'(t)\overline{u} \in \mathbb{R}^n. \tag{2.2.12}$$

Remark that the solution δu to system (2.2.11) only depends on the n independent control variables denoted by $\delta\psi = (\delta\psi_i)_{1\leq i\leq n}$. Therefore, since we originally had $n+1$ control variables $(\delta\phi_i)_{i\in\{0,..,n\}}$, it remains an extra degree of freedom. This degree of freedom ought to be designed exclusively for the stabilization of the thickness δe. We make this explicit by defining a new control variable as for any $t \geq 0$:

$$\delta\theta(t) := \sum_{i=0}^{n} \delta\phi_i(t), \tag{2.2.13}$$

such that for any $t \geq 0$:

$$\delta e(t) = \int_0^t \delta\theta(s)ds + \delta e_0 \tag{2.2.14}$$

Now we claim that the change of control variables $(\delta\phi_0, \ldots, \delta\phi_n) \to (\delta\theta, \delta\psi_1, \ldots, \delta\psi_n)$, defined according to (2.2.12) and (2.2.13) is invertible. Indeed, it can be checked that for any $t > 0$,

$$\delta\varphi(t) = \delta\psi(t) + \delta\theta(t)\overline{u},$$

and

$$\delta\phi_0(t) = \delta\theta(t) - \sum_{i=1}^{n} \left(\delta\psi_i(t) + \delta\theta(t)\overline{u}_i\right).$$

This new choice of control variables $(\delta\theta, \delta\psi)$ is more convenient for our analysis since we can now completely decouple the control analysis of the thickness and of the volume fractions respectively, as will be made clear in Section 2.5.

2.3 Stabilization of the linearized system: main results

The aim of this section is to present the main results of this work, which focuses on the stabilization of the linearized system (2.2.10)-(2.2.11). In Section 2.3.1, we introduce the precise notions of weak solutions and stability considered here. In Section 2.3.2 are stated our main theoretical results, and we decompose the problem into n *scalar* problems. Finally, in Section 2.4, we detail our backstepping strategy to stabilize the scalar problem.

2.3.1 Main definitions

We first need to specify the notion of solution to system (2.2.11) we will consider here. In the following, we are interested in the stabilization with the spatial L^2 norm, so defining an appropriate notion of weak solution in L^2 for L^2 initial data is needed for our analysis to hold. In our case, anticipating slightly on the next section, the fluxes will be defined as a closed-loop feedback of the form

$$\delta\psi(t) = \Psi(t, \delta u(t)), \tag{2.3.1}$$

where $\delta u(t) = \delta u(t, \cdot)$ is the solution function at time t defined in the space domain $(0, \overline{e}(t))$ and where the mapping Ψ is decomposed into a non-local integral part and a local multiplication operator at $x = \overline{e}(t)$ (recall the expression (2.2.8) of $\overline{e}(t)$). More precisely, the mapping Ψ will be of the following form: for almost all $t \geq 0$ and all $z \in H^1(0, \overline{e}(t))^n$,

$$\Psi(t, z) := H_{nl}(t)z + H_l(t)z, \tag{2.3.2}$$

where the family of operators $(H_{nl}(t))_{t\geq 0}$ and $(H_l(t))_{t\geq 0}$ will be required to satisfy the following properties (in fact, these conditions are necessary to give a meaning to our definition of weak solution, see Definition 3 below):

Properties of operators:

(P1) for almost all $t \geq 0$, $H_{nl}(t)$ is a continuous linear mapping from $L^2(0, \overline{e}(t))^n$ to $\mathbb{R}^n$;

(P2) for all $T > 0$, and all $z \in \left[L^2((0,T), (L^2))^n\right]_{\overline{e}}$, the mapping $(0,T) \ni t \mapsto H_{nl}(t)z(t)$ belongs to $L^2(0,T)^n$. Moreover, there exists a constant $C(T) > 0$ such that

$$\|H_{nl}(\cdot)z(\cdot)\|_{[L^2((0,T),(L^2))^n]_{\overline{e}}} \leq C(T)\|z\|_{[L^2((0,T),(L^2))^n]_{\overline{e}}};$$

(P3) for almost all $t \geq 0$, the operator $H_l(t) : H^1(0, \overline{e}(t))^n \to \mathbb{R}^n$ is defined as follows:

$$\forall z \in H^1(0, \overline{e}(t))^n, \quad H_l(t)z := K_l(t)z(\overline{e}(t)) \tag{2.3.3}$$

where $K_l \in L^\infty_{loc}\left(\mathbb{R}^*_+; \mathbb{R}^{n\times n}\right)$ is a locally bounded matrix-valued mapping.

Using the particular form of fluxes highlighted above, a weak solution can be defined by testing (2.2.11) against regular test functions that satisfy dual boundary conditions (see Definition 3 below and Appendix 2.6.1 for details). We obtain the following definition:

Definition 3 (Weak solution in L^2)**.** *Let $\delta u^0 \in L^2(0, \overline{e}_0)$. Let $(H_{nl}(t))_{t\geq 0}$ and $(H_l(t))_{t\geq 0}$ be two families of operators satisfying (P1)-(P2)-(P3). A function $\delta u \in \left[\mathcal{C}^0(\mathbb{R}_+, L^2)^n\right]_{\overline{e}}$ such that $\partial_t \delta u \in \left[L^2(\mathbb{R}_+; (H^1)')\right]_{\overline{e}}$ is said to be a L^2-weak solution to (2.2.11) with fluxes $\delta\psi$ defined by (2.3.1)-(2.3.2) if, for any $T > 0$, it satisfies:*

$$\int_0^T \int_0^{\overline{e}(t)} \delta u(t,x) \cdot \left[\partial_t v(t,x) + A(\overline{u})^T \partial_{xx}^2 v(t,x)\right] dxdt$$
$$+ \int_0^{\overline{e}_0} \delta u^0(x) \cdot v(0,x)dx + \int_0^T (H_{nl}(t)\delta u(t)) \cdot v(t,\overline{e}(t))dt = 0,$$

for any test function v that satisfies:

- $v \in \left[\left(L^2\left((0,T);H^2\right)\right)^n\right]_{\overline{e}} \cap \left[\mathcal{C}^0([0,T],L^2)^n\right]_{\overline{e}}$,
- $\partial_t v \in \left[\left(L^2\left((0,T);L^2\right)\right)^n\right]_{\overline{e}}$,
- $v(T,\cdot) = 0$,
- $A(\overline{u})^T \partial_x v(t,0) = 0$, *for almost all* $t \in (0,T)$,
- $K_l(t)^T v(t,\overline{e}(t)) - A(\overline{u})^T \partial_x v(t,\overline{e}(t)) = 0$, *for almost all* $t \in (0,T)$.

Remark 2. *One may wonder why the assumption on the time derivative is needed. In fact, we will use this assumption to ensure uniqueness in this class of solutions (see the proof of Corollary 1 based on the backstepping transformation). Nevertheless, it is likely that any L^2 solution to (2.2.11) satisfies this assumption. This would amount to prove a regularity result for (2.2.11) (or equivalently a uniqueness result in the class of L^2 solutions) that we do not provide in this work. (see however Lemma 10 in Appendix 2.6.2 about the homogeneous problem)*

Similarly, the control of the thickness $\delta\theta$ will also be defined as a closed-loop feedback of the form

$$\delta\theta(t) = \Theta(t, \delta e(t)) \tag{2.3.4}$$

where the mapping Θ will be chosen so that $\Theta \in L^1_{\text{loc}}\left(\mathbb{R}_+^*; \mathcal{C}^0(\mathbb{R})\right)$.

Let us now give precise definitions for the different notions of stabilization we consider in the present work. We start with the notion of exponential stabilization:

Definition 4 (Exponential stabilization in L^2)**.** *Let $\mu > 0$. A target state $(\overline{u},\overline{e})$ of (2.1.4) is said to be μ-*exponentially stabilizable *in L^2 if there exist constants $C_{\overline{u},\mu}, C_{\overline{e},\mu} > 0$ such that:*

a) There exist families of operators $(H_{nl}(t))_{t\geq 0}$ and $(H_l(t))_{t\geq 0}$ satisfying properties (P1)-(P2)-(P3), such that, for any perturbation $\delta u^0 \in L^2(0,\overline{e}_0)$, the linearized system (2.2.11) with the fluxes defined by (2.3.1)-(2.3.2) has a unique L^2 weak solution δu in the sense of Definition 3 and this solution satisfies:

$$\|\delta u(t)\|_{L^2(0,\overline{e}(t))} \leq C_{\overline{u},\mu} e^{-\mu t} \|\delta u^0\|_{L^2(0,e_0)}, \text{ for all } t \geq 0.$$

b) There exists a function $\Theta \in L^1_{\text{loc}}\left(\mathbb{R}_+^*; \mathcal{C}^0(\mathbb{R})\right)$ such that, for any perturbation $\delta e_0 \in \mathbb{R}$, δe is well-defined by (2.2.14) with $\delta\theta$ defined by (2.3.4) and satisfies:

$$|\delta e(t)| \leq C_{\overline{e},\mu} e^{-\mu t} |\delta e_0|, \text{ for all } t \geq 0. \tag{2.3.5}$$

Let us also give a definition of *finite time* stabilization:

Definition 5 (Finite time stabilization in L^2)**.** *Let $T > 0$. A target state $(\overline{u}, \overline{e})$ of (2.1.4) is said to be* stabilizable in finite time T *in L^2 if:*

a) There exist families of operators $(H_{nl}(t))_{t\geq 0}$ and $(H_l(t))_{t\geq 0}$ satisfying properties (P1)-(P2)-(P3), such that, for any perturbation $\delta u^0 \in L^2(0, \overline{e}_0)$, the linearized system (2.2.11) with the fluxes defined by (2.3.1)-(2.3.2) has a unique L^2 weak solution δu in the sense of Definition 3 and this solution satisfies:

i) (stability) For any $\epsilon > 0$, there exists $\nu_u > 0$ such that if $\|\delta u^0\|_{L^2(0,\overline{e}_0)} \leq \nu_u$ then for all $t \geq 0$:

$$\|\delta u(t)\|_{L^2(0,\overline{e}(t))} \leq \epsilon.$$

ii) (convergence)

$$\|\delta u(t)\|_{L^2(0,\overline{e}(t))} \to 0 \text{ as } t \to T^-.$$

b) There exists a function $\Theta \in L^1_{\text{loc}}\big((0,T); \mathcal{C}^0(\mathbb{R})\big)$ such that, for any perturbation $\delta e_0 \in \mathbb{R}$, δe is well-defined by (2.2.14) with $\delta\theta$ defined by (2.3.4) and satisfies:

i) (stability) For any $\epsilon > 0$, there exists $\nu_e > 0$ such that if $|\delta e_0| \leq \nu_e$ then for all $t \geq 0$:

$$|\delta e(t)| \leq \epsilon.$$

ii) (convergence)

$$\delta e(t) \to 0 \text{ as } t \to T^-.$$

2.3.2 Main results

Let us summarize our assumptions here. Let $(\overline{u}, \overline{e})$ be a target state of (2.1.4) (in the sense of the discussion in Section 2.2.2) such that:

Assumptions:

(A1) $\overline{u} \in \mathcal{D}$ (which implies that for all $1 \leq i \leq n$, $\overline{u}_i > 0$ and $1 - \rho_{\overline{u}} = 1 - \sum_{i=1}^n \overline{u}_i > 0$);

(A2) The diffusion matrix mapping A satisfies assumptions (H0)-(H1)-(H2). Besides, the mobility matrix mapping M defined by (2.2.3) is such that $M(\overline{u})$ is symmetric.

Let us emphasize here that, in particular, the diffusion matrix A defined by (2.2.4) in Remark 1 satisfies assumption (A2). The additional requirement that $M(\overline{u})$ is symmetric enables to guarantee that the matrix $A(\overline{u})$ is diagonalizable with positive eigenvalues:

Lemma 1. *Assume that $\overline{u}$ satisfies (A1) and that the diffusion matrix A satisfies (A2). Then it holds that $A(\overline{u})$ is diagonalizable with positive eigenvalues.*

Proof. From (2.2.3), it holds that $A(\overline{u}) = M(\overline{u})H(\overline{u})$ with $H(\overline{u}) := D^2h(\overline{u})$. The matrices $M(\overline{u})$ and $H(\overline{u})$ are both symmetric positive definite, which implies that $H(\overline{u})^{1/2}$ is well-defined and

$$A(\overline{u}) = M(\overline{u})H(\overline{u}) = H(\overline{u})^{-1/2}H(\overline{u})^{1/2}M(\overline{u})H(\overline{u})^{1/2}H(\overline{u})^{1/2}.$$

Therefore $A(\overline{u})$ is similar to the symmetric real matrix $H(\overline{u})^{1/2}M(\overline{u})H(\overline{u})^{1/2}$ that is clearly positive definite. Hence the result. □

The result of Lemma 1 enables us to decompose system (2.2.11) into n scalar problems as follows. One can write $A(\overline{u}) = Q^{-1}(\overline{u})\Sigma(\overline{u})Q(\overline{u})$, where the coefficients of the diagonal matrix $\Sigma(\overline{u})$ are the positive eigenvalues $(\sigma_1, \dots, \sigma_n)$ of $A(\overline{u})$. As a consequence, denoting by $z := Q(\overline{u})\delta u$, by z_i the ith component of z for $1 \le i \le n$ and by $z^0 := Q(\overline{u})\delta u^0$, system (2.2.11) boils down to the following set of n uncoupled scalar equations: for all $1 \le i \le n$,

$$\begin{cases} \partial_t z_i - \sigma_i \partial^2_{xx} z_i = 0, & \text{for } (t,x) \in U_{\overline{e}}, \\ \sigma_i \partial_x z_i(t, \overline{e}(t)) + \overline{v} z_i(t, \overline{e}(t)) = \delta\psi^i(t), & \text{for } t \in \mathbb{R}^*_+, \\ \sigma_i(\partial_x z_i)(t, 0) = 0, & \text{for } t \in \mathbb{R}^*_+, \\ z_i(0,x) = z_i^0(x), & \text{for } x \in (0, \overline{e}_0), \end{cases} \tag{2.3.6}$$

where we have introduced the following change of coordinates of the feedback: for all $t \ge 0$, $\delta\psi^i(t) := (Q(\overline{u})\delta\psi(t))_i$. We are now in position to state our main results.

Theorem 5. *Let $\mu > 0$. Let $(\overline{u}, \overline{e})$ be a target state and assume that assumptions (A1)-(A2) are satisfied. Then, $(\overline{u}, \overline{e})$ is μ-exponentially stabilizable in L^2 in the sense of Definition 4. More precisely, let us introduce the following functions and operators:*

- *for any $t \ge 0$ and $w \in \mathbb{R}$, $\Theta(t, w) = -\mu w$;*
- *for any $t \ge 0$, $1 \le i \le n$, $z \in H^1(0, \overline{e}(t))$ and $\lambda > 0$,*

$$H^i_{l,\lambda}(t)z := \sigma_i k^{\sigma_i}_\lambda(\overline{e}(t), \overline{e}(t))z(\overline{e}(t)),$$
$$H^i_{nl,\lambda}(t)z := \int_0^{\overline{e}(t)} \left[\sigma_i \partial_x k^{\sigma_i}_\lambda(\overline{e}(t), y) + \overline{v} k^{\sigma_i}_\lambda(\overline{e}(t), y)\right] z(y)dy,$$

where $k^{\sigma_i}_\lambda$ is the unique solution to (2.4.15) given below with $\sigma = \sigma_i$. We also define for all $t \ge 0$, $\lambda > 0$ and $z := (z_i)_{1 \le i \le n} \in H^1(0, \overline{e}(t))^n$,

$$H_{l,\lambda}(t)z := Q(\overline{u})^{-1}\left(H^i_{l,\lambda}(t)z_i\right)_{1 \le i \le n},$$
$$H_{nl,\lambda}(t)z := Q(\overline{u})^{-1}\left(H^i_{nl,\lambda}(t)z_i\right)_{1 \le i \le n}.$$

Then, there exists $\lambda > 0$ large enough such that $(\Theta, (H_{l,\lambda}(t))_{t \ge 0}, (H_{nl,\lambda}(t))_{t \ge 0})$ satisfy the conditions of Definition 4.

Elaborating on this result, we can even obtain finite time stabilization.

Theorem 6. *Let $(\overline{u}, \overline{e})$ be a target state and assume that assumptions (A1)-(A2) are satisfied. Then, it is stabilizable in any finite time $T > 0$ in L^2 in the sense of Definition 5.*

In Appendix 2.6.4 we show why the common approach which consists in directly using a basic quadratic Lyapunov function would fail to show the exponential stability in this case. This motivates our use of the backstepping approach, described in Section 2.4.

2.4 Backstepping approach

The proof of Theorem 5 and Theorem 6 relies on the use of a backstepping transformation, in conjunction with the fact that system (2.2.11) can be decomposed into n scalar uncoupled problems of the form (2.3.6). Thus, we will need to collect intermediate results on the resulting scalar equations, which is the object of the present section.

From now on, let $\tau_1 \geq 0$ and let us denote by $U_{\overline{e},\tau_1} := \bigcup_{t\in(\tau_1,+\infty)} \{t\} \times (0, \overline{e}(\tau_1))$, where $\overline{e}$ is defined in (2.2.8). Note that $U_{\overline{e},0} = U_{\overline{e}}$. Let us now fix $\sigma, \lambda > 0$ and consider the following auxiliary scalar problem:

$$\begin{cases} \partial_t \zeta_\lambda^\sigma - \sigma \partial_{xx}^2 \zeta_\lambda^\sigma = 0, & \text{for } (t,x) \in U_{\overline{e},\tau_1}, \\ \sigma \partial_x \zeta_\lambda^\sigma(t, \overline{e}(t)) + \overline{v} \zeta_\lambda^\sigma(t, \overline{e}(t)) = \delta\psi_\lambda^\sigma(t), & \text{for } t \in (\tau_1, +\infty), \\ \sigma \partial_x \zeta_\lambda^\sigma(t, 0) = 0, & \text{for } t \in (\tau_1, +\infty), \\ \zeta_\lambda^\sigma(\tau_1, x) = \zeta^{\sigma,\tau_1}(x), & \text{for } x \in (0, \overline{e}(\tau_1)), \end{cases} \tag{2.4.1}$$

for some $\zeta_\lambda^{\sigma,\tau_1} \in L^2(0, \overline{e}(\tau_1))$ and where $\delta\psi_\lambda^\sigma$ will be defined later in (2.4.11). In particular, the solution ζ_λ^σ to (2.4.1) with $\tau_1 = 0$, $\sigma = \sigma_i$, $\delta\psi_\lambda^\sigma = \delta\psi^i$ and $\zeta_\lambda^{\sigma,\tau_1} = z_i^0$ can be identified with z_i the solution to (2.3.6).

2.4.1 Backstepping transformation

In a nutshell, the general idea of backstepping is to map the original problem (2.4.1) to a *target problem* for which exponential or finite-time stability can be proven more easily, and to get the stability result using the reverse transformation. The backstepping approach usually consists in using a "spatially-causal" kernel transformation $\mathcal{T}_\lambda^\sigma$, that reads, for any $(t,x) \in U_{\overline{e},\tau_1}$:

$$g_\lambda^\sigma(t,x) := (\mathcal{T}_\lambda^\sigma \zeta_\lambda^\sigma)(t,x), \tag{2.4.2}$$

where for all $t \geq 0$, all $\xi \in L^2(0, \overline{e}(t))$,

$$(\mathcal{T}_\lambda^\sigma \zeta_\lambda^\sigma)(t,x) = (\mathcal{T}_{\lambda,t}^\sigma \zeta_\lambda^\sigma(t))(x),$$

and $\mathcal{T}_{\lambda,t}^\sigma$ is a Volterra transform of the second kind from $L^2(0, e(t))$ to itself

$$\forall x \in (0, \overline{e}(t)), \quad (\mathcal{T}_{\lambda,t}^\sigma \xi)(x) := \xi(x) - \int_0^x k_\lambda^\sigma(t; x, y) \xi(y) dy, \tag{2.4.3}$$

where k_λ^σ is the solution to the kernel problem (2.4.15) which will be introduced below and is a real-valued function defined in the triangular domain

$$D_t := \left\{(x,y) \in (\mathbb{R}_+)^2, \quad 0 < y \leq x < \overline{e}(t)\right\}. \tag{2.4.4}$$

One of the expected difficulty is that the domain of the problem depends on time and therefore $\mathcal{T}$ and the kernel k_λ^σ *a priori* depend on the time t. However, an interesting feature of our problem, that we comment about below in Section 2.4.4 and Appendix 2.6.3, is that the kernel k_λ^σ actually does not depend on the time t in the sense that it can be chosen as the restriction to D_t of a time-independent function kernel $k_\lambda^{\sigma,\infty}$ defined in a domain

$$D_\infty := \left\{(x,y) \in (\mathbb{R}_+)^2, \quad 0 < y \leq x\right\}, \tag{2.4.5}$$

namely $k_\lambda^\sigma(t) = k_\lambda^{\sigma,\infty}|_{D_t}$ for any $t \geq 0$. Naturally, it holds that for all $0 \leq t \leq t'$, $D_t \subset D_{t'} \subset D_\infty$. To alleviate the notations, in the following we will use a slight abuse of notation and denote $k_\lambda^{\sigma,\infty}$ by k_λ^σ.

Consequently, we have:

$$\forall (t,x) \in U_{\overline{e}}, \quad (\mathcal{T}_\lambda^\sigma w)(t,x) := \left(\mathcal{T}_{\lambda,t}^\sigma w(t)\right)(x) = w(t,x) - \int_0^x k_\lambda^\sigma(x,y) w(t,y) dy,$$

for any $w \in \left[\mathcal{C}^0([0,+\infty), L^2(0,1))\right]_{\overline{e}}$.

The main advantage of the transformation $\mathcal{T}_{\lambda,t}^\sigma$ is that, thanks to the triangular structure, it is always invertible provided that $k_\lambda^\sigma|_{D_t} \in L^2(D_t)$ for all $0 \leq t \leq T$ (see Lemma 2 below). The inverse transformation has then the same form and writes as follows (see Lemma 2): for any $w \in \left[\mathcal{C}^0([0,+\infty), L^2(0,1))\right]_{\overline{e}}$, let us denote by

$$\forall (t,x) \in U_{\overline{e}}, \quad (\mathcal{T}_\lambda^{\sigma,\mathrm{inv}} w)(t,x) := (\mathcal{T}_{\lambda,t}^{\sigma,\mathrm{inv}} w(t))(x) = w(t,x) + \int_0^x l_\lambda^\sigma(x,y) w(t,y) dy.$$

where for all $t \geq 0$ and all $\xi \in L^2(0,\overline{e}(t))$,

$$\forall x \in (0,\overline{e}(t)), \quad \left(\mathcal{T}_{\lambda,t}^{\sigma,\mathrm{inv}} \xi\right)(x) = \xi(x) + \int_0^x l_\lambda^\sigma(x,y)\xi(y) dy, \tag{2.4.6}$$

with l_λ^σ solution to the inverse kernel problem (2.4.16) below. Similarly to k_λ^σ, l_λ^σ is expected to depend on t but can be chosen as the restriction to D_t of a fixed kernel $l_\lambda^{\sigma,\infty}$ defined in D_∞. In the following we use again the same slight abuse of notation and denote $l_\lambda^{\sigma,\infty}$ by l_λ^σ.

We will then see that the following identity holds: for any $t \geq \tau_1$ and $x \in (0,\overline{e}(t))$

$$\zeta_\lambda^\sigma(t,x) = (\mathcal{T}_\lambda^{\sigma,\mathrm{inv}} g_\lambda^\sigma)(t,x) = \left(\mathcal{T}_{\lambda,t}^{\sigma,\mathrm{inv}} g_\lambda^\sigma(t)\right)(x), \tag{2.4.7}$$

Formally, the strategy to identify the set of equations satisfied by k_λ^σ and l_λ^σ is to differentiate (2.4.2) in time in space and to write that ζ_λ^σ and g_λ^σ must satisfy respectively the initial problem (2.4.1) and the target problem (2.4.8) in order to obtain a set of necessary conditions on the kernels k_λ^σ and l_λ^σ (see (2.4.15)-(2.4.16) below).

2.4.2 Target problem

We consider the following target problem:

$$\begin{cases} \partial_t g_\lambda^\sigma - \sigma \partial_{xx}^2 g_\lambda^\sigma + \lambda g_\lambda^\sigma = 0, \text{ for } (t,x) \in U_{\overline{e},\tau_1}, \\ \sigma \partial_x g_\lambda^\sigma(t,\overline{e}(t)) + \overline{v} g_\lambda^\sigma(t,\overline{e}(t)) = 0, \text{ for } t \in (\tau_1, +\infty), \\ \sigma \partial_x g_\lambda^\sigma(t,0) = 0, \text{ for } t \in (\tau_1, +\infty), \\ g_\lambda^\sigma(\tau_1, x) = g_\lambda^{\sigma,\tau_1}(x), \text{ for } x \in (0, \overline{e}(\tau_1)), \end{cases} \tag{2.4.8}$$

that is similar to the original problem (2.4.1) but with homogeneous boundary conditions, an additional *damping term* λg_λ^σ and an initial condition $g_\lambda^{\sigma,\tau_1} \in L^2(0, \overline{e}(\tau_1))$.

We introduce here a notion of weak L^2 solution to (2.4.8). To this aim, we introduce the set D^{targ} of test functions $v : U_{\overline{e},\tau_1} \to \mathbb{R}$ satisfying:

(i) $v \in \left[\left(L^2\left((\tau_1, T); H^2\right)\right)\right]_{\overline{e}} \cap \left[\mathcal{C}^0([\tau_1, T], L^2)\right]_{\overline{e}}$,

(ii) $\partial_t v \in \left[\left(L^2\left((\tau_1, T); L^2\right)\right)\right]_{\overline{e}}$,

(iii) $v(T, \cdot) = 0$,

(iv) $\sigma \partial_x v(t, 0) = 0$, for almost all $t \in (\tau_1, T)$,

(v) $\sigma \partial_x v(t, \overline{e}(t)) = 0$, for almost all $t \in (\tau_1, T)$.

Definition 6. *Let $g_\lambda^{\sigma,\tau_1} \in L^2(0, \overline{e}(\tau_1))$. A function $g_\lambda^\sigma \in \left[\mathcal{C}^0([\tau_1, +\infty), L^2)\right]_{\overline{e}}$ such that $\partial_t g_\lambda^\sigma \in \left[L^2((\tau_1, +\infty); (H^1)')\right]_{\overline{e}}$ is said to be a L^2-weak solution of (2.4.8) if, for any $T > \tau_1$, it satisfies:*

$$\begin{aligned} a^{\text{targ}}(g_\lambda^\sigma, v) := & \int_{\tau_1}^T \int_0^{\overline{e}(t)} g_\lambda^\sigma(t,x) \left[\partial_t v(t,x) + \sigma \partial_{xx}^2 v(t,x) - \lambda v(t,x)\right] dxdt \\ & + \int_0^{\overline{e}(\tau_1)} g_\lambda^{\sigma,\tau_1}(x) v(\tau_1, x) dx = 0, \end{aligned} \tag{2.4.9}$$

for any test function $v \in D^{\text{targ}}$.

Problem (2.4.8) is actually exponentially stable with decay rate λ, that can be chosen arbitrarily large here (see Appendix 2.6.2):

Proposition 2 (Well-posedness and exponential stability of the target equation)**.** *Let $\tau_1 \geq 0$, $\sigma, \lambda > 0$ and $g_\lambda^{\sigma,\tau_1} \in L^2(0, \overline{e}(\tau_1))$. Then, there exists a unique weak L^2 solution $g_\lambda^\sigma \in \mathcal{C}^0([\tau_1, +\infty), L^2(0, \overline{e}(t)))$ to (2.4.8) in the sense of Definition 6, and it holds that, for any $t \geq \tau_1$:*

$$\|g_\lambda^\sigma(t)\|_{L^2(0,\overline{e}(t))} \leq e^{-\lambda(t-\tau_1)} \|g_\lambda^{\sigma,\tau_1}\|_{L^2(0,\overline{e}(\tau_1))}. \tag{2.4.10}$$

2.4.3 Expression of the feedback and weak solution

Let us first explain here how we can derive an expression for the feedback control $\delta\psi_\lambda^\sigma$. Assume for now k_λ^σ and ζ_λ^σ are smooth and differentiate (2.4.2) with respect to x at $x = \overline{e}(t)$. One finds:

$$\partial_x g_\lambda^\sigma(t,\overline{e}(t)) = \partial_x \zeta_\lambda^\sigma(t,\overline{e}(t)) - k_\lambda^\sigma(\overline{e}(t),\overline{e}(t))\zeta_\lambda^\sigma(t,\overline{e}(t)) - \int_0^{\overline{e}(t)} \partial_x k_\lambda^\sigma(\overline{e}(t),y)\zeta_\lambda^\sigma(t,y)dy.$$

Then, combining with (2.4.2) and considering the second equation of (2.4.8), namely $\sigma\partial_x g_\lambda^\sigma(t,\overline{e}(t)) + \overline{v}g_\lambda^\sigma(t,\overline{e}(t)) = 0$ and the boundary condition at $x = \overline{e}(t)$ in (2.4.1), one must impose the following expression of the feedback, which depends on the kernel k_λ^σ: for all $t \geq \tau_1$,

$$\delta\psi_\lambda^\sigma(t) := \sigma k_\lambda^\sigma(\overline{e}(t),\overline{e}(t))\zeta_\lambda^\sigma(t,\overline{e}(t)) + \int_0^{\overline{e}(t)} \left[\sigma\partial_x k_\lambda(\overline{e}(t),y) + \overline{v}k_\lambda(\overline{e}(t),y)\right]\zeta_\lambda^\sigma(t,y)dy. \tag{2.4.11}$$

Let us already remark that this feedback is of the form

$$\delta\psi_\lambda^\sigma(t) = H_{l,\lambda}^\sigma(t)\zeta_\lambda^\sigma(t) + H_{nl,\lambda}^\sigma(t)\zeta_\lambda^\sigma(t), \tag{2.4.12}$$

where, for any $t \geq 0$ and $\xi \in H^1(0,\overline{e}(t))$, the operators are given by

$$\begin{aligned} H_{nl,\lambda}^\sigma(t)\xi &= \int_0^{\overline{e}(t)} \left[\sigma\partial_x k_\lambda^\sigma(\overline{e}(t),y) + \overline{v}k_\lambda^\sigma(\overline{e}(t),y)\right]\xi(y)dy, \\ H_{l,\lambda}^\sigma(t)\xi &= \sigma k_\lambda^\sigma(\overline{e}(t),\overline{e}(t))\xi(\overline{e}(t)). \end{aligned} \tag{2.4.13}$$

Assuming now that the feedback is of the form (2.4.12), we can give a rigorous definition of weak-L^2 solutions to problem (2.4.1) provided that the family of operators $(H_{nl,\lambda}^\sigma(t))_{t\geq 0}$ and $(H_{l,\lambda}^\sigma(t))_{t\geq 0}$ satisfy properties (P1')-(P2')-(P3') below, which are scalar versions of properties (P1)-(P2)-(P3).

Scalar properties of operators:

(P1') for almost all $t \geq 0$, $H_{nl,\lambda}^\sigma(t)$ is a continuous linear mapping from $L^2(0,\overline{e}(t))$ to $\mathbb{R}$;

(P2') for all $T > 0$, and all $z \in \left[L^2((0,T),L^2)\right]_{\overline{e}}$, the mapping $(0,T) \ni t \mapsto H_{nl,\lambda}^\sigma(t)z(t)$ belongs to $L^2(0,T)$. Moreover, there exists a constant $C = C(T,\sigma,\lambda) > 0$ such that

$$\left\|H_{nl,\lambda}^\sigma(\cdot)z(\cdot)\right\|_{[L^2((0,T),L^2)]_{\overline{e}}} \leq C\|z\|_{[L^2((0,T),L^2)]_{\overline{e}}};$$

(P3') for almost all $t \geq 0$, the operator $H_{l,\lambda}^\sigma(t) : H^1(0,\overline{e}(t)) \to \mathbb{R}$ is defined as follows:

$$\forall z \in H^1(0,\overline{e}(t)), \quad H_{l,\lambda}^\sigma(t)z := K_{l,\lambda}^\sigma(t)z(\overline{e}(t))$$

where $K_{l,\lambda}^\sigma \in L_{loc}^\infty\left(\mathbb{R}_+^*\right)$.

We are then in a position to give the definition of weak-L^2 solutions to (2.4.1), by analogy with Definition 3. To this aim, we introduce the set D^{ini} of test functions $w : U_{\overline{e},\tau_1} \to \mathbb{R}$ satisfying:

(i) $w \in \left[\left(L^2\left((\tau_1, T); H^2\right)\right)\right]_{\overline{e}} \cap \left[\mathcal{C}^0([\tau_1, T], L^2)\right]_{\overline{e}}$,

(ii) $\partial_t w \in \left[\left(L^2\left((\tau_1, T); L^2\right)\right)\right]_{\overline{e}}$,

(iii) $w(T, \cdot) = 0$,

(iv) $\sigma \partial_x w(t, 0) = 0$, for almost all $t \in (\tau_1, T)$,

(v) $K_l(t) w(t, \overline{e}(t)) - \sigma \partial_x w(t, \overline{e}(t)) = 0$, for almost all $t \in (\tau_1, T)$.

Definition 7 (Weak solution in L^2 to (2.4.1))**.** *Let $\zeta_\lambda^{\sigma,\tau_1} \in L^2(0, \overline{e}(\tau_1))$. Let $(H_{nl,\lambda}^\sigma(t))_{t\geq 0}$ and $(H_{l,\lambda}^\sigma(t))_{t\geq 0}$ be two families of operators satisfying (P1')-(P2')-(P3'). A function $\zeta_\lambda^\sigma \in \left[\mathcal{C}^0([\tau_1, +\infty), L^2)\right]_{\overline{e}}$ such that $\partial_t \zeta_\lambda^\sigma \in \left[L^2((\tau_1, +\infty); (H^1)')\right]_{\overline{e}}$ is said to be a L^2-weak solution to (2.4.1) with fluxes $\delta\psi_\lambda^\sigma$ defined by (2.4.12) if, for any $T > \tau_1$, it satisfies:*

$$\begin{aligned} a^{\text{ini}}(\zeta_\lambda^\sigma, w) := \int_{\tau_1}^{T} \int_0^{\overline{e}(t)} \zeta_\lambda^\sigma(t,x) \left[\partial_t w(t,x) + \sigma \partial_{xx}^2 w(t,x)\right] dxdt \\ + \int_0^{\overline{e}(\tau_1)} \zeta_\lambda^{\sigma,\tau_1}(x) w(\tau_1, x) dx + \int_{\tau_1}^{T} (H_{nl}(t)\zeta_\lambda^\sigma(t)) w(t, \overline{e}(t)) dt = 0, \end{aligned} \tag{2.4.14}$$

for any test function $w \in D^{\text{ini}}$.

2.4.4 Kernel definition and properties

Now that we have an *a priori* expression for the feedback (2.4.11), it remains to derive the full problems satisfied by the kernels k_λ^σ and l_λ^σ. We consider the following problems (recall the definitions of the triangular domains (2.4.4) and (2.4.5)):

$$\begin{cases} \partial_{xx}^2 k_\lambda^\sigma(x,y) - \partial_{yy}^2 k_\lambda^\sigma(x,y) = \dfrac{\lambda}{\sigma} k_\lambda^\sigma(x,y) & (x,y) \in D_\infty, \\ \partial_y k_\lambda^\sigma(x,0) = 0 & x \in (0, +\infty), \\ k_\lambda^\sigma(x,x) = -\dfrac{\lambda}{2\sigma} x & x \in (0, +\infty), \end{cases} \tag{2.4.15}$$

$$\begin{cases} \partial_{xx}^2 l_\lambda^\sigma(x,y) - \partial_{yy}^2 l_\lambda^\sigma(x,y) = -\dfrac{\lambda}{\sigma} l_\lambda^\sigma(x,y) & (x,y) \in D_\infty, \\ \partial_y l_\lambda^\sigma(x,0) = 0 & x \in (0, \infty), \\ l_\lambda^\sigma(x,x) = -\dfrac{\lambda}{2\sigma} x & x \in (0, \infty), \end{cases} \tag{2.4.16}$$

with the notation $\frac{d}{dx} f(x,x) := \partial_x f(x,x) + \partial_y f(x,x)$. It appears that the two problems are related through

$$k_\lambda^\sigma = -l_{-\lambda}^\sigma. \tag{2.4.17}$$

It is rigorously justified below in Lemmas 3 and 4 that these kernels indeed meet our expectations. Let us however comment here about the derivation of these kernel problems:

- First, the derivation is done in Appendix 2.6.3 assuming that the kernels depend on t. In order to explicit the time dependence, one needs to rescale the kernel, which leads to a dynamical boundary problem set in a fixed domain (see (2.6.9)). Searching for solutions with separate variables, as in (2.6.10), one finds the stationary equations (2.6.11).
- Second, one remarks that any solution to the obtained problem in D_T is in fact a solution to the same problem set in D_t for any $0 \leq t < T$, thanks to the structure of the boundary conditions. Therefore, it suffices to look for a solution in D_∞, hence (2.4.15)-(2.4.16).

Thanks to the structure of the backstepping transformation, we can connect the stability of the two problems: let g_λ^σ be the solution to (2.4.8) in the sense of Proposition 2. Then, assuming that (2.4.16) has a solution, the function ζ_λ^σ defined by (2.4.7) can be shown to be a solution to (2.4.1) (see Lemma 4 below) and it holds that for all $t \geq \tau_1$,

$$\begin{aligned}\|\zeta_\lambda^\sigma(t)\|_{L^2(0,\bar{e}(t))} &\leq \left(1 + \|l_\lambda^\sigma\|_{L^2(D_t)}\right) \|g_\lambda^\sigma(t)\|_{L^2(0,\bar{e}(t))} \\ &\leq \left(1 + \|l_\lambda^\sigma\|_{L^2(D_t)}\right) e^{-\lambda(t-\tau_1)} \|g_\lambda^{\sigma,\tau_1}\|_{L^2(0,\bar{e}(\tau_1))} \\ &\leq \left(1 + \|l_\lambda^\sigma\|_{L^2(D_t)}\right) \left(1 + \|k_\lambda^\sigma\|_{L^2(D_{\tau_1})}\right) e^{-\lambda(t-\tau_1)} \|\zeta^{\sigma,\tau_1}\|_{L^2(0,\bar{e}(\tau_1))}.\end{aligned} \tag{2.4.18}$$

Hence, to get the desired stability, the remaining key point of the analysis is the control of $\|l_\lambda^\sigma\|_{L^2(D_t)}$ with respect to time. For this, we study the following problem, for $\alpha \in \mathbb{R}$,

$$\begin{cases} \partial_{xx}^2 k^\alpha(x,y) - \partial_{yy}^2 k^\alpha(x,y) = \alpha k^\alpha(x,y) & (x,y) \in D_\infty, \\ \partial_y k^\alpha(x,0) = 0 & x \in (0,\infty), \\ k^\alpha(x,x) = -\dfrac{\alpha}{2} x & x \in (0,\infty), \end{cases} \tag{2.4.19}$$

of which (2.4.15) and (2.4.16) are instances. We consider the following definition of weak solution to (2.4.19):

Definition 8. *A function $k^\alpha : D_\infty \to \mathbb{R}$ is said to be a weak solution to (2.4.19) if and only if the two following conditions are satisfied:*

(i) the function $\overline{k}^\alpha : (0,+\infty)^2 \to \mathbb{R}$ defined such that

$$\overline{k}^\alpha(x,y) := \begin{cases} k^\alpha(x,y) & \text{if } (x,y) \in D_\infty := \{0 < y \leq x < \infty\}, \\ -\frac{\alpha}{2} x & \text{otherwise} \end{cases}$$

is such that, for any $L > 0$, the function $\overline{k}_L^\alpha := \overline{k}^\alpha|_{[0,L]^2}$ is such that

$$\begin{aligned} \overline{k}_L^\alpha &\in \mathcal{C}^0([0,L], H^1(0,L)), \\ \partial_x \overline{k}_L^\alpha &\in \mathcal{C}^0([0,L], L^2(0,L)), \\ \partial_{xx} \overline{k}_L^\alpha &\in \mathcal{C}^0([0,L], H^1(0,L)'); \end{aligned}$$

(ii) for all $L > 0$ and for all $v, w \in H^1(0, L)$,

$$
\begin{aligned}
&-\int_0^L \left(\int_0^x \partial_x k^\alpha(x,y)v(y)\,dy\right)\partial_x w(x)\,dx + w(L)\int_0^L \partial_x k^\alpha(L,y)v(y)\,dy \\
&+\int_0^L \int_0^x \partial_y k^\alpha(x,y)\partial_y v(y)\,dy w(x)\,dx \\
&= \alpha \int_0^L \left(\int_0^x k^\alpha(x,y)v(y)\,dy\right) w(x)\,dx \\
&+ \frac{\alpha}{2}\int_0^L v(x)w(x)\,dx.
\end{aligned}
$$

Well-posedness and estimates for (2.4.15) and (2.4.16) are achieved in the following proposition, which is proven in Section 2.5.1.

Proposition 3. *Let $\sigma > 0$. For any $\lambda \geq 0$, there exists a unique weak solution k^σ_λ (resp. l^σ_λ) (in the sense of Definition 8) to the kernel problem (2.4.15) (resp. (2.4.16)). Moreover, there exist $\lambda_\sigma > 0$ and constants $C, c > 0$ independent of σ such that, for any $\lambda \geq \lambda_\sigma$, $t \geq 0$ and $x \in (0, \overline{e}(t))$:*

$$
\int_0^x \left(|k^\sigma_\lambda(x,y)|^2 + |\nabla k^\sigma_\lambda(x,y)|^2\right)\,dy \leq Ce^{c\overline{e}(t)\sqrt{\lambda/\sigma}}, \tag{2.4.20}
$$

$$
\int_0^x \left(|l^\sigma_\lambda(x,y)|^2 + |\nabla l^\sigma_\lambda(x,y)|^2\right)\,dy \leq C\left(\frac{\lambda}{\sigma}\right)^4 e^{c\overline{e}(t)}. \tag{2.4.21}
$$

Remark 3. *An immediate consequence of (2.4.20)-(2.4.21) is that for any $t \geq 0$, $k^\sigma_\lambda|_{D_t} \in H^1(D_t)$, $l^\sigma_\lambda|_{D_t} \in H^1(D_t)$ and*

$$
\|k^\sigma_\lambda\|^2_{H^1(D_t)} \leq Ce^{\widetilde{c}\overline{e}(t)\sqrt{\lambda/\sigma}}, \tag{2.4.22}
$$

$$
\|l^\sigma_\lambda\|^2_{H^1(D_t)} \leq C\left(\frac{\lambda}{\sigma}\right)^2 e^{\widetilde{c}\overline{e}(t)}. \tag{2.4.23}
$$

Remark 4. *It was shown in ([179], Lemma 3.2) that the kernel solutions obtained in Proposition 3 are more regular, namely C^2. The proof is based on an integral reformulation and a series representation formula. We have chosen to adopt a weak framework here since on the one hand, it is an appropriate framework to derive estimates (2.4.22)-(2.4.23) and on the other hand, it shows that our strategy can be extended to equations with space-dependent coefficients [92].*

2.4.5 Main auxiliary results

Next, we check that the kernels defined as solutions to (2.4.15)-(2.4.16) indeed map (2.4.1) to (2.4.8) through the transformation $\mathcal{T}^\sigma_\lambda$ and the other way around. In fact, we

need to check that the formal computations performed for the derivation of the kernel problems can be adapted to the case when we have to consider weak L^2 solutions in the sense of Definitions 3 and 6.

We start by stating in Lemma 2 that for all $\lambda, \sigma > 0$ and $t \geq 0$, the transformation $\mathcal{T}^{\sigma}_{\lambda,t} : L^2(0, \overline{e}(t)) \to L^2(0, \overline{e}(t))$ associated to the unique kernel solution to (2.4.15) is one-to-one, and that it can be inverted from $L^2(0, \overline{e}(t))$ to its image, with inverse given by $\mathcal{T}^{\sigma,\text{inv}}_{\lambda,t}$. The proof of Lemma 2 in the case of Dirichlet boundary conditions is provided in [92] (Lemma 4). We omit the proof here, which is very similar. We also refer to [179] for the invertibility of the transformation with Neumann boundary conditions (Lemma 3.3).

Lemma 2. *Let $\lambda, \sigma > 0$ and $t \geq 0$. Then, $\mathcal{T}^{\sigma,\text{inv}}_{\lambda,t} \circ \mathcal{T}^{\sigma}_{\lambda,t} = \mathcal{T}^{\sigma}_{\lambda,t} \circ \mathcal{T}^{\sigma,\text{inv}}_{\lambda,t} = \text{Id}_{L^2(0,\overline{e}(t))}$.*

Then in Lemma 3, we check that this transformation indeed transforms (2.4.1) into (2.4.8) when the boundary term $\delta\psi^{\sigma}_{\lambda}$ in (2.4.1) is defined in (2.4.12)-(2.4.13).

Lemma 3. *Let $\sigma > 0$, let $\lambda \geq \lambda_\sigma$ where λ_σ is defined in Proposition 3, $\tau_1 \geq 0$ and $\zeta^{\sigma,\tau_1}_{\lambda} \in L^2(0, \overline{e}(\tau_1))$. Let k^{σ}_{λ} be the unique weak solution to (2.4.15) in the sense of Definition 8. Assume that ζ^{σ}_{λ} is a weak-L^2 solution to (2.4.1) in the sense of Definition 7 where $H^{\sigma}_{l,\lambda}$ and $H^{\sigma}_{nl,\lambda}$ are defined by (2.4.13) and $\delta\psi_{\lambda}$ by (2.4.12). For all $t \geq \tau_1$, define $g^{\sigma}_{\lambda}(t) := \mathcal{T}^{\sigma}_{\lambda,t}\zeta^{\sigma}_{\lambda}(t)$ where $\mathcal{T}^{\sigma}_{\lambda,t}$ is defined by (2.4.3). Then g^{σ}_{λ} is the unique weak L^2 solution to (2.4.8) in the sense of Definition 6 with $g^{\sigma,\tau_1}_{\lambda} = \mathcal{T}^{\sigma}_{\lambda,\tau_1}\zeta^{\sigma,\tau_1}_{\lambda}$.*

The objective of Lemma 4 is to state the following point: let g^{σ}_{λ} be the solution to the target problem, then $\zeta^{\sigma}_{\lambda} := \mathcal{T}^{\sigma,\text{inv}}_{\lambda} g^{\sigma}_{\lambda}$ is a solution to the original problem.

Lemma 4. *Let $\sigma > 0$, let $\lambda \geq \lambda_\sigma$ where λ_σ is defined in Proposition 3, $\tau_1 \geq 0$ and $g^{\sigma,\tau_1}_{\lambda} \in L^2(0, \overline{e}(\tau_1))$. Let l^{σ}_{λ} be the unique weak solution to (2.4.16). Let g^{σ}_{λ} be the unique weak-L^2 solution to (2.4.8) in the sense of Proposition 2.*

For all $t \geq \tau_1$, define $\zeta^{\sigma}_{\lambda}(t) := \mathcal{T}^{\sigma,\text{inv}}_{\lambda,t} g^{\sigma}_{\lambda}(t)$ where $\mathcal{T}^{\sigma,\text{inv}}_{\lambda,t}$ is defined in (2.4.6). Then, ζ_{λ} is a weak-L^2 solution to (2.4.1) with $\zeta^{\sigma,\tau_1}_{\lambda} = \mathcal{T}^{\sigma,\text{inv}}_{\lambda,\tau_1} g^{\sigma,\tau_1}_{\lambda}$, $\delta\psi^{\sigma}_{\lambda}$ defined by (2.4.12) and $(H^{\sigma}_{l,\lambda}(t))_{t\geq 0}, (H^{\sigma}_{nl,\lambda}(t))_{t\geq 0}$ defined by (2.4.13).

The proofs of Lemmas 3 and 4 are postponed to Section 2.5.2. Lemma 4 together with Propositions 2 and 3 yield the existence of at least one weak-L^2 solution to (2.4.1) for any $\zeta^{\sigma,\tau_1}_{\lambda} \in L^2(0, \overline{e}(\tau_1))$ provided that $\lambda \geq \lambda_\sigma$, and this solution satisfies the stability estimate (2.4.24). Lemmas 2 and 4 yield uniqueness of this solution. As a consequence, the feedback control (2.4.11) stabilizes (2.4.1) exponentially with an arbitrary decay provided λ is chosen large enough. The object of Corollary 1 is to summarize these points.

Corollary 1. *Let $\sigma > 0$, $\tau_1 \geq 0$, $\lambda \geq \lambda_\sigma$ where λ_σ is defined in Proposition 3 and $\zeta^{\sigma,\tau_1}_{\lambda} \in L^2(0, \overline{e}(\tau_1))$. Then, there exists a unique weak-L^2 solution to problem (2.4.1) in the sense of Definition 7 with $\delta\psi^{\sigma}_{\lambda}$ defined by (2.4.12) and operators $(H^{\sigma}_{nl,\lambda}(t))_{t\geq\tau_1}$ and*

$(H^\sigma_{l,\lambda}(t))_{t\geq\tau_1}$ *defined by* (2.4.13)*. Moreover, there exist constants* $C, c > 0$ *independent of* λ*,* σ *and* t *such that this solution satisfies, for any* $t \geq \tau_1$*:*

$$\|\zeta^\sigma_\lambda(t)\|_{L^2(0,\overline{e}(t))} \leq C\left(1+\left(\frac{\lambda}{\sigma}\right)^2\right) e^{c\overline{e}(\tau_1)\sqrt{\lambda/\sigma}+c\overline{e}(t)-\lambda(t-\tau_1)}\|\zeta^{\sigma,\tau_1}_\lambda\|_{L^2(0,\overline{e}(\tau_1))}. \tag{2.4.24}$$

Proof. Existence and estimate: Let k^σ_λ and l^σ_λ be the kernels defined in Proposition 3. Since $k^\sigma_\lambda|_{D_{\tau_1}} \in L^2(D_{\tau_1})$, one can define $g^{\sigma,\tau_1}_\lambda := \mathcal{T}^\sigma_{\lambda,\tau_1}\zeta^{\sigma,\tau_1}_\lambda \in L^2((0,\overline{e}(\tau_1)))$. Then by Proposition 2, there exists a unique weak-L^2 solution g^σ_λ to (2.4.8) with initial condition $g^{\sigma,\tau_1}_\lambda$, and this solution satisfies (2.4.10). Since, for any $t \geq \tau_1$, $l^\sigma_\lambda|_{D_t} \in L^2(D_t)$, one can define $\zeta^\sigma_\lambda(t) := \mathcal{T}^{\sigma,\mathrm{inv}}_{\lambda,t} g^\sigma_\lambda(t)$ and by Lemma 4, it defines a solution to (2.4.1) associated to operators $(H^\sigma_{nl,\lambda}(t))_{t\geq\tau_1}$ and $(H^\sigma_{l,\lambda}(t))_{t\geq\tau_1}$. Moreover, estimate (2.4.24) follows from the definition of $\mathcal{T}^{\sigma,\mathrm{inv}}_\lambda$ together with the estimates (2.4.10) and (2.4.21):

$$\begin{aligned}
\|\zeta^\sigma_\lambda(t)\|_{L^2(0,\overline{e}(t))} &\leq \left(1+\|l^\sigma_\lambda(t)\|_{L^2(D_t)}\right)\left(1+\|k^\sigma_\lambda(\tau_1)\|_{L^2(D_{\tau_1})}\right) e^{-\lambda(t-\tau_1)}\|\zeta^{\sigma,\tau_1}\|_{L^2(0,\overline{e}(\tau_1))} \\
&\leq \left(1+C\left(\frac{\lambda}{\sigma}\right)^2 e^{c\overline{e}(t)}\right)\left(1+Ce^{c\overline{e}(\tau_1)\sqrt{\lambda/\sigma}}\right) e^{-\lambda(t-\tau_1)}\|\zeta^{\sigma,\tau_1}_\lambda\|_{L^2(0,\overline{e}(\tau_1))} \\
&\leq \tilde{C}\left(1+\left(\frac{\lambda}{\sigma}\right)^2\right) e^{c\overline{e}(\tau_1)\sqrt{\lambda/\sigma}+c\overline{e}(t)-\lambda(t-\tau_1)}\|\zeta^{\sigma,\tau_1}_\lambda\|_{L^2(0,\overline{e}(\tau_1))}
\end{aligned}$$

Uniqueness: take two weak-L^2 solutions to (2.4.1) ζ_1 and ζ_2. Then by Lemma 3, it holds:

$$\mathcal{T}^\sigma_\lambda(\zeta_1-\zeta_2) = 0,$$

but Lemma 2 yields:

$$\zeta_1 = \zeta_2.$$

□

2.5 Proofs

2.5.1 Proof of Proposition 3

We begin by proving a few preliminary lemmas. In the following, the variable x should be interpreted as the time variable of a wave equation.

Lemma 5. *Let* $\alpha \in \mathbb{R}$*,* $L > 0$ *and* $f \in L^2((0,L)^2)$*. Then, there exists a unique solution* $K \in \mathcal{C}^0([0,L], H^1(0,L))$ *such that* $\partial_x K \in \mathcal{C}^0([0,L], L^2(0,L))$ *and* $\partial_{xx}K \in L^2((0,L),(H^1(0,L))')$ *solution to the equation*

$$\begin{cases} \partial_{xx}K(x,y) - \partial_{yy}K(x,y) = \alpha K(x,y) + f(x,y), & \text{for } (x,y)\in(0,L)^2, \\ \partial_y K(x,0) = \partial_y K(x,L) = 0, & \text{for } x\in(0,L), \\ K(0,y) = \partial_x K(0,y) = 0, & \text{for } y\in(0,L), \end{cases} \tag{2.5.1}$$

in the sense that, for all $v \in H^1(0,L)$, for almost all $x \in (0,L)$,

$$\begin{aligned}\langle \partial_{xx}K(x,\cdot), v\rangle_{H^1(0,L)',H^1(0,L)} + \int_0^L \partial_y K(x,y)\partial_y v(y)\,dy \\ = \alpha \int_0^L K(x,y)v(y)\,dy + \int_0^L f(x,y)v(y)\,dy.\end{aligned} \tag{2.5.2}$$

Moreover, there exists a constant $C > 0$ independent of α and L such that for almost any $x \in (0,L)$,

$$\int_0^L \left(|K(x,y)|^2 + |\nabla K(x,y)|^2\right) dy \le (1+L^2)e^{C\max([\alpha]_+^{1/2},1)L}\|f\|^2_{L^2((0,L)^2)}, \tag{2.5.3}$$

where $[\alpha]_+ := \max(\alpha, 0)$ denotes the positive part of α.

Proof. The existence and uniqueness of a solution K to problem (2.5.1) in the sense of (2.5.2) such that $K \in \mathcal{C}^0([0,L], H^1(0,L))$, $\partial_x K \in \mathcal{C}^0([0,L], L^2(0,L))$ and $\partial_{xx}K \in L^2((0,L),(H^1(0,L))')$ is a direct consequence of [49][Theorem 10.14,p.345]. Let us now prove estimate (2.5.3).

Step 1 (smooth f): Let us first assume that f satisfies the additional regularity constraint $\partial_x f \in L^2((0,L)^2)$. Then differentiating the equation with respect to x as in the proof of [124][Theorem 5,p.389], it can be checked that $\partial_{xx}K \in L^\infty((0,L), L^2(0,L))$, $\partial_x K \in L^\infty((0,L), H^1(0,L))$ and $K \in L^\infty((0,L), H^2(0,L))$. In particular, for almost all $x \in (0,L)$, $\partial_{xx}K(x,\cdot) \in L^2(0,L)$, $\partial_x K(x,\cdot) \in H^1(0,L)$ and $K(x,\cdot) \in H^2(0,L)$.

Taking $v = \partial_x K(x,\cdot)$ as a test function in (2.5.2) yields that for almost all $x \in (0,L)$,

$$\begin{aligned}&\langle \partial_{xx}K(x,\cdot), \partial_x K(x,\cdot)\rangle_{H^1(0,L)',H^1(0,L)} + \int_0^L \partial_y K(x,y)\partial_{xy}K(x,y)\,dy \\ &= \alpha \int_0^L K(x,y)\partial_x K(x,y)\,dy + \int_0^L f(x,y)\partial_x K(x,y)\,dy.\end{aligned}$$

This yields, using the Aubin-Lions theorem, that

$$\begin{aligned}\frac{1}{2}\frac{d}{dx}\left(\int_0^L \left(|\partial_x K(x,y)|^2 + |\partial_y K(x,y)|^2\right) dy\right) = \frac{\alpha}{2}\frac{d}{dx}\left(\int_0^L |K(x,y)|^2\,dy\right) \\ + \int_0^L f(x,y)\partial_x K(x,y)\,dy.\end{aligned} \tag{2.5.4}$$

Now, using the fact that $\partial_y K(0,y) = 0$ (since $K(0,y) = 0$ for almost all $y \in (0,L)$) and the fact that $f(x,y)\partial_x K(x,y) \le \frac{1}{2}(f(x,y)^2 + \partial_x K(x,y)^2)$ and integrating (2.5.4) between 0 and x, we obtain that for almost all $x \in (0,L)$:

$$\begin{aligned}\int_0^L \left[|\partial_x K(x,y)|^2 + |\partial_y K(x,y)|^2\right] dy \le \alpha \int_0^L |K(x,y)|^2 dy \\ + \int_0^x \int_0^L \left[|\partial_x K(s,y)|^2 + |\partial_y K(s,y)|^2\right] dy\,ds + \|f\|^2_{L^2((0,L)^2)}.\end{aligned} \tag{2.5.5}$$

Case 1: If $\alpha \leq 0$, an immediate Gronwall argument yields that for almost all $x \in (0, L)$:

$$\int_0^L \left[|\partial_x K(x,y)|^2 + |\partial_y K(x,y)|^2\right] dy \leq e^x \|f\|^2_{L^2((0,L)^2)} \leq e^L \|f\|^2_{L^2((0,L)^2)}. \tag{2.5.6}$$

Case 2: If $\alpha > 0$, we perform a change of variables: let us define, for all $\hat{x} \in (0, \alpha^{1/2}L)$,

$$\hat{K}(\hat{x}, y) = K(\alpha^{-1/2}\hat{x}, y),$$

such that

$$\partial_x \hat{K}(\hat{x}, y) = \alpha^{-1/2}\partial_x K(\alpha^{-1/2}\hat{x}, y).$$

Then for all $\hat{x} \in (0, \alpha^{1/2}L)$, rewrite (2.5.5) with $x = \alpha^{-1/2}\hat{x}$ as

$$\begin{aligned}\int_0^L \left[|\partial_x K(\alpha^{-1/2}\hat{x}, y)|^2 + |\partial_y K(\alpha^{-1/2}\hat{x}, y)|^2\right] dy &\leq \alpha \int_0^L |K(\alpha^{-1/2}\hat{x}, y)|^2 dy \\ &+ \int_0^{\alpha^{-1/2}\hat{x}} \int_0^L \left[|\partial_x K(s,y)|^2 + |\partial_y K(s,y)|^2\right] dy\, ds + \|f\|^2_{L^2((0,L)^2)}.\end{aligned}$$

Performing the change of variable $\hat{s} = \alpha^{1/2}s$ in the double integral on the right-hand side, and dividing everything by α, one gets

$$\begin{aligned}&\int_0^L \left[\left|\partial_x \hat{K}(\hat{x}, y)\right|^2 + \alpha^{-1}\left|\partial_y \hat{K}(\hat{x}, y)\right|^2\right] dy \leq \int_0^L \left|\hat{K}(\hat{x}, y)\right|^2 dy \\ &+ \alpha^{-1/2}\int_0^{\hat{x}} \int_0^L \left[\left|\partial_x \hat{K}(\hat{s}, y)\right|^2 + \alpha^{-1}\left|\partial_y \hat{K}(\hat{s}, y)\right|^2\right] dy\, d\hat{s} + \alpha^{-1}\|f\|^2_{L^2((0,L)^2)}.\end{aligned} \tag{2.5.7}$$

Let us define for almost all $\hat{x} \in (0, \alpha^{1/2}L)$

$$V_1(\hat{x}) = \int_0^L \left[\left|\partial_x \hat{K}(\hat{x}, y)\right|^2 + \alpha^{-1}\left|\partial_y \hat{K}(\hat{x}, y)\right|^2\right] dy \text{ and } V_2(\hat{x}) = \int_0^L \left|\hat{K}(\hat{x}, y)\right|^2 dy.$$

The previous estimate can be equivalently rewritten as: for almost all $\hat{x} \in (0, \alpha^{1/2}L)$

$$V_1(\hat{x}) \leq V_2(\hat{x}) + \alpha^{-1/2}\int_0^{\hat{x}} V_1(s)\, ds + \alpha^{-1}\|f\|^2_{L^2}.$$

Notice also that

$$V_2'(\hat{x}) = 2\int_0^L \partial_x \hat{K}(\hat{x}, y)\hat{K}(\hat{x}, y) dy \leq 2V_1(\hat{x})^{1/2}V_2(\hat{x})^{1/2} \leq V_1(\hat{x}) + V_2(\hat{x}),$$

so that

$$V_1(\hat{x}) + V_2'(\hat{x}) \leq 3V_2(\hat{x}) + 2\alpha^{-1/2}\int_0^{\hat{x}} V_1(s) ds + 2\alpha^{-1}\|f\|^2_{L^2}.$$

We are now in the position to use a Gronwall-type argument. Set $g(\hat{x}) := \int_0^{\hat{x}} V_1(s)\,ds + V_2(\hat{x})$. The previous estimate then reads as: for almost any $\hat{x} \in (0, \alpha^{1/2}L)$

$$g'(\hat{x}) \leq C_\alpha g(\hat{x}) + D_\alpha \|f\|_{L^2}^2.$$

with

$$\begin{aligned} C_\alpha &:= \max(3, 2\alpha^{-1/2}), \\ D_\alpha &:= 2\alpha^{-1}. \end{aligned}$$

Therefore,

$$g(\hat{x}) \leq D_\alpha \|f\|_{L^2}^2 \hat{x} e^{C_\alpha \hat{x}}.$$

Now rewrite (2.5.7) in terms of V_1, V_2: for almost any $\hat{x} \in (0, \alpha^{1/2}L)$

$$\begin{aligned} V_1(\hat{x}) &= \int_0^L \left[\left| \partial_x \hat{K}(\hat{x}, y) \right|^2 + \alpha^{-1} \left| \partial_y K(\hat{x}, y) \right|^2 \right] dy \\ &\leq V_2(\hat{x}) + \alpha^{-1/2} \int_0^{\hat{x}} V_1(s)\,ds + \alpha^{-1} \|f\|_{L^2}^2. \end{aligned}$$

Thus,

$$\begin{aligned} &\alpha^{-1} \int_0^L \left[|\partial_x K(\hat{x}, y)|^2 + |\partial_y K(\hat{x}, y)|^2 \right] dy = V_1(\hat{x}) \\ &\leq \max(1, \alpha^{-1/2}) g(\hat{x}) + \alpha^{-1} \|f\|_{L^2}^2 \\ &\leq \alpha^{-1} \|f\|_{L^2}^2 \left(1 + 2\max(1, \alpha^{-1/2}) \hat{x} e^{C_\alpha \hat{x}} \right) \\ &\leq \alpha^{-1} \|f\|_{L^2}^2 \left(1 + 2\max(\alpha^{1/2}, 1) L e^{\max(3\alpha^{1/2}, 2)L} \right) \\ &\leq \alpha^{-1} \|f\|_{L^2}^2 \left(\left(1 + 2\max(\alpha^{1/2}, 1) L \right) e^{\max(3\alpha^{1/2}, 2)L} \right) \\ &\leq \alpha^{-1} \|f\|_{L^2}^2 e^{3\max(3\alpha^{1/2}, 2)L}. \end{aligned}$$

We thus finally obtain that for almost all $x \in (0, L)$

$$\int_0^L \left[|\partial_x K(x, y)|^2 + |\partial_y K(x, y)|^2 \right] dy \leq \|f\|_{L^2}^2 e^{\max(6\alpha^{1/2}, 4)L}. \tag{2.5.8}$$

Therefore, combining (2.5.6) and (2.5.8) we have proven so far that, for $\alpha \in \mathbb{R}$,

$$\int_0^L \left[|\partial_x K(x, y)|^2 + |\partial_y K(x, y)|^2 \right] dy \leq e^{C \max([\alpha]_+^{1/2}, 1)L} \|f\|_{L^2((0,L)^2)}^2. \tag{2.5.9}$$

Thanks to the null initial conditions ($x = 0$) it holds for almost any $(x, y) \in (0, L)^2$

$$K(x, y) = \int_0^x \partial_x K(z, y) dz \leq \sqrt{L} \sqrt{\int_0^L |\partial_x K(z, y)|^2 dz}$$

Integrate over $y \in (0, L)$ the square of this inequality: for almost any $x \in (0, L)$

$$\int_0^L |K(x,y)|^2 dy \leq L \int_0^L \int_0^L |\partial_x K(z,y)|^2 dydz \leq L^2 e^{C \max([\alpha]_+^{1/2},1)L} \|f\|^2_{L^2((0,L)^2)},$$

where we used (2.5.9) for the last inequality. Hence the result when f is a smooth function.

Step 2 (approximation): Let us now turn to the case when $f \in L^2((0,L)^2)$. Then, there exists a sequence $(f_n)_{n\in\mathbb{N}}$ of functions in $C_c^\infty((0,L)^2)$ such that $\|f_n - f\|_{L^2((0,L)^2)} \xrightarrow{n\to\infty} 0$. Let us denote by K_n the unique solution of (2.5.1) with $f = f_n$ for all $n \in \mathbb{N}$. By standard results on the wave equation (see [124][Theorem 5,p.410]), there exists a constant $C > 0$ independent of n such that for all $n \in \mathbb{N}$

$$\|K_n - K\|_{L^\infty((0,L),H^1(0,L))} + \|\partial_x K_n - \partial_x K\|_{L^\infty((0,L),L^2(0,L))} \leq C\|f_n - f\|_{L^2((0,L))}.$$

Thus, passing to the limit $n \to +\infty$ in the inequality

$$\int_0^L \left(|K_n(x,y)|^2 + |\nabla K_n(x,y)|^2\right) dy \leq (1+L^2) e^{C \max([\alpha]_+^{1/2},1)L} \|f_n\|^2_{L^2((0,L)^2)},$$

which holds for almost all $x \in (0, L)$ yields the desired result.

□

Lemma 6. *In the framework of Lemma 5, assume in addition that in (2.5.1),*

$$\text{Supp } f \subset D_L := \left\{(x,y) \in (0,L)^2,\ 0 < y \leq x < L\right\}.$$

Then it holds that

$$K(x,y) = 0 \text{ a.e in } (0,L)^2 \setminus D_L. \tag{2.5.10}$$

Proof. Consider the restriction of the H^1 energy: for almost any $x \in (0, L)$,

$$E(x) := \frac{1}{2} \int_x^L \left(K^2(x,y) + (\partial_x K)^2(x,y) + (\partial_y K)^2(x,y)\right) dy.$$

Assume first that f is smooth in the sense that $\partial_x f \in L^2((0,L)^2)$.
Then, the function E is absolutely continuous, and it holds that

$$\begin{aligned} E'(x) = &\int_x^L \left[\partial_x K(x,y)K(x,y) + \partial_{xx}K(x,y)\partial_x K(x,y) + \partial_{xy}K\partial_y K(x,y)\right] dy \\ &- \frac{1}{2}\left(K^2(x,x) + (\partial_x K)^2(x,x) + (\partial_y K)^2(x,x)\right). \end{aligned}$$

Integrating by parts the last term yields

$$\int_x^L (\partial_{xy}K(x,y)\partial_y K(x,y))dy = -\int_x^L \partial_x K(x,y)\partial_{yy}K(x,y)\, dy - \partial_x K(x,x)\partial_y K(x,x).$$

Using the fact that K is a solution of (2.5.1), and that Supp $f \subset D_L = \{0 < y \leq x < L\}$, we obtain:

$$\begin{aligned}
E'(x) &= (\alpha+1)\int_x^L \partial_x K(x,y)K(x,y)dy - \frac{1}{2}K^2(x,x) \\
&- \frac{1}{2}\left((\partial_x K)^2(x,x) + (\partial_y K)^2(x,x) + 2\partial_x K(x,x)\partial_y K(x,x)\right) \\
&\leq (\alpha+1)\int_x^L \partial_x K(x,y)K(x,y)dy \\
&= -(\alpha+1)\int_x^L \partial_x K(x,y)\int_y^L \partial_y K(x,s)\,ds\,dy \\
&+ (\alpha+1)K(x,L)\int_x^L \partial_x K(x,y)dy.
\end{aligned}$$

The Cauchy-Schwarz inequality enables to bound the first term by $2|\alpha+1|(L-x)E(x)$ and the second term by $|\alpha+1||K(x,L)|\sqrt{L-x}(2E(x))^{1/2}$. Then, we use the one-dimensional Sobolev inequality on $y \to K(x,y)$ to deal with $K(x,L)$:

$$\begin{aligned}
|K(x,L)| &\leq \sqrt{2}\max\left(\sqrt{L-x}, \frac{1}{\sqrt{L-x}}\right)\left(\int_x^L K(x,y)^2 + (\partial_y K)^2(x,y)dy\right)^{1/2} \\
&\leq 2\max\left(\sqrt{L-x}, \frac{1}{\sqrt{L-x}}\right)E(x)^{1/2}.
\end{aligned}$$

Finally, we obtain that there exists $C > 0$ such that for almost all $x \in (0,L)$,

$$E'(x) \leq C|\alpha+1|\max(1, L-x)E(x),$$

and since $E(0) = 0$ a Gronwall argument yields that $E(x) = 0$ for all $x \in [0,L]$. Hence (2.5.10) holds.

Lastly, reasoning as in Step 2 of the proof of Lemma 5 by a density argument, we can easily check that the result holds true for arbitrary $f \in L^2((0,L)^2)$. □

We are now in position to prove Proposition 3.

Proof of Proposition 3. Let us begin to prove that there exists a unique weak solution k^α to (2.4.19) in the sense of Definition 8, for any $\alpha \in \mathbb{R}$. Let $L > 0$.

Existence: Denote by $K^\alpha(x,y) := k^\alpha(x,y) + \frac{\alpha}{2}x$ for all $(x,y) \in D_L$. Then, it holds that K^α is solution to

$$\begin{cases}
\partial^2_{xx}K^\alpha(x,y) - \partial^2_{yy}K^\alpha(x,y) = \alpha K^\alpha(x,y) - \dfrac{\alpha^2}{2}x & (x,y) \in D_L, \\
\partial_y K^\alpha(x,0) = 0 & x \in (0,L), \\
K^\alpha(x,x) = 0 & x \in (0,L),
\end{cases} \tag{2.5.11}$$

and it is equivalent to solve one problem or the other. Now, using Lemmas 5 and 6, we obtain that the restriction of the unique weak solution $K = \widetilde{K}^\alpha$ to (2.5.1) with $f(x,y) = f^\alpha(x,y) = -\frac{\alpha^2}{2}x\mathbb{1}_{D_L}(x,y)$ to D_L is a solution K^α to (2.5.11). Besides, from Lemma 6, it holds that $K = 0$ in $(0,L)^2 \setminus D_L$. In particular, it holds that K satisfies the weak formulation: for almost all $x \in (0,L)$ and all $v \in H^1(0,L)$,

$$\begin{aligned}&\langle \partial_{xx}K(x,\cdot), v\rangle_{H^1(0,L)',H^1(0,L)} + \int_0^x \partial_y K(x,y)\partial_y v(y)\,dy\\ &= \alpha \int_0^x \left(K(x,y) - \frac{\alpha}{2}x\right) v(y)\,dy.\end{aligned}$$

As a consequence, for all $w \in H^1(0,L)$, it holds that

$$\begin{aligned}&\int_0^L \langle \partial_{xx}K(x,\cdot), v\rangle_{H^1(0,L)',H^1(0,L)} w(x)\,dx + \int_0^L \int_0^x \partial_y K(x,y)\partial_y v(y)\,dy\, w(x)\,dx\\ &= \alpha \int_0^L \left(\int_0^x \left(K(x,y) - \frac{\alpha}{2}x\right) v(y)\,dy\right) w(x)\,dx.\end{aligned} \tag{2.5.12}$$

Using the fact that

$$\begin{aligned}\int_0^L \langle \partial_{xx}K(x,\cdot), v\rangle_{H^1(0,L)',H^1(0,L)} w(x)\,dx &= -\int_0^L \left(\int_0^L \partial_x K(x,y), v(y)\,dy\right) \partial_x w(x)\,dx\\ &\quad + w(L)\int_0^L \partial_x K(L,y)v(y)\,dy\\ &\quad - w(0)\int_0^L \partial_x K(0,y)v(y)\,dy,\end{aligned}$$

together with the fact that

$$\partial_x K(0,y) = 0$$

we obtain that

$$\begin{aligned}\int_0^L \langle \partial_{xx}K(x,\cdot), v\rangle_{H^1(0,L)',H^1(0,L)} w(x)\,dx &= -\int_0^L \left(\int_0^L \partial_x K(x,y)v(y)\,dy\right) \partial_x w(x)\,dx\\ &\quad + w(L)\int_0^L \partial_x K(L,y)v(y)\,dy\\ &= -\int_0^L \left(\int_0^x \partial_x K(x,y)v(y)\,dy\right) \partial_x w(x)\,dx\\ &\quad + w(L)\int_0^L \partial_x K(L,y)v(y)\,dy.\end{aligned}$$

Combining the previous equality with (2.5.12) gives

$$
\begin{aligned}
&-\int_0^L \left(\int_0^x \partial_x K v(y)\,dy\right)\partial_x w(x)\,dx + w(L)\int_0^L \partial_x K^\alpha(L,y)v(y)\,dy\\
&+\int_0^L\int_0^x \partial_y K(x,y)\partial_y v(y)\,dy w(x)\,dx\\
&=\alpha\int_0^L\left(\int_0^x\left(K(x,y)-\frac{\alpha}{2}x\right)v(y)\,dy\right)w(x)\,dx.
\end{aligned}
$$

Finally, since $k^\alpha = K - \frac{\alpha}{2}x$ in D_L, we obtain that k^α is solution to the following weak formulation: for all $v, w \in H^1(0,L)$,

$$
\begin{aligned}
&-\int_0^L \left(\int_0^x \partial_x k^\alpha(x,y)v(y)\,dy\right)\partial_x w(x)\,dx + w(L)\int_0^L \partial_x k^\alpha(L,y)v(y)\,dy\\
&+\int_0^L\int_0^x \partial_y k^\alpha(x,y)\partial_y v(y)\,dy w(x)\,dx\\
&=\alpha\int_0^L\left(\int_0^x k^\alpha(x,y)v(y)\,dy\right)w(x)\,dx\\
&-\frac{\alpha}{2}\int_0^L\left(\int_0^x v(y)\,dy\right)\partial_x w(x)\,dx + \frac{\alpha}{2}w(L)\int_0^L v(y)\,dy\\
&=\alpha\int_0^L\left(\int_0^x k^\alpha(x,y)v(y)\,dy\right)w(x)\,dx\\
&+\frac{\alpha}{2}\int_0^L v(x)w(x)\,dx,
\end{aligned}
$$

where the last equality follows from integration by parts in the x variable. We thus obtain the existence of a weak solution to (2.4.19) in the sense of Definition 8.

Uniqueness: Let us now prove the uniqueness of the solution for this problem. Assume there exist two solutions k_1^α and k_2^α and denote by $\hat{k} := k_1^\alpha - k_2^\alpha$ their difference. Then $\hat{k}$ satisfies the homogeneous equation associated to (2.4.19). Since $\hat{k}$ has null trace on the diagonal $x = y$, it can be extended by 0 to the square $(0,L)^2$. But then one can check that it satisfies the assumptions of Lemma 5 without source term. Hence $\hat{k} = 0$. Uniqueness is proved.

Estimates: Furthermore, Lemma 5 yields the following estimate for almost all $x \in (0,L)$

$$
\int_0^L \left(|\widetilde{K}^\alpha(x,y)|^2 + |\nabla\widetilde{K}^\alpha(x,y)|^2\right)dy \le (1+L^2)e^{C\max([\alpha]_+^{1/2},1)L}\|f^\alpha\|^2_{L^2((0,L)^2)}.
$$

This yields that for almost all $x \in (0,L)$,

$$
\int_0^x \left(|K^\alpha(x,y)|^2 + |\nabla K^\alpha(x,y)|^2\right)dy \le (1+L^2)e^{C\max([\alpha]_+^{1/2},1)L}\|f^\alpha\|^2_{L^2((0,L)^2)},
$$

Since $\|f^\alpha\|^2_{L^2((0,L)^2)} \leq (\alpha L)^4$, and $K^\alpha(x,y) = k^\alpha(x,y) - \frac{\alpha}{2}x$, we obtain that

$$\begin{aligned}
&\int_0^x \left(|k^\alpha(x,y)|^2 + |\nabla k^\alpha(x,y)|^2\right) dy \\
&\leq 2\int_0^x \left(|K^\alpha(x,y)|^2 + |\nabla K^\alpha(x,y)|^2\right) dy + 2\left[\frac{\alpha^2}{12}x^3 + x\frac{\alpha^2}{4}\right] \\
&\leq C_0\left(\alpha^2(L^3+L) + \alpha^4 L^4(1+L^2)e^{C\max([\alpha]_+^{1/2},1)L}\right),
\end{aligned}$$

where $C_0 > 0$ is a constant independent of α and L.

We are now in a position to conclude the proof of Proposition 3. For any $\lambda, \sigma > 0$, we define k^σ_λ a weak solution to (2.4.15) as follows: for all $t \geq 0$, $k^\sigma_\lambda|_{D_t}$ is defined as k^α with $L = \overline{e}(t)$ and $\alpha = \frac{\lambda}{\sigma}$. One can easily check from the previous results that k^σ_λ is thus well-defined and unique and is a weak solution to (2.4.15). l^σ_λ is defined from k^σ_λ according to (2.4.17). To get the desired estimates, it is now sufficient to apply the previously obtained estimates with $L = \overline{e}(t)$ and $\alpha = \frac{\lambda}{\sigma} > 0$ for k^σ_λ and $\alpha = -\frac{\lambda}{\sigma} < 0$ for l^σ_λ. To this aim, we consider $\lambda \geq \lambda_\sigma := \sigma$. Taking into account the fact that $\overline{e}(t) \geq \overline{e}_0$ for all $t \geq 0$ then yields the existence of constants $c, C > 0$ independent of t, λ and σ such that

$$\int_0^x \left(|k^\sigma_\lambda(x,y)|^2 + |\nabla k^\sigma_\lambda(x,y)|^2\right) dy \leq Ce^{c\overline{e}(t)\sqrt{\lambda/\sigma}},$$

and

$$\int_0^x \left(|l^\sigma_\lambda(x,y)|^2 + |\nabla l^\sigma_\lambda(x,y)|^2\right) dy \leq C\left(\frac{\lambda}{\sigma}\right)^4 e^{c\overline{e}(t)}.$$

Hence, (2.4.20) and (2.4.21) hold.

□

2.5.2 Proofs of Lemmas 3 and 4

We begin with the following lemma, from which we will easily deduce Lemmas 3 and 4. The sets D^{targ} and D^{ini} are respectively defined before Definitions 6 and 7.

Lemma 7. *Let σ, λ, τ_1 and some initial conditions $\zeta^{\sigma,\tau_1}_\lambda, g^{\sigma,\tau_1}_\lambda$ be defined as in Lemmas 3 and 4. Assume that some functions $\zeta, g \in \left[L^2(0,T;H^1)\right]_{\overline{e}}$ such that $\partial_t\zeta, \partial_t g \in \left[L^2(0,T;(H^1)')\right]_{\overline{e}}$ are related to each other by the relation: for any $t \geq \tau_1$, $g(t) = \mathcal{T}^\sigma_{\lambda,t}\zeta(t)$ (or, equivalently, from Lemma 2, $\zeta(t) = \mathcal{T}^{\sigma,\text{inv}}_{\lambda,t}g(t)$). Then the following assertions hold:*

i) The linear operator $\mathcal{G} : \left[L^2((0,T),L^2)\right]_{\overline{e}} \to \left[L^2((0,T),L^2)\right]_{\overline{e}}$ defined for any $f \in \left[L^2((0,T),L^2)\right]_{\overline{e}}$ by

$$\mathcal{G}f(t,y) = f(t,y) - \int_y^{\overline{e}(t)} k^\sigma_\lambda(x,y)f(t,x)\,dx, \qquad \text{for a.a. } t \in (0,T),\ x \in (0,\overline{e}(t)), \tag{2.5.13}$$

is invertible from D^{targ} to D^{ini}.

ii) For any test function $v \in D^{\text{targ}}$, it holds

$$a^{\text{targ}}(g, v) = a^{\text{ini}}(\zeta, \mathcal{G}v),$$

where a^{ini} and a^{targ} are given respectively by (2.4.14) and (2.4.9).

iii) As a consequence of i) and ii), for any test function $w \in D^{\text{ini}}$, it holds

$$a^{\text{targ}}(g, \mathcal{G}^{-1}w) = a^{\text{ini}}(\zeta, w).$$

Proof. Let $\lambda, \sigma > 0$. To simplify, we denote in the sequel $k := k_\lambda^\sigma$.

i) Let $v \in D^{\text{targ}}$ and differentiate (2.5.13). It holds for almost any $t \geq 0, y \in (0, \overline{e}(T))$,

$$\partial_y(\mathcal{G}v)(t, y) = \partial_y v(t, y) + k(y, y)v(t, y) - \int_y^{\overline{e}(t)} \partial_y k(x, y)v(t, x)dx$$

The previous equality holds in $\left[L^2(0, T; L^2)\right]_{\overline{e}}$ since

$$v \in \left[L^2(0, T; H^2)\right]_{\overline{e}} \subset \left[L^2(0, T; L^\infty)\right]_{\overline{e}},$$

and the function $(0, \overline{e}(t)) \ni y \mapsto k(y, y)$ belongs to $H^1(0, \overline{e}(t))$. Besides, the quantity $\|\partial_y k(x, \cdot)\|_{L^2(0,x)}$ is bounded uniformly in x for $x \in (0, \overline{e}(t))$. Differentiate once again:

$$\begin{aligned}\partial_{yy}^2(\mathcal{G}v)(t, y) =& \partial_{yy}^2 v(t, y) + \left(\frac{d}{dy}k(y, y)\right) v(t, y) + k(y, y)\partial_y v(t, y) + \partial_y k(y, y)v(t, y) \\ &- \langle \partial_{yy}^2 k(\cdot, y), v(t)\rangle_{(H^1(y,\overline{e}(t)))', H^1(y,\overline{e}(t))}.\end{aligned}$$

All the terms on the right-hand-side belong to $\left[L^2(0, T; L^2)\right]_{\overline{e}}$. Therefore $\mathcal{G}v \in \left[L^2(0, T; H^2)\right]_{\overline{e}}$. It is then clear that

$$\mathcal{G}v \in D^{\text{ini}},$$

since in particular

$$\sigma\partial_y(\mathcal{G}v)(t, \overline{e}(t)) = 0 + \sigma k(\overline{e}(t), \overline{e}(t))v(t, \overline{e}(t)) - 0 = K_l(t)(\mathcal{G}v)(t, e(t)).$$

Therefore the range of $\mathcal{G}$ is a subset of D^{ini}. Besides, $\mathcal{G}$ is invertible in L^2 from classical results on Volterra operators (see Lemma 2). Finally, just as in Lemma 2, it can be easily checked following the same lines that the inverse has a similar form, and that it is defined from D^{ini} with values in D^{targ}.

ii) Let $v \in D^{\text{targ}}$. It holds, denoting by $\phi(t,x) := \int_0^x k(x,y)\zeta(t,y)\,dy$,

$$
\begin{aligned}
a^{\text{targ}}(g,v) &= \int_{\tau_1}^T \left\langle \partial_t v(t) + \sigma\partial_{xx}^2 v(t) - \lambda v(t), g(t)\right\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t)}\,dt \\
&+ \int_0^{\overline{e}(\tau_1)} g(\tau_1,x)v(\tau_1,x)dx \\
&= \int_{\tau_1}^T \left\langle \partial_t v(t) + \sigma\partial_{xx}^2 v(t) - \lambda v(t), \zeta(t)\right\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))}\,dt \qquad (2.5.14)\\
&- \int_{\tau_1}^T \left\langle \partial_t v(t) + \sigma\partial_{xx}^2 v(t) - \lambda v(t), \phi(t)\right\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))}\,dt \\
&+ \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)v(\tau_1,x)dx - \int_0^{\overline{e}(\tau_1)} \left(\int_0^x k(x,y)\zeta(\tau_1,y)dy\right) v(\tau_1,x)dx
\end{aligned}
$$

Let us now look at the term in (2.5.14) involving the function ϕ and perform some integration by parts. Begin with the time derivative: it holds,

$$
\begin{aligned}
&\int_{\tau_1}^T \langle \partial_t v(t), \phi(t)\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))}\,dt \\
&= -\int_{\tau_1}^T \langle \partial_t \phi(t), v(t)\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))}\,dt + \int_0^{\overline{e}(\tau_1)} v(\tau_1,x)\phi(\tau_1,x)\,dx \\
&- \overline{v}\int_{\tau_1}^T \phi(t,\overline{e}(t))v(t,\overline{e}(t)) \\
&= -\int_{\tau_1}^T \int_0^{\overline{e}(t)} \langle \partial_t\zeta(t), k(x,\cdot)\rangle_{H^1(0,x)',H^1(0,x)} v(t,x)dxdt \\
&- \int_0^{\overline{e}(\tau_1)} \left(\int_0^x k(x,y)\zeta(\tau_1,y)dy\right) v(\tau_1,x)dx \\
&- \overline{v}\int_{\tau_1}^T \phi(t,\overline{e}(t))v(t,\overline{e}(t)).
\end{aligned}
$$

Now the space derivative:

$$
\begin{aligned}
&\int_{\tau_1}^T \left\langle \sigma\partial_{xx}^2 v(t), \phi(t)\right\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))}\,dt \\
&= -\int_{\tau_1}^T \int_0^{\overline{e}(t)} \left(k(x,x)\zeta(t,x) + \int_0^x \partial_x k(x,y)\zeta(t,y)dy\right)\sigma\partial_x v(t,x)dxdt \\
&= \sigma\int_{\tau_1}^T \int_0^{\overline{e}(t)} \left[\frac{d}{dx}k(x,x)\zeta(t,x) + k(x,x)\partial_x\zeta(t,x)\right] v(t,x)dxdt \\
&- \int_{\tau_1}^T v(t,\overline{e}(t))\left[\sigma k(\overline{e}(t),\overline{e}(t))\zeta(t,\overline{e}(t))\right]dt \\
&- \sigma\int_{\tau_1}^T \int_0^{\overline{e}(t)} \left(\int_0^x \partial_x k(x,y)\zeta(t,y)dy\right)\partial_x v(t,x)dxdt.
\end{aligned}
$$

Using the weak formulation of k, we obtain that for all $t \geq \tau_1$

$$
\begin{aligned}
&-\sigma \int_0^{\overline{e}(t)} \left(\int_0^x \partial_x k(x,y)\zeta(t,y)dy \right) \partial_x v(t,x)dxdt \\
&= -v(t,\overline{e}(t)) \int_0^{\overline{e}(t)} \sigma \partial_x k(\overline{e}(t),y)\zeta(t,y)\, dy \\
&-\sigma \int_0^{\overline{e}(t)} v(t,x) \left(\int_0^x \partial_y k(x,y)\partial_y \zeta(t,y)\, dy \right) dx \\
&+\lambda \int_0^{\overline{e}(t)} \int_0^x k(x,y)\zeta(t,y)\, dy v(t,x)\, dx \\
&-\frac{\lambda}{2} \int_0^{\overline{e}(t)} \zeta(t,x)\ v(t,x)\, dx.
\end{aligned}
$$

Remember that:

$$
H_{nl}(t)\zeta(t) = \int_0^{\overline{e}(t)} \left[\sigma \partial_x k(\overline{e}(t),y) + \overline{v} k(\overline{e}(t),y) \right] \zeta(t,y)dy,
$$

and now insert the two previous calculations into (2.5.14). It holds that:

$$
\begin{aligned}
a^{\text{targ}}(g,v) &= \int_{\tau_1}^T \left\langle \partial_t v(t) + \sigma \partial_{xx}^2 v(t) - \lambda v(t), \zeta(t) \right\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} \\
&+ \int_{\tau_1}^T H_{nl}(t)\zeta(t)v(t,\overline{e}(t))dt + \int_{\tau_1}^T \int_0^{\overline{e}(t)} \langle \partial_t \zeta(t), k(x,\cdot) \rangle_{(H^1(0,x))', H^1(0,x)} v(t,x)dxdt \\
&- \sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \left[\frac{d}{dx} k(x,x)\zeta(t,x) + k(x,x)\partial_x \zeta(t,x) \right] v(t,x)dxdt \\
&+ \sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \left(\int_0^x \partial_y k(x,y)\partial_y \zeta(t,y)\, dy \right) v(t,x)\, dx\, dt \\
&+ \frac{\lambda}{2} \int_{\tau_1}^T \int_0^{\overline{e}(t)} \zeta(t,x)v(t,x)\, dx \\
&+ \int_{\tau_1}^T v(t,\overline{e}(t))K_l(t)\zeta(t,\overline{e}(t))dt + \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)v(\tau_1,x)dx.
\end{aligned}
$$

Note that we have

$$
\frac{\lambda}{2} \int_0^{\overline{e}(t)} \zeta(t,x)v(t,x)\, dx = -\sigma \int_0^{\overline{e}(t)} \frac{d}{dx} k(x,x)\zeta(t,x)v(t,x)\, dx.
$$

Hence, we obtain that

$$
\begin{aligned}
a^{\mathrm{targ}}(g,v) &= \int_{\tau_1}^{T} \left\langle \partial_t v(t) + \sigma \partial_{xx}^2 v(t), \zeta(t) \right\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} \\
&+ \int_{\tau_1}^{T} H_{nl}(t)\zeta(t)v(t,\overline{e}(t))dt + \int_{\tau_1}^{T}\int_0^{\overline{e}(t)} \langle \partial_t \zeta(t), k(x,\cdot)\rangle_{(H^1(0,x))',H^1(0,x)} v(t,x)dxdt \\
&- \sigma \int_{\tau_1}^{T}\int_0^{\overline{e}(t)} k(x,x)\partial_x \zeta(t,x)v(t,x)dxdt \\
&+ \sigma \int_{\tau_1}^{T}\int_0^{\overline{e}(t)} \left(\int_0^x \partial_y k(x,y)\partial_y \zeta(t,y)\, dy \right) v(t,x)\, dx\, dt \\
&+ \int_{\tau_1}^{T} v(t,\overline{e}(t))K_l(t)\zeta(t,\overline{e}(t))dt + \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)v(\tau_1,x)dx.
\end{aligned}
$$

Let us now denote by $w := \mathcal{G}v$ and by $\psi(t,y) := \int_y^{\overline{e}(t)} k(x,y)v(t,x)\, dx$. It then holds that

$$
\begin{aligned}
a^{\mathrm{ini}}(\zeta,w) &:= \int_{\tau_1}^{T} \left\langle \partial_t w(t) + \sigma \partial_{xx}^2 w(t), \zeta(t) \right\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} dt \\
&+ \int_{\tau_1}^{T} H_{nl}(t)\zeta(t)w(t,\overline{e}(t))dt + \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)w(\tau_1,x)dx \\
&= \int_{\tau_1}^{T} \left\langle \partial_t v(t) + \sigma \partial_{xx}^2 v(t), \zeta(t) \right\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} dt \\
&+ \int_{\tau_1}^{T} H_{nl}(t)\zeta(t)v(t,\overline{e}(t))dt + \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)v(\tau_1,x)dx \\
&- \int_{\tau_1}^{T} \left\langle \partial_t \psi(t) + \sigma \partial_{xx}^2 \psi(t), \zeta(t) \right\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} dt - \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,x)\psi(\tau_1,x)dx
\end{aligned}
$$

Doing similar computations as above, we obtain that

$$
\begin{aligned}
&\int_{\tau_1}^{T} \langle \partial_t \psi(t), \zeta(t)\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} = -\int_{\tau_1}^{T} \langle \partial_t \zeta(t), \psi(t)\rangle_{H^1(0,\overline{e}(t))', H^1(0,\overline{e}(t))} \\
&- \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,y)\psi(\tau_1,y)\, dy - \overline{v} \int_{\tau_1}^{T} \zeta(t,\overline{e}(t))\psi(t,\overline{e}(t))\, dt \\
&= -\int_{\tau_1}^{T}\int_0^{\overline{e}(t)} \langle \partial_t \zeta(t), k(x,\cdot)\rangle_{(H^1(0,x))',H^1(0,x)} v(t,x)dxdt \\
&- \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,y)\psi(\tau_1,y)\, dy - \overline{v} \int_{\tau_1}^{T} \zeta(t,\overline{e}(t))\psi(t,\overline{e}(t))\, dt \\
&= -\int_{\tau_1}^{T}\int_0^{\overline{e}(t)} \langle \partial_t \zeta(t), k(x,\cdot)\rangle_{(H^1(0,x))',H^1(0,x)} v(t,x)dxdt \\
&- \int_0^{\overline{e}(\tau_1)} \zeta(\tau_1,y)\psi(\tau_1,y)\, dy.
\end{aligned}
$$

Moreover, since $\partial_y \psi(t,y) = k(y,y)v(t,y) - \int_y^{\overline{e}(t)} \partial_y k(x,y)v(t,x)\,dx$, we have

$$\begin{aligned}
&\int_{\tau_1}^T \langle \sigma \partial_{xx}\psi(t), \zeta(t)\rangle_{H^1(0,\overline{e}(t))',H^1(0,\overline{e}(t))} \\
&= -\sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \partial_y \zeta(t,y)\partial_y \psi(t,y)\,dy + \sigma \int_{\tau_1}^T \zeta(t,\overline{e}(t))k(\overline{e}(t),\overline{e}(t))v(t,\overline{e}(t)) \\
&= -\sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \partial_y \zeta(t,y)k(y,y)v(t,y)\,dy + \sigma \int_{\tau_1}^T \zeta(t,\overline{e}(t))k(\overline{e}(t),\overline{e}(t))v(t,\overline{e}(t)) \\
&+ \sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \partial_y \zeta(t,y) \left(\int_y^{\overline{e}(t)} \partial_y k(x,y)v(t,x)\,dx \right) dy \\
&= -\sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} \partial_y \zeta(t,y)k(y,y)v(t,y)\,dy + \int_{\tau_1}^T K_l(t)\zeta(t)v(t,\overline{e}(t)) \\
&+ \sigma \int_{\tau_1}^T \int_0^{\overline{e}(t)} v(t,x) \left(\int_0^x \partial_y \zeta(t,y)\partial_y k(x,y)\,dy \right) dx.
\end{aligned}$$

As a consequence, we obtain that

$$a^{\mathrm{targ}}(g,v) = a^{\mathrm{ini}}(\zeta,w).$$

Hence the desired result.

iii) The proof of (iii) is a direct consequence of (i) and (ii).

□

Now we provide the proofs of Lemmas 3 and 4.

Proof of Lemma 3 and 4. Let ζ_λ^σ be a weak-L^2 solution to (2.4.1) in the sense of Definition 7. Define now, for all $t \geq \tau_1$, $x \in (0,\overline{e}(t))$,

$$g_\lambda^\sigma(t,x) := \mathcal{T}_{\lambda,t}^\sigma \zeta_\lambda^\sigma(t,x) = \zeta_\lambda^\sigma(t,x) - \int_0^x k_\lambda^\sigma(x,y)\zeta_\lambda^\sigma(t,y)\,dy.$$

Continuity and initial data: $\zeta_\lambda^\sigma \in \left[\mathcal{C}^0([\tau_1,T];L^2)\right]_{\overline{e}}$ by assumption and the Cauchy-Schwarz inequality provides the following estimate, for any $\tau_1 \leq s,t \leq T$,

$$\left\| \int_0^x k_\lambda^\sigma(x,y)\left(\zeta_\lambda^\sigma(t,y) - \zeta_\lambda^\sigma(s,y)\right)dy \right\|_{L^2(0,\overline{e}(T))} \leq \|k_\lambda^\sigma\|_{L^2(D_T)} \|\zeta_\lambda^\sigma(t) - \zeta_\lambda^\sigma(s)\|_{L^2((0,\overline{e}(T)))},$$

which goes to 0 by assumption as t goes to s. Therefore $g_\lambda^\sigma \in \left[\mathcal{C}^0([\tau_1,T],L^2)\right]_{\overline{e}}$ as well. The initial data $g_\lambda^{\sigma,\tau_1} = \mathcal{T}_{\lambda,\tau_1}^\sigma \zeta_\lambda^{\sigma,\tau_1}$ follows from continuity and the initial data of ζ_λ^σ.

Time derivative : We want to differentiate this formula with respect to time. It gives formally for almost any $t \in (\tau_1,T)$, $x \in (0,\overline{e}(t))$

$$\partial_t g_\lambda^\sigma(t,x) = \partial_t \zeta_\lambda^\sigma(t,x) - \int_0^x k_\lambda^\sigma(x,y)\partial_t \zeta_\lambda^\sigma(t,y)dy.$$

By assumption, $\partial_t \zeta_\lambda^\sigma \in \left[L^2((\tau_1,T);(H^1)'\right]_{\overline{e}}$ and from Proposition 3 it holds that for almost all $x \in (0,\overline{e}(T))$, $k_\lambda^\sigma(x;\cdot) \in H^1(0,x)$, uniformly in x. Therefore the integral terms are well-defined as duality products:

$$\partial_t g_\lambda^\sigma(t,x) = \partial_t \zeta_\lambda^\sigma(t,x) - \langle \partial_t \zeta_\lambda^\sigma(t), k_\lambda^\sigma(x)\rangle_{(H^1(0,x))',H^1(0,x)},$$

where the second term can be estimated as:

$$\begin{aligned}\langle \partial_t \zeta_\lambda^\sigma(t), k_\lambda^\sigma(x)\rangle_{(H^1(0,x))',H^1(0,x)} &\leq \|\partial_t \zeta_\lambda^\sigma(t)\|_{(H^1(0,x))'} \|k_\lambda^\sigma(x)\|_{H^1(0,x)} \\ &\leq \|\partial_t \zeta_\lambda^\sigma(t)\|_{(H^1(0,\overline{e}(t)))'} \sup_{0\leq x\leq \overline{e}(T)} \|k_\lambda^\sigma(x)\|_{H^1(0,x)},\end{aligned}$$

where the last term is independent of x and belongs to $L^2(\tau_1,T)$ by assumption. Hence $\partial_t g_\lambda^\sigma \in \left[L^2((\tau_1,T);(H^1)')\right]_{\overline{e}}$.

Therefore, g_λ^σ and ζ_λ^σ satisfy the assumptions of Lemma 7. It follows that for any $v \in D^{\text{targ}}$, $a^{\text{targ}}(g_\lambda^\sigma, v) = 0$, so that g_λ^σ satisfies indeed Definition 6.

The proof of Lemma 4 follows the exact same lines.

□

2.5.3 Proof of Theorem 5

Fix $\mu > 0$ and $(\overline{u},\overline{e})$. We need to check all the conditions of Definitions 3-4.

Let us first deal with the thickness and remember from (2.2.10)-(2.2.13) that $\delta e'(t) = \delta\theta(t)$. The exponential stabilization of δe can then be achieved with no effort. It suffices to define $\Theta(t,w) = -\mu w$ for all $t \geq 0$ and $w \in \mathbb{R}$ to get (2.3.5) with $C_{\overline{e},\mu} = 1$.

Let us now focus on the exponential stabilization of δu with the control variables $\delta\psi$ in (2.2.11). Remember the decomposition (2.3.6) and choose $\lambda > 0$ such that $\lambda \geq \max_{1\leq i\leq n} \lambda_{\sigma_i}$ where λ_{σ_i} is defined as in Corollary 1.

Then it follows by Proposition 3 that there exists a unique solution $k_\lambda^{\sigma_i}$ (respectively $l_\lambda^{\sigma_i}$) to the kernel problem (2.4.15) (respectively to the inverse kernel problem (2.4.16)) satisfying estimates (2.4.22) and (2.4.23) with $\sigma = \sigma_i$. Then, for all $1 \leq i \leq n$, $t \geq 0$ and $z \in H^1(0,\overline{e}(t))$, let us define

$$\begin{aligned} H_{l,\lambda}^{\sigma_i}(t)z &:= \sigma_i k_\lambda^{\sigma_i}(\overline{e}(t),\overline{e}(t))z(\overline{e}(t)), \\ H_{nl,\lambda}^{\sigma_i}(t)z &= \int_0^{\overline{e}(t)} \left[\sigma_i \partial_x k_\lambda^{\sigma_i}(\overline{e}(t),y) + \overline{v} k_\lambda^{\sigma_i}(\overline{e}(t),y)\right] z(y)dy, \end{aligned} \tag{2.5.15}$$

Defining now

$$\delta\psi^{\sigma_i,\lambda}(t) := H_{l,\lambda}^{\sigma_i}(t)\zeta_\lambda^{\sigma_i}(t) + H_{nl,\lambda}^{\sigma_i}(t)\zeta_\lambda^{\sigma_i}(t),$$

it follows from Corollary 1 that there exists a unique weak-L^2 solution $\zeta_\lambda^{\sigma_i}$ to (2.4.1) in the sense of Definition 7 with $\tau_1 = 0$ and $\zeta_\lambda^{\sigma_i,0} = z_i^0$. To simplify notations, we will denote by z_i^λ the solution $\zeta_\lambda^{\sigma_i}$. Note that z_i^λ is then also solution to problem (2.3.6) with $\delta\psi^i$ given by

$$\delta\psi^i(t) = \delta\psi^{\sigma_i,\lambda}(t) := H_{l,\lambda}^{\sigma_i}(t)z_i(t) + H_{nl,\lambda}^{\sigma_i}(t)z_i(t).$$

From Corollary 1, there exist constants $C, c > 0$ independent of λ, $1 \leq i \leq n$ and t such that for any $1 \leq i \leq n$, and $t \geq 0$,

$$\|z_i^\lambda(t)\|_{L^2(0,\overline{e}(t))} \leq Ce^{c\overline{e}_0\sqrt{\lambda/\sigma_i}+c\overline{e}(t)-\lambda t}\|z_i^0\|_{L^2(0,\overline{e}_0)}.$$

It follows that there exists a $\lambda_\mu > 0$ large enough and a constant $C_\mu > 0$ that depends on $(\max_{1\leq i\leq n}\sigma_i, \lambda_\mu, \overline{e}_0)$ such that for any $t \geq 0$,

$$\|z^{\lambda_\mu}(t)\|_{L^2(0,\overline{e}(t))^n} \leq C_\mu e^{-\mu t}\|z^0\|_{L^2(0,\overline{e}_0)^n},$$

where $z^{\lambda_\mu} := (z_i^{\lambda_\mu})_{1\leq i\leq n}$ and $z^0 := (z_i^0)_{1\leq i\leq n}$. It remains to check that the operators $(H_{l,\lambda_\mu}(t))_{t\geq 0}$ and $(H_{nl,\lambda_\mu}(t))_{t\geq 0}$ defined such that, for any $t \geq 0$ and $z := (z_i)_{1\leq i\leq n} \in H^1(0,\overline{e}(t))^n$,

$$H_{l,\lambda_\mu}(t)z := Q(\overline{u})^{-1}\left(H_{l,\lambda_\mu}^{\sigma_i}(t)z_i\right)_{1\leq i\leq n},$$
$$H_{nl,\lambda_\mu}(t)z := Q(\overline{u})^{-1}\left(H_{nl,\lambda_\mu}^{\sigma_i}(t)z_i\right)_{1\leq i\leq n},$$

satisfy assumptions (P1)-(P2)-(P3). To prove this, it is sufficient to show that for all $1 \leq i \leq n$, the families of operators $(H_{l,\lambda_\mu}^{\sigma_i}(t))_{t\geq 0}$ and $(H_{nl,\lambda_\mu}^{\sigma_i}(t))_{t\geq 0}$ satisfy the scalar assumptions (P1')-(P2')-(P3').

Let $1 \leq i \leq n$. It follows from Proposition 3 that for all $t \geq 0$, the functions $(0,\overline{e}(t)) \ni y \to \partial_x k_{\lambda_\mu}^{\sigma_i}(t,\overline{e}(t),y)$ and $(0,\overline{e}(t)) \ni y \to k_{\lambda_\mu}^{\sigma_i}(t,\overline{e}(t),y)$ are well-defined almost everywhere and belong to $L^2((0,\overline{e}(t))$. As a consequence, $H_{nl,\lambda_\mu}^{\sigma_i}(t)$ defined by (2.5.15) is well-defined and satisfies (P1'). Now in order to check (P2'), for any $T > 0$, it holds by the Cauchy-Schwarz inequality that for all $z \in [L^2((0,T),L^2]_{\overline{e}}$,

$$\begin{aligned}&\|H_{nl,\lambda_\mu}^{\sigma_i}(\cdot)z(\cdot)\|_{L^2(0,T)}^2\\ &\leq \int_0^T\left(\int_0^{\overline{e}(t)}\left[\sigma\partial_x k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y)+Vk_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y)\right]^2dy\right)\|z(t)\|_{L^2(0,\overline{e}(t))}^2dt.\end{aligned}$$

But according to the uniform estimate (2.4.20) in Proposition 3, it holds that for any $0 \leq t \leq T$,

$$\int_0^{\overline{e}(t)}\left[\sigma_i\partial_x k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y)+\overline{v}k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y)\right]^2 \leq C(\sigma_i,\overline{v})e^{c\overline{e}(T)\sqrt{\lambda_\mu/\sigma_i}},$$

hence (P2').

Finally, the family $(H_{l,\lambda_\mu}^{\sigma_i}(t))_{t\geq 0}$ satisfies (P3') provided that $\mathbb{R}_+^* \ni t \to k_{\lambda_\mu}^{\sigma_i}(t,\overline{e}(t),\overline{e}(t))$ belongs to $L_{loc}^\infty\left(\mathbb{R}_+^*;\mathbb{R}\right)$. It is in fact again a consequence of Proposition 3 and the one-dimensional Sobolev inequality. Indeed, for $t \geq 0$, we then write for all $(y,\tilde{y}) \in [0,\overline{e}(t)]^2$,

$$k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y) = \int_{\tilde{y}}^y \partial_y k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),y')\,dy' + k_{\lambda_\mu}^{\sigma_i}(\overline{e}(t),\tilde{y}).$$

Integration with respect to $\tilde{y} \in [0, \overline{e}(t)]$ leads to:

$$\begin{aligned}|k^{\sigma_i}_{\lambda_\mu}(\overline{e}(t), y)| &\leq \frac{1}{\overline{e}(t)} \int_0^{\overline{e}(t)} \int_{\tilde{y}}^{y} |\partial_y k^{\sigma_i}_{\lambda_\mu}(\overline{e}(t), y')|\, dy'\, d\tilde{y} + \frac{1}{\overline{e}(t)} \int_0^{\overline{e}(t)} |k^{\sigma_i}_{\lambda_*}(\overline{e}(t), \tilde{y})| d\tilde{y} \\ &\leq C \left(\sqrt{\overline{e}(t)} + \frac{1}{\sqrt{\overline{e}(t)}} \right) e^{c\overline{e}(t)\sqrt{\lambda_\mu/\sigma_i}},\end{aligned}$$

where we have used again estimate (2.4.20) as well as Cauchy-Schwarz inequality. Hence (P3') and the proof of Theorem 5.

2.5.4 Proof of Theorem 6

Let us fix $T > 0$. Let us first explain how the function Θ can be chosen to ensure condition b) of Definition 5. The main idea is to go from the autonomous feedback $\Theta(w) = -\mu w$ to *piecewise constant* in time. Let $(t'_m)_{m\in\mathbb{N}}$ be an increasing sequence of real numbers such that $t'_0 = 0$ and $t'_m \underset{m\to\infty}{\longrightarrow} T^-$. Let $(\mu_m)_{m\in\mathbb{N}}$ be a nondecreasing sequence of positive numbers which will be made precise below and define, for all $t \geq 0$ and $w \in \mathbb{R}$,

$$\Theta(t, w) = -\mu_m w \quad \text{ if } t \in [t'_m, t'_{m+1}).$$

Then, it holds that for all $m \in \mathbb{N}$ and for all $t \in [t'_m, t'_{m+1})$,

$$|\delta e(t)| \leq e^{-\mu_m(t-t'_m)}|\delta e(t'_m)| \leq e^{-\sum_{k=0}^{m-1} \mu_k(t'_{k+1}-t'_k)}|\delta e(0)|$$

It is then clear that condition b-i) is always satisfied with this choice. Moreover, if the series $\sum_{k\in\mathbb{N}} \mu_k(t'_{k+1} - t'_k)$ diverges, then $\delta e(t) \underset{t\to T^-}{\longrightarrow} 0$. For instance, this is the case when defining $t'_m = T - \frac{1}{m}$ and $\mu_m = m$ for all $m \geq 1$. Hence b-ii).

Let us now turn to the proof of condition a) of Definition 5. Let us introduce again an increasing sequence $(t_m)_{m\in\mathbb{N}}$ of real numbers such that $t_0 = 0$ and $t_m \underset{m\to\infty}{\longrightarrow} T^-$. Let us introduce a sequence of positive numbers $(\lambda_m)_{m\in\mathbb{N}}$ such that $\lambda_m \geq \max_{1\leq i\leq n} \lambda_{\sigma_i}$ for all $m \in \mathbb{N}$, where λ_{σ_i} is defined in Proposition 3 for $\sigma = \sigma_i$. Then, for all $1 \leq i \leq n$, we define the families of operators $(H^i_{nl}(t))_{t\geq 0}$ and $(H^i_l(t))_{t\geq 0}$ as follows:

$$H^i_{nl}(t) = H^{\sigma_i}_{nl,\lambda_m}(t) \quad \text{ and } H^i_{nl}(t) = H^{\sigma_i}_{l,\lambda_m}(t) \text{ if } t \in [t_m, t_{m+1}).$$

We also define for all $t \geq 0$ and $z := (z_i)_{1\leq i\leq n} \in H^1(0, \overline{e}(t))^n$,

$$H_l(t)z := Q(\overline{u})^{-1} \left(H^i_l(t)z_i\right)_{1\leq i\leq n}, \tag{2.5.16}$$

$$H_{nl}(t)z := Q(\overline{u})^{-1} \left(H^i_{nl}(t)z_i\right)_{1\leq i\leq n}. \tag{2.5.17}$$

We wish to identify some sufficient conditions on the sequence $(\lambda_m)_{m\in\mathbb{N}}$ and $(t_m)_{m\in\mathbb{N}}$ in order to guarantee condition a) of Definition 5.

To this aim, we first prove the following lemma.

Lemma 8. *Let $(\lambda_m)_{m\in\mathbb{N}}$ be a nondecreasing sequence of positive coefficients and let $(t_m)_{m\in\mathbb{N}}$ be an increasing sequence of times such that $t_0 = 0$ and $t_m \underset{m\to\infty}{\longrightarrow} T^-$. Let us define, for $m \geq 0$, $s_m := \sum_{k=0}^{m} \lambda_k(t_{k+1} - t_k)$. Then, there exists a constant $\gamma > 0$ such that, if*

$$\forall m \in \mathbb{N}, \quad (t_{m+1} - t_m)\sqrt{\lambda_m} \geq \gamma, \tag{2.5.18}$$

then, there exists positive constants $C > 0$ and $\alpha > 0$ such that for any $m \in \mathbb{N}$ and any $t \in [t_m, t_{m+1})$,

$$\|z(t)\|_{L^2(0,\bar{e}(t))^n} \leq Ce^{-s_m+\alpha m}\|z_0\|_{L^2(0,\bar{e}_0)^n},$$

where $z := (z_i)_{1\leq i\leq n}$ with z_i the unique weak solution of (2.3.6) and $\delta\psi^i$ defined by:

$$\forall t \geq 0, \quad \delta\psi_i(t) = H_l^i(t)z_i(t) + H_{nl}^i(t)z_i(t).$$

Besides, if we assume in addition that:

$$\lim_{m\to+\infty} \frac{s_m}{m} = +\infty, \tag{2.5.19}$$

then it holds:

$$\lim_{t\to T_-} \|z(t)\|_{L^2(0,\bar{e}(t))^n} = 0, \tag{2.5.20}$$

Proof of Lemma 8. From Proposition 3, it holds that for all $1 \leq i \leq n$, for any $m \in \mathbb{N}$, for any $t \in [t_m, t_{m+1})$,

$$\|k_{\lambda_m}^{\sigma_i}(t)\|_{L^2(D_t)} \leq Ce^{c\bar{e}(t)\sqrt{\lambda_m/\sigma_i}},$$

$$\|l_{\lambda_m}^{\sigma_i}(t)\|_{L^2(D_t)} \leq C\left(\frac{\lambda_m}{\sigma_i}\right)^2 e^{c\bar{e}(t)}.$$

Fix $m \in \mathbb{N}$ and $t_m \leq t < t_{m+1}$. Denoting by $g_i(t) := \mathcal{T}_{\lambda_m,t}^{\sigma_i} z_i(t)$, it holds that

$$\begin{aligned}\|g_i(t)\|_{L^2(0,\bar{e}(t))}^2 &\leq \left(1 + \|k_{\lambda_m}^{\sigma_i}(t)\|_{L^2(D_t)}^2\right)\|z_i(t)\|_{L^2(0,\bar{e}(t))}^2 \\ &\leq Ce^{c\bar{e}(t)\sqrt{\lambda_m/\sigma_i}}\|z_i(t)\|_{L^2}^2.\end{aligned}$$

Moreover, using the fact that $z_i(t) = \mathcal{T}_{\lambda_m,t}^{\mathrm{inv},\sigma_i} g_i(t)$, we obtain that

$$\|z_i(t)\|_{L^2(0,\bar{e}(t))}^2 \leq \frac{C}{\sigma_i^4}\lambda_m^4 e^{c\bar{e}(t)}\|g_i(t)\|_{L^2(0,\bar{e}(t))}^2.$$

Besides, from Proposition 2, for any $t_m \leq \tau_1 \leq \tau_2 < t_{m+1}$, we have

$$\|g_i(\tau_2)\|_{L^2(0,\bar{e}(\tau_2))}^2 \leq e^{-2\lambda_m(\tau_2-\tau_1)}\|g_i(\tau_1)\|_{L^2(0,\bar{e}(\tau_1))}^2.$$

Since z_i and g_i are in $C([0,T], L^2)$, we can combine these inequalities as $\tau_2 \to t_{m+1}^-$ and $\tau_1 \to t_m^+$. We thus obtain, with $C > 0$ and $c > 0$ being arbitrary constants independent of

t,i and m which may change along the computations, and using the fact that $\ln(x) \leq \sqrt{x}$ for all $x > 0$,

$$\begin{aligned}
\|z_i(t_{m+1})\|^2_{L^2(0,\bar{e}(t_{m+1}))} &\leq \frac{C}{\sigma_i^4}\lambda_m^4 e^{c\bar{e}(t_{m+1})}\|g_i(t_{m+1})\|^2_{L^2(0,\bar{e}(t_{m+1}))} \\
&\leq Ce^{c\bar{e}(T)+4\ln(\lambda_m/\sigma_i)}\|g_i(t_{m+1})\|^2_{L^2(0,\bar{e}(t_{m+1}))} \\
&\leq Ce^{4\log(\lambda_m/\sigma_i)-2\lambda_m(t_{m+1}-t_m)}\|g_i(t_m)\|^2_{L^2(0,\bar{e}(t_m))} \\
&\leq Ce^{4\log(\lambda_m/\sigma_i)+c\bar{e}(t_m)\sqrt{\lambda_m/\sigma_i}-2\lambda_m(t_{m+1}-t_m)}\|z_i(t_m)\|^2_{L^2(0,\bar{e}(t_m))}, \\
&\leq Ce^{c\sqrt{\lambda_m/\sigma_i}-2\lambda_m(t_{m+1}-t_m)}\|z_i(t_m)\|^2_{L^2(0,\bar{e}(t_m))}.
\end{aligned}$$

Denoting by $\gamma := \max_{1\leq i\leq n}\frac{c}{\sqrt{\sigma_i}}$, then, if (2.5.18) holds, we obtain that for all $m \in \mathbb{N}$,

$$\|z(t_{m+1})\|^2_{L^2(0,\bar{e}(t_{m+1})} \leq Ce^{-\lambda_m(t_{m+1}-t_m)}\|z(t_m)\|^2_{L^2(0,\bar{e}(t_m))} \leq Ce^{-s_m+\alpha m}\|z_0\|^2_{L^2(0,\bar{e}_0)},$$

with $\alpha := \ln(C)$. This estimate together with (2.5.19) yields (2.5.20) and the proof of the desired result. □

We are now in position to terminate the proof of Theorem 6. Indeed, for any $\gamma > 0$, there always exist sequences $(t_m)_{m\in\mathbb{N}}$ and $(\lambda_m)_{m\in\mathbb{N}}$ that satisfy (2.5.18) and (2.5.19). Indeed, let us define, as in [92], $t_m = T - \frac{1}{m^2}$ and $\lambda_m = \gamma^2(m+1)^8$. Then, it holds that for all $m \geq 1$

$$(t_{m+1} - t_m)\sqrt{\lambda_m} = \gamma\frac{(2m+1)(m+1)^2}{m^2} \geq \gamma.$$

Besides, $(t_{m+1} - t_m)\lambda_m = \gamma^2\frac{(2m+1)(m+1)^6}{m^2}$ so that $\frac{s_m}{m} \underset{m\to+\infty}{\longrightarrow} +\infty$. Choosing such sequences, and defining the families of operators $(H_{nl}(t))_{t\geq 0}$ and $(H_l(t))_{t\geq 0}$ with (2.5.17) and (2.5.16) then yields the desired result.

Conclusion and perspectives

We have shown arbitrary small-time boundary stabilization for a class of cross-diffusion systems in a one-dimensional domain, at the level of the linearized system around uniform equilibria. The system is assumed to have an entropy structure and moreover its mobility matrix should be symmetric, so that the linearized system can be uncoupled into n independent scalar equations. Anticipating on the nonlinear stabilization, we have chosen a weak L^2 framework for the stabilization. We have adapted the backstepping technique to derive a feedback control: we have shown that, although the equation is non autonomous, it suffices to study the usual stationary kernels PDEs in a moving domain, *i.e.* the moving-domain structure is somehow transported to the kernel PDE. Besides, we have proven the well-posedness of the backstepping transformation in the framework of weak L^2 solutions and have provided quantitative estimates on the kernels with respect to time.

We intend to continue this work to get the local stabilization of the nonlinear system. We also see several closely related open problems:

- The symmetry assumption on the mobility matrix is technical. Without this assumption, one has to use the backstepping technique to stabilize the coupled linearized system (2.2.11). In consequence, one has to consider a matrix kernel k with values in $\mathbb{R}^{n\times n}$ associated to the backstepping transformation. The derivation of the (matrix) kernel equations (see the scalar derivation in Appendix 2.6.3) is complicated by the fact that $A(\overline{u})$ and k *do not commute* in general and leads to a "non-commutative version" of the kernel equations. On the other hand, the boundary conditions are unchanged since one obtains a commutation condition on the diagonal $x = y$. After the same separation of variables trick, one obtains the system:

$$\begin{cases} \partial^2_{xx}k(x,y)A(\overline{u}) - A(\overline{u})\partial^2_{yy}k(x,y) = \lambda k(x,y) & (x,y) \in \{0 < y \leq x < +\infty\}, \\ \partial_y k(x,0) = 0 & x \in (0,+\infty), \\ A(\overline{u})k(x,x) = -\dfrac{\lambda}{2}x & x \in (0,+\infty), \end{cases} \tag{2.5.1}$$

  Up to our knowledge, it is an open problem to prove well-posedness and estimates for this system when $A(\overline{u})$ is not diagonalizable.

- The extension of the present work to the related nonlinear system is currently work in progress. We expect that getting global exponential or finite-time stabilization might be difficult in this situation. However, we have good hope of proving at least exponentially fast local stabilization. The control and estimates of the higher-order terms appearing in the equation is the most delicate part of the analysis.

- It would be interesting, both mathematically and physically, to see whether it is possible to design an observer to have a control feedback that does not depend on the full state. An interesting additional direction would be to see whether the resulting observer-based control can be made robust (with respect to the propagation speeds of the system), which is not always granted (see for instance [18, 20, 29]).

- A last natural extension would be to study the stabilization of a similar system in a multidimensional context: this however requires as a first step to define a relevant multidimensional moving boundary domain model for the problem considered here. This is a very interesting problem left for future investigation.

2.6 Appendices

2.6.1 Weak formulation of the controlled linearized system in L^2

We start from the strong formulation (2.2.11) with a feedback law of the form (2.3.1)-(2.3.2). We test against a regular test function v that satisfies for all $x \in (0,T)$, $v(T,x) =$

0 and integrate with respect to time and space. Considering the moving boundary, the integration of the time derivative gives:

$$\int_0^T \int_0^{\overline{e}(t)} (\partial_t u \cdot v)(t,x)dxdt = -\int_0^T \int_0^{\overline{e}(t)} (\partial_t v \cdot u)(t,x)dxdt - \int_0^T \overline{e}(t)'(u \cdot v)(t,\overline{e}(t))dt \\ - \int_0^{\overline{e}_0} u^0(x) \cdot v(0,x)dx.$$

Recall that $\overline{e}(t)' = \overline{v} > 0$. Now we consider the space derivatives and perform two integration by parts:

$$\int_0^T \int_0^{\overline{e}(t)} A(\overline{u})\partial_{xx}^2 u \cdot v dxdt = \int_0^T A(\overline{u})\partial_x u(t,\overline{e}(t)) \cdot v(t,\overline{e}(t))dt \\ - \int_0^T \int_0^{\overline{e}(t)} A(\overline{u})\partial_x u \cdot \partial_x v dxdt \\ = \int_0^T A(\overline{u})\partial_x u(t,\overline{e}(t)) \cdot v(t,\overline{e}(t))dt + \int_0^T \int_0^{\overline{e}(t)} A(\overline{u}) u \cdot \partial_{xx}^2 v dxdt \\ - \int_0^T A(\overline{u})u(t,\overline{e}(t) \cdot \partial_x v(t,\overline{e}(t))dt + \int_0^T A(\overline{u})u(t,0) \cdot \partial_x v(t,0)dt.$$

Now we write the equality of these two quantities with the appropriate factorizations:

$$0 = \int_0^T \int_0^{\overline{e}(t)} u \cdot \left[\partial_t v + A(\overline{u})^T \partial_{xx} v\right] dxdt + \int_0^{\overline{e}_0} u^0(x) \cdot v(0,x)dx \\ - \int_0^T A(\overline{u})u(t,\overline{e}(t)) \cdot \partial_x v(t,\overline{e}(t))dt + \int_0^T A(\overline{u})u(t,0) \cdot \partial_x v(t,0)dt \\ + \int_0^T v(t,\overline{e}(t)) \cdot \left[A(\overline{u})\partial_x u(t,\overline{e}(t)) + \overline{v}u(t,\overline{e}(t))\right] dt.$$

In the last integral we recognize the boundary condition at $x = \overline{e}(t)$, that is nothing else than $\delta\psi(t) = H_{nl}(t)u(t) + K_l(t)u(t,\overline{e}(t))$. Now all the terms that do not make sense for $u \in \left[\mathcal{C}^0([0,+\infty), L^2(0,1))^n\right]_{\overline{e}}$ must vanish if this is to be true against any test function. It entails conditions on the test functions, the so-called dual boundary conditions. The first condition at $x = 0$ is:

$$\forall t \in (0,T),\ A(\overline{u})^T \partial_x v(t,0) = 0.$$

Now we examine the condition at $x = \overline{e}(t)$ where the local part of the feedback intervenes:

$$\forall t \in (0,T),\ K(t)^T v(t,\overline{e}(t)) - A(\overline{u})^T \partial_x v(t,\overline{e}(t)) = 0.$$

The remaining terms make sense for $u \in \left[\mathcal{C}^0([0,+\infty), L^2)^n\right]_{\overline{e}}$ provided:

$$v \in \left[L^2\left((0,T); H^2\right)^n\right]_{\overline{e}} \cap \left[\mathcal{C}^0([0,T], L^2)^n\right]_{\overline{e}},\ \partial_t v \in \left[L^2\left((0,T); L^2\right)^n\right]_{\overline{e}}.$$

Putting together all the conditions, we obtain Definition 3.

2.6.2 Analysis of the target problem

For the sake of the analysis, we consider the rescaled version of (2.4.8) given by the change of variables $x \to x/\overline{e}(t)$ so that the space variable is now defined in a fixed domain:

$$\begin{cases} \partial_t w - \dfrac{\sigma}{\overline{e}(t)^2}\partial^2_{xx} w - \dfrac{\overline{v}}{\overline{e}(t)} x\partial_x w + \lambda w = 0, & \text{for } (t,x) \in \mathbb{R}^*_+ \times (0,1), \\ \dfrac{\sigma}{\overline{e}(t)}\partial_x w(t,1) + \overline{v} w(t,1) = 0, & \text{for } t \in \mathbb{R}^*_+, \\ \dfrac{\sigma}{\overline{e}(t)}\partial_x w(t,0) = 0, & \text{for } t \in \mathbb{R}^*_+, \\ w(0,x) = w^0(x) := g^0(x\overline{e}_0), & \text{for } x \in (0,1), \end{cases} \tag{2.6.1}$$

and the associated notion of weak L^2 solution:

Definition 9. *A function $w \in \mathcal{C}^0([0,+\infty), L^2(0,1))$ is said to be a L^2-weak solution of (2.6.1) if for any $T > 0$, it satisfies:*

$$\int_0^T \int_0^1 w(t,x)\left[\partial_t \tilde{v}(t,x) + \frac{\sigma}{\overline{e}(t)^2}\partial^2_{xx}\tilde{v}(t,x) - \frac{\overline{v}}{\overline{e}(t)} x\partial_x \tilde{v}(t,x) - \left(\lambda + \frac{\overline{v}}{\overline{e}(t)}\right)\tilde{v}(t,x)\right] dxdt$$
$$+ \int_0^1 w(0,x)\tilde{v}(0,x)dx = 0,$$

for any test function $\tilde{v}$ that satisfies:

- $\tilde{v} \in \left(L^2\left((0,T); H^2(0,1)\right)\right) \cap \mathcal{C}^0([0,T], L^2(0,1))$,
- $\partial_t \tilde{v} \in \left(L^2\left((0,T); L^2\right)\right)$,
- $\tilde{v}(T,\cdot) = 0$,
- $\sigma\partial_x \tilde{v}(t,0) = 0, \ \forall t \in (0,T)$,
- $\sigma\partial_x \tilde{v}(t,\overline{e}(t)) = 0, \forall t \in (0,T)$.

Note that the two definitions 6 and 9 are equivalent: from the latter to the former, take a test function of the form $\overline{e}(t)v(t,\overline{e}(t)x)$ where v satisfies the assumptions in 6. The other way around, take a test function of the form $\frac{1}{\overline{e}(t)}\tilde{v}(t, \frac{x}{\overline{e}(t)})$ where $\tilde{v}$ satisfies the previous assumptions.
The problem is uniformly parabolic: for any $0 \le t \le T$

$$\frac{\sigma}{\overline{e}(t)^2} \ge \frac{\sigma}{\overline{e}(T)^2} > 0,$$

so that we expect the classical parabolic estimates and well-posedness in the space $\mathcal{C}^0([0,T], H^k(0,1))$ for any $k \in \mathbb{N}$ as soon as $w^0 \in H^k(0,1)$. In fact, we have the following a priori estimates

Lemma 9. *Assume $w^0 \in L^2((0,1))$. Any smooth solution w to (2.6.1) must satisfy the energy estimate:*

$$\begin{aligned}&\frac{1}{2}\|w\|^2_{L^\infty(0,T;L^2)} + \frac{\sigma}{\overline{e}(T)^2}\|\partial_x w\|^2_{L^2(0,T;L^2(0,1))}\\ &+\frac{\overline{v}}{2\overline{e}(T)}\int_0^T w(t,1)^2 + \left(\frac{\overline{v}}{2\overline{e}(T)}+\lambda\right)\|w\|^2_{L^2(0,T;L^2(0,1))} \leq \|w^0\|^2_{L^2(0,1)}.\end{aligned} \tag{2.6.2}$$

Furthermore, it must satisfy the stability estimate: for any $0 \leq t \leq T$

$$\|w(t)\|_{L^2(0,1)} \leq e^{-\lambda t}\|w^0\|_{L^2(0,1)} \tag{2.6.3}$$

Proof. Multiply the first equation in (2.6.1) by w and integrate by parts in space at time t. One first obtains:

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2} + \frac{\sigma}{\overline{e}(t)^2}\int_0^1 (\partial_x w)^2 + \left(\frac{\overline{v}}{2\overline{e}(t)}+\lambda\right)\\ &\int_0^1 w^2 - \frac{\sigma}{\overline{e}(t)^2}\partial_x w(t,1)w(t,1) - \frac{\overline{v}}{2\overline{e}(t)}w(t,1)^2 = 0.\end{aligned}$$

Then using the boundary conditions in (2.6.1), one gets:

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2} + \frac{\sigma}{\overline{e}(t)^2}\int_0^1 (\partial_x w)^2 + \left(\frac{\overline{v}}{2\overline{e}(t)}+\lambda\right)\int_0^1 w^2 + \frac{\overline{v}}{2\overline{e}(t)}w(t,1)^2 = 0. \tag{2.6.4}$$

It comes in particular:

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2(0,1)} \leq -\lambda\|w(t)\|^2_{L^2(0,1)},$$

from which we conclude to (2.6.3) with the Gronwall lemma. Integrating (2.6.4) with respect to time in $[0,T]$, one finds (2.6.2).

□

From these estimates, we define a notion of *energy solution* for the problem.

Definition 10. *A function $w \in \mathcal{C}^0([0,T], L^2(0,1)) \cap L^2((0,T); H^1(0,1))$ such that $\partial_t w \in L^2((0,T); (H^1(0,1))')$ is an energy solution to (2.6.1) if, for almost any time $0 \leq t \leq T$ and any function $\tilde{v} \in H^1(0,1)$, it satisfies*

$$\langle \partial_t w(t), \tilde{v}(t)\rangle_{(H^1)',H^1} + a(t; w, \tilde{v}) = 0,$$

where the bilinear form a is given by:

$$a(t; w, \tilde{v}) = \int_0^1 \left(\frac{\sigma}{\overline{e}(t)^2}\partial_x w \partial_x \tilde{v} - \frac{\overline{v}}{\overline{e}(t)} w\left(\tilde{v} + x\partial_x \tilde{v}\right) + \lambda w \tilde{v}\right) dx.$$

By construction of the weak formulation, such solutions still satisfy the previous estimates. In particular and by linearity, such a solution is unique, if it exists. The existence follows from the Galerkin method (see [49][Theorem 10.9, p.341] for a general result). This is summarized in the following proposition

Proposition 4. *Let $w^0 \in L^2(0,1)$. There exists a unique energy solution to (2.6.1). This solution satisfies (2.6.2) and (2.6.3).*

Proposition 4 gives existence to a weak L^2 solution since the energy solution is a particular one, and this solution satisfies in particular (2.6.3). But one cannot directly conclude that *any* weak L^2 satisfies (2.6.3) and deduce uniqueness from the estimate. Indeed, such an estimate cannot be deduced directly from the weak formulation in (6). Instead, we will first prove uniqueness from the weak formulation, then deduce that the only weak L^2 solution satisfies indeed the estimate.

Lemma 10. *There is at most one weak L^2 solution in the sense of Definition 9.*

Proof. Consider two such solutions $w_1, w_2 \in \mathcal{C}^0([0,T]; L^2(0,1))$. Then the difference satisfies, for any test function $\tilde{v}$ that satisfies the assumptions of Definition 9:

$$\int_0^T \int_0^1 (w_1 - w_2) \left(\partial_t \tilde{v} + \frac{\sigma}{\overline{e}(t)^2} \tilde{v} - \frac{\overline{v}}{\overline{e}(t)} x \partial_x \tilde{v} - \left(\lambda + \frac{\overline{v}}{\overline{e}(t)} \right) \tilde{v} \right) dxdt = 0$$

Now fix $S \in L^2((0,T); L^2(0,1))$ and consider the inhomogeneous dual problem with source term S:

$$\begin{cases} \partial_t \tilde{v} + \dfrac{\sigma}{\overline{e}(t)^2} \partial^2_{xx} \tilde{v} - \dfrac{\overline{v}}{\overline{e}(t)} x \partial_x \tilde{v} - \left(\lambda + \dfrac{\overline{v}}{\overline{e}(t)} \right) \tilde{v} = S, & \text{for } (t,x) \in [0,T] \times (0,1), \\ \partial_x \tilde{v}(t,1) = 0, & \text{for } t \in [0,T], \\ \partial_x \tilde{v}(t,0) = 0, & \text{for } t \in [0,T], \\ \tilde{v}(T,x) = 0, & \text{for } x \in (0,1). \end{cases}$$

Up to time reversal $t \to T - t$, this is a classical parabolic problem with smooth coefficients. Therefore, there exists a (unique) solution $\tilde{v} \in \left(L^2\left((0,T); H^2(0,1)\right)\right) \cap \mathcal{C}^0([0,T], L^2(0,1))$ and such that $\partial_t \tilde{v} \in \left(L^2\left((0,T); L^2(0,1)\right)\right)$ (the regularity is limited by $S \in L^2$). Consequently, $\tilde{v}$ can be taken as a test function against $(w_1 - w_2)$ and it holds:

$$\int_0^T \int_0^1 (w_1 - w_2) S dxdt = 0.$$

Since this is true for any $S \in L^2((0,T); L^2(0,1))$, $w_1 = w_2$ and uniqueness is proved. □

Proposition 2 follows from Proposition 4 and 10.

2.6.3 Formal derivation of the backstepping kernel problems

As explained in the remarks in Section 2.4.4, the derivation is done assuming that the kernels explicitly depend on time t, then we show they do not have to depend on t. In the spirit of Section 2.4.3, we assume that all the functions are smooth and we differentiate (2.4.2) at $x = 0$. It gives:

$$\partial_x g(t,0) = -k(t,0,0)\zeta(t,0),$$

which suggests, since $\zeta(t,0)$ is undetermined, that the kernel k should be supplied with the condition

$$k(t,0,0) = 0,$$

for the boundary condition at $x = 0$ in (2.4.8) to be satisfied.

At this stage, it is unclear how the kernel depends on time. We make it explicit by applying a rescaling in the space variable into a fixed domain. More precisely, we consider the rescaled versions of problems (2.4.1) and (2.4.8). The latter one was defined in (2.6.1) while the former is given by:

$$\begin{cases} \partial_t z - \dfrac{1}{\overline{e}(t)^2}\sigma\partial^2_{xx} z - \dfrac{\overline{v}}{\overline{e}(t)} x\partial_x z = 0, & \text{for } (t,x) \in \mathbb{R}^*_+ \times (0,1), \\ \dfrac{\sigma}{\overline{e}(t)}\partial_x z(t,1) + \overline{v} z(t,1) = \delta\psi(t), & \text{for } t \in \mathbb{R}^*_+, \\ \dfrac{\sigma}{\overline{e}(t)}\partial_x z(t,0) = 0, & \text{for } t \in \mathbb{R}^*_+, \\ z(0,x) = \zeta^0(x\overline{e}(t)), & \text{for } x \in (0,1). \end{cases} \tag{2.6.5}$$

We consider the backstepping transformation associated to these rescaled problems: for any $t \geq 0$, $x \in (0,1)$:

$$w(t,x) := z(t,x) - \int_0^x \tilde{k}(t,x,y)z(t,y)dy, \tag{2.6.6}$$

where z is a solution to (2.6.5), w a solution to (2.6.1) and $\tilde{k}$ an unknown function defined in $D_1 := \{0 < y \leq x < 1\}$. Assume everything is smooth and compute derivatives:

$$\begin{aligned} \partial_x w(t,x) &= \partial_x z(t,x) - \tilde{k}(t,x,x)z(t,x) - \int_0^x \partial_x \tilde{k}(t,x,y)z(t,y)dy, \\ \partial^2_{xx} w(t,x) &= \partial^2_{xx} z(t,x) - \partial_x\left(\tilde{k}(t,x,x)z(t,x)\right) - \partial_x\tilde{k}(t,x,x)z(t,x) \\ &\quad - \int_0^x \partial^2_{xx}\tilde{k}(t,x,y)z(t,y)dy. \end{aligned} \tag{2.6.7}$$

and:

$$\begin{aligned} \partial_t w(t,x) &= \partial_t z - \int_0^x \tilde{k}(t,x,y)\partial_t z(t,y)dy - \int_0^x \partial_t\tilde{k}(t,x,y)z(t,y)dy \\ &= \frac{\sigma}{\overline{e}(t)^2}\partial^2_{xx} z + \frac{\overline{v}}{\overline{e}(t)} x\partial_x z - \int_0^x \tilde{k}(t,x,y)\left(\frac{\sigma}{\overline{e}(t)^2}\partial^2_{yy} z + \frac{\overline{v}}{\overline{e}(t)} y\partial_y z\right)dy \\ &\quad - \int_0^x \partial_t\tilde{k}(t,x,y)z(t,y)dy \end{aligned}$$

Now use integration by parts for the integral terms in the middle. It holds:

$$\int_0^x \tilde{k}(t,x,y)y\partial_x z(t,y)dy = \tilde{k}(t,x,x)xz(t,x) - \int_0^x \partial_y(y\tilde{k}(t,x,y))z(t,y)dy,$$

and, using $\partial_x z(0) = 0$:

$$\begin{aligned}
-\int_0^x \tilde{k}(t,x,y)\partial_{yy}^2 z &= -\tilde{k}(t,x,x)\partial_x z(t,x) + \int_0^x \partial_y \tilde{k}(t,x,y)\partial_x z \\
&= -\tilde{k}(t,x,x)\partial_x z(t,x) + \Big(\partial_y \tilde{k}(t,x,x)z(t,x) - \partial_y \tilde{k}(t,x,0)z(t,0)\Big) \\
&\quad - \int_0^x \partial_{yy}^2 \tilde{k}(t,x,y)z(t,y)dy,
\end{aligned}$$

so that it holds:

$$\begin{aligned}
\partial_t w(t,x) =& \frac{\sigma}{\overline{e}(t)^2}\Big(\partial_{xx}^2 z - \tilde{k}(t,x,x)\partial_x z(t,x) + \Big(\partial_y \tilde{k}(t,x,x)z(t,x) - \partial_y \tilde{k}(t,x,0)z(t,0)\Big) \\
&- \int_0^x \partial_{yy}^2 \tilde{k}(t,x,y)z(t,y)dy\Big) \\
&+ \frac{\overline{v}}{\overline{e}(t)}\left(x\partial_x z + \int_0^x \partial_y(y\tilde{k}(t,x,y))z(t,y)dy - \tilde{k}(t,x,x)xz(x)\right) \\
&- \int_0^x \partial_t \tilde{k}(t,x,y)z(t,y)dy
\end{aligned} \tag{2.6.8}$$

Now we insert (2.6.7),(2.6.8) into the equation satisfied by w:

$$\partial_t w - \frac{\sigma}{\overline{e}(t)^2}\partial_{xx}^2 w - \frac{\overline{v}}{\overline{e}(t)}x\partial_x w + \lambda w = 0.$$

After cancellations, it remains, for any $x \in (0,1)$:

$$\begin{aligned}
0 &= \frac{\sigma}{\overline{e}(t)^2}\left(2\frac{d}{dx}\tilde{k}(t,x,x) + \lambda\right)z(x) - \partial_y \tilde{k}(t,x,0)z(0) \\
&- \int_0^x z\left(\partial_t \tilde{k} - \frac{\sigma}{\overline{e}(t)^2}(\partial_{xx}^2 \tilde{k} - \partial_{yy}^2 \tilde{k}) - \frac{\overline{v}}{\overline{e}(t)}(x\partial_x \tilde{k} + \partial_y(y\tilde{k})) + \lambda\tilde{k}\right)dy,
\end{aligned}$$

which leads to the following problem for $t > 0$

$$\begin{cases}
\partial_t \tilde{k} - \frac{\sigma}{\overline{e}(t)^2}\Big(\partial_{yy}^2 \tilde{k}(t,x,y) - \partial_{xx}^2 \tilde{k}(t,x,y)\Big) \\
\qquad - \frac{\overline{v}}{\overline{e}(t)}\left(x\partial_x \tilde{k} + y\partial_y \tilde{k} + \tilde{k}\right) + \lambda\tilde{k} = 0 & (x,y) \in \{0 < y \leq x < 1\}, \\
\frac{\sigma}{\overline{e}(t)^2}\partial_y \tilde{k}(t,x,0) = 0 & x \in (0,1), \\
\frac{2\sigma}{\overline{e}(t)^2}\frac{d}{dx}\tilde{k}(t,x,x) = -\lambda & x \in (0,1).
\end{cases} \tag{2.6.9}$$

Now we look for a solution with separate variables under the form (k does not depend explicitly on time):

$$\tilde{k}(t,x,y) = \overline{e}(t)k(x\overline{e}(t), y\overline{e}(t)). \tag{2.6.10}$$

Inserting (2.6.10) into (2.6.9), the terms in $\overline{e}(t)$ cancel each other and coming back to the original domain we obtain

$$\begin{cases} \partial^2_{xx}k(x,y) - \partial^2_{yy}k(x,y) = \dfrac{\lambda}{\sigma}k(x,y) & (x,y) \in \{0 < y \leq x < \overline{e}(t)\}, \\ \partial_y k(x,0) = 0 & x \in (0,\overline{e}(t)), \\ k(x,x) = -\dfrac{\lambda}{2\sigma}x & x \in (0,\overline{e}(t)), \end{cases} \tag{2.6.11}$$

Moreover, inserting (2.6.10) into (2.6.6), it is clear with a change of variables that the k defined from (2.6.10) enables to recover the original kernel in (2.4.2)-(2.4.3) we were looking for.

2.6.4 Failure of the basic quadratic Lyapunov approach

We show why the common approach of directly using a basic quadratic Lyapunov function would fail to provide exponential stabilization. In order to have a proper basic quadratic Lyapunov function, we work on the rescaled system (2.6.5). A basic quadratic Lyapunov function for the L^2 norm has the form, for some positive function $f \in C^2((0,1)) \cap C^1([0,1])$,

$$V(z(t,\cdot)) = \int_0^1 f(x)z(t,x)^2 dx. \tag{2.6.12}$$

Let us take V as a Lyapunov function candidate. By differentiating along C^2 solutions of (2.6.5), we have

$$\frac{d}{dt}V(z(t,\cdot)) = \int_0^1 2f(x)z\left[\frac{\sigma}{\overline{e}(t)^2}\partial^2_{xx}z + \frac{\overline{v}}{\overline{e}(t)}x\partial_x z\right]dx,$$

Integrating by parts the first term gives

$$\left[2f\frac{\sigma}{\overline{e}(t)^2}z\partial_x z\right]_0^1 - \frac{\sigma}{\overline{e}(t)^2}\int_0^1 \left[2f(x)(\partial_x z)^2 + 2f'(x)z\partial_x z\right]dx,$$

while the second terms gives

$$\left[fx\frac{\overline{v}}{\overline{e}(t)}z^2\right]_0^1 - \frac{2\overline{v}}{\overline{e}(t)}\int_0^1 \left(z^2\left(f + xf'\right) + fxz\partial_x z\right)dx.$$

Note that the last term in the previous equation is the same term we integrated by parts. Therefore putting everything together we obtain:

$$\begin{aligned}\frac{d}{dt}V(z(t,\cdot)) = &\left(\left[2f\frac{\sigma}{\overline{e}(t)^2}z\partial_x z\right]_0^1 + \left[fx\frac{\overline{v}}{\overline{e}(t)}z^2\right]_0^1\right) \\ &- \frac{\sigma}{\overline{e}(t)^2}\int_0^1 \left[2f(x)(\partial_x z)^2 + 2f'(x)z\partial_x z\right]dx - \frac{\overline{v}}{\overline{e}(t)}\int_0^1 z^2\left(f + xf'\right)dx,\end{aligned}$$

which gives, using again an integration by parts for the second term in the first integral and the boundary conditions of (2.6.5)

$$\begin{aligned}
\frac{d}{dt}V(z(t,\cdot)) &= \left(\left[2f\frac{\sigma}{\overline{e}(t)^2}z\partial_x z\right]_0^1 + \left[fx\frac{\overline{v}}{\overline{e}(t)}z^2\right]_0^1 - \left[z^2 f'\frac{\sigma}{\overline{e}(t)^2}\right]_0^1\right) \\
&- \frac{\sigma}{\overline{e}(t)^2}\int_0^1 \left[2f(x)(\partial_x z)^2 - f''(x)z^2\right]dx - \frac{\overline{v}}{\overline{e}(t)}\int_0^1 z^2\left(f + xf'\right)dx \\
&= \left(\frac{2}{\overline{e}(t)}f(1)\delta\psi(t)z(t,1) - \frac{\overline{v}}{\overline{e}(t)}z^2(t,1)) + \frac{\sigma}{\overline{e}(t)^2}\left(z(t,0)^2 f'(0) - z(t,1)^2 f'(1)\right)\right) \\
&- \frac{\sigma}{\overline{e}(t)^2}\int_0^1 \left[2f(x)(\partial_x z)^2 - f''(x)z^2\right]dx - \frac{\overline{v}}{\overline{e}(t)}\int_0^1 z^2\left(f + xf'\right)dx.
\end{aligned}$$

To have a Lyapunov function ensuring an exponential stability estimate, there has to exist $\gamma > 0$ such that the right-hand side is lower or equal than $-\gamma V$ for any $t \in [0,T]$ and any solution of (2.6.5). From that point one would typically require in the Lyapunov approach that for all $t \in [0,+\infty)$ and $Z \in C^2([0,1])$,

$$\begin{aligned}
&\left(\frac{2}{\overline{e}(t)}f(1)\delta\psi(t)Z(1) - \frac{\overline{v}}{\overline{e}(t)}Z^2(1)) + \frac{\sigma}{\overline{e}(t)^2}\left(Z(0)^2 f'(0) - Z(1)^2 f'(1)\right)\right) \\
&- \int_0^1 \left[2f(x)\frac{\sigma}{\overline{e}(t)^2}(\partial_x Z)^2 + \left(\frac{\overline{v}}{\overline{e}(t)}(f + xf') - f''(x)\frac{\sigma}{\overline{e}(t)^2} - \gamma f(x)\right)Z^2\right]dx \leq 0,
\end{aligned}$$

In particular this would be true for any $Z \in C^2([0,1])$ with compact support which implies that

$$\int_0^1 \left[2f(x)\frac{\sigma}{\overline{e}(t)^2}(\partial_x Z)^2 + \left(\frac{\overline{v}}{\overline{e}(t)}(f + xf') - f''(x)\frac{\sigma}{\overline{e}(t)^2} - \gamma f(x)\right)Z^2\right]dx \geq 0.$$

Since this has to be true for any time and any $Z \in C_c^2([0,1])$, and since $\overline{e}(t) \to +\infty$ when $t \to +\infty$, this implies that for any $x \in (0,1)$,

$$xf'(x) - \gamma f(x) \geq 0,$$

but as $f \in C^1([0,1];(0,+\infty))$ this is impossible: indeed, denoting $M = \sup_{[0,1]}(f') \in \mathbb{R}$ and $m = \inf_{[0,1]}(f) > 0$ this would imply in particular that

$$xM \geq \gamma m > 0,\ \forall x \in (0,1),$$

which would lead to a contradiction. Note that, although Lyapunov functionals of the form (2.6.12) fail here, some other Lyapunov functionals ([95, 232] or quadratic functionals with time-dependent weights) may manage to provide rapid stabilization results for this system.

Chapter 3

On a cross-diffusion Cahn-Hilliard system

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3.1 Introduction

The aim of this work is the study of a multispecies degenerate Ginzburg-Landau energy and its relation to a system of cross-diffusion Cahn-Hilliard equations which was recently studied in [118]. The latter model describes the evolution of a multicomponent mixture where cross-diffusion effects between the different species are taken into account, and where only one species does separate from the others. This is motivated by multiphase systems where miscible entities may coexist in one single phase, see [166] for examples. Within this phase, cross-diffusion between the different species is taken into account in order to correctly account for finite size effects that may occur at high concentrations.
We assume that the mixture occupies an open, smooth and bounded domain $\Omega \subset \mathbb{R}^d$ with $d = 1, 2, 3$ and that there are $n + 1$ species in the mixture. We denote by $u_i(x, t)$,

$i = 0, \dots, n$, the volume fraction of the ith species at point $x \in \Omega$ and time $t \geq 0$ and set $\boldsymbol{u} = (u_0, \dots, u_n)$. The dynamics of the system is governed by the free energy functional

$$E(\boldsymbol{u}) := \int_\Omega \left[\sum_{i=0}^{n} (u_i \ln u_i - u_i + 1) + \frac{\varepsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0) \right] dx, \tag{3.1.1}$$

where ε and β are positive constants. Denoting by $\boldsymbol{\mu} = D_{\boldsymbol{u}} E(\boldsymbol{u})$ the chemical potential, the corresponding evolution system formally reads as

$$\partial_t \boldsymbol{u} = \operatorname{div}(M(\boldsymbol{u}) \nabla \boldsymbol{\mu}) \quad \text{in } \Omega \times (0, +\infty), \tag{3.1.2}$$

where $M : \mathbb{R}^{n+1} \to \mathbb{R}^{(n+1)\times(n+1)}$ is a degenerate mobility matrix. More precisely, for every $i \neq j = 0, \dots, n$, let K_{ij} be positive real numbers satisfying $K_{ij} = K_{ji}$, then for $\boldsymbol{u} \in \mathbb{R}^{n+1}_+$, it has entries

$$\begin{aligned} M_{ij}(\boldsymbol{u}) &:= -K_{ij} u_i u_j && \text{for all } i \neq j = 0, \dots, n, \\ M_{ii}(\boldsymbol{u}) &:= \sum_{0 \leq k \neq i \leq n} K_{ik} u_i u_k && \text{for all } i = 0, \dots, n. \end{aligned} \tag{3.1.3}$$

As expected, due to their interpretation as volume fractions, the quantities u_i must satisfy

$$0 \leq u_i(x,t) \leq 1 \quad \text{for all } i = 0, \dots, n \quad \text{and} \quad \sum_{i=0}^{n} u_i(x,t) = 1 \text{ for a.e. } x \in \Omega,\ t \in (0, +\infty), \tag{3.1.4}$$

and the constraint on the sum is referred to as the volume-filling constraint. The evolution system is supplemented with no-flux boundary conditions as well as initial conditions consistent with the constraints. The main result from [118] is the existence of a solution to a suitable weak formulation of this problem. The aim of this paper is twofold. First, we study some solutions to the stationary problem

$$0 = \operatorname{div}(M(\boldsymbol{u}) \nabla \boldsymbol{\mu}) \quad \text{in } \Omega. \tag{3.1.5}$$

In general, the analysis of this system of coupled, degenerate elliptic equations is by no means straightforward. In this work, motivated by the gradient flow structure of the time-dependent equation highlighted above, we focus our study on the set of local minimizers of the energy functional (3.1.1). The latter are natural candidates for solutions to (3.1.5), in the sense that one naturally expects that solutions of the time-dependent system should converge in the long time limit to one of these local minimizers. We acknowledge here that other stationary solutions may exist, but stress on the fact that local energy minimizers are of particular physical relevance for the present system. When the parameters are chosen such that the energy functional is convex, the unique minimizers are constants and we show that solutions to the evolution problem (3.1.2) converge to them exponentially fast.

In the non-convex case, the dynamics is much more complex which leads us to the second aim of the paper: we introduce a finite volume scheme that preserves the structure

of the continuous time-dependent system. The simulations demonstrate the capability of the scheme and allow to explore the dynamics for arbitrary parameter regimes.

Let us briefly review previous contributions on the respective components of our model.

Cross-diffusion systems with size exclusion

Systems of partial differential equations with cross-diffusion have gained a lot of interest in recent years [171, 76, 77, 177, 156] and appear in many applications, for instance the modelling of population dynamics of multiple species [54] or cell sorting as well as chemotaxis-like applications [203, 202].

Ginzburg-Landau Energy

In the case $n = 1$, which implies $u_0 = 1 - u_1$, (3.1.1) reduces to the classical Ginzburg-Landau energy with singular potential as introduced in [58]. The works [140, 139] study the structure of energy minimizers to the functional

$$E_{\mathrm{GL}}(v) = \int_\Omega \frac{1}{2}|\nabla v|^2 + \frac{1}{4}(1 - v^2)^2 \, dx,$$

when the system size is large and the mean value of the phase parameter v is close to -1. The authors study the case when constant stationary states are local but not global minimizers and estimate the size of the energy barrier, i.e. the difference of the energy at the respective states. In particular, the authors prove bounds on the minimizers using suitable competitors which inspired part of the construction in the proof of Theorem 7.

Cahn-Hilliard equation

The scalar Cahn-Hilliard equation with constant mobility was introduced in [58] as a model for phase separation. It is indeed the H^{-1}-gradient flow to (3.1.1) for two species. Existence of weak solutions was first shown in e.g. [122, 56] in the case of constant mobility, and later extended to degenerate, concentration dependent mobilities [120]. Regarding the long-time behaviour, for a constant mobility and in one spatial dimension, the authors in [200] show that for initial data with bounded distance to a so-called kink state, algebraic convergence to equilibrium holds. This was further improved in [199]. We also refer to [1, 213, 214] for long-time analysis in the case of logarithmic nonlinearity. More details can be found in the review [195] and the monograph [190].

Multi-species Cahn-Hilliard systems have been studied in several earlier works and usually consider an energy functional of the form

$$E(\boldsymbol{u}) := \int_\Omega \Big[\Psi(\boldsymbol{u}) + \frac{1}{2}\nabla \boldsymbol{u} \cdot \Gamma \nabla \boldsymbol{u}\Big] dx, \tag{3.1.6}$$

for some symmetric positive semi-definite matrix $\Gamma \in \mathbb{R}^{(n+1)\times(n+1)}$ and bulk free-energy functional Ψ. In [121], Elliott and Luckhaus proved a global existence result for such a multiphase Cahn-Hilliard system with constant mobility and $\Gamma = \gamma \mathrm{I}$ for some $\gamma > 0$.

In [119], the authors generalized their result to the case of a degenerate concentration-dependent mobility matrix with a positive definite matrix Γ while [52] study a system of Cahn-Hilliard/Allen-Cahn equations with cross-kinetic coupling. Recently, in [43], the authors proposed a novel hierarchy of multispecies Cahn-Hilliard systems which are consistent with the standard two-species Cahn-Hilliard system, and which read as the model introduced above with Γ positive definite, a particular Ψ and for a constant mobility matrix. Numerical methods for such systems were proposed and analyzed in several contributions, see e.g. [132, 230, 78, 22].

Concerning coupled cross-diffusion Cahn-Hilliard systems, other than [118], the only work we are aware of is [150], which treats the case where all species aim to separate, i.e. the case when Γ in (3.1.6) is positive definite.

Structure-preserving finite volume schemes.

The finite volume method is a classical discretization method to approximate conservation laws, see a pedagogical introduction in [128]. It is a natural physical requirement for a discretization method to preserve as much as possible of the structure of the continuous problem such as conservation laws, nonnegativity or dissipation. In addition, such properties can be mathematically useful, since they enable to "transfer" the mathematical analysis to the discrete level. A method that preserves the dissipation of an energy (resp. entropy) is often called "energy-stable" (resp. entropy-stable). Following the success of the entropy method, there has been considerable effort in order to preserve the entropy structure of scalar parabolic equations [35, 70, 63] and parabolic systems [60, 62, 61, 65, 164, 162, 101, 161, 64, 146, 157] at the discrete level. See also a review of energy-stable schemes for the Cahn-Hilliard equation in [44].

3.1.1 Contributions and outline

Our work makes the following contributions

- Proving existence and uniform lower and upper bounds for the local minimizers of (3.1.1) in the $L^\infty(\Omega)^{n+1}$ topology. We emphasise that the latter, in contrast to the results of [118], requires a construction which has to preserve not only the constraints (3.1.4) but also the mass of the competitor (candidate for lower energy in the contradiction argument), which significantly complicates the argument.

- Gaining regularity of the minimizers from the Euler-Lagrange system, we show that they qualify as classical solutions to the stationary system. We also show that the Euler-Lagrange equation for the void species decouples, revealing a strong link with the single-species energy.

- We study the convexity properties of (3.1.1) and are able to give explicit quantitative bounds. In a particular parameters regime, we show that the minimizers are constant and that solutions to the dynamical system converge exponentially

fast to them, for arbitrary initial data with finite energy. We give explicit rates of convergence.

- We introduce a two-point finite volume scheme that approximates the evolution problem (3.1.2), preserving the constraints (3.1.4). The discrete free energy is shown to be nonincreasing, adapting the convex-concave splitting of [118] to the discrete case. We provide numerical simulations to illustrate the behaviour of the scheme and to investigate the variety of stationary solutions in the long-time limit.

Remark 5 (Nonlocal and potential contributions to the energy)**.** *We remark that most of the results of this work remain valid, after minor modifications, if potential or non-local interaction terms of the form*

$$\int_\Omega V_i(x)u_i(x)\,dx \qquad or \qquad c_{ij}\int_\Omega u_i L * u_j\,dx$$

are added to the energy. Here, for all $0 \le i \le n$, $V_i : \Omega \to \mathbb{R}$ *is a given potential and* $L : \Omega \to \mathbb{R}$ *is an interaction kernel. All these functions must be sufficiently smooth. With these additions, existence of minimizers (Lemma 11), strict bounds (Theorem 7) hold without any changes. First order optimality conditions have to be adapted and the regularity of solutions (Theorem 8) is limited by the regularity of* L *and* $V := (V_i)_{0\le i\le n}$. *Under suitable assumptions on the matrix* $C = (c_{ij})_{0\le i,j\le n}$ *the numerical scheme can be adapted and still preserves the structure.*

The paper is organised as follows: Section 3.2 contains an analysis of properties of the energy functional and establishes the link with stationary solutions. Section 3.3 is dedicated to the large-time asymptotics in a globally stable regime. Section 3.4 is devoted to the introduction of a structure preserving finite volume scheme and some numerical results are presented in Section 3.5.

3.1.2 The model

We now present the system under consideration in full detail. For $\varepsilon > 0$ and $\beta > 0$ we consider the energy functional given by (3.1.1). We define formally the chemical potentials as variational derivatives of the energy by

$$\mu_i := D_{u_i}E(\boldsymbol{u}) = \ln u_i \qquad \text{for all } i = 1,\dots,n, \tag{3.1.7}$$

as well as

$$\mu_0 := D_{u_0}E(\boldsymbol{u}) = \ln u_0 - \varepsilon\Delta u_0 + \beta(1-2u_0), \tag{3.1.8}$$

so that $\boldsymbol{\mu} := (\mu_0, \mu_1, \dots, \mu_n) = D_{\boldsymbol{u}}E(\boldsymbol{u})$. Furthermore, we introduce the auxiliary variables

$$w_i = \ln u_i - \ln u_0,\ i = 1,\dots,n, \tag{3.1.9}$$

as well as

$$w_0 := -\varepsilon\Delta u_0 + \beta(1-2u_0). \tag{3.1.10}$$

With these definitions, (3.1.2) can be rewritten as

$$\begin{aligned}\partial_t u_i &= \operatorname{div}\left(\sum_{0\le j\ne i\le n} K_{ij}u_iu_j\nabla(\mu_i-\mu_j)\right)\\ &= \operatorname{div}\left(\sum_{0\le j\ne i\le n} K_{ij}u_iu_j\nabla(w_i-w_j)\right)\\ &= \operatorname{div}\left(\sum_{0\le j\ne i\le n} K_{ij}(u_j\nabla u_i-u_i\nabla u_j)-K_{i0}u_iu_0\nabla w_0\right),\end{aligned} \tag{3.1.11}$$

for $i=1,\dots,n$ and

$$\begin{aligned}\partial_t u_0 &= \operatorname{div}\left(\sum_{j=1}^{n} K_{0j}u_0u_j\nabla(\mu_0-\mu_j)\right)\\ &= \operatorname{div}\left(\sum_{j=1}^{n} K_{0j}u_0u_j\nabla(w_0-w_j)\right)\\ &= \operatorname{div}\left(\sum_{j=1}^{n} K_{0j}(u_j\nabla u_0-u_0\nabla u_j+u_0u_j\nabla w_0)\right).\end{aligned} \tag{3.1.12}$$

The conservative form (3.1.2) together with the zero-flux boundary conditions suggest that the mass of each species is conserved along the evolution. Therefore, given fixed masses $m_0,\dots,m_n>0$ such that $\sum_{j=0}^{n} m_j=|\Omega|$, we will look for solutions to (3.1.5) in the admissible set

$$\begin{aligned}\mathcal{A}_m := \Bigg\{\boldsymbol{u} := (u_0,\dots,u_n)\in (L^\infty(\Omega))^{n+1} :\ u_i\ge 0,\ \int_\Omega u_i\,dx = m_i,\ i=0,\dots,n,\\ \sum_{j=0}^{n} u_j = 1 \text{ a.e. in } \Omega \text{ and } u_0\in H^1(\Omega)\Bigg\}.\end{aligned}$$

Note that $\mathcal{A}_m$ is non-empty, convex, and that for any $\boldsymbol{u}\in\mathcal{A}_m$, it holds $0\le u_i\le 1$ for all $i=0,\dots,n$.

3.2 Minimizers of the energy functional

In this section we use the direct method of the calculus of variations to prove the existence of minimizers to the energy (3.1.1) over the set $\mathcal{A}_m$:

$$\min_{\boldsymbol{u}\in\mathcal{A}_m} E(\boldsymbol{u}). \tag{3.2.1}$$

Arguing by means of competitors, we further obtain strict bounds which then allow for higher regularity by making use of the optimality conditions. In consequence, minimizers are solutions to the stationary problem (3.1.5).

Lemma 11. *Let $E\colon \mathcal{A}_m \to \mathbb{R}$ be defined by (3.1.1). Then, E has at least one minimizer.*

Proof. We apply the direct method of calculus of variations. First, using the non-negativity of the function $[0,1] \ni x \mapsto x \ln x - x + 1$, together with the fact that $|\nabla v_0|^2 \geq 0$ and that $v_0(1-v_0) \geq 0$ for any $\boldsymbol{v} = (v_0, \dots, v_n) \in \mathcal{A}_m$, we obtain that E is nonnegative on $\mathcal{A}_m$. Moreover, it is clear that $\mathcal{A}_m$ contains constant solutions with finite energy. Thus, there exists a minimizing sequence $\left(\boldsymbol{v}^{(p)}\right)_{p\in\mathbb{N}} \subset \mathcal{A}_m$ such that $E\left(\boldsymbol{v}^{(p)}\right)$ is bounded and

$$\lim_{p\to\infty} E\big(\boldsymbol{v}^{(p)}\big) = \inf_{\mathcal{A}_m} E.$$

In particular, we have that $\left(\left\|\nabla v_0^{(p)}\right\|_{L^2(\Omega)}\right)_{p\in\mathbb{N}}$ is bounded as well. Therefore, without relabelling, up to the extraction of a subsequence, there exists $u_0 \in H^1(\Omega)$ such that $\nabla v_0^{(p)} \rightharpoonup \nabla u_0$ weakly in $L^2(\Omega)$, and thanks to the uniform L^∞-bound we have $v_0^{(p)} \to u_0$ strongly in $L^q(\Omega)$ for every $1 \leq q < \infty$ and a.e. in Ω. Furthermore, since $v_i^{(p)}$ is bounded in $L^2(\Omega)$ by construction, it follows that, up to the extraction of a subsequence, for all $i = 1, \dots, n$, there exists $u_i \in L^2(\Omega)$ such that $v_i^{(p)} \rightharpoonup u_i$ weakly in $L^2(\Omega)$. We also easily obtain that $0 \leq u_i \leq 1$ almost everywhere on Ω. Then the convexity of the integrands together with the strong continuity of the functional (dominated convergence) imply the lower-semicontinuity

$$\int_\Omega u_i \ln u_i \, dx \leq \liminf_{p\to\infty} \int_\Omega v_i^{(p)} \ln v_i^{(p)} \, dx$$

as well as

$$\int_\Omega |\nabla u_0|^2 \, dx \leq \liminf_{p\to\infty} \int_\Omega \left|\nabla v_0^{(p)}\right|^2 \, dx.$$

Furthermore, the weak convergence in $L^2(\Omega)$ yields

$$\int_\Omega \big(-v_i^{(p)} + 1\big) \, dx \to \int_\Omega \big(-u_i + 1\big) \, dx \quad \text{for all } i = 0, \dots, n,$$

while the strong convergence gives

$$\int_\Omega v_0^{(p)}\big(1 - v_0^{(p)}\big) \, dx \to \int_\Omega u_0 \left(1 - u_0\right) \, dx.$$

This implies

$$E(\boldsymbol{u}) \leq \liminf_{p\to\infty} E(\boldsymbol{v}^{(p)}) = \inf_{\mathcal{A}_m} E,$$

and that $\int_\Omega u_i \, dx = m_i$ for $i = 0, \dots, n$. Finally, the weak convergence in $L^2(\Omega)$ also yields that $\sum_{i=0}^{n} u_i = 1$ almost everywhere in Ω so that $\boldsymbol{u} \in \mathcal{A}_m$. The conclusion follows. □

Remark 6. *We point out that the uniqueness of the minimizer is neither guaranteed nor expected, due to the non-convexity of the energy functional.*

A remarkable property is that the minimizers are in the interior of the set $\mathcal{A}_m$, i.e. they strictly satisfy the box constraints in (3.1.4). This is shown by constructing suitable competitors in the following theorem.

Theorem 7. *Let E be the energy functional given by (3.1.1). Then, there exists a constant $\delta > 0$ such that for every local minimizer $\boldsymbol{u} \in \mathcal{A}_m$ of E for the $L^\infty(\Omega)^{n+1}$ topology, it holds that*

$$\delta \leq u_i \quad a.e, \text{ for all } i = 0, \dots, n,$$

which, together with the volume-filling constraint in (3.1.4), implies the upper bound

$$u_i \leq 1 - n\delta \quad a.e, \text{ for all } i = 0, \dots, n.$$

Proof. Let $\boldsymbol{u} := (u_0, \dots, u_n) \in \mathcal{A}_m$ be a local minimizer of E for the $L^\infty(\Omega)^{n+1}$ topology, i.e. there exists $\epsilon > 0$ such that for all $\boldsymbol{v} := (v_0, \dots, v_n) \in \mathcal{A}_m$ with $\|\boldsymbol{v} - \boldsymbol{u}\|_{L^\infty(\Omega)} := \max_{i=0,\dots,n} \|v_i - u_i\|_{L^\infty(\Omega)} \leq \epsilon$, necessarily $E(\boldsymbol{v}) \geq E(\boldsymbol{u})$ holds. In order to prove the assertion, we proceed as follows: first we show that there exists $\delta_0 > 0$ such that $\delta_0 \leq u_0 \leq 1 - \delta_0$. Then we proceed to show that there exists $\delta_i > 0$ such that $\delta_i \leq u_i$ for $i = 1, \dots, n$. Finally, $\delta := \min(\delta_0, \delta_1, \dots, \delta_n)$ is the constant that appears in the statement.

<u>Step 1: $\delta_0 \leq u_0$</u>. Arguing by contradiction, we assume that for all $\min\left(\epsilon, \dfrac{m_0}{2|\Omega|}\right) \geq \delta > 0$ the set

$$\mathcal{C}_\delta = \{x \in \Omega : \, u_0(x) < \delta\}$$

is such that $|\mathcal{C}_\delta| > 0$. We further define the set

$$\mathcal{C}_{\text{avg}} := \left\{ x \in \Omega \; : \; u_0(x) > \frac{m_0}{|\Omega|} \right\},$$

i.e. the part of Ω on which u_0 strictly exceeds its average. Note that

$$\mathcal{C}_{\frac{m_0}{2|\Omega|}} \cap \mathcal{C}_{\text{avg}} = \emptyset \quad \text{and} \quad \left|\mathcal{C}_{\frac{m_0}{2|\Omega|}}\right| > 0$$

imply $|\mathcal{C}_{\text{avg}}| > 0$. We then define, for all $0 \leq \lambda \leq 1$, the perturbed function

$$u_0^{\delta,\lambda} = \begin{cases} \delta & \text{in } \mathcal{C}_\delta \\ (1-\lambda)u_0 + \lambda \frac{m_0}{|\Omega|} & \text{in } \mathcal{C}_{\text{avg}} \\ u_0 & \text{otherwise,} \end{cases}$$

which satisfies $0 \leq u_0^{\delta,\lambda} \leq 1$ and $u_0^{\delta,\lambda} \in H^1(\Omega)$. Moreover, for any $0 \leq \lambda \leq \epsilon/2$, it holds that $\|u_0 - u_0^{\delta,\lambda}\|_{L^\infty(\Omega)} \leq \epsilon$. Observe that

$$\int_\Omega u_0^{\delta,0} \, dx = \int_{\mathcal{C}_\delta} \delta \, dx + \int_{\Omega \setminus \mathcal{C}_\delta} u_0 \, dx > \int_{\mathcal{C}_\delta} u_0 \, dx + \int_{\Omega \setminus \mathcal{C}_\delta} u_0 \, dx = m_0,$$

while on the other hand

$$\begin{aligned}\int_\Omega u_0^{\delta,\lambda}\,dx &= \int_{\mathcal{C}_\delta} \delta\,dx + \int_{\Omega\setminus(\mathcal{C}_\delta\cup\mathcal{C}_{\text{avg}})} u_0\,dx + \lambda\int_{\mathcal{C}_{\text{avg}}} \frac{m_0}{|\Omega|}\,dx + (1-\lambda)\int_{\mathcal{C}_{\text{avg}}} u_0\,dx \\ &= \delta|\mathcal{C}_\delta| + \int_{\Omega\setminus\mathcal{C}_\delta} u_0\,dx + \lambda\int_{\mathcal{C}_{\text{avg}}}\left(\frac{m_0}{|\Omega|} - u_0\right)dx.\end{aligned}$$

In order to estimate the last integral of the previous equality we observe that

$$\begin{aligned}0 &= \int_\Omega \left(\frac{m_0}{|\Omega|} - u_0\right)dx \\ &= \int_{\mathcal{C}_{\frac{m_0}{2|\Omega|}}} \left(\frac{m_0}{|\Omega|} - u_0\right)dx + \int_{\Omega\setminus(\mathcal{C}_{\frac{m_0}{2|\Omega|}}\cup\mathcal{C}_{\text{avg}})} \left(\frac{m_0}{|\Omega|} - u_0\right)dx + \int_{\mathcal{C}_{\text{avg}}} \left(\frac{m_0}{|\Omega|} - u_0\right)dx \\ &\geq \frac{m_0}{2|\Omega|}|\mathcal{C}_{\frac{m_0}{2|\Omega|}}| + \int_{\mathcal{C}_{\text{avg}}} \left(\frac{m_0}{|\Omega|} - u_0\right)dx,\end{aligned}$$

which implies

$$\int_{\mathcal{C}_{\text{avg}}} \left(\frac{m_0}{|\Omega|} - u_0\right)\,dx \leq -\frac{m_0}{2|\Omega|}|\mathcal{C}_{\frac{m_0}{2|\Omega|}}|.$$

Then, from the previous calculations, we conclude that for any $0 < \delta < \min\left(\epsilon, \frac{m_0}{2|\Omega|}\right)$ and any $\lambda \in [0, \epsilon/2]$,

$$\int_\Omega u_0^{\delta,\lambda}\,dx \leq \left(\delta - \lambda\frac{m_0}{2|\Omega|}\right)|\mathcal{C}_{\frac{m_0}{2|\Omega|}}| + m_0. \tag{3.2.2}$$

Let us now assume that δ is chosen so that $\delta < \frac{\epsilon m_0}{4|\Omega|}$. Then, it holds that

$$\int_\Omega u_0^{\delta,\epsilon/2}\,dx \leq \left(\delta - \epsilon\frac{m_0}{4|\Omega|}\right)|\mathcal{C}_{\frac{m_0}{2|\Omega|}}| + m_0 < m_0.$$

Thus, for all $0 < \delta < \frac{\epsilon m_0}{4|\Omega|}$, there exists $\lambda_\delta^* \in (0, \epsilon/2)$ such that the function $u_0^\delta := u_0^{\delta,\lambda_\delta^*}$ satisfies

$$\int_\Omega u_0^\delta\,dx = m_0. \tag{3.2.3}$$

Furthermore, it holds from (3.2.2) that λ_δ^* necessarily satisfies $\lambda_\delta^* \leq \frac{2|\Omega|\delta}{m_0}$, so that $\lim_{\delta\to 0}\lambda_\delta^* = 0$.

While the constructed u_0^δ preserves the mass constraint, the volume-filling constraint is no longer valid. To recover them we have to modify at least one of the other species. To this end, we make the following observation: in the set $\mathcal{C}_\delta$, it holds that

$$\sum_{i=1}^n u_i = 1 - u_0 \geq 1 - \delta.$$

Therefore, denoting by $\overline{u} := \max_{i=1,\dots,n} u_i$, we necessarily have

$$\overline{u} \geq \frac{1-\delta}{n} \text{ in } \mathcal{C}_\delta \quad \text{and} \quad \overline{u} \leq \sum_{i=1}^{n} u_i = 1 - u_0 \leq 1 - \frac{m_0}{|\Omega|} \text{ in } \mathcal{C}_{\text{avg}}. \tag{3.2.4}$$

Let us now define for almost all $x \in \Omega$

$$\bar{k}(x) := \min\left\{k = 1, \dots, n, \quad u_k(x) = \max_{i=1,\dots,n} u_i(x)\right\}$$

so that $\overline{u}(x) = u_{\bar{k}(x)}(x)$ almost everywhere on Ω. Let us then denote for all $k = 1, \dots, n$, $\mathcal{C}_\delta^k := \{x \in \mathcal{C}_\delta,\ \bar{k}(x) = k\}$ so that $\mathcal{C}_\delta = \bigcup_{k=1}^{n} \mathcal{C}_\delta^k$ and $\mathcal{C}_\delta^k \cap \mathcal{C}_\delta^{k'} = \emptyset$ as soon as $k \neq k'$. By definition, it then holds that

$$u_k = \overline{u} \text{ in } \mathcal{C}_\delta^k. \tag{3.2.5}$$

On the one hand, let us introduce

$$m_{0,k}^\delta := \int_{\mathcal{C}_\delta^k} (u_0^\delta - u_0)\, dx.$$

Then, it holds that $0 \leq m_{0,k}^\delta \leq \delta|\mathcal{C}_\delta^k| \leq \delta|\Omega|$. On the other hand, from the definition of u_0^δ and from the calculations above, it holds that

$$\int_{\mathcal{C}_{\text{avg}}} (u_0 - u_0^\delta)\, dx = \int_{\mathcal{C}_\delta} (u_0^\delta - u_0)\, dx = \sum_{k=1}^{n} m_{0,k}^\delta.$$

Therefore, using Lemma 16, there always exist measurable subsets $\mathcal{C}_{\text{avg}}^{\delta,k}$ for $k = 1, \dots, n$ such that

- $\bigcup_{k=1}^{n} \mathcal{C}_{\text{avg}}^{\delta,k} = \mathcal{C}_{\text{avg}}$;
- $\mathcal{C}_{\text{avg}}^{\delta,k} \cap C_{\text{avg}}^{\delta,k'} = \emptyset$ as soon as $k \neq k'$;
- $\int_{\mathcal{C}_{\text{avg}}^{\delta,k}} (u_0 - u_0^\delta)\, dx = m_{0,k}^\delta = -\int_{\mathcal{C}_\delta^k} (u_0 - u_0^\delta)\, dx$.

We can then define for all $k = 1, \dots, n$ the perturbed function u_k^δ in the following way:

$$u_k^\delta = \begin{cases} u_k + (u_0 - u_0^\delta) & \text{in } \mathcal{C}_\delta^k \cup \mathcal{C}_{\text{avg}}^{\delta,k} \\ u_k & \text{otherwise.} \end{cases} \tag{3.2.6}$$

It can then be easily checked that $\|u_k^\delta - u_k\|_{L^\infty(\Omega)} \leq \epsilon$ for δ arbitrarily small. Moreover, as a consequence of (3.2.4) and (3.2.5), for δ small enough, it holds for all $k = 1, \dots, n$,

$$0 \leq \frac{1-\delta}{n} - \delta \leq u_k^\delta = u_k + (u_0 - u_0^\delta) \leq u_k \leq 1 \text{ in } \mathcal{C}_\delta^k.$$

On the other hand, using again (3.2.4) and (3.2.5), we can estimate

$$0 \le u_k \le u_k^\delta = u_k + (u_0 - u_0^\delta) = u_k + \lambda_\delta^*\Big(u_0 - \frac{m_0}{|\Omega|}\Big) \le 1 - \frac{m_0}{|\Omega|} + \lambda_\delta^*\Big(1 - \frac{m_0}{|\Omega|}\Big) \text{ in } \mathcal{C}_{\text{avg}}^{\delta,k}.$$

Since $\lambda_\delta^* \underset{\delta\to 0}{\longrightarrow} 0$, choosing δ small enough implies that $\lambda_\delta^*(1 - m_0/|\Omega|) < m_0/|\Omega|$ and therefore $u_k^\delta \le 1$ in $\mathcal{C}_{\text{avg}}^{\delta,k}$. Furthermore,

$$\int_\Omega u_k^\delta \, dx = \int_\Omega u_k \, dx + \int_{\mathcal{C}_{\text{avg}}^{\delta,k} \cup \mathcal{C}_\delta^k} (u_0 - u_0^\delta) \, dx = \int_\Omega u_k \, dx. \tag{3.2.7}$$

Finally, we observe that, almost everywhere in Ω,

$$\sum_{i=1}^n u_i^\delta = \sum_{i=1}^n u_i + (u_0 - u_0^\delta),$$

holds so that $\sum_{i=0}^n u_i^\delta = \sum_{i=0}^n u_i = 1$. From this, we conclude that $\boldsymbol{u}^\delta := (u_0^\delta, \dots, u_n^\delta)$ lies in the set $\mathcal{A}_m$ and satisfies $\|\boldsymbol{u} - \boldsymbol{u}^\delta\|_{L^\infty(\Omega)^{n+1}} \le \epsilon$ for δ small enough.

We now show that for $\delta \ll 1$, it holds $E(\boldsymbol{u}^\delta) < E(\boldsymbol{u})$ strictly, which gives us the desired contradiction. Firstly, let us note that $|\nabla u_0^\delta| \le |\nabla u_0|$, which gives

$$\begin{aligned} E(\boldsymbol{u}^\delta) - E(\boldsymbol{u}) \le \int_\Omega \sum_{i=0}^n \Big((u_i^\delta \ln u_i^\delta - u_i \ln u_i) - (u_i^\delta - u_i) \Big) \, dx \\ + \beta \int_\Omega \Big(u_0^\delta (1 - u_0^\delta) - u_0(1 - u_0) \Big) \, dx \end{aligned}$$

To estimate this difference, we first observe that (3.2.3)-(3.2.7) imply

$$\int_\Omega (u_i^\delta - u_i) \, dx = 0 \quad \text{for } i = 0, \dots, n.$$

Using the convexity of $x \mapsto x \ln x$ and the concavity of $x \mapsto x(1-x)$ allows to further estimate

$$\begin{aligned} E(\boldsymbol{u}^\delta) - E(\boldsymbol{u}) &\le \sum_{k=1}^n \int_\Omega \Big(\ln u_k^\delta + 1\Big)(u_k^\delta - u_k) \, dx + \int_\Omega \Big(\ln u_0^\delta + 1\Big)(u_0^\delta - u_0) \, dx \\ &\quad + \beta \int_\Omega (1 - 2u_0)(u_0^\delta - u_0) \, dx \\ &=: \Delta E_1 + \Delta E_2 + \Delta E_3. \end{aligned} \tag{3.2.8}$$

To estimate ΔE_1 we first observe that

$$\begin{aligned} \Delta E_1 &= \sum_{k=1}^n \int_\Omega \Big(\ln u_k^\delta + 1\Big)(u_k^\delta - u_k) \, dx = \sum_{k=1}^n \int_{\mathcal{C}_\delta^k \cup \mathcal{C}_{\text{avg}}^{\delta,k}} \Big(\ln u_k^\delta + 1\Big)(u_0 - u_0^\delta) \, dx \\ &= \sum_{k=1}^n \int_{\mathcal{C}_\delta^k \cup \mathcal{C}_{\text{avg}}^{\delta,k}} - \ln u_k^\delta (u_0^\delta - u_0) \, dx. \end{aligned} \tag{3.2.9}$$

The quantity $-\ln u_k^\delta$ is nonnegative in $\mathcal{C}_\delta^k \cup \mathcal{C}_{\text{avg}}^{\delta,k}$ while $(u_0^\delta - u_0)$ is nonnegative in C_δ^k and nonpositive in $\mathcal{C}_{\text{avg}}^{\delta,k}$, and furthermore (3.2.4) gives

$$-\ln u_k = -\ln(\overline{u}) \leq -\ln\left(\frac{1-\delta}{n}\right) \leq -\ln\left(\frac{1}{n}\left(1-\frac{m_0}{2|\Omega|}\right)\right) \text{ in } \mathcal{C}_\delta^k.$$

Therefore (3.2.9) reduces to

$$\Delta E_1 \leq -\ln\left(\frac{1}{n}\left(1-\frac{m_0}{2|\Omega|}\right)\right)\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx.$$

In order to estimate the second term on the right-hand side of (3.2.8) we first observe that in the set $\mathcal{C}_{\text{avg}}$ it holds $\ln u_0^\delta \geq \ln(m_0/|\Omega|)$, while due to the mass conservation we have

$$\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx = -\int_{\mathcal{C}_{\text{avg}}}(u_0^\delta - u_0)\,dx. \tag{3.2.10}$$

It follows that

$$\begin{aligned}\Delta E_2 &= \int_\Omega \ln u_0^\delta(u_0^\delta - u_0)\,dx \leq \ln\delta\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx + \ln(m_0/|\Omega)|\int_{\mathcal{C}_{\text{avg}}}(u_0^\delta - u_0)\,dx\\ &= (\ln\delta - \ln(m_0/|\Omega|))\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx.\end{aligned}$$

Finally, for the last term in (3.2.8) we use the fact that $-1 \leq 1-2u_0 \leq 1$ and (3.2.10) again to have

$$\begin{aligned}\Delta E_3 &\leq \beta\int_\Omega(1-2u_0)(u_0^\delta - u_0)\,dx \leq \beta\int_\Omega|u_0^\delta - u_0|\,dx\\ &\leq \beta\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx - \beta\int_{\mathcal{C}_{\text{avg}}}(u_0^\delta - u_0)\,dx = 2\beta\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx.\end{aligned} \tag{3.2.11}$$

Summarising we have

$$E(\boldsymbol{u}^\delta) - E(\boldsymbol{u}) \leq \left[\ln\delta - \ln(m_0/|\Omega|) - \ln\left(\frac{1}{n}\left(1-\frac{m_0}{2|\Omega|}\right)\right) + 2\beta\right]\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx.$$

Thus, since $\int_{\mathcal{C}_\delta}(u_0^\delta - u_0)\,dx > 0$ for all $\delta > 0$, taking δ sufficiently small so that the constant in front of this integral becomes negative yields the desired contradiction.

Step 2: $u_0 \leq 1-\delta_0$. We argue again by contradiction and assume that for all $\min\left(\epsilon, \frac{m_0}{2|\Omega|}\right) \geq \delta > 0$ the set

$$\widetilde{\mathcal{C}}_\delta = \{x \in \Omega : u_0(x) > 1-\delta\}$$

is such that $|\widetilde{\mathcal{C}}_\delta| > 0$. We further define the set

$$\widetilde{\mathcal{C}}_{\text{avg}} := \left\{ x \in \Omega \ : \ u_0(x) < \frac{m_0}{|\Omega|} \right\},$$

i.e. the part of Ω on which u_0 is strictly below its average. As before we argue that $|\widetilde{\mathcal{C}}_\delta| > 0$ for all $\delta > 0$ arbitrarily small implies $|\widetilde{\mathcal{C}}_{\text{avg}}| > 0$. We then define, for $0 \leq \lambda \leq 1$, the perturbed function

$$\tilde{u}_0^{\delta,\lambda} = \begin{cases} 1-\delta & \text{in } \widetilde{\mathcal{C}}_\delta \\ \lambda u_0 + (1-\lambda)\frac{m_0}{|\Omega|} & \text{in } \widetilde{\mathcal{C}}_{\text{avg}} \\ u_0 & \text{otherwise,} \end{cases}$$

and arguing as in the previous step we show that for all $\frac{\epsilon m_0}{4|\Omega|} > \delta > 0$ there exists $\lambda_\delta^* \in (0, \epsilon/2)$ such that the function $\tilde{u}_0^\delta := \tilde{u}_0^{\delta,\lambda_\delta^*}$ has the same mass as u_0 and satisfies $\|u_0 - \tilde{u}_0^\delta\|_{L^\infty(\Omega)} \leq \epsilon$. We then observe that it holds

$$\sum_{i=1}^n u_i = 1 - u_0 \geq 1 - \frac{m_0}{|\Omega|} \quad \text{in } \widetilde{\mathcal{C}}_{\text{avg}},$$

which implies that the function $\overline{u} := \max_{i=1,\dots,n} u_i$ must satisfy

$$\overline{u} \geq \frac{1}{n}\Big(1 - \frac{m_0}{|\Omega|}\Big) \text{ in } \widetilde{\mathcal{C}}_{\text{avg}} \quad \text{and} \quad \overline{u} \leq \sum_{i=1}^n u_i = 1 - u_0 \leq \delta \text{ in } \widetilde{\mathcal{C}}_\delta.$$

For almost all $x \in \Omega$, we denote by $\tilde{k}(x) := \min\big\{k = 1, \dots, n, \ u_k(x) = \max_{i=1,\dots,n} u_i(x)\big\}$. Moreover, for all $k = 1, \dots, n$ we denote by $\widetilde{\mathcal{C}}_\delta^k := \Big\{x \in \widetilde{\mathcal{C}}_\delta, \ \tilde{k}(x) = k\Big\}$ so that $\widetilde{\mathcal{C}}_\delta = \bigcup_{k=1}^n \widetilde{\mathcal{C}}_\delta^k$ and $\widetilde{\mathcal{C}}_\delta^k \cap \widetilde{\mathcal{C}}_\delta^{k'} = \emptyset$ as soon as $k \neq k'$. By definition, it then holds that

$$u_k = \overline{u} \ \text{ in } \widetilde{\mathcal{C}}_\delta^k.$$

By the mass conservation property

$$\int_{\widetilde{\mathcal{C}}_{\text{avg}}} (u_0 - \tilde{u}_0^\delta)\, dx = \int_{\widetilde{\mathcal{C}}_\delta} (\tilde{u}_0^\delta - u_0)\, dx, \tag{3.2.12}$$

for all $\delta > 0$ sufficiently small, using again Lemma 16, there exist measurable subsets $\widetilde{\mathcal{C}}_{\text{avg}}^{\delta,k} \subset \widetilde{\mathcal{C}}_{\text{avg}}$ for all $k = 1, \dots, n$ such that

- $\widetilde{\mathcal{C}}_{\text{avg}} = \bigcup_{k=1}^n \widetilde{\mathcal{C}}_{\text{avg}}^{\delta,k}$;
- $\widetilde{\mathcal{C}}_{\text{avg}}^{\delta,k} \cap \widetilde{\mathcal{C}}_{\text{avg}}^{\delta,k'} = \emptyset$ as soon as $k \neq k'$;

- $\int_{\widetilde{\mathcal{C}}^{\delta,k}_{\text{avg}}} (u_0 - \tilde{u}_0^\delta)\, dx = \int_{\widetilde{\mathcal{C}}^k_\delta} (\tilde{u}_0^\delta - u_0)\, dx$.

Thus, for δ sufficiently small, for all $k = 1, \dots, n$, we define the function

$$\tilde{u}_k^\delta = \begin{cases} u_k + (u_0 - u_0^\delta) & \text{in } \widetilde{\mathcal{C}}^k_\delta \cup \widetilde{\mathcal{C}}^{\delta,k}_{\text{avg}} \\ u_k & \text{otherwise} \end{cases}$$

which is such that $0 \le \tilde{u}_k^\delta \le 1$ and $\displaystyle\int_\Omega \tilde{u}_k^\delta \, dx = \int_\Omega u_k \, dx$. Using similar arguments as in Step 1, we obtain that for δ sufficiently small, $\tilde{\boldsymbol{u}}^\delta := (\tilde{u}_0^\delta, \dots, \tilde{u}_n^\delta) \in \mathcal{A}_m$ and $\|\tilde{\boldsymbol{u}}^\delta - \boldsymbol{u}\|_{L^\infty(\Omega)^{n+1}} \le \epsilon$. Moreover, it holds that

$$\begin{aligned} E(\tilde{\boldsymbol{u}}^\delta) - E(\boldsymbol{u}) \le \sum_{k=1}^n \int_\Omega \ln \tilde{u}_k^\delta (\tilde{u}_k^\delta - u_k)\, dx + \int_\Omega \ln \tilde{u}_0^\delta (\tilde{u}_0^\delta - u_0)\, dx \\ + \beta \int_\Omega (1 - 2u_0)(\tilde{u}_0^\delta - u_0)\, dx =: \Delta E_1 + \Delta E_2 + \Delta E_3. \end{aligned}$$

To estimate ΔE_1 we first observe that

$$-\ln u_k \begin{cases} \le -\ln\left(\frac{1}{n}(1 - \frac{m_0}{|\Omega|})\right) & \text{in } \widetilde{\mathcal{C}}^{\delta,k}_{\text{avg}} \\ \ge -\ln \delta & \text{in } \widetilde{\mathcal{C}}^k_\delta. \end{cases}$$

Thus we can estimate

$$\begin{aligned} \Delta E_1 &= \sum_{k=1}^n \int_\Omega \ln \tilde{u}_k^\delta (\tilde{u}_k^\delta - u_{\bar{k}})\, dx = \sum_{k=1}^n \int_{\widetilde{\mathcal{C}}^{\delta,k}_{\text{avg}} \cup \widetilde{\mathcal{C}}^k_\delta} \ln \tilde{u}_k^\delta (\tilde{u}_k^\delta - u_{\bar{k}})\, dx \\ &= -\sum_{k=1}^n \left[\int_{\widetilde{\mathcal{C}}^k_\delta} \ln \tilde{u}_k^\delta (\tilde{u}_0^\delta - u_0)\, dx - \int_{\mathcal{C}^{\delta,k}_{\text{avg}}} \left(\ln \tilde{u}_k^\delta + 1\right)(\tilde{u}_0^\delta - u_0)\, dx \right] \\ &\le \left[-\ln \delta + \ln\left(\frac{1}{n}(1 - \frac{m_0}{|\Omega|})\right)\right] \int_{\mathcal{C}_\delta} (\tilde{u}_0^\delta - u_0)\, dx, \end{aligned}$$

where we used (3.2.12) to obtain the last inequality.

The second integral ΔE_2 in (3.2.8) can be estimated via

$$\Delta E_2 = \int_\Omega \ln \tilde{u}_0^\delta (\tilde{u}_0^\delta - u_0)\, dx \le \ln(1-\delta) \int_{\widetilde{\mathcal{C}}_\delta} (\tilde{u}_0^\delta - u_0)\, dx + \ln(m_0/|\Omega)| \int_{\widetilde{\mathcal{C}}_{\text{avg}}} (\tilde{u}_0^\delta - u_0)\, dx,$$

where we used $\ln(\tilde{u}_0^\delta) \le \ln(m_0/|\Omega|)$ in $\widetilde{\mathcal{C}}_{\text{avg}}$. Using again (3.2.12), we obtain

$$\Delta E_2 \le (\ln(1-\delta) - \ln(m_0/|\Omega|)) \int_{\mathcal{C}_\delta} (\tilde{u}_0^\delta - u_0)\, dx.$$

Estimating the concave part ΔE_3 as in (3.2.11) and collecting all terms eventually yields

$$\begin{aligned} &E(\tilde{\boldsymbol{u}}^\delta) - E(\boldsymbol{u}) \\ &\le \left[-\ln \delta + \ln\left(\frac{1}{n}\left(1 - \frac{m_0}{|\Omega|}\right)\right) + \ln(1-\delta) - \ln(m_0/|\Omega|) + 2\beta \right] \int_{\widetilde{\mathcal{C}}_\delta} (\tilde{u}_0^\delta - u_0)\, dx. \end{aligned}$$

As the integral on the right-hand side is strictly negative but the coefficient in front of it becomes positive for δ sufficiently small, we again reach the desired contradiction.

Step 3: $\delta \leq u_i$, $i = 1, \dots n$. To fix the ideas let us assume that $i = 1$. While the proof uses the same construction as in Step 1, it is crucial to make sure that the index $\bar{k}(x)$ used to construct the sets $\mathcal{C}_\delta^k$ and the functions such as in (3.2.6) is such that $\bar{k}(x)$ is never equal to 0, as applying (3.2.6) to define u_0^δ with $k = 0$ would yield a function u_0^δ which does not belong to $H^1(\Omega)$ and thus renders the value of the energy to be infinity. To this end, we may use the upper bound on u_0 established at Step 2 of the proof to calculate

$$\sum_{j \neq 0,1} u_j = 1 - u_0 - u_1 \geq (\delta_0 - \delta) \quad \text{in the set } \mathcal{C}_{\delta,1} := \{x \in \Omega \ : \ u_1(x) < \delta\}.$$

As δ_0 from Steps 1 and 2 is fixed at this point, choosing $\delta < \delta_0$ we can go on from here to ensure that, defining $\bar{k}(x) := \min\{k = 2, \dots, n, \quad u_k(x) = \max_{i=2,\dots,n} u_i(x)\}$, we have that $u_{\bar{k}(x)}(x) > (\delta_0 - \delta)/n$ almost everywhere in $\mathcal{C}_{\delta,1}$. Then, arguing as in Step 1 gives the existence of $\delta_1 > 0$ such that $\delta_1 \leq u_1$. As the choice $i = 1$ was arbitrary it follows that the argument can then be applied to any other u_j, using the same construction as just done for u_1.

Step 4: Conclusion. We then observe that the parameter $\delta := \min(\delta_0, \delta_1, \dots, \delta_n)$ satisfies all the properties in the statement, and therefore the conclusion follows. □

Thanks to these uniform bounds and arguing by elliptic regularity, we can derive first order optimality conditions as given by the following theorem.

Theorem 8. *Let $\boldsymbol{u} \in \mathcal{A}_m$ be a local minimizer of the energy (3.1.1) in the $L^\infty(\Omega)^{n+1}$ topology. Then $u_0 \in H^2(\Omega)$ and is solution to*

$$\begin{aligned} -\varepsilon \Delta u_0 &= \ln \frac{1-u_0}{u_0} - \beta(1-2u_0) - \frac{1}{|\Omega|} \int_\Omega \left(\ln \frac{1-u_0}{u_0} - \beta(1-2u_0) \right) dx, && \text{in } \Omega, \\ \frac{\partial u_0}{\partial n} &= 0, && \text{on } \partial\Omega. \end{aligned} \tag{3.2.13}$$

Moreover, it holds

$$u_i = \frac{m_i}{|\Omega| - m_0}(1 - u_0), \quad i = 1, \dots, n. \tag{3.2.14}$$

In addition, $\boldsymbol{u}$ is an element of $(C^\infty(\overline{\Omega}))^{n+1}$ and a classical solution to (3.1.5).

Proof. Step 1: establishing (3.2.13) and (3.2.14). Given $\boldsymbol{\psi} := (\psi_1, \dots, \psi_n) \in (C^\infty(\overline{\Omega}))^n$, set

$$\nu_i := \psi_i - \frac{1}{|\Omega|} \int_\Omega \psi_i \, dx \quad \text{for all } i = 1, \dots, n. \tag{3.2.15}$$

Fix now $r > 0$, consider the perturbations

$$u_{r,i} := u_i + r\nu_i \quad \text{for all } i = 1, \dots, n,$$

and set

$$u_{r,0} := 1 - \sum_{i=1}^{n} u_{r,i} = 1 - \sum_{i=1}^{n} u_i - r \sum_{i=1}^{n} \nu_i = u_0 + r\nu_0, \quad \text{with } \nu_0 := -\sum_{i=1}^{n} \nu_i.$$

We then set $\boldsymbol{\nu} := (\nu_0, \dots, \nu_n)$, from which $\boldsymbol{u}_r = \boldsymbol{u} + r\boldsymbol{\nu}$ and in turn $\boldsymbol{u}_r \in \mathcal{A}_m$ for r sufficiently small, due to the strict lower and upper bounds of minimizers shown in Theorem 7, so that $E(\boldsymbol{u}) \leq E(\boldsymbol{u}_r)$. We now want to calculate the variation of E, that is,

$$\lim_{r \to 0} \frac{E(\boldsymbol{u}_r) - E(\boldsymbol{u})}{r}.$$

Note that, thanks again to the strict bounds of Theorem 7, we obtain uniform L^∞-bounds on $\ln u_i, \ln u_{r,i}$, for any $i = 0, \dots, n$ and for r sufficiently small. Therefore, we can use dominated convergence to calculate

$$0 \leq \lim_{r \to 0} \frac{E(\boldsymbol{u}_r) - E(\boldsymbol{u})}{r} = \int_\Omega \sum_{i=1}^{n} \Big[\Big(\ln u_i - \ln u_0 - \beta(1 - 2u_0) \Big) \nu_i - \varepsilon \nabla u_0 \cdot \nabla \nu_i \Big] \, dx,$$

for all such ν_i. We repeat the same argument for $-\boldsymbol{\nu}$ and then use (3.2.15) to eventually infer, using Fubini theorem,

$$\begin{aligned} 0 = &\int_\Omega \sum_{i=1}^{n} \Big[\Big(\ln u_i - \ln u_0 - \beta(1 - 2u_0) \Big) \psi_i - \varepsilon \nabla u_0 \cdot \nabla \psi_i \Big] dx \\ &- \int_\Omega \Big(\frac{1}{|\Omega|} \int_\Omega \ln u_i - \ln u_0 - \beta(1 - 2u_0) \, dy \Big) \psi_i \, dx \end{aligned}$$

for every $\boldsymbol{\psi} = (\psi_1, \dots, \psi_n) \in (\mathcal{C}^\infty(\overline{\Omega}))^n$. Setting

$$\lambda_i = \frac{1}{|\Omega|} \int_\Omega \ln u_i - \ln u_0 - \beta(1 - 2u_0) \, dy,$$

we obtain that for any $i = 1, \dots, n$, for any $\varphi \in H^1(\Omega)$,

$$\int_\Omega \Big[\ln u_i - \ln u_0 - \beta(1 - 2u_0) \Big] \varphi \, dx - \varepsilon \int_\Omega \nabla u_0 \cdot \nabla \varphi \, dx = \lambda_i \int_\Omega \varphi \, dx. \tag{3.2.16}$$

Thanks to the uniform bounds of Theorem 7, we know that

$$\ln u_i - \lambda_i - \ln u_0 - \beta(1 - 2u_0) \in L^2(\Omega) \quad \text{for all } i = 1, \dots, n,$$

therefore, using standard elliptic regularity theory (see, e.g., [224]), we get from (3.2.16) that $u_0 \in H^2(\Omega)$. This in turn implies that the Euler-Lagrange system is satisfied in strong form as follows

$$-\varepsilon \Delta u_0 = \ln u_i - \lambda_i - \ln u_0 - \beta(1 - 2u_0) \quad \text{a.e. in } \Omega, \text{for all } i = 1, \dots, n. \tag{3.2.17}$$

Let us now proceed to eliminate the Lagrange multipliers from the equations. We write (3.2.17) for any pair of indexes $i \neq k \in \{1, \dots, n\}$ and take the difference of the corresponding expressions. This gives

$$\ln u_i - \ln u_k = \lambda_i - \lambda_k, \tag{3.2.18}$$

that is,

$$u_k = u_i e^{\lambda_k - \lambda_i}.$$

Solving this equation for u_i by using the volume-filling constraint gives

$$u_i = \frac{e^{\lambda_i}}{\sum\limits_{k=1}^{n} e^{\lambda_k}}(1 - u_0). \tag{3.2.19}$$

Inserting (3.2.19) in (3.2.17), the Euler-Lagrange system reduces to the following PDE on u_0 together with n Lagrange multipliers

$$-\varepsilon \Delta u_0 = \ln \frac{1 - u_0}{u_0} - \beta(1 - 2u_0) - \ln \left(\sum_{k=1}^{n} e^{\lambda_k} \right), \quad \text{in } \Omega, \tag{3.2.20}$$

together with the boundary condition

$$\frac{\partial u_0}{\partial n} = 0, \quad \text{on } \partial\Omega. \tag{3.2.21}$$

Integrating (3.2.20) over Ω, together with (3.2.21), gives

$$\ln \left(\sum_{k=1}^{n} e^{\lambda_k} \right) = \frac{1}{|\Omega|} \int_\Omega \ln \frac{1 - u_0}{u_0} - \beta(1 - 2u_0)\, dx =: \lambda_0.$$

Then integrating (3.2.19) over Ω we obtain that

$$e^{\lambda_i} = \frac{m_i}{|\Omega| - m_0} e^{\lambda_0}, \quad i = 1, \dots, n,$$

and in turn (3.2.14).

Step 2: establishing (3.1.5). First, it follows from (3.2.13) combined with the uniforms bounds on u_0 that, by elliptic regularity, u_0 is smooth in Ω, and as a consequence of (3.2.14), $\boldsymbol{u}$ is smooth as well. Secondly, it is enough to show that u_i satisfies (3.1.11) for $i = 1, \dots, n$, since then (3.1.12) is automatically satisfied thanks to the volume-filling constraint. Remark that, rewriting (3.2.17) and (3.2.18) with the notations (3.1.9)-(3.1.10) leads to

$$\begin{aligned} w_i - w_0 &= \lambda_i, && i = 1, \dots, n, \\ w_i - w_j &= \lambda_i - \lambda_j, && i \neq j = 1, \dots, n. \end{aligned}$$

Taking into account that $\boldsymbol{u}$ is independent of time and using the previous relations, we obtain from (3.1.11) that

$$\begin{aligned}
&\operatorname{div}\left(\sum_{0\le j\neq i\le n} K_{ij}u_iu_j\nabla(w_i-w_j)\right)\\
&\quad=\operatorname{div}\left(\sum_{1\le j\neq i\le n} K_{ij}u_iu_j\nabla(w_i-w_j)+K_{i0}u_iu_0\nabla(w_i-w_0)\right)\\
&\quad=\operatorname{div}\left(\sum_{1\le j\neq i\le n} K_{ij}u_iu_j\nabla(\lambda_i-\lambda_j)+K_{i0}u_iu_0\nabla\lambda_i\right)\\
&\quad=0,
\end{aligned}$$

which concludes the proof. □

Let us make a few comments on the result that we have established here. First, we have proved that any local minimizer of the energy functional E for the $L^\infty(\Omega)^{n+1}$ topology is indeed a solution to the stationary problem (3.1.5). Of course, we do not expect the converse to be true, in the sense that there may exist other solutions to (3.1.5) which are not local minimizers of the energy functional E. However, because of the gradient flow structure of the time-dependent system (3.1.2), it is natural to conjecture that solutions to this system will converge in the long-time limit to some stationary states that are local minimizers of E. We are not able to prove this claim here, but give some numerical evidence in Section 3.5.

Second, thanks to Theorem 8, we can study the properties of the local minimizers of E by studying the scalar equation (3.2.13), which is now the first-order Euler-Lagrange equation of the *single-species* Cahn-Hilliard energy

$$E_0(u_0)=\int_\Omega\left[u_0\ln u_0+(1-u_0)\ln(1-u_0)+\frac{\varepsilon}{2}|\nabla u_0|^2+\beta u_0(1-u_0)\right]\,dx. \tag{3.2.22}$$

3.3 Convexity properties and long-time behaviour

In this section we present some results obtained on the behaviour of solutions to the time-dependent system (3.1.2) in the case when the parameters ε and β are chosen such that the functional E is convex. While this range of parameter values may not be practically relevant for some physical applications where separation effects dominate over diffusion, we nevertheless believe that the present analysis is instructive and might be seen as a useful preliminary step towards the study of the long-time behaviour of solutions to (3.1.2) in the general case. We first give explicit conditions on the parameters ε and β for E to be convex. We then prove that, in a stable regime, solutions of the time-dependent system converge exponentially fast to the minimizer of E, which is proved to be unique in this setting.

3.3.1 Convexity properties

Let us now study convexity properties of the energy (3.1.1). We begin by recalling the famous Poincaré-Wirtinger inequality: there exists a constant $C_p > 0$ such that for all $v \in H^1(\Omega)$,

$$\int_\Omega \Big(v - \frac{1}{|\Omega|}\int_\Omega v\,dy\Big)^2\,dx \le C_p \int_\Omega |\nabla v|^2\,dx, \tag{3.3.1}$$

as well as the logarithmic-Sobolev inequality on bounded domains, [108, Lemma 1],

$$\int f\log f\,dx \le C_{\text{sob}}\int_\Omega |\nabla\sqrt{f}|^2\,dx, \text{ for every } f \in H^1(\Omega;\mathbb{R}_+) \text{ s.t. } \int_\Omega f\,dx = 1, \tag{3.3.2}$$

where the constant C_{sob} depends on d and Ω, only. We then have the following lemma:

Lemma 12 (Convexity of the free energy)**.** *Let $n \ge 1$ and C_p be the Poincaré constant in (3.3.1). Assume that*

$$\frac{1}{2m_0} + \frac{1}{|\Omega|}\Big(\frac{\varepsilon}{2C_p} - \beta\Big) \ge 0. \tag{3.3.3}$$

Then, the energy functional (3.1.1) is convex in the set $\mathcal{A}_m$. If $n = 1$, the result holds under the weaker condition

$$\frac{|\Omega|}{2m_0(|\Omega| - m_0)} + \frac{1}{|\Omega|}\Big(\frac{\varepsilon}{2C_p} - \beta\Big) \ge 0. \tag{3.3.4}$$

Moreover, whenever the inequalities are strict, the energy is strictly convex.

Proof. Let $\boldsymbol{u} := (u_0, \dots, u_n), \boldsymbol{v} := (v_0, \dots, v_n) \in \mathcal{A}_m$. This in particular implies that

$$\int_\Omega u_i\,dx = \int_\Omega v_i\,dx \quad \text{for all } i = 0, \dots, n.$$

We want to estimate from below the quantity

$$E(\boldsymbol{u}) - E(\boldsymbol{v}) - E'(\boldsymbol{v})(\boldsymbol{u} - \boldsymbol{v}) = \sum_{i=0}^n \int_\Omega u_i \ln\frac{u_i}{v_i} + \frac{\varepsilon}{2}|\nabla(u_0 - v_0)|^2 - \beta(u_0 - v_0)^2\,dx.$$

The first terms can be estimated thanks to the Csiszár–Kullback–Pinsker inequality [226] as

$$\int_\Omega u_i \ln\frac{u_i}{v_i}\,dx \ge \frac{1}{2m_i}\left(\int_\Omega |u_i - v_i|\,dx\right)^2, \quad i = 0, \dots, n,$$

while the gradient term is estimated using the Poincaré inequality (3.3.1). We obtain

$$\begin{aligned} &E(\boldsymbol{u}) - E(\boldsymbol{v}) - E'(\boldsymbol{v})(\boldsymbol{u} - \boldsymbol{v}) \\ &\ge \sum_{i=0}^n \frac{1}{2m_i}\left(\int_\Omega |u_i - v_i|dx\right)^2 + \Big(\frac{\varepsilon}{2C_p} - \beta\Big)\left(\int_\Omega |u_0 - v_0|^2 dx\right) \\ &\ge \sum_{i=0}^n \frac{1}{2m_i}\left(\int_\Omega |u_i - v_i|dx\right)^2 + \frac{1}{|\Omega|}\Big(\frac{\varepsilon}{2C_p} - \beta\Big)\left(\int_\Omega |u_0 - v_0|dx\right)^2, \end{aligned} \tag{3.3.5}$$

where we applied Jensen's inequality. If $n = 1$, using $u_1 = 1 - u_0, m_1 = |\Omega| - m_0$, we obtain

$$E(\boldsymbol{u}) - E(\boldsymbol{v}) - E'(\boldsymbol{v})(\boldsymbol{u} - \boldsymbol{v}) \geq \left(\frac{|\Omega|}{2m_0(|\Omega| - m_0)} + \frac{1}{|\Omega|}\left(\frac{\varepsilon}{2C_p} - \beta\right)\right) \left(\int_\Omega |u_0 - v_0| \, dx\right)^2$$

thus condition (3.3.4) ensures convexity. However, when $n \geq 2$, one cannot easily take advantage of the terms $\sum_{i=1}^{n} \frac{1}{2m_i} \left(\int_\Omega |u_i - v_i| dx\right)^2$. Therefore, using only the fact that they are nonnegative, one obtains from (3.3.5) that

$$E(\boldsymbol{u}) - E(\boldsymbol{v}) - E'(\boldsymbol{v})(\boldsymbol{u} - \boldsymbol{v}) \geq \left(\frac{1}{2m_0} + \frac{1}{|\Omega|}\left(\frac{\varepsilon}{2C_p} - \beta\right)\right) \left(\int_\Omega |u_0 - v_0| \, dx\right)^2,$$

which gives again the convexity of E under condition (3.3.3). □

When applicable, it follows from strict convexity that both the minimization problem and the Euler-Lagrange equation (3.2.13) have a unique solution. Moreover, the constant state $u_0 = \frac{m_0}{|\Omega|}$ always solves (3.2.13). This leads to the following corollary.

Corollary 2 (Uniqueness of the minimizer)**.** *Whenever condition*

$$\frac{1}{2m_0} + \frac{1}{|\Omega|}\left(\frac{\varepsilon}{2C_p} - \beta\right) > 0$$

holds, the minimization problem (3.2.1) *has a unique solution, given by the constant states*

$$u_i^\infty = \frac{m_i}{|\Omega|} \quad \textit{for all } i = 0, \ldots, n. \tag{3.3.6}$$

3.3.2 Large-time asymptotics in the stable regime

We discuss now the large-time asymptotics of the evolution system (3.1.2) in the framework of Corollary 2, i.e. when the energy admits a unique (constant) minimizer. We aim to show that $\boldsymbol{u}$ converges exponentially fast to this unique minimizer, for arbitrary large initial data with finite relative energy.

It follows from [118, Theorem 2.1] that, for any initial condition in $\mathcal{A}_m$, the system admits a weak solution $\boldsymbol{u} = (u_0, u_1, \ldots, u_n)$ that satisfies the constraints (3.1.4) and such that (see [118, Definition 2.1] for more details),

- $u_i \in L^2((0,T); H^1(\Omega))$ for all $i = 1, \ldots, n$;
- $u_0 \in L^2((0,T); H^2(\Omega))$;
- $\partial_t u_i \in L^2((0,T); (H^1(\Omega))')$ for all $i = 0, \ldots, n$;

Let $\boldsymbol{u}^\infty := (u_0^\infty, \dots, u_n^\infty)$ be defined by (3.3.6). The relative energy functional is defined as, for all $\boldsymbol{u} := (u_0, \dots, u_n) \in \mathcal{A}_m$,

$$\begin{aligned} RE[\boldsymbol{u} \,|\, \boldsymbol{u}^\infty] &= E(\boldsymbol{u}) - E(\boldsymbol{u}^\infty) - E'(\boldsymbol{u}^\infty)(\boldsymbol{u} - \boldsymbol{u}^\infty) \\ &= \int_\Omega \left[\sum_{i=0}^n u_i \ln \frac{u_i}{u_i^\infty} + \frac{\varepsilon}{2} |\nabla(u_0 - u_0^\infty)|^2 - \beta(u_0 - u_0^\infty)^2 \right] dx. \end{aligned} \tag{3.3.7}$$

Our result is stated in the next theorem.

Theorem 9 (Global exponential stability of the constant steady state)**.** *Let $\boldsymbol{u}^\infty$ be given by (3.3.6) and let $\boldsymbol{u}^0 \in \mathcal{A}_m$ be an initial condition such that $\boldsymbol{u}^0 \in H^2(\Omega)^{n+1}$ and*

$$RE[\boldsymbol{u}^0 \,|\, \boldsymbol{u}^\infty] < \infty.$$

Let $\boldsymbol{u}$ be a weak solution to (3.1.2) as constructed in [118]. Then, $\boldsymbol{u}$ satisfies

$$RE[\boldsymbol{u}(t) \,|\, \boldsymbol{u}^\infty] \le e^{-\lambda t} RE[\boldsymbol{u}^0 \,|\, \boldsymbol{u}^\infty], \ t > 0, \tag{3.3.8}$$

with the rate

$$\lambda = 4k \min\left(\frac{1}{C_{\text{sob}}}, \frac{1}{C_p} - \frac{2\beta}{\varepsilon} \right) \tag{3.3.9}$$

with $k := \min_{0 \le i \ne j \le n} K_{ij} > 0$, C_p and C_{sob} being the constants in (3.3.1) and (3.3.2), respectively. Furthermore, under the condition

$$\frac{\varepsilon}{2C_p} - \beta > 0, \tag{3.3.10}$$

it holds, for all $i = 0, \dots, n$,

$$\|u_i(t) - u_i^\infty\|^2_{L^1(\Omega)} \le RE[\boldsymbol{u}(t) \,|\, \boldsymbol{u}^\infty] \le e^{-\lambda t} RE[\boldsymbol{u}^0 \,|\, \boldsymbol{u}^\infty] \to 0 \quad \text{as } t \to +\infty, \ .$$

Remark 7. *The global stability condition (3.3.10) is stronger than the convexity condition on the energy (3.3.3) as it does not take the mass into account.*

We recall here some results proved in [118] and in particular the construction of a weak solution to the time-dependent system. The method consists in introducing a time-discrete regularised version of the evolution system, together with a suitable weak formulation. More precisely, the following theorem holds:

Theorem 10 (Theorem 3.1 from [118])**.** *Define the sets*

$$\mathcal{A} := \left\{ \overline{u} := (u_i)_{1 \le i \le n} \in (L^\infty(\Omega))^n : \ u_i \ge 0, \, i = 1, \dots, n, \ u_0 := 1 - \sum_{i=1}^n u_i \ge 0 \right\}$$

and

$$\mathcal{B} := \left\{ \overline{\phi} := (\phi_i)_{1 \le i \le n} \in (L^\infty(\Omega))^n \ : \ \phi_0 := -\sum_{i=1}^n \phi_i \in H^1(\Omega) \right\},$$

and let $\tau > 0$ be a discrete time step, let $p \in \mathbb{N}$, and let $\overline{u}^p \in \mathcal{A} \cap (H^2(\Omega))^n$. Then, there exists a solution $(\overline{u}^{p+1}, \overline{\bar{w}}^{p+1}) \in (\mathcal{A} \cap (H^2(\Omega))^n) \times (H^2(\Omega))^n$ to the following coupled system: for all $1 \le i \le n$, for all $\phi_i \in H^2(\Omega)$,

$$\begin{aligned}\int_\Omega \frac{u_i^{p+1} - u_i^p}{\tau} \phi_i \, dx &= -\tau \langle \bar{w}_i^{p+1}, \phi_i \rangle_{H^2(\Omega)} \\ &- \int_\Omega \Big(\sum_{1 \le j \ne i \le n} K_{ij} u_i^{p+1} u_j^{p+1} \nabla(\bar{w}_i^{p+1} - \bar{w}_j^{p+1}) + K_{i0} u_i^{p+1} u_0^{p+1} \nabla \bar{w}_i^{p+1} \Big) \cdot \nabla \phi_i \, dx,\end{aligned} \tag{3.3.11}$$

and for all $\boldsymbol{\psi} = (\psi_i)_{1 \le i \le n} \in \mathcal{B} \cap (L^\infty(\Omega))^n$,

$$\sum_{i=1}^n \int_\Omega (\ln u_i^{p+1} - \ln u_0^{p+1}) \psi_i + \varepsilon \nabla u_0^{p+1} \cdot \nabla \psi_0 dx = \sum_{i=1}^n \int_\Omega \Big(\bar{w}_i^{p+1} + \beta(1 - 2u_0^p) \Big) \psi_i dx, \tag{3.3.12}$$

where $u_0^p = 1 - \sum_{i=1}^n u_i^p$. Moreover, the function $\overline{u}^{p+1}$ satisfies the following property: there exists $\delta_p > 0$ such that

$$u_i^{p+1} \ge \delta_p, \quad \text{for all } 1 \le i \le n, \quad \text{and} \quad u_0^{p+1} := 1 - \sum_{i=1}^n u_i^{p+1} \ge \delta_p, \quad \text{a.e. in } (0,T) \times \Omega.$$

Proof of Theorem 9. Let $\boldsymbol{u}^0 := (u_0^0, \dots, u_n^0) \in \mathcal{A}_m \cap H^2(\Omega)^{n+1}$. For a given value of time step $\tau > 0$, and starting from $\overline{u}^0 := (u_1^0, \dots, u_n^0)$, we consider the sequence $(\overline{u}^p)_{p \in \mathbb{N}}$ of discrete iterates given by Theorem 10. For all $p \in \mathbb{N}$, we then define $\boldsymbol{u}^p = (u_0^p, \overline{u}^p)$ where $u_0^p := 1 - \sum_{i=1}^n u_i^p$. We first note that they enjoy enough regularity to define the following quantities for all $p \ge 0$, using $\overline{\overline{w}}^{p+1} := (\overline{w}_1^{p+1}, \dots, \overline{w}_n^{p+1})$,

$$\begin{aligned} w_0^{p+1/2} &:= -\varepsilon \Delta u_0^{p+1} + \beta(1 - 2u_0^p), \\ w_i^{p+1} &:= \overline{w}_i^{p+1} + w_0^{p+1/2}, \quad \text{for } i = 1, \dots, n, \\ \boldsymbol{w}^{p+1} &:= (w_i^{p+1})_{1 \le i \le n}. \end{aligned}$$

Then, one can define the piecewise constant interpolation $\boldsymbol{u}^{(\tau)}$ as well as its time-shifted version $\sigma_\tau \boldsymbol{u}^{(\tau)}$: for all $p \in \mathbb{N} \setminus \{0\}$, define the discrete time $t_p = p\tau$ and, for all $t \in (t_p, t_{p+1}]$,

$$\boldsymbol{u}^{(\tau)}(t) = \boldsymbol{u}^{p+1}, \ \sigma_\tau \boldsymbol{u}^{(\tau)}(t) = \boldsymbol{u}^{p-1}, \ \boldsymbol{w}^{(\tau)}(t) = \boldsymbol{w}^{p+1},$$

together with $\boldsymbol{u}^{(\tau)}(0) = \boldsymbol{u}^0$. For any $t \in (0, \infty)$, we also define $P^{(\tau)}(t) \in \mathbb{N} \setminus \{0\}$ to be the lowest integer such that $t_{P^{(\tau)}} \ge t$. Choosing $\phi_i = \bar{w}_i^{p+1} = w_i^{p+1} - w_0^{p+1/2}$ in (3.3.11) one obtains a discrete (relative) energy-energy dissipation inequality and the authors showed in the proofs of [118, Lemmas 4.2, 4.3, 4.4] that the terms in the dissipation can be

estimated, which yields the following inequality, for all $t > 0$,

$$\begin{aligned}
&RE[\boldsymbol{u}^{(\tau)}(t) \,|\, \boldsymbol{u}^\infty] - RE[\boldsymbol{u}^0 \,|\, \boldsymbol{u}^\infty] \\
&\le -k \sum_{i=0}^n \int_0^t \int_\Omega \frac{|\nabla u_i^{(\tau)}|^2}{u_i^{(\tau)}} \, dxds + \sum_{p=0}^{P^{(\tau)}(t)-1} 4k\beta\tau \|\nabla u_0^{p+1}\|_{L^2(\Omega)} \|\nabla u_0^p\|_{L^2(\Omega)} \\
&\quad - 2k\varepsilon \int_0^t \int_\Omega |\Delta u_0^{(\tau)}|^2 \, dxds - k \int_0^t \int_\Omega u_0^{(\tau)}(1-u_0^{(\tau)}) |\nabla w_0^{(\tau)}|^2 \, dxds \\
&- \tau \int_0^t \sum_{i=1}^n \|w_i^{(\tau)} - w_0^{(\tau)}\|_{H^2(\Omega)}^2 \, ds.
\end{aligned}$$

Considering the nonnegativity of the two last terms, and using the inequality

$$\sum_{p=0}^{P^{(\tau)}(t)-1} 4k\beta\tau \|\nabla u_0^{p+1}\|_{L^2(\Omega)} \|\nabla u_0^p\|_{L^2(\Omega)} \le 2k\beta \int_0^t \left(\|\nabla u_0^{(\tau)}\|_{L^2(\Omega)}^2 + \|\nabla \sigma_\tau u_0^{(\tau)}\|_{L^2(\Omega)}^2 \right) ds,$$

the energy inequality rewrites

$$\begin{aligned}
&RE[\boldsymbol{u}^{(\tau)}(t) \,|\, \boldsymbol{u}^\infty] - RE[\boldsymbol{u}^0 \,|\, \boldsymbol{u}^\infty] \le -4k \sum_{i=0}^n \int_0^t \int_\Omega |\nabla \sqrt{u_i^{(\tau)}}|^2 \, dxds \\
&- 2k\varepsilon \int_0^t \int_\Omega |\Delta u_0^{(\tau)}|^2 \, dxds + 2k\beta \int_0^t \left(\|\nabla u_0^{(\tau)}\|_{L^2(\Omega)}^2 + \|\sigma_\tau \nabla u_0^{(\tau)}\|_{L^2(\Omega)}^2 \right) ds.
\end{aligned}$$

We use the logarithmic Sobolev inequality (3.3.2), together with the following estimate, which we prove for any $v \in H^2(\Omega)$ with $\partial_n v = 0$ on $\partial\Omega$: denoting by $m = \frac{1}{|\Omega|} \int_\Omega v \, dx$, it holds that

$$\begin{aligned}
\int_\Omega |\nabla v|^2 \, dx &= \int_\Omega |\nabla (v-m)|^2 \, dx = -\int_\Omega (u-m)\Delta(u-m) \\
&\le \left(\int_\Omega (u-m)^2 \right)^{1/2} \left(\int_\Omega (\Delta(u-m))^2 \right)^{1/2} \\
&\le \left(C_p \int_\Omega |\nabla(u-m)|^2 \right)^{1/2} \left(\int_\Omega (\Delta(u-m))^2 \right)^{1/2} \\
&\le \frac{1}{2} \int_\Omega |\nabla u|^2 \, dx + \frac{C_p}{2} \int_\Omega (\Delta u)^2
\end{aligned}$$

i.e.

$$\forall v \in H^2(\Omega) \text{ with } \partial_n v = 0 \text{ on } \partial\Omega, \quad \int_\Omega |\nabla v|^2 \, dx \le C_p \int_\Omega (\Delta v)^2 \, dx.$$

We thus obtain, using the fact that for all $p \in \mathbb{N}$, $u_0^{p+1} \in H^2(\Omega)$ is such that $\partial_n u_0^{p+1} = 0$

(this is a consequence of the weak variational fomulation (3.3.12)):

$$RE[\boldsymbol{u}^{(\tau)}(t)\,|\,\boldsymbol{u}^\infty] - RE[\boldsymbol{u}^0\,|\,\boldsymbol{u}^\infty] \leq -\frac{4k}{C_{\text{sob}}}\int_0^t\int_\Omega\sum_{i=0}^n u_i^{(\tau)}\ln\frac{u_i^{(\tau)}}{u_i^\infty}\,dxds$$
$$-\frac{2k\varepsilon}{C_{\text{P}}}\int_0^t\|\nabla u_0^{(\tau)}\|^2_{L^2(\Omega)}\,ds + 2k\beta\int_0^t\|\nabla u_0^{(\tau)}\|^2_{L^2(\Omega)} + \|\sigma_\tau\nabla u_0^{(\tau)}\|^2_{L^2(\Omega)}\,ds.$$

We need to pass to the limit as $\tau\to 0^+$ before estimating further. On the one hand, using the analysis of [118], it holds that $(u_0^{(\tau)})_{\tau>0}$ and $(\sigma_\tau u_0^{(\tau)})_{\tau>0}$ converge strongly to u_0 in $L^2((0,t);H^1(\Omega))$, so we can pass to the limit in the three gradient terms. On the other hand, $(u_i^{(\tau)})_{\tau>0}$ converges strongly to u_i in $L^2((0,t);L^2(\Omega))$ for any $i=1,\dots,n$, so by the continuity of the function $[0,1]\ni x\mapsto x\ln x$ and Lebesgue dominated convergence theorem, we can pass to the limit in the mixing terms, and therefore in the entire energy itself as well. We obtain

$$\begin{aligned}RE[\boldsymbol{u}(t)\,|\,\boldsymbol{u}^\infty] - RE[\boldsymbol{u}^0\,|\,\boldsymbol{u}^\infty] &\leq -\frac{4k}{C_{\text{sob}}}\int_0^t\int_\Omega\sum_{i=0}^n u_i\ln\frac{u_i}{u_i^\infty}\,dxds\\ &\quad -4k(\frac{\varepsilon}{2C_p}-\beta)\int_0^t\|\nabla u_0\|^2_{L^2(\Omega)}\,ds\\ &\leq -4k\min\left(\frac{1}{C_{\text{sob}}},\frac{1}{C_p}-\frac{2\beta}{\varepsilon}\right)\int_0^t RE[\boldsymbol{u}(t)\,|\,\boldsymbol{u}^\infty]\,ds,\end{aligned}$$

so that applying an integral version of Gronwall inequality gives (3.3.8)-(3.3.9). Moreover, under the same condition, the Poincaré and the Csiszár-Kullback inequalities (see [155]) show that the relative energy (3.3.7) dominates the square of the L^1-norm, hence the conclusion. □

Remark 8. *Note that the scope of the previous result is restricted to a regime where the system evolution is mainly diffusion-driven. In particular, the system does not enjoy phase separation. The dynamics outside of this regime is more relevant, but also much more difficult to study. Some constant states may become unstable, leading to the concepts of* spinodal region *and* spinodal decomposition *(see Figure 3.5). This phenomenon has been studied in the context of the single-species Cahn-Hilliard equation [195] and for Cahn-Hilliard systems [131]. It is an interesting perspective to study it for cross-diffusion-Cahn-Hilliard systems, which we postpone to future work.*

3.4 Finite volume scheme

We introduce a two-point finite volume scheme to solve (3.1.2) and study its large-time asymptotics. In the next subsection, we introduce a suitable discretization of the space-time domain and useful notations. Then we present our scheme and prove several properties related to the preservation of the structure of the continuous system.

3.4.1 Mesh and notations

An admissible mesh of Ω is a triplet $(\mathcal{T}, \mathcal{E}, (x_K)_{K\in\mathcal{T}})$ such that the following conditions are fulfilled.

(i) Each control volume (or cell) $K \in \mathcal{T}$ is non-empty, open, polyhedral and convex. We assume that

$$K \cap L = \emptyset \text{ if } K, L \in \mathcal{T} \text{ with } K \neq L, \qquad \text{while } \bigcup_{K\in\mathcal{T}} \overline{K} = \overline{\Omega}.$$

(ii) Each face $\sigma \in \mathcal{E}$ is closed and is contained in a hyperplane of $\mathbb{R}^d$, with positive $(d-1)$-dimensional Hausdorff (or Lebesgue) measure denoted by $m_\sigma = \mathcal{H}^{d-1}(\sigma) > 0$. We assume that $\mathcal{H}^{d-1}(\sigma \cap \sigma') = 0$ for $\sigma, \sigma' \in \mathcal{E}$ unless $\sigma = \sigma'$. For all $K \in \mathcal{T}$, we assume that there exists a subset $\mathcal{E}_K$ of $\mathcal{E}$ such that $\partial K = \bigcup_{\sigma\in\mathcal{E}_K} \sigma$. Moreover, we suppose that $\bigcup_{K\in\mathcal{T}} \mathcal{E}_K = \mathcal{E}$. Given two distinct control volumes $K, L \in \mathcal{T}$, the intersection $\overline{K} \cap \overline{L}$ either reduces to a single face $\sigma \in \mathcal{E}$ denoted by $K|L$, or its $(d-1)$-dimensional Hausdorff measure is 0.

(iii) The cell-centers $(x_K)_{K\in\mathcal{T}}$ satisfy $x_K \in K$, and are such that, if $K, L \in \mathcal{T}$ share a face $K|L$, then the vector $x_L - x_K$ is orthogonal to $K|L$.

We denote by m_K the d-dimensional Lebesgue measure of the control volume K. The set of the faces is partitioned into two subsets: the set $\mathcal{E}_{\text{int}}$ of the interior faces defined by

$$\mathcal{E}_{\text{int}} = \{\sigma \in \mathcal{E} \mid \sigma = K|L \text{ for some } K, L \in \mathcal{T}\},$$

and the set $\mathcal{E}_{\text{ext}} = \mathcal{E} \setminus \mathcal{E}_{\text{int}}$ of the exterior faces defined by $\mathcal{E}_{\text{ext}} = \{\sigma \in \mathcal{E} \mid \sigma \subset \partial\Omega\}$. For a given control volume $K \in \mathcal{T}$, we also define $\mathcal{E}_{K,\text{int}} = \mathcal{E}_K \cap \mathcal{E}_{\text{int}}$ (respectively $\mathcal{E}_{K,\text{ext}} = \mathcal{E}_K \cap \mathcal{E}_{\text{ext}}$) the set of its faces that belong to $\mathcal{E}_{\text{int}}$ (respectively $\mathcal{E}_{\text{ext}}$). For such a face $\sigma \in \mathcal{E}_{K,\text{int}}$, we may write $\sigma = K|L$, meaning that $\sigma = \overline{K} \cap \overline{L}$, where $L \in \mathcal{T}$. Given $\sigma \in \mathcal{E}$, we let

$$d_\sigma := \begin{cases} |x_K - x_L| & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ |x_K - x_\sigma| & \text{if } \sigma \in \mathcal{E}_{K,\text{ext}}, \end{cases} \qquad \text{and} \qquad \tau_\sigma = \frac{m_\sigma}{d_\sigma}.$$

In what follows, we use boldface notations for any vector-valued quantity, typically for elements of $\mathbb{R}^{n+1}$, $\mathbb{R}^{|\mathcal{T}|}$, $\mathbb{R}^{|\mathcal{E}|}$, $(\mathbb{R}^{|\mathcal{T}|})^{n+1}$ and $(\mathbb{R}^{|\mathcal{E}|})^{n+1}$. Moreover, we use uppercase letters to denote discrete quantities, in contrast to lowercase letters used in the previous sections for functions. Given any discrete scalar field $\boldsymbol{V} = (V_K)_{K\in\mathcal{T}} \in \mathbb{R}^{|\mathcal{T}|}$, we define for all cell $K \in \mathcal{T}$ and interface $\sigma \in \mathcal{E}_K$ the mirror value $V_{K\sigma}$ of V_K across σ by setting:

$$V_{K\sigma} = \begin{cases} V_L & \text{if } \sigma = K|L \in \mathcal{E}_{\text{int}}, \\ V_K & \text{if } \sigma \in \mathcal{E}_{\text{ext}}. \end{cases}$$

We also define the oriented and absolute jumps of $\boldsymbol{V}$ across any edge by

$$D_{K\sigma}\boldsymbol{V} = V_{K\sigma} - V_K, \qquad \text{and} \qquad D_\sigma\boldsymbol{V} = |D_{K\sigma}\boldsymbol{V}|, \quad \forall K \in \mathcal{T},\ \forall \sigma \in \mathcal{E}_K.$$

Note that in the above definition, for all $\sigma \in \mathcal{E}$, the definition of $D_\sigma \boldsymbol{V}$ does not depend on the choice of the element $K \in \mathcal{T}$ such that $\sigma \in \mathcal{E}_K$. Therefore, it can be checked that the following discrete integration by parts formula holds, for any $\boldsymbol{V}, \boldsymbol{W} \in \mathbb{R}^{|\mathcal{T}|}$:

$$\sum_{K\in\mathcal{T}} \sum_{\sigma\in\mathcal{E}_\mathcal{K}} D_{K\sigma}\boldsymbol{W}.V_K = -\sum_{\sigma\in\mathcal{E}_{\text{int}}} D_{K\sigma}\boldsymbol{W}.D_{K\sigma}\boldsymbol{V}. \tag{3.4.1}$$

Concerning the time discretization of $(0,T)$, we consider $P_T \in \mathbb{N}^*$ and an increasing infinite family of times $0 < t_0 < t_1 < \cdots < t_{P_T} = T$ and we set $\Delta t_p = t_p - t_{p-1}$ for $p \in \{1, \cdots, P_T\}$.

3.4.2 Numerical Scheme

Let $\boldsymbol{u}^0 = (u_0^0, \ldots, u_n^0) \in \mathcal{A}_m$ be an initial condition satisfying the constraints (3.1.4). It is discretized on the mesh $\mathcal{T}$ as

$$\boldsymbol{U}^0 = \left(U_{i,K}^0\right)_{K\in\mathcal{T},0\le i\le n}$$

by setting

$$U_{i,K}^0 = \frac{1}{m_K}\int_K u_i^0(x)\,dx, \quad \forall K \in \mathcal{T};\ i = 0, \ldots, n. \tag{3.4.2}$$

Assume that $\boldsymbol{U}^p = \left(U_{i,K}^p\right)_{K\in\mathcal{T},0\le i\le n}$ is given for some $p \in \mathbb{N}$, then we have to define how to compute the discrete volume fractions $\boldsymbol{U}^{p+1} = \left(U_{i,K}^{p+1}\right)_{K\in\mathcal{T},0\le i\le n}$. For $q = p, p+1$ and $i = 0, \ldots, n$, we introduce the notation $\boldsymbol{U}_i^q := \left(U_{i,K}^q\right)_{K\in\mathcal{T}}$. We also introduce discrete fluxes $\boldsymbol{J}_\mathcal{E}^{p+1} = \left(J_{i,K\sigma}^{p+1}\right)_{K\in\mathcal{T},\sigma\in\mathcal{E}_K,0\le i\le n}$, which are based on edge values $U_{i,\sigma}^{p+1}$ for all $\sigma \in \mathcal{E}, i = 0, \ldots, n$. For any $K \in \mathcal{T}$ such that $\sigma \in \mathcal{E}_K$, the definition of $U_{i,\sigma}^{p+1}$ makes use of the values $U_{i,K}^{p+1}$ and $U_{i,K\sigma}^{p+1}$ but is independent of the choice of K. The edge volume fractions are then defined through a logarithmic mean as follows

$$U_{i,\sigma}^{p+1} = \begin{cases} 0 & \text{if } \min(U_{i,K}^{p+1}, U_{i,K\sigma}^{p+1}) \le 0, \\ U_{i,K}^{p+1} & \text{if } 0 < U_{i,K}^{p+1} = U_{i,K\sigma}^{p+1}, \\ \frac{U_{i,K}^{p+1} - U_{i,K\sigma}^{p+1}}{\ln(U_{i,K}^{p+1}) - \ln(U_{i,K\sigma}^{p+1})} & \text{otherwise.} \end{cases} \tag{3.4.3a}$$

This choice is motivated by a discrete chain rule property: for any $i = 0, \ldots, n$, $K \in \mathcal{T}$, $\sigma \in \mathcal{E}_K$, if $U_{i,K}^{p+1}, U_{i,K\sigma}^{p+1} > 0$ then

$$D_{K\sigma}\boldsymbol{U}_i^{p+1} = U_{i,\sigma}^{p+1} D_{K\sigma}\ln(\boldsymbol{U}_i^{p+1}). \tag{3.4.3b}$$

We employ a time discretization relying on the backward Euler scheme:

$$m_K \frac{U_{i,K}^{p+1} - U_{i,K}^p}{\Delta t_p} + \sum_{\sigma\in\mathcal{E}_{K,\text{int}}} J_{i,K\sigma}^{p+1} = 0, \quad \forall K \in \mathcal{T},\ i = 0, \ldots, n, \tag{3.4.3c}$$

and the discrete fluxes are adapted from formulas (3.1.11)-(3.1.12) as

$$\begin{aligned} J_{i,K\sigma}^{p+1} &= -\tau_\sigma \sum_{0\le j\neq i\le n} K_{ij}\left(U_{j,\sigma}^{p+1} D_{K\sigma}\boldsymbol{U}_i^{p+1} - U_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{U}_j^{p+1}\right) \\ &\quad + \tau_\sigma K_{i0} U_{i,\sigma}^{p+1} U_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{W}_0^{p+\frac{1}{2}},\ i=1,\dots,n, \\ J_{0,K\sigma}^{p+1} &= -\tau_\sigma \sum_{i=1}^{n} K_{i0}\left(U_{i,\sigma}^{p+1} D_{K\sigma}\boldsymbol{U}_0^{p+1} - U_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{U}_i^{p+1}\right) \\ &\quad - \tau_\sigma \sum_{i=1}^{n} K_{i0} U_{i,\sigma}^{p+1} U_{0,\sigma}^{p+1} D_{K\sigma}\boldsymbol{W}_0^{p+\frac{1}{2}}, \end{aligned} \tag{3.4.3d}$$

where the auxiliary variable w_0 is discretized from (3.1.10) as $\boldsymbol{W}_0^{p+1/2} = \left(W_{0,K}^{p+1/2}\right)_{K\in\mathcal{T}}$, where for any $K\in\mathcal{T}$,

$$W_{0,K}^{p+\frac{1}{2}} = -\frac{\varepsilon}{m_K}\sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} \tau_\sigma D_{K\sigma}\boldsymbol{U}_0^{p+1} + \beta(1-2U_{0,K}^p). \tag{3.4.3e}$$

Note that, in the latter formula, we apply the same convex-concave splitting as in [131]: the convex part of the energy is discretized implicitly while the concave part is discretized explicitly. This well-known technique is crucial in order to recover free energy dissipation at the discrete level [132], see the proof of Proposition 5.

Remark 9. *Rather than defining the system (3.4.3c) for all $i=0,\dots,n$ and then check that it holds $\sum_{i=0}^n U_{i,K}^{p+1} = 1$ for any $K\in\mathcal{T}$, $p\in\mathbb{N}$, one could have written only n equations and define $U_{0,K}^{p+1} = 1-\sum_{i=1}^n U_{i,K}^{p+1}$ (it is the chosen approach to define weak continuous solutions). However, it is important* not to *define the value on the edges $U_{0,\sigma}^{p+1}$ as $1-\sum_{i=1}^n U_{i,\sigma}^{p+1}$ but rather as the logarithmic mean according to (3.4.3a). In doing so, the saturation constraint does not necessarily hold on the edges anymore, but one can recover free energy dissipation.*

3.4.3 Elements of numerical analysis

Lemma 13 (Mass conservation)**.** *For all $p\in\mathbb{N}$, it holds*

$$\sum_{K\in\mathcal{T}} m_K U_{i,K}^{p+1} = \int_\Omega u_i^0(x)dx,\ i=0,\dots,n.$$

Proof. Summing (3.4.3c) over $K\in\mathcal{T}$ leads to:

$$\sum_{K\in\mathcal{T}} m_K(U_{i,K}^{p+1}-U_{i,K}^p) = -\Delta t_p \sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} J_{i,K\sigma}^{p+1},\ i=0,\dots,n,$$

and this quantity is null because of cancellations on both sides of $\sigma\in\mathcal{E}_{\mathrm{int}}$. The conclusion follows by induction and using (3.4.2). □

Lemma 14 (Volume-filling constraint)**.** *Let $p \in \mathbb{N}$ and assume that $\boldsymbol{U}^p = \left(U_{i,K}^p\right)_{K\in\mathcal{T},0\le i\le n}$ satisfies the volume-filling constraint $\sum_{j=0}^n U_{j,K}^p = 1$, for any $K \in \mathcal{T}$. Then any solution $\boldsymbol{U}^{p+1}$ to the scheme (3.4.3) satisfies it as well.*

Proof. Fix $K \in \mathcal{T}$ and sum (3.4.3c) over $i = 0, \dots, n$. Then on the one hand we have the sum of the cross-diffusion contributions

$$\tau_\sigma \sum_{i=0}^n \sum_{j=0}^n K_{ij} \left(U_{j,\sigma}^{p+1} D_{K\sigma} \boldsymbol{U}_i^{p+1} - U_{i,\sigma}^{p+1} D_{K\sigma} \boldsymbol{U}_j^{p+1} \right)$$

that cancels thanks to the symmetry of the coefficients K_{ij}. On the other hand, it is clear by construction that the Cahn-Hilliard term in $J_{0,K\sigma}^{p+1}$ exactly compensates the sum of the Cahn-Hilliard terms in the n other fluxes. Therefore, one obtains

$$m_K \frac{1}{\Delta t_p} \sum_{i=0}^n \left(U_{i,K}^{p+1} - U_{i,K}^p \right) = 0.$$

□

Lemma 15 (Weak positivity property)**.** *Let $p \in \mathbb{N}$ and assume that $\boldsymbol{U}^p$ is nonnegative. Then any solution $\boldsymbol{U}^{p+1}$ to the scheme is nonnegative. If moreover $\boldsymbol{U}^p$ is positive, then any solution $\boldsymbol{U}^{p+1}$ is positive as well.*

Proof. We begin by proving nonnegativity. Fix $i \in \{0, \dots, n\}$. Reason by contradiction and assume that $\boldsymbol{U}_i^{p+1}$ has a (strictly) negative minimum $U_{i,K}^{p+1}$ in the cell $K \in \mathcal{T}$. The conservation scheme (3.4.3c) in the cell K gives that

$$m_K \frac{U_{i,K}^{p+1} - U_{i,K}^p}{\Delta t_p} = - \sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} J_{i,K\sigma}^{p+1},$$

and using that $\boldsymbol{U}_i^p$ is nonnegative we get that

$$\sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} J_{i,K\sigma}^{p+1} > 0. \tag{3.4.4}$$

But using that, for any $\sigma \in \mathcal{E}_{K,\mathrm{int}}$, $U_{i,\sigma}^{p+1} = 0$ by definition (3.4.3a), several terms cancel in the fluxes formula (3.4.3d), and we get

$$\sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} \left(-\tau_\sigma \sum_{0\le j\ne i\le n} K_{ij} U_{j,\sigma}^{p+1} D_{K\sigma} \boldsymbol{U}_i^{p+1} \right) > 0,$$

but since $K_{ij}, U_{j,\sigma}^{p+1}, D_{K\sigma}\boldsymbol{U}_i^{p+1}, \tau_\sigma \ge 0$, we obtain a contradiction. Therefore $\boldsymbol{U}_i^{p+1} \ge 0$. If $\boldsymbol{U}_i^p$ is furthermore (strictly) positive then we can assume the minimum $U_{i,K}^{p+1}$ to be only nonnegative and still obtain (3.4.4), so the same reasoning gives $\boldsymbol{U}_i^{p+1} > 0$. □

Thanks to the previous lemma, the chain rule (3.4.3b) is always valid provided the initial condition is positive everywhere. We make this assumption in the following. As a consequence, we can define the discrete chemical potentials (see (3.1.7)-(3.1.8)) as follows: for any $K \in \mathcal{T}$,

$$\mu_{i,K}^{p+1} = \ln(U_{i,K}^{p+1}),\ i = 1, \dots, n, \tag{3.4.5}$$

and

$$\mu_{0,K}^{p+1} = \ln(U_{0,K}^{p+1}) + W_{0,K}^{p+\frac{1}{2}}. \tag{3.4.6}$$

For all $i = 0, \dots, n$, we introduce $\boldsymbol{\mu}_i^{p+1} := (\mu_{i,K}^{p+1})_{K\in\mathcal{T}}$. The discrete fluxes (3.4.3d) can thus be rewritten in the following entropy form (independently of the discretization formula (3.4.3e)):

$$J_{i,K\sigma}^{p+1} = -\tau_\sigma \sum_{0\le j\ne i\le n} K_{ij} U_{i,\sigma}^{p+1} U_{j,\sigma}^{p+1} D_{K\sigma}\left(\boldsymbol{\mu}_i^{p+1} - \boldsymbol{\mu}_j^{p+1}\right),\ i = 0, \dots, n. \tag{3.4.7}$$

This latter formulation of the fluxes is at the core of the discrete free energy dissipation inequality. Let us define, according to (3.1.1), the following discrete free energy functionals: for all $\boldsymbol{V} = (V_{i,K})_{0\le i\le n, K\in\mathcal{T}}$,

$$\begin{aligned}
E_{\mathcal{T}}(\boldsymbol{V}) &:= E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{V}) + E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{V}),\\
E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{V}) &:= \sum_{i=0}^{n}\sum_{K\in\mathcal{T}} m_K(V_{i,K}\ln(V_{i,K}) - V_{i,K} + 1) + \frac{\varepsilon}{2}\sum_{\sigma\in\mathcal{E}_{\mathrm{int}},\ \sigma=K|L} \tau_\sigma |D_{K\sigma}\boldsymbol{V}_0|^2,\\
E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{V}) &:= \beta \sum_{K\in\mathcal{T}} m_K V_{0,K}(1 - V_{0,K}),
\end{aligned} \tag{3.4.8}$$

with $\boldsymbol{V}_0 = (V_{0,K})_{K\in\mathcal{T}}$. Their differentials at $\boldsymbol{U} = (U_{i,K})_{0\le i\le n, K\in\mathcal{T}}$ are given by

$$\begin{aligned}
DE_{\mathrm{conv},\mathcal{T}}(\boldsymbol{U})\cdot\boldsymbol{V} &= \sum_{i=0}^{n}\sum_{K\in\mathcal{T}} m_K \ln(U_{i,K})V_{i,K} + \varepsilon \sum_{\sigma\in\mathcal{E}_{\mathrm{int}},\ \sigma=K|L} \tau_\sigma D_{K\sigma}\boldsymbol{U}_0 D_{K\sigma}\boldsymbol{V}_0,\\
DE_{\mathrm{conc},\mathcal{T}}(\boldsymbol{U})\cdot\boldsymbol{V} &= \beta\sum_{K\in\mathcal{T}} m_K(1 - 2U_{0,K})V_{0,K}.
\end{aligned} \tag{3.4.9}$$

Remark that, by convexity (resp. concavity), it holds, for $p \in \mathbb{N}$:

$$\begin{aligned}
E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{U}^{p+1}) - E_{\mathrm{conv},\mathcal{T}}(\boldsymbol{U}^p) &\le DE_{\mathrm{conv},\mathcal{T}}(\boldsymbol{U}^{p+1})\cdot(\boldsymbol{U}^{p+1} - \boldsymbol{U}^p),\\
E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{U}^{p+1}) - E_{\mathrm{conc},\mathcal{T}}(\boldsymbol{U}^p) &\le DE_{\mathrm{conc},\mathcal{T}}(\boldsymbol{U}^p)\cdot(\boldsymbol{U}^{p+1} - \boldsymbol{U}^p).
\end{aligned} \tag{3.4.10}$$

We establish a discrete free energy dissipation inequality, as stated in the next proposition. Recall the definition (3.1.3) of the mobility matrix.

Proposition 5. *Let $p \in \mathbb{N}$ and $\boldsymbol{U}^p$ be (strictly) positive. Then any solution $\boldsymbol{U}^{p+1}$ to the scheme satisfies*

$$E_{\mathcal{T}}(\boldsymbol{U}^{p+1}) - E_{\mathcal{T}}(\boldsymbol{U}^p) + \Delta t_p \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} \tau_\sigma (D_{K\sigma}\boldsymbol{\mu}^{p+1})^T M(\boldsymbol{U}_\sigma^{p+1}) D_{K\sigma}\boldsymbol{\mu}^{p+1} \le 0, \tag{3.4.11}$$

where $\boldsymbol{U}_\sigma^{p+1} = \left(U_{i,\sigma}^{p+1}\right)_{0\le i\le n}$. *In particular, since* $M(\boldsymbol{U}_\sigma^{p+1})$ *is always a positive semi-definite matrix, it holds*

$$E_{\mathcal{T}}(\boldsymbol{U}^{p+1}) \le E_{\mathcal{T}}(\boldsymbol{U}^p) \le E_{\mathcal{T}}(\boldsymbol{U}^0).$$

Proof. Multiply equations (3.4.3c) by $\Delta t_p \mu_{i,K}^{p+1}$ and sum over all species $i = 0, ..., n$ and all cells $K \in \mathcal{T}$:

$$\sum_{i=0}^{n}\sum_{K\in\mathcal{T}} m_K \left(U_{i,K}^{p+1} - U_{i,K}^p\right)\mu_{i,K}^{p+1} = -\Delta t_p \sum_{i=0}^{n}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} J_{i,K\sigma}^{p+1}\mu_{i,K}^{p+1}. \tag{3.4.12}$$

On the left-hand side, we obtain using the definitions (3.4.5)-(3.4.6) of the discrete chemical potentials:

$$\begin{aligned}\sum_{i=0}^{n}\sum_{K\in\mathcal{T}} m_K \left(U_{i,K}^{p+1} - U_{i,K}^p\right)\mu_{i,K}^{p+1} &= \sum_{K\in\mathcal{T}}\sum_{i=0}^{n} m_K \left(U_{i,K}^{p+1} - U_{i,K}^p\right)\ln U_{i,K}^{p+1} \\ &\quad + \sum_{K\in\mathcal{T}} m_K \left(U_{0,K}^{p+1} - U_{0,K}^p\right) W_{0,K}^{p+\frac{1}{2}},\end{aligned}$$

where we obtain two different contributions that we want to identify to derivatives of the discrete energies (3.4.9). The first term identifies to the Boltzmann part, taken at $\boldsymbol{U}^{p+1}$, against $(\boldsymbol{U}^{p+1} - \boldsymbol{U}^p)$. Using the definition (3.4.3e) of $W_{0,K}^{p+\frac{1}{2}}$ and using the discrete integration by part formula (3.4.1), the second term can be expressed as:

$$\begin{aligned}&\sum_{K\in\mathcal{T}} m_K \left(U_{0,K}^{p+1} - U_{0,K}^p\right) W_{0,K}^{p+\frac{1}{2}} \\ &= -\varepsilon \sum_{K\in\mathcal{T}} (U_{0,K}^{p+1} - U_{0,K}^p) \sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} \tau_\sigma D_{K\sigma}\boldsymbol{U}_0^{p+1} + \beta \sum_{K\in\mathcal{T}} m_K (U_{0,K}^{p+1} - U_{0,K}^p)(1 - 2U_{0,K}^p), \\ &= \varepsilon \sum_{\sigma\in\mathcal{E}_{\mathrm{int}}} \tau_\sigma D_{K\sigma}\boldsymbol{U}_0^{p+1} D_{K\sigma}\left(\boldsymbol{U}_0^{p+1} - \boldsymbol{U}_0^p\right) + \beta \sum_{K\in\mathcal{T}} m_K (U_{0,K}^{p+1} - U_{0,K}^p)(1 - 2U_{0,K}^p),\end{aligned}$$

where we identified the Cahn-Hilliard contributions of (3.4.9), respectively taken at $\boldsymbol{U}^{p+1}$ and $\boldsymbol{U}^p$, against $\boldsymbol{U}^{p+1} - \boldsymbol{U}^p$. Putting everything together, we can identify the total derivative of the energy:

$$\begin{aligned}\sum_{i=0}^{n}\sum_{K\in\mathcal{T}} m_K \left(U_{i,K}^{p+1} - U_{i,K}^p\right)\mu_{i,K}^{p+1} &= DE_{\mathrm{conv},\mathcal{T}}(\boldsymbol{U}^{p+1}) \cdot \left(\boldsymbol{U}^{p+1} - \boldsymbol{U}^p\right) \\ &\quad + DE_{\mathrm{conc},\mathcal{T}}(\boldsymbol{U}^p) \cdot \left(\boldsymbol{U}^{p+1} - \boldsymbol{U}^p\right),\end{aligned}$$

and we conclude from (3.4.12), using the convexity (resp. concavity) inequalities (3.4.10), that:

$$E_{\mathcal{T}}(\boldsymbol{U}^{p+1}) - E_{\mathcal{T}}(\boldsymbol{U}^p) \le -\Delta t_p \sum_{i=0}^{n}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} J_{i,K\sigma}^{p+1}\mu_{i,K}^{p+1}.$$

On the other hand, using the entropy form of the fluxes (3.4.7), the right-hand side reads:

$$
\begin{aligned}
&-\sum_{i=0}^{n}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} J_{i,K\sigma}^{p+1}\mu_{i,K}^{p+1} \\
&\quad=\sum_{i=0}^{n}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_{K,\mathrm{int}}} \tau_\sigma\left(\sum_{0\le j\ne i\le n} K_{ij}U_{i,\sigma}^{p+1}U_{j,\sigma}^{p+1}D_{K\sigma}(\boldsymbol{\mu}_j^{p+1}-\boldsymbol{\mu}_i^{p+1})\right)\mu_{i,K}^{p+1}.
\end{aligned}
$$

Using once again integration by parts, this is equal to

$$
-\sum_{\sigma\in\mathcal{E}_{\mathrm{int}}}\tau_\sigma\sum_{i=0}^{n}\sum_{0\le j\ne i\le n} K_{ij}U_{i,\sigma}^{p+1}U_{j,\sigma}^{p+1}D_{K\sigma}(\boldsymbol{\mu}_i^{p+1}-\boldsymbol{\mu}_j^{p+1})D_{K\sigma}\boldsymbol{\mu}_i^{p+1},
$$

and having in mind the expression of the mobility matrix (3.1.3), we finally obtain

$$
-\sum_{i=0}^{n}\sum_{K\in\mathcal{T}}\sum_{\sigma\in\mathcal{E}_K} J_{i,K\sigma}^{p+1}\mu_{i,K}^{p+1} = -\sum_{\sigma\in\mathcal{E}_{\mathrm{int}}}\tau_\sigma(D_{K\sigma}\boldsymbol{\mu}^{p+1})^T M(\boldsymbol{U}_\sigma^{p+1})D_{K\sigma}\boldsymbol{\mu}^{p+1}.
$$

We have obtained (3.4.11). □

3.5 Numerical Simulations

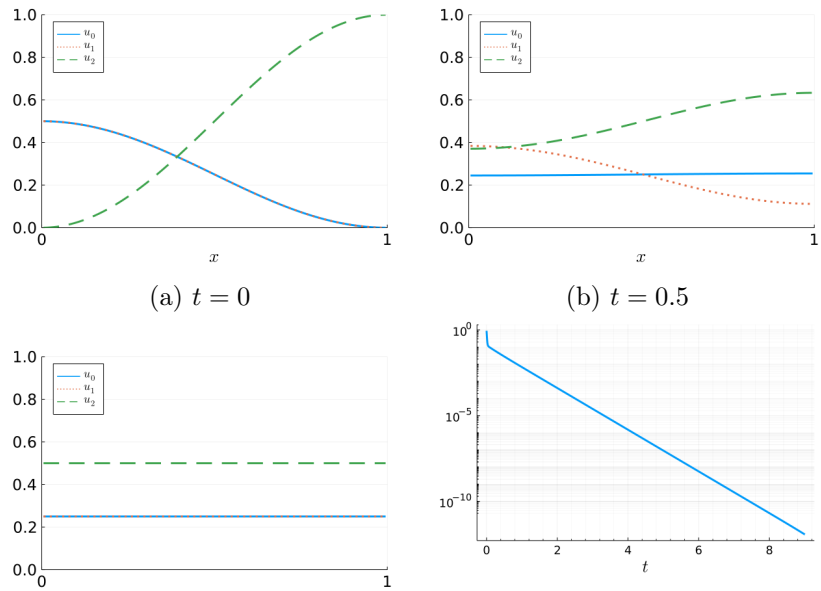
The numerical scheme has been implemented in the Julia language. At each time step, the nonlinear system is solved using Newton's method with stopping criterion $\|\boldsymbol{U}^{p,k+1}-\boldsymbol{U}^{p,k}\|_\infty \le 10^{-10}$ and adaptive time stepping. We always consider the case $n=2$ of three species and the cross-diffusion coefficients are chosen to be $K_{01}=K_{10}=0.2$, $K_{12}=K_{21}=0.1$, $K_{02}=K_{20}=1$ (diagonal coefficients do not play any role). We study the dynamics for different values of ε and β and different initial conditions, with a particular focus on the stationary solutions obtained in the long-time asymptotics and the shape of the free energy over time.

3.5.1 One-dimensional simulations

We consider the domain $(0,1)$, a uniform mesh of 100 cells, a maximal time step $\Delta t_1 = 10^{-3}$ and three initial profiles defined as smooth perturbations of a constant state: for $x\in(0,1)$,

$$
u_0^0(x)=u_1^0(x)=\frac{1}{4}\left(1+\kappa\cos(k\pi x)\right),\ u_2^0(x)=1-u_0^0(x)-u_1^0(x),
$$

where the perturbation is parametrized by its amplitude $\kappa\in(0,1)$ and frequency $k\in\mathbb{N}^*$, making sure that the box constraints in (3.1.4) are respected. Note that the mass is preserved by the perturbation, so that it holds $m_0=\int_\Omega u_0^0\,dx = 0.25$. Moreover, the Poincaré constant of the domain is $C_p=1$.



(a) $t = 0$

(b) $t = 0.5$

(c) $T_1 = 10$

(d) $RE[\boldsymbol{u}(t) \,|\, \boldsymbol{u}^\infty] = E(\boldsymbol{u}(t)) - E(\boldsymbol{u}^\infty)$

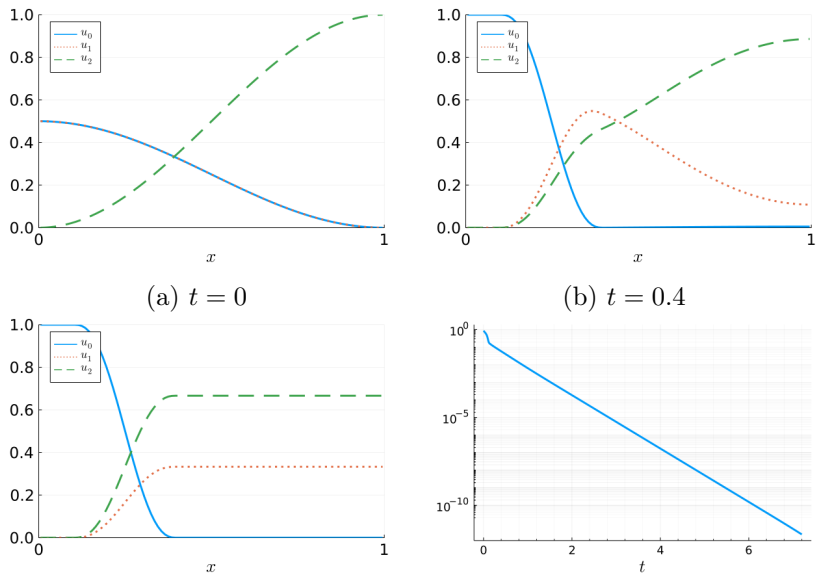
Figure 3.1: Profiles along time in the globally stable case. $\varepsilon = 4, \beta = 1, \kappa = k = 1$.

We begin by illustrating Theorem 9 and we denote by $\boldsymbol{U}^\infty$ the discrete constant state defined according to (3.3.6). We first consider $\varepsilon = 4, \beta = 1$ so that condition (3.3.10) is satisfied. Starting from various initial conditions, we always observe a diffusive behaviour with exponential convergence to $\boldsymbol{U}^\infty$, which confirms the globally stable behaviour. In Figure 3.1, we give some snapshots of the evolution and plot the discrete relative free energy $RE_\mathcal{T}[\boldsymbol{U}^p \,|\, \boldsymbol{U}^\infty] = E_\mathcal{T}(\boldsymbol{U}^p) - E_\mathcal{T}(\boldsymbol{U}^\infty)$ (see (3.4.8)) over the discrete time, starting from a specific initial condition and with time horizon $T_1 = 10$. For $\varepsilon = 0.5, \beta = 2$, (3.3.10) is not anymore satisfied, but the simulations behave similarly. Note that the convexity condition (3.3.3) on the energy reads

$$2 + \frac{\varepsilon}{2} - \beta \geq 0,$$

and is verified in this case. It seems that this condition is more determinant for the dynamics than (3.3.10).

We are now interested in the unstable regime and consider $\varepsilon = 0.1, \beta = 10$, so that both (3.3.10) and (3.3.3) are widely violated. In Figure 3.2, we display the results of the dynamics starting from the same initial condition as before and with a time horizon $T_2 = 8$. We observe convergence to a non-constant stationary solution with a diffuse segregation interface and exponential decrease to 0 of the quantity $E_\mathcal{T}(\boldsymbol{U}^p) - E_\mathcal{T}(\boldsymbol{U}^{P_{T_2}})$ over the discrete time. Let us make two remarks about this quantity: first, in contrast to the stable situation, we can only measure the difference with respect to the final solution $\boldsymbol{U}^{P_{T_2}}$, since we do not know *a priori* the limit of the dynamics. Second, since the limit is not homogeneous in space, the quantity $E_\mathcal{T}(\boldsymbol{U}^p) - E_\mathcal{T}(\boldsymbol{U}^{P_{T_2}})$ differs by a linear term from



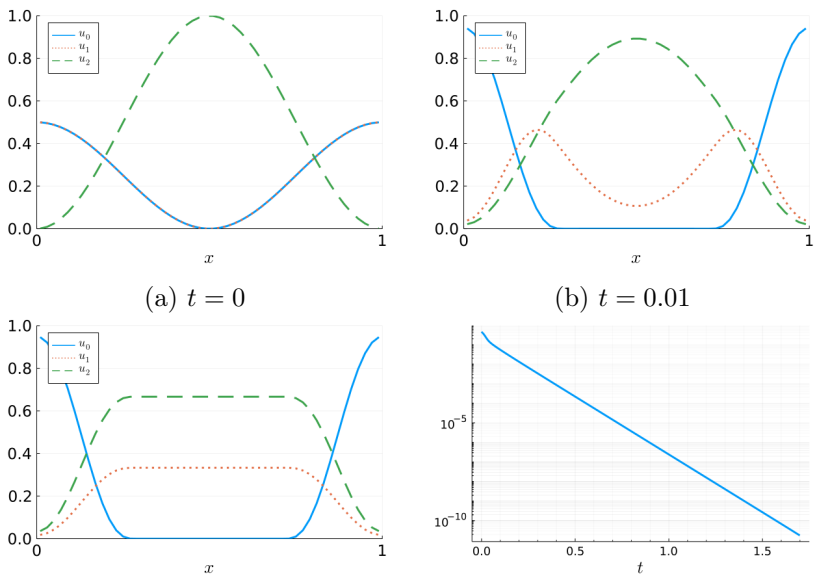
(a) $t = 0$ (b) $t = 0.4$

(c) $T_2 = 8$ (d) $E(\boldsymbol{u}(t)) - E(\boldsymbol{u}(T_2))$

Figure 3.2: Profiles along time in the non-convex case. $\varepsilon = 0.1, \beta = 10, \kappa = k = 1$.

an approximation of the relative energy (3.3.7). In Figure 3.3, we display the results of the dynamics starting from an initial condition with higher frequency $k = 2$ over a time horizon $T_3 = 2$. We observe exponential convergence to another stationary solution, for which the free energy is smaller. Note that, in accordance with the results of Theorem 7, diffusion prevents the profiles from being exactly zero somewhere, and we always observe a $\delta > 0$ such that all profiles are uniformly bounded between δ and $1 - \delta$.

Finally, we provide numerical evidence that, in the general regime, the solution should converge to a local minimizer of the energy. Although the property of being a local minimizer cannot be easily verified numerically, one can use Theorem 8 and verify that the obtained numerical stationary solutions satisfy a discrete version of the optimality conditions (3.2.13)-(3.2.14). In Figure 3.4, we plot, for the two previous simulations, the L^∞ norm of the residual of this system over time and observe exponential convergence to 0, which indicates that the solution converges to a critical point of the energy.



(a) $t = 0$ (b) $t = 0.01$

(c) $T_3 = 2$ (d) $E(\boldsymbol{u}(t)) - E(\boldsymbol{u}(T_3))$

Figure 3.3: Profiles along time in the non-convex case. $\varepsilon = 0.1, \beta = 10, \kappa = 1, k = 2$.

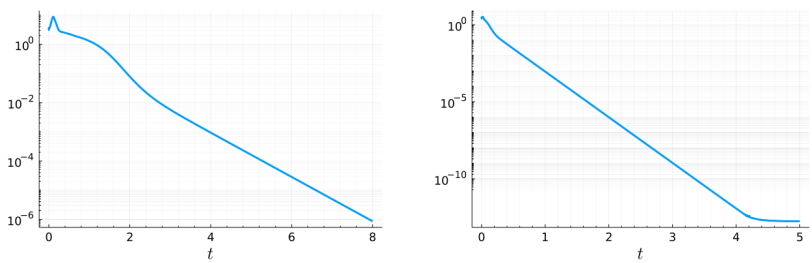


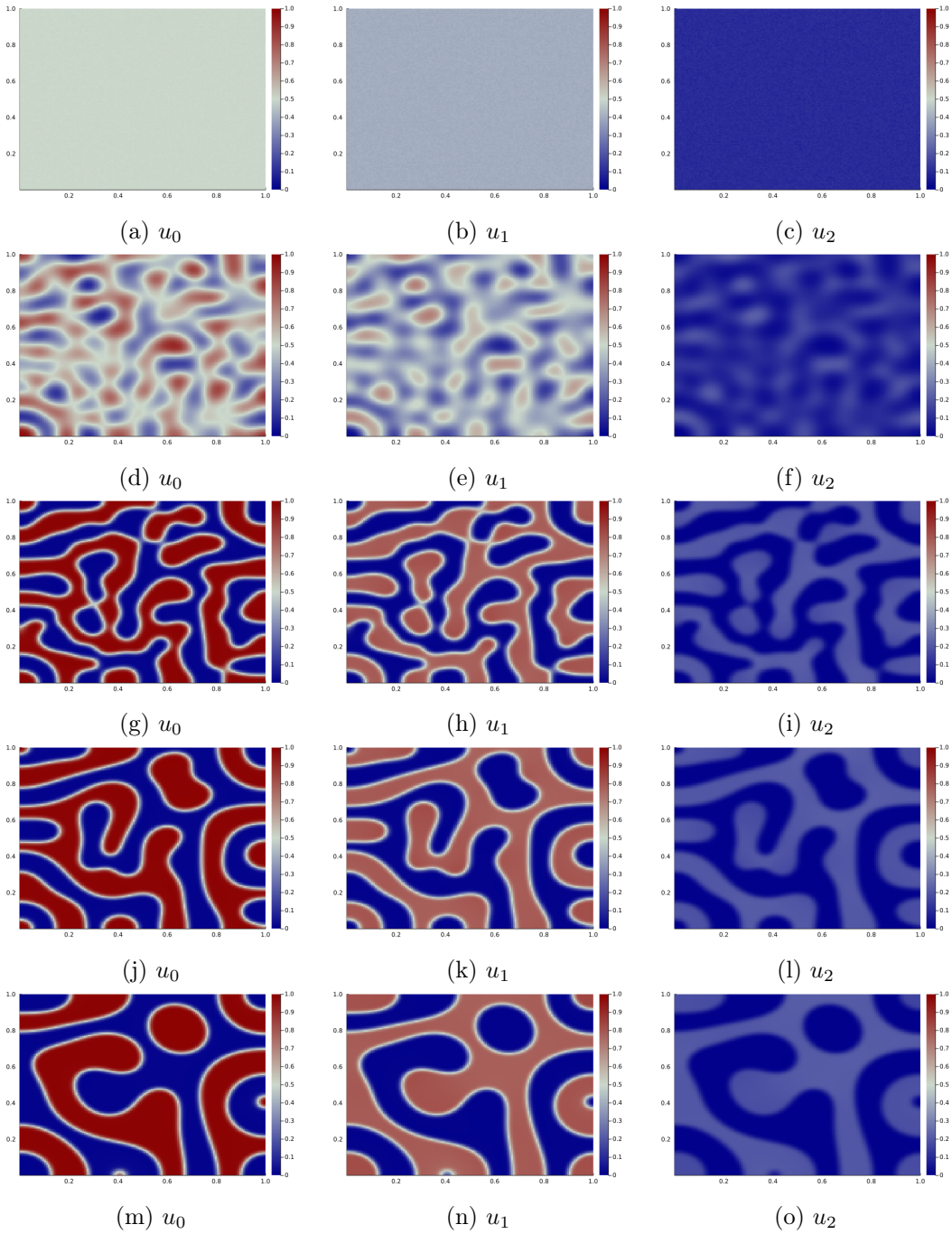
Figure 3.4: Residual of the Euler-Lagrange system in the case $k = 1$ (left) and $k = 2$ (right).

3.5.2 Two-dimensional simulations

We consider the domain $(0,1)^2$, a uniform mesh of 150^2 squares and a maximal time step $\Delta t_2 = 5 \times 10^{-3}$. We want to observe spinodal decomposition, so we pick initial profiles defined by random perturbation of constant states: for $(x,y) \in (0,1)^2$,

$$\begin{aligned} u_0^0(x,y) &= 0.5 + 2\kappa \left(\eta_0(x,y) - \frac{1}{2} \right), \\ u_1^0(x,y) &= 0.4 + 2\kappa \left(\eta_1(x,y) - \frac{1}{2} \right), \\ u_2^0(x,y) &= 1 - u_0^0(x,y) - u_1^0(x,y), \end{aligned}$$

where, for any $(x,y) \in (0,1)^2$, $\eta_0(x,y)$ and $\eta_1(x,y)$ are independent noises drawn uniformly in $(0,1)$ and $\kappa = 10^{-2}$. We choose the parameters $\varepsilon = 10^{-3}, \beta = 5$. The results of the simulation are given in Figure 3.5. As expected, u_0 quickly separates from the two other species. Then on a slower time scale, the effect of cross-diffusion homogenizes u_1 and u_2 to the constant states. Finally, the coarsening process happens on a much slower time scale, minimizing the interface energy.



(a) u_0 (b) u_1 (c) u_2

(d) u_0 (e) u_1 (f) u_2

(g) u_0 (h) u_1 (i) u_2

(j) u_0 (k) u_1 (l) u_2

(m) u_0 (n) u_1 (o) u_2

Figure 3.5: Spinodal decomposition successively at times $t = 0, 0.06, 0.13, 0.49, 1.5$.

3.6 Appendix

Lemma 16. *Let $\Omega \subset \mathbb{R}^d$ be a measurable bounded domain and let $u \in L^1(\Omega)$ be such that $u \geq 0$ almost everywhere on Ω. Let $M := \int_\Omega u\,dx$, $n \in \mathbb{N}^*$ and $m_1, \ldots, m_n \in \mathbb{R}_+$ such that*

$$M := \sum_{k=1}^{n} m_k.$$

Then there exist n measurable subsets $\Omega_k \subset \Omega$ for $k = 1, \ldots, n$ such that

- $\bigcup_{k=1}^{n} \Omega_k = \Omega$;
- $\Omega_k \cap \Omega_{k'} = \emptyset$ *as soon as* $k \neq k'$;
- $\int_{\Omega_k} u\,dx = m_k$.

Proof. Let $x_1 \in \Omega$ and consider the function $f : \mathbb{R}_+ \to \mathbb{R}_+$ defined as:

$$\forall r \geq 0, \quad f(r) := \int_{\Omega \cap B_r} u\,dx.$$

Then, it can be easily seen that f is continuous using the Lebesgue convergence theorem, non-decreasing, such that $f(0) = 0$ and that there exists $R > 0$ such that for all $r \geq R$, $f(r) = M$. This implies that there exists $r_1 \geq 0$ such that $f(r_1) = m_1$, and we defined $\Omega_1 = \Omega \cap B_{r_1}$. The other sets $\Omega_2, \ldots, \Omega_n$ can be constructed using exactly the same procedure by induction on the set $\Omega \setminus \Omega_1$. $\square$

Chapter 4

Cross-diffusion systems coupled by a moving interface

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4.1 Introduction

We propose and study an extension of the mathematical model introduced in [24] to describe a physical vapor deposition process used in particular for the fabrication of semiconducting thin film layers in the photovoltaic industry. The process can be described as follows: a wafer is introduced in a hot chamber where chemical elements are injected under gaseous form. As the latter deposit on the substrate, a heterogeneous solid layer grows upon it. Because of the high temperature conditions, diffusion occurs in the bulk until the wafer is taken out and the system is frozen. There are two essential features in the problem: the evolution of the surface of the film and the diffusion of the

various species due to high temperature conditions. In the series of works [24, 25, 68], the authors introduced and studied a one-dimensional moving-boundary cross-diffusion model where only the evolution of the solid layer was considered. The latter is composed of n different chemical species and occupies a domain of the form $(0, X(t))$, where $X(t) > 0$ denotes the thickness of the film at time $t > 0$. For any $i \in \{1, \dots, n\}$, the flux of atoms of species i absorbed at the surface of the solid film layer at time t is denoted by $F_i(t)$. For all $t > 0$ and $x \in (0, X(t))$, denoting by $c_i(t, x)$ the local volumic fraction of species i at point $x \in (0, X(t)$ and time t and setting $\boldsymbol{F}(t) = (F_i(t))_{1 \le i \le n}$ and $\boldsymbol{c}(t, x) := (c_i(t, x))_{1 \le i \le n}$, the resulting moving-boundary cross-diffusion system reads as

$$\partial_t \boldsymbol{c}(t, x) - \partial_x(\boldsymbol{A}_s(\boldsymbol{c})\partial_x \boldsymbol{c})(t, x) = 0, \text{ for } t > 0 \text{ and } x \in (0, X(t)), \tag{4.1.1}$$

for some cross-diffusion matrix function $\boldsymbol{A}_s : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ describing the diffusion in the solid phase, together with the boundary conditions

$$(\boldsymbol{A}_s(\boldsymbol{c})\partial_x \boldsymbol{c})(t, 0) = 0, \tag{4.1.2}$$

$$(\boldsymbol{A}_s(\boldsymbol{c})\partial_x \boldsymbol{c})(t, X(t)) + X'(t)\boldsymbol{c}(t, X(t)) = \boldsymbol{F}(t), \tag{4.1.3}$$

and appropriate initial conditions. In other words, no-flux boundary conditions are assumed on the bottom ($x = 0$) part of the thin film layer while (4.1.3) expresses the fact that the flux of the ith species absorbed on the upper part of the layer (corresponding to $x = X(t)$) is given by $F_i(t)$. The evolution of the thickness of the layer is assumed to be driven by the following equation

$$X'(t) = \sum_{i=1}^{n} F_i(t). \tag{4.1.4}$$

In [24, 25], the absorbed fluxes $\boldsymbol{F}(t)$ are assumed to be explicitly known, which is of course not realistic since the values of these fluxes depend on the interaction between the gaseous and the solid phase in the hot chamber. A more realistic model thus has to account for the evolution of the gaseous phase and of how the deposition occurs at the interface between the two phases. This work is a first attempt to build a more evolved model taking into account the evolution of the gaseous phase and its interaction with the solid phase. For the sake of simplicity, we only consider here an isolated system (no incoming fluxes in the hot chamber) in order to mainly focus on the moving-interface coupling. The present paper is then devoted to the theoretical and numerical analysis of the proposed system.

Let us present some related contributions from the literature before highlighting the novel contributions of the present work. Cross-diffusion systems have gained significant interest from the mathematical community in the last twenty years. Indeed, it has been understood in the seminal works [77, 53, 159, 160, 156] that many of these systems have a variational entropy structure, which enables to obtain appropriate estimates in order to prove the existence of weak solutions and to study convergence to equilibrium. In particular, many contributions study theoretical and numerical aspects of the Stefan-Maxwell system [38, 41, 160, 40, 145, 61] and of the size-exclusion system [53, 156, 62,

147] that we both consider in this work as typical applications. The variational entropy structure was extended to reaction-diffusion systems of mass-action type in [186], and to bulk-interface systems in [142], see also the related works [188, 181, 112, 192]. However, all these contributions are restricted to a fixed domain.
Similar problems posed in moving-boundary domains were investigated in previous works by the authors: in [24], the existence of global weak solutions to the system (4.1.1)-(4.1.2)-(4.1.3) was proved and the long-time asymptotics were studied in the case of constant fluxes F. The rapid stabilization of the associated linearized system was studied in [68]. A similar moving-boundary parabolic system was introduced and studied in [5, 6, 4] to model concrete carbonation. In [72], the authors introduced a finite volume scheme approximating the system, using a rescaling to a fixed domain, and proved its convergence towards a continuous weak solution. Additionally, the long-time regime of the approximated moving-interface was studied in [237] (see also the thesis [238]). In [208], the authors studied a scalar parabolic problem in a one-dimensional moving-boundary domain, using Wasserstein gradient flows methods. This approach was adapted to a more complex model in [185]. The authors of [39] studied Stefan-Maxwell reaction-diffusion in moving-boundary domains of arbitrary dimension. Their model, though more complex, is very much related to ours, but they do not seem to include energy dissipation through the interface and are more interested in dynamical aspects than numerical considerations. We also refer to the monograph [209] for mathematical tools related to quasilinear parabolic problems in moving-boundary domains.

Our work makes the following contributions:

- In Section 4.2, we introduce a new moving-interface cross-diffusion system and highlight its variational entropy structure. The latter implies the thermodynamics consistency of the model and lays the foundations for a rigorous mathematical analysis. The stationary states are identified and insights are given concerning the long-time behaviour.

- In Section 4.3, a finite-volume scheme is introduced to approximate the system. In contrast to the scheme designed in [72], we do not rescale the system to a fixed domain but rather discretize the moving-interface following a cut-cell approach. Thus the main novelty lies in the numerical treatment of the moving interface

- We present some results of numerical analysis of the scheme in Section 4.4. We prove the existence of at least one discrete solution to the scheme at each time step and that this solution preserves the full structure of the continuous system. In particular, updating the interface and the mesh preserves the decay of the entropy at the discrete level. The proofs require some more technicalities with respect to the situation of a fixed domain.

- Numerical results are given in Section 4.5, illustrating the properties of the model and the good behaviour of the scheme. These results also support conjectures concerning the long-time behaviour.

4.2 Moving-interface coupled model

This section is devoted to the presentation and analysis of the continuous system we consider in this work. The model is first broadly presented in Section 4.2.1 while technical assumptions on the cross-diffusion matrices together with relevant examples are given in Section 4.2.2. The entropy structure of the system is formally investigated in Section 4.2.3. Finally, Section 4.2.4 is devoted to the characterization of the stationary states and to a discussion about the long-time asymptotics.

4.2.1 Presentation of the model

Let $\Omega = (0,1)$ be the physical domain containing both the solid and gaseous phases. For all $t \geq 0$, let $X(t) \in [0,1]$ denote the position at time t of the interface between the two phases. More precisely, at time t, the solid phase occupies the domain $(0, X(t))$ and the gaseous phase occupies the domain $(X(t), 1)$. We adopt the convention that if $X(t) = 0$ (respectively $X(t) = 1$), then the domain is entirely composed of a gaseous (respectively solid) phase. The map $X : \mathbb{R}_+ \ni t \mapsto X(t) \in [0,1]$ is assumed to be absolutely continuous. We denote by $Q := \mathbb{R}_+ \times \Omega$ the time-space domain of the problem. We consider n different chemical species represented by their densities of molar concentration. More precisely, for all $i \in \{1, \dots, n\}$, $c_i(t,x)$ represents the density of molar concentration of species i at time $t \geq 0$ and point $x \in \Omega$ and we set $\boldsymbol{c}(t,x) := (c_i(t,x))_{i \in \{1,\dots,n\}}$. From a modelling perspective, it is natural to expect that so-called volume-filling constraints are satisfied, i.e. for almost all $(t,x) \in Q$, the vector $\boldsymbol{c}(t,x)$ is expected to belong to the set

$$\mathcal{A} := \left\{ (c_1, \dots, c_n) \in \mathbb{R}^n_+, \ \sum_{i=1}^n c_i = 1 \right\}. \tag{4.2.1}$$

The volume-filling constraints arise from size exclusion effects in the solid phase and from isobaric assumptions in the gas mixture (see Examples 1 and 2 and Remark 10 in Section 4.2.2 below). We assume that initial conditions for the model are given such that, at time $t = 0$,

$$X(0) = X^0 \text{ and } \boldsymbol{c}(0,x) = \boldsymbol{c}^0(x), \tag{4.2.2a}$$

for some $X^0 \in \Omega$ and $\boldsymbol{c}^0 \in L^\infty(\Omega; \mathcal{A})$. Now, for almost all $(t,x) \in Q$ and all $i \in \{1, \dots, n\}$, we denote by $J_i(t,x) \in \mathbb{R}$ the molar flux of species i at time t and point $x \in \Omega$, and set $\boldsymbol{J}(t,x) := (J_1(t,x), \dots, J_n(t,x))^T$. The local conservation of matter inside the solid and gaseous phase respectively reads as

$$\partial_t \boldsymbol{c} + \partial_x \boldsymbol{J} = 0, \text{ a.e. in } Q. \tag{4.2.2b}$$

Let us also denote by

$$Q_s := \{(t,x) \in Q, \ x \in (0, X(t))\} \quad \text{and} \quad Q_g := \{(t,x) \in Q, \ x \in (X(t), 1)\},$$

the time-space domain associated to the solid and gaseous phase respectively. Cross-diffusion phenomena are modelled by a diffusion matrix-valued mapping $\boldsymbol{A}_s : \mathbb{R}^n \to \mathbb{R}^{n \times n}$

(resp. $\boldsymbol{A}_g : \mathbb{R}^n \to \mathbb{R}^{n\times n}$) in the solid (resp. gaseous) phase, as

$$\begin{aligned} \boldsymbol{J} &= -\boldsymbol{A}_s(\boldsymbol{c})\partial_x \boldsymbol{c}, \text{ a.e. in } Q_s, \\ \boldsymbol{J} &= -\boldsymbol{A}_g(\boldsymbol{c})\partial_x \boldsymbol{c}, \text{ a.e. in } Q_g. \end{aligned} \tag{4.2.2c}$$

We require that the diffusion mappings $\boldsymbol{A}_s$ and $\boldsymbol{A}_g$ satisfy some assumptions which will be made precise below in Section 4.2.2. On the boundary of the full domain Ω, zero-flux boundary conditions are imposed, i.e.

$$\boldsymbol{J}(t,0) = \boldsymbol{J}(t,1) = 0, \text{ for a.a. } t \geq 0. \tag{4.2.2d}$$

In addition, we assume that $\boldsymbol{J}$ and $\boldsymbol{c}$ are regular enough in order to define their trace on the boundary of Q_s and Q_g respectively. More precisely, for all $t \geq 0$ such that $X(t) \in (0,1)$, we assume that we can define for all $i \in \{1,\dots,n\}$,

$$J_i^s(t) := J_i(t, X(t)^-),\ J_i^g(t) := J_i(t, X(t)^+),\ c_i^s(t) := c_i(t, X(t)^-),\ c_i^g(t) := c_i(t, X(t)^+),$$

and set $\boldsymbol{c}^s(t) := (c_i^s(t))_{i\in\{1,\dots,n\}}$, $\boldsymbol{c}^g(t) := (c_i^g(t))_{i\in\{1,\dots,n\}}$, $\boldsymbol{J}^s(t) := (J_i^s(t))_{i\in\{1,\dots,n\}}$, $\boldsymbol{J}^g(t) := (J_i^g(t))_{i\in\{1,\dots,n\}}$. To complete the definition of the model, it now remains to introduce (i) the evolution of the position of the interface $X(t)$ and (ii) the flux boundary conditions at this interface. To this aim, we use a flux vector $\boldsymbol{F}(t) = (F_i(t))_{i\in\{1,\dots,n\}}$ which accounts for phase transition mechanisms located at the vicinity of the moving interface between the solid and gaseous phases. We focus in this work on interface fluxes of Butler-Volmer type. More precisely, we introduce some constant reference chemical potentials $\boldsymbol{\mu}^{*,s} := (\mu_i^{*,s})_{i\in\{1,\dots,n\}}, \boldsymbol{\mu}^{*,g} := (\mu_i^{*,g})_{i\in\{1,\dots,n\}} \in \mathbb{R}^n$ and define the constants

$$\beta_i^* := \exp\left([\![\mu_i^*]\!]\right), \quad [\![\mu_i^*]\!] := \mu_i^{*,g} - \mu_i^{*,s} \quad \forall i \in \{1,\dots,n\}. \tag{4.2.2e}$$

Then, the vector $\boldsymbol{F}(t)$ is defined for all $t \geq 0$ such that $X(t) \in (0,1)$ by

$$F_i(t) = \frac{1}{\sqrt{\beta_i^*}} c_i^g(t) - \sqrt{\beta_i^*} c_i^s(t),\ \forall i \in \{1,\dots,n\}. \tag{4.2.2f}$$

and by $F_i(t) = 0$ for all $i \in \{1,\dots,n\}$ for all $t \geq 0$ such that $X(t) = 0$ or $X(t) = 1$. Note that (4.2.2f) is a trivial case of the law of mass action.

Then, the evolution of the location of the interface is defined as, for almost all $t \geq 0$,

$$X'(t) = \sum_{i=1}^n F_i(t). \tag{4.2.2g}$$

Notice that, if there exists $t_0 \geq 0$ such that $X(t_0) = 0$ (respectively $X(t_0) = 1$), then $X(t) = 0$ (respectively $X(t) = 1$) for all $t \geq t_0$, and the system boils down to a simple cross-diffusion systems with no-flux boundary conditions on the boundary of the whole domain Ω and diffusion matrix given by $\boldsymbol{A}_g$ (respectively $\boldsymbol{A}_s$). We define

$$T := \sup\{t \in \mathbb{R}_+,\ X(t) \in (0,1)\}$$

so that $X(t) \in (0,1)$ if and only if $t \in [0,T)$. Then, for all $0 \leq t < T$, we impose the following boundary conditions across the moving interface

$$-\boldsymbol{J}^s(t) + X'(t)\boldsymbol{c}^s(t) = -\boldsymbol{J}^g(t) + X'(t)\boldsymbol{c}^g(t) = \boldsymbol{F}(t). \tag{4.2.2h}$$

Note that this implies in particular that for almost all $0 \leq t < T$,

$$[\![\boldsymbol{J}(t)]\!] - X'(t)[\![\boldsymbol{c}(t)]\!] = 0, \tag{4.2.3}$$

where

$$[\![\boldsymbol{J}(t)]\!] = \boldsymbol{J}^g(t) - \boldsymbol{J}^s(t) \quad \text{and} \quad [\![\boldsymbol{c}(t)]\!] = \boldsymbol{c}^g(t) - \boldsymbol{c}^s(t).$$

Let us point out that conservation of matter follows from the local conservation equation (4.2.2b), the zero-flux conditions on the fixed boundary and the conservative condition (4.2.3) (which was designed accordingly). Indeed, taking into account the discontinuity of the fluxes and concentrations at the interface, it holds that for any $i \in \{1, \dots, n\}$ and almost all $t \geq 0$,

$$\begin{aligned}
\frac{d}{dt}\left(\int_0^1 c_i(t)\right) &= \frac{d}{dt}\left(\int_0^{X(t)} c_i(t) + \int_{X(t)}^1 c_i(t)\right) \\
&= \int_0^{X(t)} \partial_t c_i(t) + \int_{X(t)}^1 \partial_t c_i(t) - X'(t)[\![c_i(t)]\!] \\
&= -\int_0^{X(t)} \partial_x J_i(t) - \int_{X(t)}^1 \partial_x J_i(t) - X'(t)[\![c_i(t)]\!] \\
&= [\![J_i(t)]\!] - X'(t)[\![c_i(t)]\!] \\
&= 0,
\end{aligned}$$

where $[\![c_i(t)]\!] = c_i^g(t) - c_i^s(t)$ and $[\![J_i(t)]\!] = J_i^g(t) - J_i^s(t)$.

4.2.2 Assumptions on cross-diffusion matrices

The aim of this section is to summarize the assumptions that $\boldsymbol{A}_s$ and $\boldsymbol{A}_g$ must satisfy for the coupled interface system presented in the previous section to enjoy the entropy structure that will be highlighted in the next section. Let us define

$$\mathcal{V}_0 := \left\{ \boldsymbol{z} = (z_1, \dots, z_n) \in \mathbb{R}^n,\ \sum_{i=1}^n z_i = 0 \right\}.$$

We make the following two assumptions: for all $\alpha = s, g$,

(A1) for all $\boldsymbol{c} \in \mathcal{A} \cap (\mathbb{R}_+^*)^n$, $\boldsymbol{A}_\alpha(\boldsymbol{c})\,(\mathcal{V}_0) \subset \mathcal{V}_0$.

(A2) There exists $C_\alpha > 0$ and $m_1, \dots, m_n \leq 2$ such that for all $\boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}} \in \mathcal{A} \cap (\mathbb{R}_+^*)^n$ and all $\boldsymbol{z} = (z_i)_{i\in\{1,\dots,n\}} \in \mathcal{V}_0$,

$$\boldsymbol{z}^T \boldsymbol{A}_\alpha(\boldsymbol{c}) \boldsymbol{H}(\boldsymbol{c})^{-1} \boldsymbol{z} \geq C_\alpha \sum_{i=1}^n c_i^{m_i} |z_i|^2,$$

where $|\cdot|$ denotes the Euclidean norm of $\mathbb{R}^n$ and where

$$\boldsymbol{H}(\boldsymbol{c}) = \operatorname{diag}\left(\frac{1}{c_1}, \dots, \frac{1}{c_n}\right).$$

Let us make a few remarks before giving explicit examples of diffusion matrices satisfying conditions (A1)-(A2). First, let us point out here that, if $\boldsymbol{A}_s$ and $\boldsymbol{A}_g$ are chosen so that (A1) is satisfied, then in the light of (4.2.2b)-(4.2.2c) this implies, at least on the formal level, that $\sum_{i=1}^n J_i(t,x) = 0$ and $\sum_{i=1}^n c_i(t,x) = 1$ for almost all $(t,x) \in Q$. Second, let us mention that condition (A2) implies that the cross-diffusion system associated to a pure (gaseous or solid) phase enjoys an entropy structure in the sense of [156] associated to the logarithmic free energy functional with free energy density defined by

$$\forall \boldsymbol{c} := (c_i)_{i\in\{1,\dots,n\}} \in \mathcal{A}, \quad h(\boldsymbol{c}) := \sum_{i=1}^n c_i \log c_i.$$

Let us point out in particular that $\boldsymbol{H}(\boldsymbol{c})$ is the Hessian of h at vector $\boldsymbol{c} \in \mathcal{A} \cap (\mathbb{R}_+^*)^n$. In the following for all $\boldsymbol{c} \in \mathcal{A} \cap (\mathbb{R}_+^*)^n$, we denote by

$$\boldsymbol{M}_\alpha(\boldsymbol{c}) = \boldsymbol{A}_\alpha(\boldsymbol{c}) \boldsymbol{H}^{-1}(\boldsymbol{c}). \tag{4.2.4}$$

the so-called *mobility matrix* of the phase α.

We give in the following two typical examples of diffusion mappings which satisfy conditions (A1) and (A2). We will use them throughout the rest of the article.

Example 1 (solid phase): We consider here the diffusion mapping introduced in [24]. More precisely, for all $i, j \in \{1, \dots, n\}$, we introduce some cross-diffusion coefficients $\kappa_{ij}^s = \kappa_{ji}^s > 0$ (with $\kappa_{ii}^s = 0$ by convention). For all $\boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}} \in \mathbb{R}^n$, the diffusion matrix $\boldsymbol{A}_s(\boldsymbol{c}) \in \mathbb{R}^{n\times n}$ is defined by

$$\begin{aligned} (\boldsymbol{A}_s)_{ii}(\boldsymbol{c}) &= \sum_{j\neq i} \kappa_{ij}^s c_j, \ i \in \{1, \dots, n\}, \\ (\boldsymbol{A}_s)_{ij}(\boldsymbol{c}) &= -\kappa_{ij}^s c_i, \ i \neq j \in \{1, \dots, n\}. \end{aligned} \tag{4.2.5}$$

First, it can be easily checked that for all $\boldsymbol{c} \in \mathcal{A}$, $\boldsymbol{A}_s(\boldsymbol{c})$ satisfies condition (A1). Moreover, it can be checked that $\boldsymbol{A}_s$ satisfies condition (A2) with $m_i = 1$ for any $i \in \{1, \dots, n\}$ and we refer the reader to [24, Lemma 1] for a proof.

Example 2 (gaseous phase): For all $i, j \in \{1, \dots, n\}$, we introduce some (inverse) cross-diffusion coefficients $\kappa_{ij}^g = \kappa_{ji}^g > 0$ (with $\kappa_{ii}^g = 0$ by convention). In the gaseous phase, the fluxes are implicitly defined via the Stefan-Maxwell linear system [38]

$$\widetilde{\boldsymbol{A}}_g(\boldsymbol{c})\boldsymbol{J} = -\partial_x \boldsymbol{c} \text{ and } \boldsymbol{J} \in \mathcal{V}_0, \text{ a.e. in } Q_g, \tag{4.2.6}$$

where for all $\boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}}$, the diffusion matrix $\widetilde{\boldsymbol{A}}_g(\boldsymbol{c}) \in \mathbb{R}^{n\times n}$ is defined by

$$\begin{aligned} \left(\widetilde{\boldsymbol{A}}_g\right)_{ii}(\boldsymbol{c}) &= \sum_{j\neq i} \kappa_{ij}^g c_j, \ i \in \{1, \dots, n\}, \\ \left(\widetilde{\boldsymbol{A}}_g\right)_{ij}(\boldsymbol{c}) &= -\kappa_{ij}^g c_i, \ i \neq j \in \{1, \dots, n\}. \end{aligned} \tag{4.2.7}$$

Notice that the expression of $\widetilde{\boldsymbol{A}}_g(\boldsymbol{c})$ is similar to the one of $\boldsymbol{A}_s(\boldsymbol{c})$. The matrix $\widetilde{\boldsymbol{A}}_g(\boldsymbol{c})$ is not invertible in general, but it holds that for all $\boldsymbol{c} \in \mathcal{A} \cap \left(\mathbb{R}_+^*\right)^n$, $\widetilde{\boldsymbol{A}}_g(\boldsymbol{c})\left(\mathcal{V}_0\right) \subset \mathcal{V}_0$ and the restriction $\widetilde{\boldsymbol{A}}_g(\boldsymbol{c})|_{\mathcal{V}_0}$ defines an invertible linear mapping from $\mathcal{V}_0$ onto $\mathcal{V}_0$ (see [38, Section 5]). As a consequence, for all $\boldsymbol{c} \in \mathcal{A} \cap (\mathbb{R}_+^*)^n$, there exists a unique matrix $\boldsymbol{A}_g(\boldsymbol{c}) \in \mathbb{R}^{n\times n}$ so that

$$\boldsymbol{A}_g(\boldsymbol{c})z = \begin{cases} \widetilde{\boldsymbol{A}}_g(\boldsymbol{c})|_{\mathcal{V}_0}^{-1}\boldsymbol{z} & \text{if } \boldsymbol{z} \in \mathcal{V}_0, \\ 0 & \text{if } \boldsymbol{z} \in (\mathcal{V}_0)^\perp. \end{cases}$$

The relationship (4.2.6) can then be rewritten as

$$\boldsymbol{J} = -\boldsymbol{A}_g(\boldsymbol{c})\partial_x \boldsymbol{c}, \text{ a.e. in } Q_g, \tag{4.2.8}$$

It can then easily be checked that $\boldsymbol{A}_g$ satisfies condition (A1). The proof that its satisfies condition (A2) with $m_i = 1$ for any $i \in \{1, \dots, n\}$ can be found in [160, Lemma 2.4].

Remark 10 (Physical variables)**.** *In [24], the system in the solid phase is written in terms of volume fraction variables, and the volume-filling constraints originates from size exclusion effects. Since we work here with molar concentrations, we should rather write* $\sum_{j=1}^n v_j c_j = 1$ *in* $(0, X)$*, where the* v_j *are constant molar volumes, but we normalize these constants to one to simplify. In [38], the volume-filling constraint in the Stefan-Maxwell model follows from isobaric conditions in the mixture. Let us point out that, although void can be modelled in the solid layer as one particular species accounting for vacancies at the microscopic level and represented by its volume fraction in the continuous limit, the Stefan-Maxwell model, because it is written in terms of molar concentrations of an incompressible mixture, does not address void (or free volume), see for example [198].*

4.2.3 Entropy structure

The aim of this section is to highlight the entropy structure of the coupled model introduced in Sections 4.2.1 and 4.2.2. For any $\boldsymbol{c} \in L^\infty(\Omega; \mathcal{A})$ and $X \in [0, 1]$, the coupled free energy functional is defined by

$$\mathcal{H}(\boldsymbol{c}, X) = \int_0^X h_s(\boldsymbol{c}) + \int_X^1 h_g(\boldsymbol{c}), \tag{4.2.9}$$

with free energy densities given by, for $\alpha \in \{s, g\}$,

$$\forall \boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}} \in \mathcal{A}, \quad h_\alpha(\boldsymbol{c}) = \sum_{i=1}^{n} c_i(\log(c_i) - \mu_i^{*,\alpha}) - c_i + 1. \tag{4.2.10}$$

For all $\boldsymbol{c} := (c_i)_{i\in\{1,\dots,n\}} \in \mathcal{A}$, the chemical potentials are defined as

$$\mu_i^\alpha(\boldsymbol{c}) = \log(c_i) - \mu_i^{*,\alpha}, \quad \forall i \in \{1, \dots, n\}. \tag{4.2.11}$$

Note that $\partial_x \boldsymbol{\mu}^\alpha(\boldsymbol{c}) = \partial_x \log(\boldsymbol{c})$ for $\alpha \in \{s, g\}$. Then differentiating formally the free energy with respect to time and using (4.2.4), we obtain the free energy dissipation equality: for almost all $t \geq 0$,

$$\begin{aligned} \frac{d}{dt}\mathcal{H}(\boldsymbol{c}(t), X(t)) &+ \int_0^{X(t)} \partial_x \log(\boldsymbol{c}(t))^T \boldsymbol{M}_s(\boldsymbol{c}(t))\partial_x \log(\boldsymbol{c}(t)) \\ &+ \int_{X(t)}^1 \partial_x \log(\boldsymbol{c}(t))^T \boldsymbol{M}_g(\boldsymbol{c}(t))\partial_x \log(\boldsymbol{c}(t)) + \boldsymbol{F}(t)^T [\![\boldsymbol{\mu}(t)]\!] = 0, \end{aligned} \tag{4.2.12}$$

where

$$[\![\boldsymbol{\mu}(t)]\!] = \begin{cases} \boldsymbol{\mu}^g(t) - \boldsymbol{\mu}^s(t), & \text{if } t \in [0, T) \text{ with } \boldsymbol{\mu}^g(t) := \boldsymbol{\mu}^g(\boldsymbol{c}^g(t)) \text{ and } \boldsymbol{\mu}^s(t) := \boldsymbol{\mu}^s(\boldsymbol{c}^s(t)), \\ 0, & \text{otherwise.} \end{cases}$$

First, since, for $\alpha \in \{s, g\}$, $\boldsymbol{A}_\alpha$ satisfies condition (A2), it holds that, almost everywhere in Q_α,

$$(\partial_x \log(\boldsymbol{c})^T \boldsymbol{M}_\alpha(\boldsymbol{c})\partial_x \log(\boldsymbol{c}) \geq C_\alpha \sum_{i=1}^{n} c_i^{m_i} |\partial_x \log(c_i)|^2 \geq C_\alpha \sum_{i=1}^{n} \frac{1}{c_i^{2-m_i}} |\partial_x c_i|^2 \geq C_\alpha |\partial_x \boldsymbol{c}|^2, \tag{4.2.13}$$

where in the last inequality we used the fact that, for any $i \in \{1, \dots, n\}$, $m_i \leq 2$ and $c_i \leq 1$. Furthermore, for almost all $t \in (0, T)$, the Butler-Volmer fluxes (4.2.2f) can be reinterpreted, using (4.2.11), as, for $i \in \{1, \dots, n\}$,

$$F_i(t) = c_i^g(t) \exp\left(-\frac{1}{2}[\![\mu_i^*]\!]\right) - c_i^s(t) \exp\left(\frac{1}{2}[\![\mu_i^*]\!]\right) = 2\sqrt{c_i^s(t) c_i^g(t)} \sinh\left(\frac{1}{2}[\![\mu_i(t)]\!]\right), \tag{4.2.14}$$

which guarantees that, for almost any $t \geq 0$,

$$\boldsymbol{F}(t)^T [\![\boldsymbol{\mu}(t)]\!] \geq 0.$$

As a consequence, the free energy is a Lyapunov functional of the coupled system, in the sense that for almost all $t \geq 0$,

$$\frac{d}{dt}\mathcal{H}(\boldsymbol{c}(t), X(t)) \leq 0.$$

Note that, given the definition of the free energy density (4.2.10), this property guarantees the preservation of nonnegativity of the concentrations along the dynamics.

Let us now go a step further in the analysis of the variational structure of the interface potentials (4.2.2f) with respect to the free energy (4.2.9). In the series of works [186, 142, 181], the mass action law was associated to a quadratic gradient structure with respect to $\mathcal{H}$. Later, the authors of [2, 3, 189] tried to derive this structure from microscopic systems using large deviations theory. Interestingly, they did not recover the previously known quadratic structure, but discovered a new generalized (non-quadratic) gradient structure. We choose to use this structure in this work. More precisely, let us introduce an auxiliary function, defined on the real line as

$$\phi(x) = 4\left(\cosh\left(\frac{x}{2}\right) - 1\right), \ \forall x \in \mathbb{R}.$$

This function is smooth, strictly convex, nonnegative and such that $\phi(0) = 0$. Its derivative is given by

$$\phi'(x) = 2\sinh\left(\frac{x}{2}\right), \ \forall x \in \mathbb{R},$$

and ϕ' is bijective from $\mathbb{R}$ to $\mathbb{R}$. The convex conjugate of ϕ is given by (see [3, Section 5a])

$$\phi^*(z) = \sup_{x\in\mathbb{R}}\{xz - \phi(x)\} = 2z\log\left(\frac{z+\sqrt{z^2+4}}{2}\right) - 2\sqrt{z^2+4} + 4, \ \forall z \in \mathbb{R}.$$

The Fenchel-Young duality states that $z = \phi'(x)$ if and only if

$$\phi(x) + \phi^*(z) = zx, \tag{4.2.15}$$

so that

$$\phi^*(\phi'(x)) = x\phi'(x) - \phi(x), \ x \in \mathbb{R},$$

which implies, by strict convexity of ϕ, the fact that $\phi(0) = 0$ and that $\phi' : \mathbb{R} \to \mathbb{R}$ is bijective, that $\phi^* \geq 0$ in $\mathbb{R}$ and $\phi^*(z) = 0$ if and only if $z = 0$.

Let us now remark that the Butler-Volmer fluxes (4.2.14) are related to ϕ via the following relationship

$$\phi'\left([\![\mu_i]\!]\right) = \frac{F_i}{\sqrt{c_i^g c_i^s}}, \ i \in \{1, \dots, n\}.$$

As a consequence, applying (4.2.15) to $x := [\![\mu_i]\!]$, it holds that for any $i \in \{1, \dots, n\}$,

$$\sqrt{c_i^s c_i^g}\left(\phi([\![\mu_i]\!]) + \phi^*\left(\frac{F_i}{\sqrt{c_i^s c_i^g}}\right)\right) = F_i[\![\mu_i]\!].$$

Therefore, one can rewrite (4.2.12) as

$$\begin{aligned}\mathcal{H}(\boldsymbol{c}(t), X(t)) &+ \int_0^t \int_0^{X(\tau)} (\partial_x \log(\boldsymbol{c}(\tau)))^T \boldsymbol{M}_s(\boldsymbol{c}(\tau))\partial_x \log(\boldsymbol{c}(\tau))\, dx d\tau \\ &+ \int_0^t \int_{X(\tau)}^1 (\partial_x \log(\boldsymbol{c}(\tau)))^T \boldsymbol{M}_g(\boldsymbol{c}(\tau))\partial_x \log(\boldsymbol{c}(\tau))\, dx d\tau \\ &+ \int_0^t \sum_{i=1}^n \sqrt{c_i^s(\tau)c_i^g(\tau)}\left(\phi([\![\mu_i(\tau)]\!]) + \phi^*\left(\frac{F_i(\tau)}{\sqrt{c_i^s(\tau)c_i^g(\tau)}}\right)\right) d\tau = 0.\end{aligned} \tag{4.2.16}$$

This relation is not yet satisfying, since it may degenerate when $c_i^s, c_i^g = 0$. To circumvent this issue, we use on the one hand the estimates (4.2.13) on the diffusion terms, and on the other hand the fact that it holds

$$\sqrt{c_i^s c_i^g}\left(\phi([\![\mu_i]\!]) + \phi^*\left(\frac{F_i}{\sqrt{c_i^s c_i^g}}\right)\right) \geq \sqrt{c_i^s c_i^g}\phi^*\left(\frac{F_i}{\sqrt{c_i^s c_i^g}}\right) \geq \phi^*(F_i) \geq 0.$$

The first inequality follows from the nonnegativity of ϕ and the second from the convexity of ϕ^* combined with $\phi^*(0) = 0$. We have derived the *weak dissipation inequality*: for some $C_s, C_g > 0$,

$$\begin{aligned}\mathcal{H}(\boldsymbol{c}(t), X(t)) + C_s \int_0^t \int_0^{X(\tau)} |\partial_x \boldsymbol{c}(\tau)|^2 \, dx d\tau + C_g \int_0^t \int_{X(\tau)}^1 |\partial_x \boldsymbol{c}(\tau)|^2 \, dx d\tau \\ + \int_0^t \sum_{i=1}^n \phi^*(F_i(\tau)) \, d\tau \leq \mathcal{H}(\boldsymbol{c}^0, X^0).\end{aligned} \tag{4.2.17}$$

Remark 11 (Extension of the model)**.** *The derivation of the dissipation equality* (4.2.12) *shows that, in fact, a more general equality holds:*

$$\begin{aligned}\frac{d}{dt}\mathcal{H}(\boldsymbol{c}(t), X(t)) + \int_0^{X(t)} \partial_x \log(\boldsymbol{c}(t))^T \boldsymbol{M}_s(\boldsymbol{c}(t)) \partial_x \log(\boldsymbol{c}(t)) \\ + \int_{X(t)}^1 \partial_x \log(\boldsymbol{c}(t))^T \boldsymbol{M}_g(\boldsymbol{c}(t)) \partial_x \log(\boldsymbol{c}(t)) + \boldsymbol{F}(t)^T [\![\boldsymbol{\mu}(t)]\!] = X'(t) \, [\![\pi(\boldsymbol{c})]\!] \, ,\end{aligned}$$

where we have introduced the thermodynamic pressure, for $\alpha \in \{s, g\}$,

$$\pi^\alpha(\boldsymbol{c}) = \boldsymbol{c} \cdot \boldsymbol{\mu}^\alpha(\boldsymbol{c}) - h(\boldsymbol{c}). \tag{4.2.18}$$

The term $X'(t) \, [\![\pi(\boldsymbol{c})]\!]$ happens to be null in our case, but we have identified three different contributions to free energy dissipation: the two first terms account for bulk diffusion; the term $\boldsymbol{F}(t)^T [\![\boldsymbol{\mu}]\!]$ accounts for reactions at the interface, driven by a jump of chemical potentials; the last term $X'(t)[\![\pi(\boldsymbol{c})]\!]$ accounts for a displacement of the interface driven by a jump of pressure. It is worth noticing that, if the volume-filling constraints were not normalized to the same constant in (4.2.1) *(which would be physically relevant, since the molar volumes are not expected to be equal in the two phases), then there would be a (constant) nonzero contribution of $[\![\pi(\boldsymbol{c})]\!]$ to the dissipation of the free energy. To go further in the modelling, one may question the relevance of the isobaric assumption (or incompressibility) in the context of vapor deposition. This assumption led to the saturation constraint in the gas phase, and is fundamental for the Stefan-Maxwell model. Going beyond it would lead us to implement a different model to describe a* compressible *fluid mixture. In this model, the pressure π may become a proper time-dependent variable, and equation* (4.2.12) *would suggest defining an evolution law for the location of the interface of the form*

$$X' = \partial_\pi \psi(\boldsymbol{c}^s, \boldsymbol{c}^g, [\![\pi]\!]),$$

for some function $\psi : \left\{ \begin{array}{ccc} \mathcal{A} \times \mathcal{A} \times \mathbb{R} & \to & \mathbb{R} \\ (\boldsymbol{c}_1, \boldsymbol{c}_2, \pi) & \mapsto & \psi(\boldsymbol{c}_1, \boldsymbol{c}_2, \pi) \end{array} \right.$ *to ensure dissipation. This goes beyond the scope of this work.*

4.2.4 Stationary states and long-time asymptotics

One deduces from the weak dissipation inequality (4.2.17) that stationary solutions $(\bar{\boldsymbol{c}}, \bar{X})$ must be such that $\bar{\boldsymbol{c}}$ is equal to a constant vector $\bar{\boldsymbol{c}}^s := (\bar{c}_i^s)_{i\in\{1,\dots,n\}} \in \mathcal{A}$ in $(0, \bar{X})$ and another constant vector $\bar{\boldsymbol{c}}^g := (\bar{c}_i^g)_{i\in\{1,\dots,n\}} \in \mathcal{A}$ in $(\bar{X}, 1)$. Moreover, if $\bar{X} \in (0,1)$, $\overline{F}_i := \frac{1}{\sqrt{\beta_i^*}}\bar{c}_i^g - \sqrt{\beta_i^*}\bar{c}_i^s$ should be equal to 0 for any $i \in \{1,\dots,n\}$. We set $\boldsymbol{m}^0 := \int_\Omega \boldsymbol{c}^0$ (remember that $\boldsymbol{c}^0$ is the initial condition of $\boldsymbol{c}$ given by (4.2.2a)), and denote by m_i^0 the ith component of $\boldsymbol{m}^0$ for all $i \in \{1,\dots,n\}$.

Definition 11. *A state $(\bar{\boldsymbol{c}}^s, \bar{\boldsymbol{c}}^g, \bar{X}) \in \mathcal{A} \times \mathcal{A} \times [0,1]$ is said to be a stationary state of model (4.2.2) if and only if*

(i) for all $i \in \{1,\dots,n\}$, $\bar{X}\bar{c}_i^s + (1-\bar{X})\bar{c}_i^g = m_i^0$ (mass conservation);

(ii) if $\bar{X} = 0$ (respectively $\bar{X} = 1$), then $\bar{\boldsymbol{c}}^s = 0$ (respectively $\bar{\boldsymbol{c}}^g = 0$) (convention in the pure phase case);

(iii) if $\bar{X} \in (0,1)$, $\overline{F}_i := \frac{1}{\sqrt{\beta_i^*}}\bar{c}_i^g - \sqrt{\beta_i^*}\bar{c}_i^s = 0$ (zero-flux in the two-phase case).

We characterize the set of stationary states of (4.2.2) in the sense of Definition 11, as stated in Proposition 6.

Proposition 6 (Stationary states)**.** *Let us assume that $m_i^0 > 0$ for all $i \in \{1,\dots,n\}$. In addition to the trivial pure phase stationary states $(\boldsymbol{m}^0, 0, 1)$ and $(0, \boldsymbol{m}^0, 0)$, we can characterize the set of stationary states of model (4.2.2) (in the sense of Definition 11) as follows:*

Case 1: *If $\beta_i^* = 1$ for all $i \in \{1,\dots,n\}$, then the set of non-trivial stationary states is equal to the set of vectors of the form $(\boldsymbol{m}^0, \boldsymbol{m}^0, \bar{X})$ with $\bar{X} \in (0,1)$.*

Case 2: *If there exists $i_0 \in \{1,\dots,n\}$ such that $\beta_{i_0}^* \neq 1$, then there exists a non-trivial stationary solution (i.e. such that $\bar{X} \in (0,1)$) if and only if*

$$\min\left(\sum_{i=1}^n m_i^0\beta_i^*, \sum_{i=1}^n m_i^0\frac{1}{\beta_i^*}\right) > 1. \tag{4.2.19}$$

In addition, if (4.2.19) is satisfied, then this non-trivial stationary state is unique.

Proof. Since the initial condition $\boldsymbol{c}^0$ is assumed to belong to $L^\infty(\Omega;\mathcal{A})$, this implies that $\sum_{i=1}^n m_i^0 = 1$. Moreover, it can be easily proved that for all $x \in \mathbb{R}_+^*$, $x + \frac{1}{x} \geq 2$ with equality if and only if $x = 1$. As a consequence, it holds that

$$\sum_{i=1}^n m_i^0(\beta_i^* + \frac{1}{\beta_i^*}) \geq 2,$$

with equality if and only if $\beta_i^* = 1$ for all $i \in \{1, \dots, n\}$. We can thus distinguish two cases:

Case 1: For all $i \in \{1, \dots, n\}$, $\beta_i^* = 1$. Then, it holds that

$$\sum_{i=1}^{n} m_i^0 \beta_i^* = \sum_{i=1}^{n} m_i^0 \frac{1}{\beta_i^*} = 1.$$

Case 2: There exists $i_0 \in \{1, \dots, n\}$ such that $\beta_{i_0}^* \neq 1$. Then, it holds that

$$\sum_{i=1}^{n} m_i^0 (\beta_i^* + \frac{1}{\beta_i^*}) > 2.$$

In this proof, we consider each case separately.

Case 1: Let $(\bar{\boldsymbol{c}}^s, \bar{\boldsymbol{c}}^g, \bar{X}) \in \mathcal{A} \times \mathcal{A} \times (0,1)$ be a non-trivial stationary state of model (4.2.2) in the sense of Definition 11. Then, from (iii), it holds that for all $i \in \{1, \dots, n\}$, $\overline{F}_i = \bar{c}_i^g - \bar{c}_i^s = 0$, which yields $\bar{\boldsymbol{c}}^s = \bar{\boldsymbol{c}}^g$. Now, the mass conservation property (i) implies necessarily that $\bar{\boldsymbol{c}}^s = \bar{\boldsymbol{c}}^g = \boldsymbol{m}^0$. Conversely, for any $\bar{X} \in (0,1)$, $(\boldsymbol{m}_0, \boldsymbol{m}_0, \bar{X})$ can be easily checked to be a stationary state of model (4.2.2).

Case 2: Let $(\bar{\boldsymbol{c}}^s, \bar{\boldsymbol{c}}^g, \bar{X}) \in \mathcal{A} \times \mathcal{A} \times (0,1)$ be a non-trivial stationary state of model (4.2.2) in the sense of Definition 11. Let us first prove that for all $i \in \{1, \dots, n\}$, $\bar{c}_i^g > 0$ and $\bar{c}_i^s > 0$, reasoning by contradiction. Indeed, if for instance there exists $i_0 \in \{1, \dots, n\}$ such that $\bar{c}_{i_0}^g = 0$, the fact that $\overline{F}_{i_0} = 0$ yields that $\bar{c}_{i_0}^s = 0$ as well. This yields a contradiction with the fact that

$$\bar{X} \bar{c}_{i_0}^s + (1 - \bar{X}) \bar{c}_{i_0}^g = m_{i_0}^0 > 0.$$

Now, it is easy to see that (i) and (iii) are satisfied if and only if

$$\forall i \in \{1, \dots, n\}, \quad \bar{c}_i^g = \beta_i^* \bar{c}_i^s \text{ and } \bar{c}_i^s = \frac{m_i^0}{\bar{X} + \beta_i^*(1 - \bar{X})}. \tag{4.2.20}$$

As a consequence, $(\bar{\boldsymbol{c}}^s, \bar{\boldsymbol{c}}^g, \bar{X})$ is a stationary state in the sense of Definition 11 if and only if $\bar{X}$ is a solution in $(0,1)$ to

$$\sum_{i=1}^{n} \frac{m_i^0}{\bar{X} + \beta_i^*(1 - \bar{X})} = 1. \tag{4.2.21}$$

In addition, for any solution $\bar{X} \in (0,1)$ to (4.2.21), $\bar{\boldsymbol{c}}^g$ and $\bar{\boldsymbol{c}}^s$ are necessarily given by (4.2.20), which immediately implies that $\sum_{i=1}^{n} \bar{c}_i^s = \sum_{i=1}^{n} \bar{c}_i^g = 1$ and thus that $\bar{\boldsymbol{c}}^g$ and $\bar{\boldsymbol{c}}^s$ belong to $\mathcal{A}$. It thus remains to characterize the set of solution $\bar{X} \in (0,1)$ to (4.2.21). Let us introduce

$$\varphi : \left\{ \begin{array}{ccc} [0,1] & \to & \mathbb{R} \\ x & \mapsto & \sum_{i=1}^{n} \frac{m_i^0}{x + \beta_i^*(1-x)} - 1. \end{array} \right. \tag{4.2.22}$$

Then, the function φ is $\mathcal{C}^\infty$ on $[0,1]$ and its first and second-order derivatives are respectively given by

$$\forall x \in [0,1], \quad \varphi'(x) = -\sum_{i=1}^{n} \frac{(1-\beta_i^*)m_i^0}{(x+\beta_i^*(1-x))^2} \text{ and } \varphi''(x) = 2\sum_{i=1}^{n} \frac{(1-\beta_i^*)^2 m_i^0}{(x+\beta_i^*(1-x))^3}.$$

Then, the function φ enjoys the following properties. First, it can be easily seen that $\varphi''(x) > 0$ for all $x \in [0,1]$, the strict positivity stemming from the fact that there exists at least one index $i_0 \in \{1,\dots,n\}$ such that $\beta_{i_0}^* \neq 1$. Hence φ is strictly convex. Second, it holds that $\varphi(1) = \sum_{i=1}^n m_i^0 - 1 = 0$. Thus, there exists at least one solution $\bar{X} \in (0,1)$ to the equation $\varphi(\bar{X}) = 0$ if and only if

$$\varphi(0) > 0 \text{ and } \varphi'(1) > 0, \tag{4.2.23}$$

and the solution is then unique. The desired result is then obtained by remarking that (4.2.23) is equivalent to (4.2.19). □

Let us now make some remarks on the dynamics. Under condition (4.2.19), we expect the two-phases stationary state to be the only stable one, and the solution to converge exponentially to this state. Note, however, that this convergence can by no means hold for any initial condition, but at best for *close enough* initial conditions. Indeed, the interface dynamics only depends on the *local* concentrations around the interface. In consequence, there is no reason for the interface to be monotone over time (think of very slow diffusion), and, since the value of $X(t)$ might reach 0 or 1 for some time t, the dynamics may get "trapped" in a one-phase solution, even when (4.2.19) holds. Thus, it seems difficult to predict to which state the dynamics converges for any initial condition, since it certainly does not depend only on the quantities involved in condition (4.2.19). On the other hand, if (4.2.19) is violated, the system should converge to one of the one-phase solutions, depending on which quantity violates the condition. We refer to the numerical results in Section 4.5 and highlight the difficulties in the analysis below.

Letting time go to infinity in the weak dissipation inequality (4.2.17), we expect weak solutions to converge to the previously identified set of stationary points. First remark that the free energy functional is uniformly bounded from below by a real constant $C \in \mathbb{R}$, so that the time-integrated dissipation terms in (4.2.17) are nonnegative and uniformly bounded from above. Thus, as time goes to infinity, the integrals in time must remain bounded, which implies that, necessarily,

$$\int_0^{X(t)} |\partial_x \boldsymbol{c}|^2, \ \int_{X(t)}^1 |\partial_x \boldsymbol{c}|^2, \ \sum_{i=1}^n \phi^*(F_i(t)) \to 0 \text{ as } t \to \infty. \tag{4.2.24}$$

From the last convergence, we get an alternative: either $\lim_{t\to+\infty} X(t) = 0$ (resp. 1), and we deduce convergence to the one-phase gas (resp. solid) stationary state, either $X(t) \in (0,1)$ for any $t \geq 0$, then $F_i(t)$ is given for any time by the formula (4.2.2f) for any $i \in \{1,\dots,n\}$ and, if we knew in addition that $X(t)$ converges to a constant $\bar{X} \in (0,1)$,

then we could use the conclusions of Proposition 6. However, the convergence of the interface is not granted and we cannot directly conclude.

This difficulty leads us to consider the dynamics of a simplified model. Assuming that diffusion is infinitely fast in comparison to the interface reactions, our system amounts to a system of ordinary differential equations. More precisely, we assume for the moment that all the components are uniform in space and still denoted by $\boldsymbol{c}^s(t), \boldsymbol{c}^g(t)$. Then, the masses are simply defined by $\boldsymbol{m}^s(t) = \boldsymbol{c}^s(t)X(t)$, $\boldsymbol{m}^g(t) = \boldsymbol{m}^0 - \boldsymbol{m}^s(t)$ and the dynamics reduces to the system of ordinary differential equations

$$\frac{d}{dt}\boldsymbol{m}^s(t) = \boldsymbol{F}(t). \tag{4.2.25}$$

We intend to perform a stability analysis of the above ODE system in the future.

4.3 Finite volume scheme

This section is devoted to the finite volume approximation of system (4.2.2). In Section 4.3.1, we introduce a space-time discretization of the domain and some useful notations. The scheme is presented in two steps: in Section 4.3.2, we discretize the conservation laws, while Section 4.3.3 is devoted to the mesh displacement.

In this section, we restrict ourselves to the case where the cross-diffusion mapping for the solid (respectively gaseous) phase is given by Example 1 (respectively Example 2) of Section 4.2.2.

4.3.1 Discretization

We consider $N \in \mathbb{N}^*$ reference cells of uniform size $\Delta x = \frac{1}{N}$. The $N+1$ edge vertices are denoted by $0 = x_{\frac{1}{2}} \leq x_{\frac{3}{2}} \leq \cdots \leq x_{N+\frac{1}{2}} = 1$. More precisely, $x_{K+\frac{1}{2}} = K\Delta x$ for all $K \in \{0, \ldots, N\}$. We consider a time horizon $T > 0$ and a time discretization with mesh parameter Δt defined such that $N_T \Delta t = T$ with $N_T \in \mathbb{N}^*$. The concentrations are discretized as $\boldsymbol{c}^p_{\Delta x} = (c^p_{i,K})_{i\in\{1,\ldots,n\},\ K\in\{1,\ldots,N\}}$ for $p \in \{0, \ldots, N_T\}$. The interface is time-discretized as X^p for $p \in \{0, \ldots, N_T\}$, and we denote by $K^p \in \{0, \ldots, N\}$ the lowest integer such that $|x_{K^p+\frac{1}{2}} - X^p| \leq |x_{K+\frac{1}{2}} - X^p|$ for all $K \in \{0, \ldots, N\}$. For all $p \geq 1$, at time $t^{p-1} = (p-1)\Delta t$, the mesh is locally modified around X^{p-1}. More precisely, for all $K \in \{1, \ldots, N\}$, we denote by C^{p-1}_K the Kth cell of the mesh defined by

$$C^{p-1}_K := \begin{cases} (x_{K-\frac{1}{2}}, x_{K+\frac{1}{2}}) & \text{if } K < K^{p-1} \text{ or } K > K^{p-1}+1, \\ (x_{K^{p-1}-\frac{1}{2}}, X^{p-1}) & \text{if } K = K^{p-1}, \\ (X^{p-1}, x_{K^{p-1}+\frac{3}{2}}) & \text{if } K = K^{p-1}+1. \end{cases}$$

We refer to the initial configuration in Figure 4.1, where the interface cell is assumed to be the Kth one (instead of K^{p-1}) to alleviate the notation. The size of the cell C^{p-1}_K is

then denoted by Δ_K^{p-1} for all $K \in \{1, \dots, N\}$:

$$\Delta_K^{p-1} = \begin{cases} (X^{p-1} - x_{K^{p-1}-\frac{1}{2}}) & \text{if } K = K^{p-1}, \\ (x_{K^{p-1}+\frac{3}{2}} - X^{p-1}) & \text{if } K = K^{p-1}+1, \\ \Delta x & \text{otherwise.} \end{cases} \tag{4.3.1}$$

With this notation, a constraints-compatible initial condition $\boldsymbol{c}^0 \in L^\infty(\Omega; \mathcal{A})$ is naturally discretized as $c_{i,K}^0 = \frac{1}{\Delta_K^0} \int_{C_K^0} c_i^0 \, dx$ for any $i \in \{1, \dots, n\}$, $K \in \{1, \dots, N\}$. Starting from the knowledge of $(\boldsymbol{c}_{\Delta x}^{p-1}, X^{p-1})$, our scheme consists in

i) solving the conservation laws and updating the interface position, leading to the intermediate solution denoted by $(\boldsymbol{c}_{\Delta x}^{p,\star}, X^p)$.

ii) updating the cells of the mesh $(C_K^p)_{K \in \{1,\dots,N\}}$ and post-processing the interface concentrations into the final values $\boldsymbol{c}_{\Delta x}^p$.

4.3.2 Conservation laws

The conservation laws (4.2.2b) are discretized implicitly as, for $K \in \{1, \dots, N\}, i \in \{1, \dots, n\}$,

$$\frac{1}{\Delta t}(\Delta_K^{p,\star} c_{i,K}^{p,\star} - \Delta_K^{p-1} c_{i,K}^{p-1}) + J_{i,K+\frac{1}{2}}^{p,\star} - J_{i,K-\frac{1}{2}}^{p,\star} = 0, \tag{4.3.2a}$$

where we have introduced the numerical fluxes and the quantity (see the intermediate mesh in Figure 4.1 where $K := K^{p-1}$)

$$\Delta_K^{p,\star} = \begin{cases} (X^p - x_{K^{p-1}-\frac{1}{2}}) & \text{if } K = K^{p-1}, \\ (x_{K^{p-1}+\frac{3}{2}} - X^p) & \text{if } K = K^{p-1}+1, \\ \Delta x & \text{otherwise.} \end{cases} \tag{4.3.2b}$$

We can impose conditions on the time step Δt to guarantee that the new position of the interface X^p still belongs to $(x_{K^{p-1}-\frac{1}{2}}, x_{K^{p-1}+\frac{3}{2}})$. These conditions are made explicit in the next section and we assume that they hold here. The aim of the term $\frac{1}{\Delta t}(\Delta_K^{p,\star} c_{i,K}^{p,\star} - \Delta_K^{p-1} c_{i,K}^{p-1})$ for $K = K^{p-1}$ in (4.3.2a) is to yield the approximation

$$\begin{aligned} \frac{d}{dt}\left(\int_{x_{K^{p-1}-\frac{1}{2}}}^{X(t)} c_i(t)\right)_{|t=t^p} &\approx \frac{1}{\Delta t}\left(\int_{x_{K^{p-1}-\frac{1}{2}}}^{X(t^p)} c_i(t^p) - \int_{x_{K^{p-1}-\frac{1}{2}}}^{X(t^{p-1})} c_i(t^{p-1})\right) \\ &\approx \frac{1}{\Delta t}\left(\int_{x_{K^{p-1}-\frac{1}{2}}}^{X^p} c_{i,K^{p-1}}^{p,\star} - \int_{x_{K^{p-1}-\frac{1}{2}}}^{X^{p-1}} c_{i,K^{p-1}}^{p-1}\right) \\ &= \frac{1}{\Delta t}(\Delta_{K^{p-1}}^{p,\star} c_{i,K^{p-1}}^{p,\star} - \Delta_{K^{p-1}}^{p-1} c_{i,K^{p-1}}^{p-1}). \end{aligned}$$

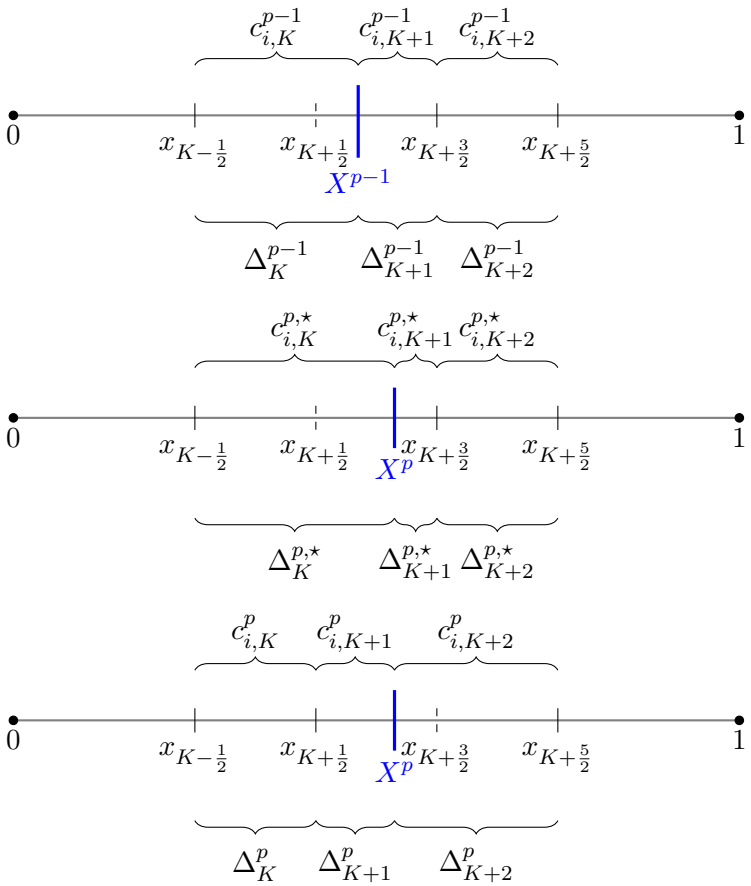


Figure 4.1: A virtual mesh displacement between $t^{p-1} = (p-1)\Delta t$ and $t^p = p\Delta t$, where $K := K^{p-1}$.

Similarly, the aim of the term $\frac{1}{\Delta t}(\Delta_K^{p,\star} c_{i,K}^{p,\star} - \Delta_K^{p-1} c_{i,K}^{p-1})$ for $K = K^{p-1} + 1$ in (4.3.2a) is to yield an approximation of $\dfrac{d}{dt}\left(\displaystyle\int_{X(t)}^{x_{K^{p-1}+\frac{3}{2}}} c_i(t)\right)$. The zero-flux conditions at the boundary of the domain $\Omega = (0,1)$ are discretized as:

$$\forall i \in \{1,\dots,n\},\ J_{i,\frac{1}{2}}^{p,\star} = J_{i,N+\frac{1}{2}}^{p,\star} = 0.$$

We are thus left with the definition of the fluxes $\boldsymbol{J}_{K+\frac{1}{2}}^{p,\star} := \left(J_{i,K+\frac{1}{2}}^{p,\star}\right)_{i\in\{1,\dots,n\}}$ for all $K \in \{1,\dots,N-1\}$. To this aim, we need to introduce the edge concentrations $\boldsymbol{c}_{K+\frac{1}{2}}^{p,\star}$ for all $K \in \{1,\dots,N-1\}$, defined through a logarithmic mean as

$$c_{i,K+\frac{1}{2}}^{p,\star} = \begin{cases} 0 & \text{if } \min(c_{i,K}^{p,\star}, c_{i,K+1}^{p,\star}) \le 0, \\ c_{i,K}^{p,\star} & \text{if } 0 < c_{i,K}^{p,\star} = c_{i,K+1}^{p,\star}, \\ \frac{c_{i,K}^{p,\star} - c_{i,K+1}^{p,\star}}{\log(c_{i,K}^{p,\star}) - \log(c_{i,K+1}^{p,\star})} & \text{otherwise.} \end{cases} \tag{4.3.2c}$$

Let us also introduce the finite difference notation, for all $K \in \{1,\dots,N-1\}$, and any $\boldsymbol{c} = (\boldsymbol{c}_K)_{K\in\{1,\dots,N\}} \in (\mathbb{R}^q)^N$ with any $q \in \mathbb{N}^*$,

$$D_{K+\frac{1}{2}}\boldsymbol{c} := \boldsymbol{c}_{K+1} - \boldsymbol{c}_K.$$

Then, Definition (4.3.2c) yields a discrete chain rule: for any $i \in \{1,\dots,n\}$, $K \in \{1,\dots,N-1\}$, if $c_{i,K}^{p,\star}, c_{i,K+1}^{p,\star} > 0$, then

$$D_{K+\frac{1}{2}}\boldsymbol{c}_i^{p,\star} = c_{i,K+\frac{1}{2}}^{p,\star} D_{K+\frac{1}{2}} \log(\boldsymbol{c}_i^{p,\star}). \tag{4.3.2d}$$

We define, for $\alpha \in \{s,g\}$, the coefficients $\kappa^{*,\alpha} = \min_{ij} \kappa_{ij}^{\alpha} > 0$, $\bar{\kappa}_{ij}^{\alpha} = \kappa_{ij}^{\alpha} - \kappa^{*,\alpha} \ge 0$ and, for all $\boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}} \in \mathbb{R}^n$, we define the matrices $\bar{\boldsymbol{A}}_\alpha(\boldsymbol{c}) \in \mathbb{R}^{n\times n}$ similarly to (4.2.5) by

$$(\bar{\boldsymbol{A}}_\alpha)_{ii}(\boldsymbol{c}) = \sum_{j\neq i} \bar{\kappa}_{ij}^{\alpha} c_j,\ i \in \{1,\dots,n\},$$
$$(\bar{\boldsymbol{A}}_\alpha)_{ij}(\boldsymbol{c}) = -\bar{\kappa}_{ij}^{\alpha} c_i,\ i \neq j \in \{1,\dots,n\}.$$

Then the bulk fluxes in the solid domain are discretized as (similarly to [62])

$$\Delta x J_{i,K+\frac{1}{2}}^{p,\star} = -\kappa^{*,s} D_{K+\frac{1}{2}}\boldsymbol{c}_i^{p,\star} - \sum_{j=1}^{n} \bar{\kappa}_{ij}^{s}\left(c_{j,K+\frac{1}{2}}^{p,\star} D_{K+\frac{1}{2}}\boldsymbol{c}_i^{p,\star} - c_{i,K+\frac{1}{2}}^{p,\star} D_{K+\frac{1}{2}}\boldsymbol{c}_j^{p,\star}\right),$$

for all $1 \le K < K^{p-1}$, which rewrites in compact form as

$$\Delta x \boldsymbol{J}_{K+\frac{1}{2}}^{p,\star} = -\widehat{\boldsymbol{A}}_s(\boldsymbol{c}_{K+\frac{1}{2}}^{p,\star}) D_{K+\frac{1}{2}}\boldsymbol{c}^{p,\star},\ \forall 1 \le K < K^{p-1}, \tag{4.3.2e}$$

where

$$\forall \boldsymbol{c} \in \mathbb{R}^n, \quad \widehat{\boldsymbol{A}}_s(\boldsymbol{c}) := \bar{\boldsymbol{A}}_s(\boldsymbol{c}) + \kappa^{*,s} I, \tag{4.3.2f}$$

with $I \in \mathbb{R}^{n\times n}$ the identity matrix. The bulk fluxes in the gas phase (4.2.6) are defined similarly as in the scheme proposed in [61], introducing for all $\boldsymbol{c} \in \mathcal{A}$,

$$\widehat{\boldsymbol{A}}_g(\boldsymbol{c}) := \left(\bar{\boldsymbol{A}}_g(\boldsymbol{c}) + \kappa^{*,g} I\right)^{-1}, \tag{4.3.2g}$$

so that

$$\Delta x \boldsymbol{J}^{p,\star}_{K+\frac{1}{2}} = -\widehat{\boldsymbol{A}}_g\left(\boldsymbol{c}^{p,\star}_{K+\frac{1}{2}}\right) D_{K+\frac{1}{2}}\boldsymbol{c}^{p,\star},\ \forall K^{p-1} < K \leq N-1. \tag{4.3.2h}$$

The interface potentials (4.2.2f) are discretized as

$$F^{p,\star}_i = c^{p,\star}_{i,(K^{p-1}+1)} \exp\left(\frac{\mu^{*,s}_i - \mu^{*,g}_i}{2}\right) - c^{p,\star}_{i,K^{p-1}} \exp\left(\frac{\mu^{*,g}_i - \mu^{*,s}_i}{2}\right),\ \forall i \in \{1,\dots,n\}, \tag{4.3.2i}$$

and we define

$$\boldsymbol{J}^{p,\star}_{K^{p-1}+\frac{1}{2}} := -\boldsymbol{F}^{p,\star}, \tag{4.3.2j}$$

where $\boldsymbol{F}^{p,\star} := \left(F^{p,\star}_i\right)_{i\in\{1,\dots,n\}}$. This expression stems from the fact that, on the continuous level, it holds using (4.2.2) that

$$\begin{aligned}\frac{d}{dt}\left(\int_{x_{K^{p-1}-\frac{1}{2}}}^{X(t)} \boldsymbol{c}(t)\right) &= X'(t)\boldsymbol{c}^s(t) + \int_{x_{K^{p-1}-\frac{1}{2}}}^{X(t)} \partial_t \boldsymbol{c}(t),\\ &= X'(t)\boldsymbol{c}^s(t) - \boldsymbol{J}^s(t) + \boldsymbol{J}(t, x_{K^{p-1}-\frac{1}{2}}),\\ &= \boldsymbol{F}(t) + \boldsymbol{J}(t, x_{K^{p-1}-\frac{1}{2}}).\end{aligned}$$

Finally, (4.2.2g) is discretized as

$$X^p = X^{p-1} + \Delta t \sum_{i=1}^{n} F^{p,\star}_i. \tag{4.3.2k}$$

A solution to (4.3.2) is denoted by $(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p)$.

4.3.3 Post-processing

Once the new value of the interface location X^p has been determined, the updated value of the integer K^p can be determined. The mesh has then to be updated, together with the discretized values of the concentrations accordingly.

First note that, if for all $1 \leq K \leq N$, $\boldsymbol{c}^{p,*}_K := \left(c^{p,*}_{i,K}\right)_{i\in\{1,\dots,n\}} \in \mathcal{A}$ (we prove in Lemma 17 below that it is indeed the case), this implies the uniform bound on the interface fluxes $|F^{p,\star}_i| \leq 2|\cosh(\frac{1}{2}[\![\mu^*_i]\!])|$, for any $i \in \{1,\dots,n\}$. Therefore, we obtain from (4.3.2k), defining

$$C_{\boldsymbol{\mu}^*} := \max_{i\in\{1,\dots,n\}} 2|\cosh(\frac{1}{2}[\![\mu^*_i]\!])| > 0, \tag{4.3.3}$$

for all $p \in \mathbb{N}^*$,

$$|X^p - X^{p-1}| \leq C_{\boldsymbol{\mu}^*} \Delta t.$$

Assuming then that $\Delta t > 0$ is chosen in order to ensure the condition

$$\Delta t \leq \frac{\Delta x}{2C_{\boldsymbol{\mu}^*}}, \tag{4.3.4}$$

we obtain that, necessarily, for all $p \in \mathbb{N}^*$, $|X^p - X^{p-1}| \leq \frac{1}{2}\Delta x$, which in particular ensures that $|K^p - K^{p-1}| \leq 1$ and that X^p belongs to $(x_{K^{p-1}-\frac{1}{2}}, x_{K^{p-1}+\frac{3}{2}})$ (see Figure 4.1 with $K := K^{p-1}$).

If $K^p = K^{p-1}$, then we can directly iterate the scheme with $\boldsymbol{c}^p_{\Delta x} = \boldsymbol{c}^{p,\star}_{\Delta x}$. Otherwise, let us assume that $K^p = K^{p-1} + 1 < N$, the case $K^p = K^{p-1} - 1 > 1$ being treated similarly. We perform the following steps (see the final mesh in Figure 4.1 where the notation $K := K^{p-1}$ is used):

i) *Projection:* The value $c^{p,\star}_{i,K^{p-1}}$ is assigned to the virtual cell $(x_{K^{p-1}-\frac{1}{2}}, X^p)$. We assign this value to both the fixed cell $C^p_{K^{p-1}} = (x_{K^{p-1}-\frac{1}{2}}, x_{K^{p-1}+\frac{1}{2}})$ and the new interface cell $C^p_{K^{p-1}+1} = C^p_{K^p} = (x_{K^{p-1}+\frac{1}{2}}, X^p)$:

$$c^p_{i,K^{p-1}} = c^p_{i,K^{p-1}+1} := c^{p,\star}_{i,K^{p-1}}. \tag{4.3.5}$$

ii) *Average:* We define the value in the cell $C^p_{K^{p-1}+2} = (X^p, x_{K^{p-1}+2})$ as the following average:

$$c^p_{i,K^{p-1}+2} = c^p_{i,K^p+1} := \frac{1}{\Delta x + \Delta^{p,\star}_{K^{p-1}+1}} \left[\Delta^{p,\star}_{K^{p-1}+1} c^{p,\star}_{i,K^{p-1}+1} + \Delta x \; c^{p,\star}_{i,K^{p-1}+2}\right]. \tag{4.3.6}$$

iii) For all $1 \leq K \leq N$, such that $K \neq K^{p-1}, K^{p-1}+1, K^{p-1}+2$, $c^p_{i,K} = c^{p,\star}_{i,K}$.

In the limit cases where $K^p = N$ (resp. $K^p = 1$), in agreement with the continuous model, we consider that only a single phase remains in the system, and definitely set $X^p = 1$ (resp. $X^p = 0$).

The scheme (4.3.2)-(4.3.5)-(4.3.6) is now complete and referred to as (S).

4.4 Elements of numerical analysis of the finite volume scheme

The aim of this section is to gather some elements of numerical analysis of the finite volume scheme presented in Section 4.3. We present here some properties of the scheme on a fixed grid, the convergence of the scheme when discretization parameters go to zero being work in progress.

4.4.1 Non-negativity and volumic constraints

To prove the *a priori* nonnegativity of the concentrations and the volume-filling constraint, we need to slightly modify the scheme (S) as described below. For all $x \in \mathbb{R}$, we set $x^+ := \max(0, x)$ and $x^\diamond := \max(0, \min(1, x))$. We then introduce a modified scheme, which we denote hereafter by $(\widetilde{S})$. Starting from $(\boldsymbol{c}_{\Delta x}^{p-1}, X^{p-1}) \in \mathcal{A}^N \times (0,1)$, and assuming that $1 < K^{p-1} < N$, we first compute $(\boldsymbol{c}_{\Delta x}^{p,\star}, X^p) \in (\mathbb{R}^n)^N \times (0,1)$ solution to (4.3.2) up to the following modifications:

(i) Equation (4.3.2j) is replaced by

$$\boldsymbol{J}^{p,\star}_{K^{p-1}+\frac{1}{2}} = -\widetilde{\boldsymbol{F}}^{p,\star} \tag{4.4.1}$$

where $\widetilde{\boldsymbol{F}}^{p,\star} = \left(\widetilde{F}_i^{p,\star}\right)_{i\in\{1,\dots,n\}}$ with, for all $i \in \{1,\dots,n\}$,

– if $\min\left(\sum_{i=1}^n \left(c_{i,K^{p-1}}^{p,\star}\right)^\diamond, \sum_{i=1}^n \left(c_{i,K^{p-1}+1}^{p,\star}\right)^\diamond\right) > 0$,

$$\widetilde{F}_i^{p,\star} = \min\left(\sum_{i=1}^n \left(c_{i,K^{p-1}}^{p,\star}\right)^\diamond, \sum_{i=1}^n \left(c_{i,K^{p-1}+1}^{p,\star}\right)^\diamond\right) \times \left[\left(c_{i,(K^{p-1}+1)}^{p,\star}\right)^\diamond \exp\left(\frac{\mu_i^{*,s} - \mu_i^{*,g}}{2}\right) - \left(c_{i,K^{p-1}}^{p,\star}\right)^\diamond \exp\left(\frac{\mu_i^{*,g} - \mu_i^{*,s}}{2}\right)\right];$$

– otherwise,

$$\widetilde{F}_i^{p,\star} = \left(c_{i,(K^{p-1}+1)}^{p,\star}\right)^\diamond \exp\left(\frac{\mu_i^{*,s} - \mu_i^{*,g}}{2}\right) - \left(c_{i,K^{p-1}}^{p,\star}\right)^\diamond \exp\left(\frac{\mu_i^{*,g} - \mu_i^{*,s}}{2}\right);$$

(ii) Equation (4.3.2a) is modified by

$$\frac{1}{\Delta t}(\widetilde{\Delta}_K^p c_{i,K}^{p,\star} - \Delta_K^{p-1} c_{i,K}^{p-1}) + J_{i,K+\frac{1}{2}}^{p,\star} - J_{i,K-\frac{1}{2}}^{p,\star} = 0, \tag{4.4.2}$$

where

$$\widetilde{\Delta}_K^p = \begin{cases} (X^{p,s} - x_{K^{p-1}-\frac{1}{2}}) & \text{if } K = K^{p-1}, \\ (x_{K^{p-1}+\frac{3}{2}} - X^{p,g}) & \text{if } K = K^{p-1}+1, \\ \Delta x & \text{otherwise,} \end{cases} \tag{4.4.3}$$

with

$$X^{p,s} := X^{p-1} + \Delta t G^p(\boldsymbol{c}_{K^{p-1}}^{p,\star}),\ X^{p,g} := X^{p-1} + \Delta t G^p(\boldsymbol{c}_{K^{p-1}+1}^{p,\star}), \tag{4.4.4}$$

where for all $\boldsymbol{c} = (c_i)_{i\in\{1,\dots,n\}}$,

$$G^p(\boldsymbol{c}) := \begin{cases} \left(\sum_{i=1}^n c_i^+\right)^{-1} \sum_{i=1}^n \widetilde{F}_i^{p,\star}, & \text{if } \sum_{i=1}^n c_i^+ > 0, \\ 0, & \text{otherwise.} \end{cases}$$

The resulting modified scheme is referred to as $(\widetilde{S})$ while we still denote a possible solution by $(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p)$ (resp.$(\boldsymbol{c}^{p}_{\Delta x}, X^p)$ after post-processing). We prove existence of a solution to $(\widetilde{S})$ that satisfies the positivity of the concentrations and the volume-filling constraint, and is therefore a solution to the original scheme (S). Lemma 17 provides some *a priori* estimates fulfilled by a solution to $(\widetilde{S})$. From now on and in all the rest of the section, we assume that the time step Δt satisfies the following assumption:

$$\Delta t < \frac{\Delta x}{2C^*_{\boldsymbol{\mu}}}, \tag{4.4.5}$$

where $C^*_{\boldsymbol{\mu}}$ was defined in (4.3.3). Then, we have the following results.

Lemma 17. *Let $p \in \mathbb{N} \setminus \{0\}$. Let $(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1})$ be such that for all $1 \leq K \leq N$, $\boldsymbol{c}^{p-1}_K := (c^{p-1}_{i,K})_{i\in\{1,\dots,n\}}$ belongs to $\mathcal{A}$. Let $(\boldsymbol{c}^{p}_{\Delta x}, X^{p,s}, X^{p,g})$ be a solution to $(\widetilde{S})$. Then it holds that*

$$\begin{aligned} c^p_{i,K} &> 0,\ \forall i \in \{1,\dots,n\},\ \forall K \in \{1,\dots,N\}, \\ \sum_{i=1}^n c^p_{i,K} &= 1,\ \forall K \in \{1,\dots,N\}, \\ \sum_{K=1}^N \Delta^p_K c^p_{i,K} &= \sum_{K=1}^N \Delta^{p-1}_K c^{p-1}_{i,K},\ \forall i \in \{1,\dots,n\}. \end{aligned}$$

In particular, $X^{p,s} = X^{p,g} =: X^p$ and $(\boldsymbol{c}^p_{\Delta x}, X^p)$ is then also a solution to (S).

Proof. Let us prove the positivity of $\boldsymbol{c}^{p,\star}_{\Delta x}$ (hence of $\boldsymbol{c}^p_{\Delta x}$). Let us reason by contradiction and assume that there exists $i \in \{1,\dots,n\}$ and $K \in \{1,\dots,N\}$ such that

$$c^{p,\star}_{i,K} = \min_{j\in\{1,\dots n\}} \min_{L\in\{1,\dots,N\}} c^{p,\star}_{j,L}$$

is such that $c^{p,\star}_{i,K} \leq 0$. First, let us point out that the assumption on Δt and the expression of the fluxes $\widetilde{\boldsymbol{F}}^{p,\star}$ imply that $\widetilde{\Delta}^p_K > 0$ for all $1 \leq K \leq N$. In addition, the conservation laws (4.3.2a) read

$$\frac{1}{\Delta t}(\widetilde{\Delta}^p_K c^{p,\star}_{i,K} - \Delta^{p-1}_K c^{p-1}_{i,K}) = J^{p,\star}_{i,K-\frac{1}{2}} - J^{p,\star}_{i,K+\frac{1}{2}},$$

from which it follows that

$$J^{p,\star}_{i,K-\frac{1}{2}} - J^{p,\star}_{i,K+\frac{1}{2}} \leq 0.$$

If $K \neq K^{p-1}$ and $K \neq K^{p-1}+1$, the cell C^{p-1}_K is a bulk cell, and thanks to the specific choice (4.3.2c), it follows from the analysis in [62, Lemma 3.1] and [61, Lemma 3.1] that $J^{p,\star}_{i,K-\frac{1}{2}}$ and $-J^{p,\star}_{i,K+\frac{1}{2}}$ are nonnegative, which implies that

$$J^{p,\star}_{i,K-\frac{1}{2}} = J^{p,\star}_{i,K+\frac{1}{2}} = 0,$$

and in turn that

$$D_{K-\frac{1}{2}} c_i^{p,\star} = D_{K+\frac{1}{2}} c_i^{p,\star} = 0.$$

In [62, Lemma 3.1] and [61, Lemma 3.1], the contradiction follows from iterating the argument in the neighboring cells and reaching the conclusion that the entire mass is nonpositive, using the connexity of the domain. We only need to check that the argument can be adapted to the interface cell. Let us assume then that the nonpositive minimum occurs in the interface cell $C^{p-1}_{K^{p-1}}$ from which we get

$$J^{p,\star}_{i,K^{p-1}-\frac{1}{2}} - \widetilde{F}_i^{p,\star} \leq 0.$$

Besides, if $\min\left(\sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}}\right)^\diamond, \sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}+1}\right)^\diamond\right) > 0$,

$$\begin{aligned}
\widetilde{F}_i^{p,\star} &= \min\left(\sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}}\right)^\diamond, \sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}+1}\right)^\diamond\right) \\
&\quad \times \left(c^{p,\star}_{i,K^{p-1}}\right)^\diamond \exp\left(\frac{\mu_i^{*,g} - \mu_i^{*,s}}{2}\right) - \left(c^{p,\star}_{i,(K^{p-1}+1)}\right)^\diamond \exp\left(\frac{\mu_i^{*,s} - \mu_i^{*,g}}{2}\right) \\
&= -\min\left(\sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}}\right)^\diamond, \sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}+1}\right)^\diamond\right) \left(c^{p,\star}_{i,(K^{p-1}+1)}\right)^\diamond \exp\left(\frac{\mu_i^{*,s} - \mu_i^{*,g}}{2}\right) \leq 0,
\end{aligned}$$

so we conclude as before that $\widetilde{F}_i^{p,\star} = 0$, which implies that $\left(c^{p,\star}_{i,(K^{p-1}+1)}\right)^\diamond = 0$ and in turn that $c^{p,\star}_{i,(K^{p-1}+1)} \leq 0$. We reach the same conclusion in the case when

$$\min\left(\sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}}\right)^\diamond, \sum_{i=1}^n \left(c^{p,\star}_{i,K^{p-1}+1}\right)^\diamond\right) = 0.$$

The same argument being valid when reasoning in the interface cell $C^{p-1}_{K^{p-1}+1}$, we have proven that $\boldsymbol{c}^{p,\star}_{i,\Delta x} > 0$.

Let us now turn to the volume-filling constraint. Using formula (4.4.3), it holds

$$\widetilde{\Delta}^p_{K^{p-1}} = \Delta^{p-1}_{K^{p-1}} + \Delta t \left(\sum_{i=1}^n c^{p,\star}_{i,K^{p-1}}\right)^{-1} \sum_{i=1}^n \widetilde{F}_i^{p,\star}.$$

and

$$\widetilde{\Delta}^p_{K^{p-1}+1} = \Delta^{p-1}_{K^{p-1}+1} - \Delta t \left(\sum_{i=1}^n c^{p,\star}_{i,K^{p-1}+1}\right)^{-1} \sum_{i=1}^n \widetilde{F}_i^{p,\star}.$$

We sum the conservation laws (4.3.2a) over $i \in \{1, \ldots, n\}$. We obtain in $C^{p-1}_{K^{p-1}}$ (resp. in

$C^{p-1}_{K^{p-1}+1}$):

$$\frac{1}{\Delta t}\left(\widetilde{\Delta}^p_{K^{p-1}}\sum_{i=1}^n c^{p,\star}_{i,K^{p-1}} - \Delta^{p-1}_{K^{p-1}}\sum_{i=1}^n c^{p-1}_{i,K^{p-1}}\right) - \sum_{i=1}^n \widetilde{F}^{p,\star}_i - \sum_{i=1}^n J^{p,\star}_{i,K^{p-1}-\frac{1}{2}}$$
$$= \frac{\Delta^{p-1}_{K^{p-1}}}{\Delta t}\left(\sum_{i=1}^n c^{p,\star}_{i,K^{p-1}} - 1\right) - \kappa^{*,s}\sum_{i=1}^n D_{K^{p-1}-\frac{1}{2}}\boldsymbol{c}^{p,\star}_i = 0.$$

In consequence, we obtain that the field $(\eta_K)_{K\in\{1,\dots,N\}}$ defined by $\eta_K = \sum_{i=1}^n c^{p,\star}_{i,K} - 1$ is the solution to a backward TPFA Euler scheme for the heat equation, with diffusion coefficient $\kappa^{*,s}$ in the solid phase and $(\kappa^{*,g})^{-1}$ in the gaseous phase (the two phases decouple). As a consequence, we thus obtain that $\sum_{i=1}^n c^{p,\star}_{i,K} = 1$ for all $K \in \{1,\dots,N\}$. This implies that $X^{p,s} = X^{p,g} = X^p$, $\widetilde{\Delta}^p_K = \Delta^{p,\star}_K$ for any $K \in \{1,\dots,N\}$ and $\widetilde{\boldsymbol{F}}^{p,\star} = \boldsymbol{F}^{p,\star}$, so that $(\boldsymbol{c}^p_{\Delta x}, X^p)$ is a solution to the original scheme (S).

Concerning conservation of matter, it follows from summing the conservation laws (4.3.2a) over the cells K and the fact that the fluxes are locally conservative that, for any $i \in \{1,\dots,n\}$,

$$\sum_{K=1}^N \Delta^{p,\star}_K c^{p,\star}_{i,K} = \sum_{K=1}^N \Delta^{p-1}_K c^{p-1}_{i,K}.$$

If $K^p = K^{p-1}$, the result follows immediately. Otherwise, fix $i \in \{1,\dots,n\}$, and let us prove that the quantity $\sum_{K=1}^N \Delta^p_K c^p_{i,K} - \sum_{K=1}^n \Delta^{p,\star}_K c^{p,\star}_{i,K}$ is null. Observe first that, from the post-processing formulas (see Figure 4.1), we only have to study the difference in the cells $C^{p-1}_{K^{p-1}}, C^{p-1}_{K^{p-1}+1}, C^{p-1}_{K^{p-1}+2}$. Then compute, setting $K := K^{p-1}$,

$$\begin{aligned}
&\Delta^p_K c^p_{i,K} + \Delta^p_{K+1} c^p_{i,K+1} + \Delta^p_{K+2} c^p_{i,K+2}\\
&= \Delta x\, c^p_{i,K} + (X^p - x_{K+\frac{1}{2}}) c^p_{i,K+1} + (x_{K+\frac{5}{2}} - X^p) c^p_{i,K+2}\\
&= \Delta x\, c^{p,\star}_{i,K} + (X^p - x_{K+\frac{1}{2}}) c^{p,\star}_{i,K} + \left[(x_{K+\frac{3}{2}} - X^p) c^{p,\star}_{i,K+1} + \Delta x\; c^{p,\star}_{i,K+2}\right]\\
&= (X^p - x_{K-\frac{1}{2}}) c^{p,\star}_{i,K} + (x_{K+\frac{3}{2}} - X^p) c^{p,\star}_{i,K+1} + \Delta x\, c^{p,\star}_{i,K+2}\\
&= \Delta^{p,\star}_K c^{p,\star}_{i,K} + \Delta^{p,\star}_{K+1} c^{p,\star}_{i,K+1} + \Delta^{p,\star}_{K+2} c^{p,\star}_{i,K+2},
\end{aligned}$$

where we used formulas (4.3.5)-(4.3.6) in the second equality. The result follows.

□

4.4.2 Discrete free energy dissipation inequality

Let us introduce the notation, for any $K \in \{1,\dots,N\}$,

$$\alpha^p_K = \begin{cases} s, & \text{if } K \le K^p,\\ g, & \text{if } K > K^p, \end{cases} \tag{4.4.6}$$

so that the discrete version of the free energy functional (4.2.9) reads

$$\mathcal{H}^p\left(\boldsymbol{c}^p_{\Delta x}, X^p\right) = \sum_{K=1}^{N} \Delta^p_K h_{\alpha^p_K}(\boldsymbol{c}^p_K) = \sum_{K\leq K^p} \Delta^p_K h_s(\boldsymbol{c}^p_K) + \sum_{K>K^p} \Delta^p_K h_g(\boldsymbol{c}^p_K). \tag{4.4.7}$$

Note that, besides the explicit dependence on $(\boldsymbol{c}^p_{\Delta x}, X^p)$, the functional depends implicitly on p through the interface cell K^p (resp. through α^p_K). We eliminate this dependence by introducing the interpolation operator $\mathcal{I}_{\Delta^p}$ that maps $\boldsymbol{c}^p_{\Delta x}$ into the (vector-valued) piecewise constant function, defined in $(0,1)$, that interpolates the values $\boldsymbol{c}^p_{\Delta x}$ on the mesh defined by $(\Delta^p_K)_{K\in\{1,\dots,N\}}$. We can now connect the discrete energy functional to its continuous counterpart (4.2.9) as

$$\mathcal{H}^p\left(\boldsymbol{c}^p_{\Delta x}, X^p\right) = \mathcal{H}\left(\mathcal{I}_{\Delta^p}\left(\boldsymbol{c}^p_{\Delta x}\right), X^p\right). \tag{4.4.8}$$

Following the modifications of the diffusion matrices (4.3.2f)-(4.3.2g), we define the modified mobility matrices in the spirit of (4.2.4) as, for any $\boldsymbol{c} \in (\mathcal{A}\cap\mathbb{R}^*_+)$,

$$\begin{aligned} \widehat{\boldsymbol{M}}_s(\boldsymbol{c}) &= \widehat{\boldsymbol{A}}_s(\boldsymbol{c})\boldsymbol{H}^{-1}(\boldsymbol{c}), \\ \widehat{\boldsymbol{M}}_g(\boldsymbol{c}) &= \widehat{\boldsymbol{A}}_g(\boldsymbol{c})\boldsymbol{H}^{-1}(\boldsymbol{c}). \end{aligned} \tag{4.4.9}$$

The positivity result of Lemma 17 implies that the chain rule is valid for any $p \geq 1$ and therefore the fluxes (4.3.2e)-(4.3.2h) can be rewritten in mobility form as

$$\begin{aligned} \Delta x \boldsymbol{J}^{p,\star}_{K+\frac{1}{2}} &= -\widehat{\boldsymbol{M}}_s(\boldsymbol{c}^{p,\star}_{K+\frac{1}{2}}) D_{K+\frac{1}{2}} \log(\boldsymbol{c}^{p,\star}),\ \forall 1 \leq K < K^{p-1}, \\ \Delta x \boldsymbol{J}^{p,\star}_{K+\frac{1}{2}} &= -\widehat{\boldsymbol{M}}_g(\boldsymbol{c}^{p,\star}_{K+\frac{1}{2}}) D_{K+\frac{1}{2}} \log(\boldsymbol{c}^{p,\star}),\ \forall K^{p-1} < K \leq N-1. \end{aligned} \tag{4.4.10}$$

We are ready to prove a discrete version of the free energy dissipation relation (4.2.12), as stated in the next lemma.

Lemma 18. *Let $(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1})$ be such that $\boldsymbol{c}^{p-1}_{\Delta x} \geq 0$ and $\sum_{i=1}^n c^{p-1}_{i,K} = 1$ for any $K \in \{1,\dots,N\}$. Let $(\boldsymbol{c}^p_{\Delta x}, X^p)$ be a solution to $(\widetilde{S})$. It holds*

$$\begin{aligned} &\mathcal{H}^p(\boldsymbol{c}^p_{\Delta x}, X^p) + \frac{\Delta t}{\Delta x} \sum_{K\neq K^{p-1}} (D_{K+\frac{1}{2}} \log(\boldsymbol{c}^{p,\star}))^T \boldsymbol{M}_{\alpha^{p-1}_K}(c^{p,\star}_{K+\frac{1}{2}}) D_{K+\frac{1}{2}} \log(\boldsymbol{c}^{p,\star}) \\ &+ \Delta t \sum_{i=1}^n F^{p,\star}_i D_{K^{p-1}+\frac{1}{2}} \left[\log(\boldsymbol{c}^{p,\star}_i) - \mu^*_i\right] \leq \mathcal{H}^{p-1}(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1}) \end{aligned} \tag{4.4.11}$$

In particular, $\mathcal{H}^p(\boldsymbol{c}^p_{\Delta x}, X^p) \leq \mathcal{H}^{p-1}(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1})$.

Proof. In the same spirit as in the proof of matter conservation, we first introduce the intermediate energy quantity

$$\mathcal{H}^{p-1}(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p) = \sum_{K=1}^{N} \Delta^p_K h_{\alpha^{p-1}_K}(\boldsymbol{c}^{p,\star}_K) = \sum_{K\leq K^{p-1}} \Delta^{p,\star}_K h_s(\boldsymbol{c}^{p,\star}_K) + \sum_{K>K^{p-1}} \Delta^{p,\star}_K h_g(\boldsymbol{c}^{p,\star}_K).$$

Using the expression of the entropy density (4.2.10) and conservation of matter, it holds

$$\mathcal{H}^{p-1}(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p) - \mathcal{H}^{p-1}(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1}) = \sum_{K=1}^{N}\sum_{i=1}^{n}\left(\Delta^{p,\star}_K c^{p,\star}_{i,K}\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right) - \Delta^{p-1}_K c^{p-1}_{i,K}\left(\log(c^{p-1}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)\right).$$

On the other hand, multiplying the conservation laws (4.3.2a) by the quantity $\Delta t\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)$, we obtain

$$\begin{aligned}&\sum_{i=1}^{n}\sum_{K=1}^{N}\left(\Delta^{p,\star}_K c^{p,\star}_{i,K} - \Delta^{p-1}_K c^{p-1}_{i,K}\right)\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)\\ &= \Delta t\sum_{i=1}^{n}\sum_{K=1}^{N}\left(J^{p,\star}_{i,K-\frac{1}{2}} - J^{p,\star}_{i,K+\frac{1}{2}}\right)\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right).\end{aligned} \tag{4.4.12}$$

Using the mobility form of the bulk fluxes (4.4.10) and applying discrete integration by parts, the right-hand side of (4.4.12) can be reformulated as

$$\begin{aligned}&-\Delta t\sum_{i=1}^{n}\sum_{K=1}^{N}\left(J^{p,\star}_{i,x_{K-\frac{1}{2}}} - J^{p,\star}_{i,x_{K+\frac{1}{2}}}\right)\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)\\ &= -\frac{\Delta t}{\Delta x}\sum_{K\neq K^{p-1}}(D_{K+\frac{1}{2}}\log(\boldsymbol{c}^{p,\star}))^T\boldsymbol{M}_{\alpha_K^{p-1}}(c^{p,\star}_{K+\frac{1}{2}})D_{K+\frac{1}{2}}\log(\boldsymbol{c}^{p,\star})\\ &-\Delta t\sum_{i=1}^{n}F_i^{p,\star}D_{K^{p-1}+\frac{1}{2}}\left[\log(\boldsymbol{c}_i^{p,\star}) - \mu_i^*\right].\end{aligned}$$

On the other hand, the convexity of the functional $c \to c\log c$ implies that

$$\begin{aligned}&\sum_{i=1}^{n}\sum_{K=1}^{N}\left(\Delta^{p,\star}_K c^{p,\star}_{i,K} - \Delta^{p-1}_K c^{p-1}_{i,K}\right)\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)\\ &\geq \sum_{K=1}^{N}\sum_{i=1}^{n}\left(\Delta^{p,\star}_K c^{p,\star}_{i,K}\left(\log(c^{p,\star}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right) - \Delta^{p-1}_K c^{p-1}_{i,K}\left(\log(c^{p-1}_{i,K}) - \mu_i^{*,\alpha_K^{p-1}}\right)\right)\\ &= \mathcal{H}^{p-1}(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p) - \mathcal{H}^{p-1}(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1}),\end{aligned}$$

so inserting the two previous equations in (4.4.12) gives

$$\begin{aligned}&\mathcal{H}^{p-1}(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p) + \frac{\Delta t}{\Delta x}\sum_{K\neq K^{p-1}}(D_{K+\frac{1}{2}}\log(\boldsymbol{c}^{p,\star}))^T\boldsymbol{M}_{\alpha_K^{p-1}}(c^{p,\star}_{K+\frac{1}{2}})D_{K+\frac{1}{2}}\log(\boldsymbol{c}^{p,\star})\\ &+\Delta t\sum_{i=1}^{n}F_i^{p,\star}D_{K^{p-1}+\frac{1}{2}}\left[\log(\boldsymbol{c}_i^{p,\star}) - \mu_i^*\right] \leq \mathcal{H}^{p-1}(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1})\end{aligned} \tag{4.4.13}$$

It remains to prove the inequality

$$\mathcal{H}^p(\boldsymbol{c}^p_{\Delta x}, X^p) \leq \mathcal{H}^{p-1}(\boldsymbol{c}^{p,\star}_{\Delta x}, X^p),$$

or equivalently

$$\mathcal{H}\left(\mathcal{I}_{\Delta^p_K}\left(\boldsymbol{c}^p_{\Delta x}\right), X^p\right) \leq \mathcal{H}\left(\mathcal{I}_{\Delta^{p,\star}_K}\left(\boldsymbol{c}^{p,\star}_{\Delta x}\right), X^p\right).$$

The latter stems from the convexity of $\mathcal{H}$ with respect to its first argument and the fact that $\mathcal{I}_{\Delta^p_K}\left(\boldsymbol{c}^p_{\Delta x}\right)$ is obtained from $\mathcal{I}_{\Delta^{p,\star}_K}\left(\boldsymbol{c}^{p,\star}_{\Delta x}\right)$ by projection (4.3.5) and convex combination (4.3.6).The proof is complete. □

4.4.3 Existence of a discrete solution

We are now in position to prove the existence of at least one discrete solution to the scheme (S), thanks to the lemmas that were established in the previous sections.

Proposition 7. *Let* $(\boldsymbol{c}^{p-1}_{\Delta x}, X^{p-1})$ *be such that* $\boldsymbol{c}^{p-1}_{\Delta x} \geq 0$ *and* $\sum_{i=1}^n c^{p-1}_{i,K} = 1$ *for any* $K \in \{1, \dots, N\}$. *There exists a solution* $(\boldsymbol{c}^p_{\Delta x}, X^p)$ *to* $(\widetilde{S})$.

Proof. The proof uses the topological degree theory and in particular the properties of the degree listed in [107, Theorem 3.1]. The idea is to continuously deform our coupled system to two independent systems for which we know respectively that a solution exists, while ensuring that some *a priori* estimates remain valid along the path. In fact, only the nonnegativity and volume-filling estimates are needed, since they provide boundedness in l^∞ norm. Let us detail the argument. The system $(\widetilde{S})$ is only deformed in the interface cells as, for $i \in \{1, \dots, n\}$,

$$\begin{cases} \dfrac{X^{p,s}_\lambda - x_{K^{p-1}-\frac{1}{2}}}{\Delta t}\left(c^\lambda_{i,K^{p-1}} - c^{p-1}_{i,K^{p-1}}\right) - \lambda \widetilde{F}^\lambda_i - J^\lambda_{i,K^{p-1}-\frac{1}{2}} = 0, \\ \dfrac{x_{K^{p-1}+\frac{3}{2}} - X^{p,g,\lambda}}{\Delta t}\left(c^\lambda_{i,K^{p-1}+1} - c^{p-1}_{i,K^{p-1}+1}\right) + J^\lambda_{i,K^{p-1}+\frac{3}{2}} + \lambda \widetilde{F}^\lambda_i = 0, \\ X^{p,s}_\lambda = X^{p-1} + \lambda \Delta t G(c^\lambda_{K^{p-1}}), \\ X^{p,g}_\lambda = X^{p-1} + \lambda \Delta t G(c^\lambda_{K^{p-1}+1}). \end{cases} \tag{4.4.14}$$

which, together with the rest of scheme $(\widetilde{S})$, define the scheme $(\widetilde{S}_\lambda)$. We denote by $h(\lambda, \boldsymbol{c}) \in \mathbb{R}^N$ the residual associated to the scheme $(\widetilde{S}_\lambda)$. For $\lambda = 0$, the interface cells equations decouple and we obtain two independent nonlinear systems defined on a fixed boundary domain with zero-flux boundary conditions, for which we know that a solution exists ([62, Proposition 3.3] and [61, Proposition 3.4]). For $\lambda = 1$, we get the scheme $(\widetilde{S})$, for which we have already proven positivity and volume-filling constraint in Lemma 17. The proof can be directly adapted to the case $\lambda \in [0, 1)$, so that any solution $\boldsymbol{c}^\lambda_{\Delta x}$ to the scheme $(\widetilde{S}_\lambda)$ satisfies $\boldsymbol{c}^\lambda_{\Delta x} > 0$ and $\sum_{i=1}^n c^\lambda_{i,K} = 1$ for any $K \in \{1, \dots, N\}$.

Since the set $\mathcal{A}$ is not open, the topological degree cannot be directly applied and we define, for $\eta > 0$, the open set

$$\mathcal{A}_\eta := \left\{\boldsymbol{u} \in \mathbb{R}^N, \inf_{\boldsymbol{v} \in \mathcal{A}} \|\boldsymbol{u} - \boldsymbol{v}\|_{l^\infty} \leq \eta.\right\}$$

The residual $[0,1] \times \mathcal{A}_\eta \ni (\lambda, \boldsymbol{c}) \to h(\lambda, \boldsymbol{c})$ is clearly a continuous function, and moreover, the estimates give that any solution $\boldsymbol{c}_{\Delta x}^\lambda$ to $h(\lambda, \boldsymbol{c}_{\Delta x}^\lambda) = 0$ lies in $\mathcal{A}$ and therefore in the interior of $\mathcal{A}_\eta$. These two ingredients allow to conclude that the topological degree of $(h_\lambda, \mathcal{A}_\eta, 0)$ is constant with respect to λ and therefore equal to 1 when $\lambda = 1$, which gives existence of a solution to $(\widetilde{S})$.

□

As a direct corollary, we obtain the existence of an admissible discrete solution to the scheme (4.3.2), satisfying all the previously established *a priori* estimates.

4.5 Numerical results

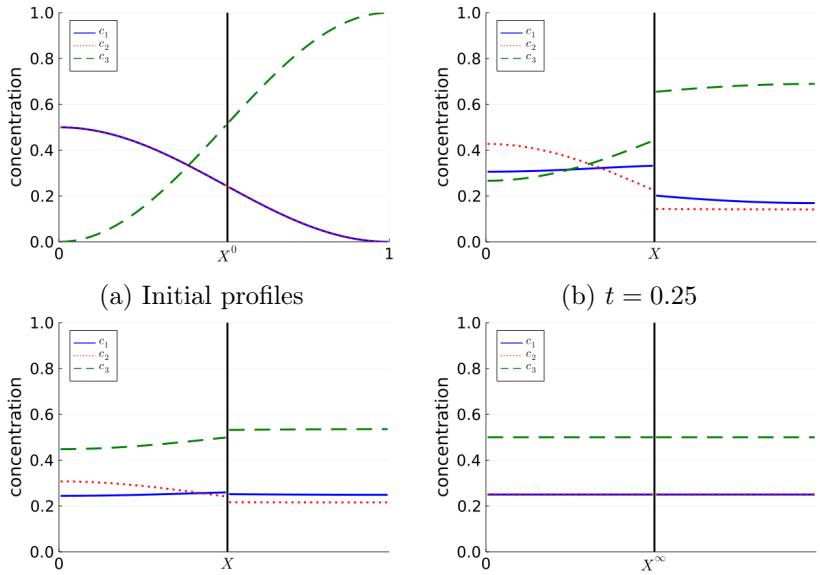
The numerical scheme has been implemented in the Julia language. The nonlinear system is solved with Newton method, with stopping criterion $\|\boldsymbol{c}_{\Delta x}^{p,k+1} - \boldsymbol{c}_{\Delta x}^{p,k}\|_\infty \leq 10^{-12}$ and adaptive time stepping based on the CFL condition (4.3.4). We fix an initial interface $X^0 = 0.51$ and consider smooth initial concentrations

$$c_1^0(x) = c_2^0(x) = \frac{1}{4}\left(1 + \cos(\pi x)\right), \; c_3^0(x) = \frac{1}{2}\left(1 - \cos(\pi x)\right)$$

that are suitably discretized on a uniform mesh of $N = 100$ cells. The cross-diffusion coefficients are taken equal in each phase, with values $\kappa_{12} = \kappa_{21} = 0.2$, $\kappa_{23} = \kappa_{32} = 0.1$, $\kappa_{13} = \kappa_{31} = 1$ and the numerical diffusion parameters are $\kappa^{*,s} = \kappa^{*,g} = 0.1$ (but remember that the cross-diffusion matrices of each phase are morally inverse of each other). The solid reference chemical potential is chosen such that $\boldsymbol{\mu}^{*,s} = 0$, so that the interface dynamics only depends on $\boldsymbol{\beta}^* = \exp(\boldsymbol{\mu}^{*,g})$. We always consider the time horizon $T = 5$.

Our first test case is devoted to the trivial situation $\boldsymbol{\beta}^* \equiv 1$. We start from a time step $\Delta t_1 = 8 \times 10^{-4}$. Snapshots of the simulation are presented in Figure 4.2, where we verify that, although discontinuities appear across the interface, the interface itself does not move, and the system converges to constant concentrations in the entire domain. Exponential decay of the relative free energy $\mathcal{H}(\boldsymbol{c}_{\Delta x}^p, X^p) - \mathcal{H}(\boldsymbol{c}^\infty, X^\infty)$ is shown in Figure 4.6a. Note that, in this case, the phases are only distinguished by different speeds of convergence to equilibrium.

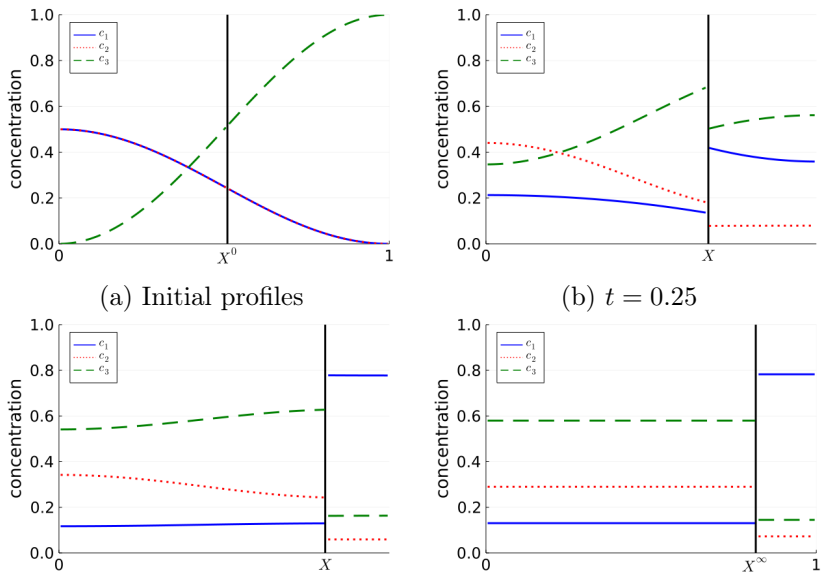
In our second test case, we choose $\boldsymbol{\beta}^* = [6, 0.25, 0.25]$, so as to fulfill the equilibrium condition (4.2.19), and an initial time step $\Delta t_2 = 6 \times 10^{-4}$. The simulation is presented in Figure 4.3, where we observe the interface evolution and convergence in the long-time limit to the two-phase stationary solution defined by Proposition 6. To study the long-time asymptotics, we first compute accurately the stationary solution $(\boldsymbol{c}^\infty, X^\infty)$ (we construct the function φ defined in (4.2.22) and solve $\varphi(X^\infty) = 0$ with Newton's method). Then, in addition to the relative free energy, we study the relative interface $|X^\infty - X^p|$ over time, see Figure 4.6b, where we observe exponential convergence and decrease of both functionals. In particular, our scheme is well-balanced and preserves the asymptotics of the continuous system.



(a) Initial profiles (b) $t = 0.25$

(c) $t = 1.0$ (d) Stationary profiles

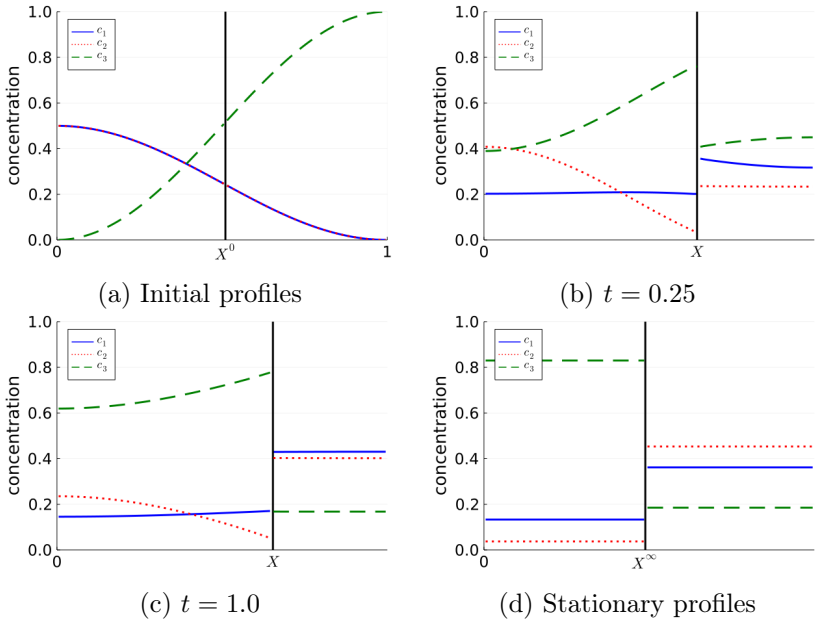
Figure 4.2: Trivial case: no interface movement



(a) Initial profiles (b) $t = 0.25$

(c) $t = 1.0$ (d) Stationary profiles

Figure 4.3: Equilibrium case with monotone interface



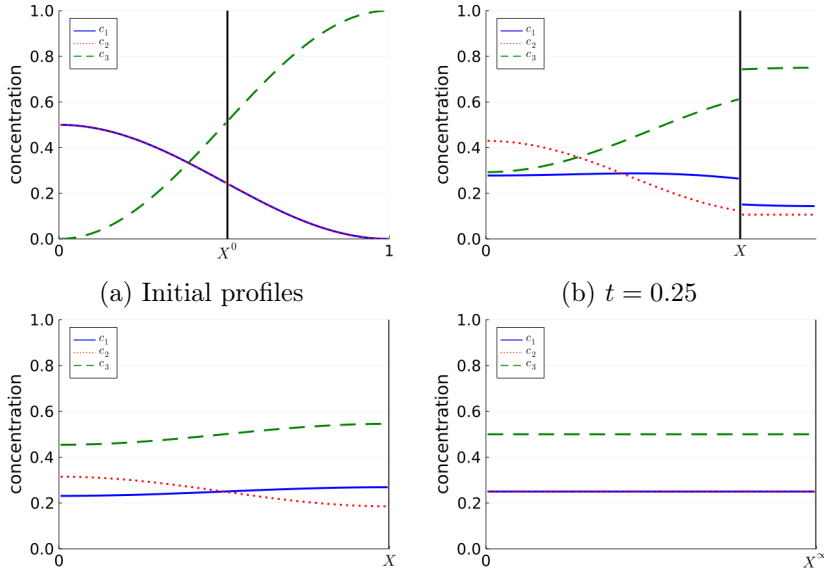
(a) Initial profiles (b) $t = 0.25$

(c) $t = 1.0$ (d) Stationary profiles

Figure 4.4: Equilibrium case with non-monotone interface

Note that, in the previous case, the interface evolves monotonously and $|X^\infty - X^p| = X^\infty - X^p$. However, modifying $\boldsymbol{\beta}^*$, we can easily construct a test case where the interface is not monotone along the evolution, see Figures 4.4 and 4.6c. Finally, we verify that, as soon as $\boldsymbol{\beta}^* \not\equiv 1$ violates (4.2.19), then the system converges to a one-phase solution, see Figures 4.5 and 4.6d.

Our final test case is devoted to a convergence analysis with respect to the size of the mesh. We consider a fixed time step $\Delta t_2 = 10^{-4}$, a final time $T_2 = 0.25$, uniform meshes from 2^3 to 2^{10} cells and we compare the different solutions with respect to a reference solution computed on a finer grid of 2^{11} cells. The space-time (resp. time) L^1 error on the concentrations (resp. on the interface) are displayed in Figure 4.7. One clearly observes convergence, at first order in space for the concentrations. These results should be compared with the second order accurate one-phase schemes [62, 61]. On the one hand, it is plausible that the interface treatment induces the loss of order. On the other hand, the discrete $L^1((0,1))$ space distance we use to compare solutions is not perfectly adapted since the solutions are defined in slightly different domains. Rescaling all quantities might offer more insights into the convergence properties.



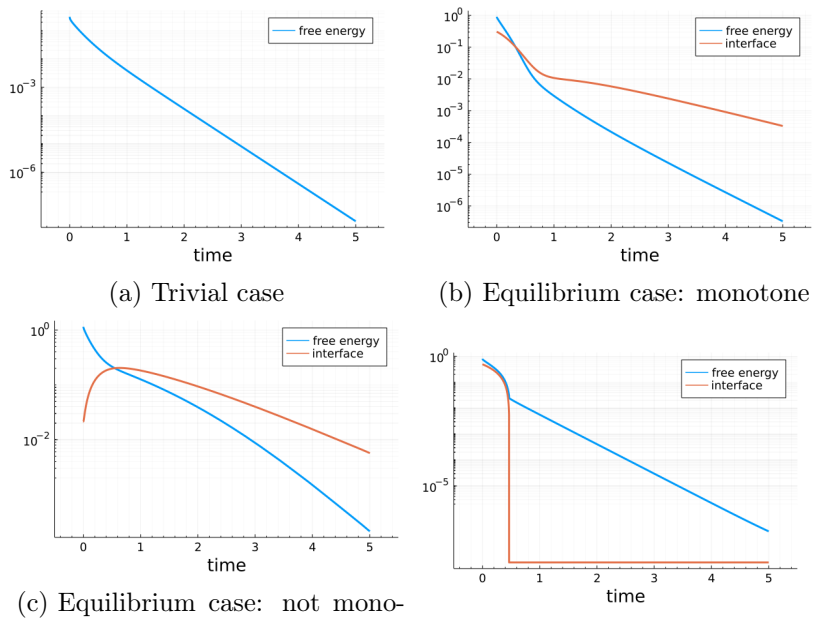
(a) Initial profiles

(b) $t = 0.25$

(c) $t = 1.0$

(d) Stationary profiles

Figure 4.5: Non-equilibrium case



(a) Trivial case

(b) Equilibrium case: monotone

(c) Equilibrium case: not monotone

(d) Non-equilibrium case

Figure 4.6: $\mathcal{H}(\boldsymbol{c}^p_{\Delta x}, X^p) - \mathcal{H}(\boldsymbol{c}^\infty, X^\infty)$ and $|X^\infty - X^p|$ for different test cases

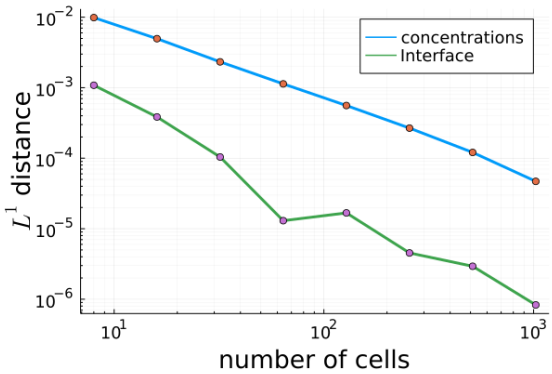


Figure 4.7: Convergence analysis of the solution under space grid refinement

4.6 Perspectives

Let us mention in this section some perspectives related to the present work. Of course, a natural question is to prove the convergence of the finite volume scheme presented here to some weak solution of the model (4.2.2), which would yield in particular the existence of a weak solution to the model. For any $x \in [0,1]$, we introduce the broken Sobolev space

$$H^1_{b,x} := \left\{u \in L^2(0,1),\ u|_{(0,x)} \in H^1(0,x), \quad u|_{(x,1)} \in H^1(x,1)\right\}.$$

For any $u \in H^1_{b,x}$, we also denote by

$$\|u\|_{H^1_{b,x}} := \sqrt{\|u\|^2_{L^2(0,1)} + \|u'\|^2_{L^2(0,x)} + \|u'\|^2_{L^2(x,1)}}.$$

Notice that, since for all $x \in [0,1]$, $H^1(0,1) \subset H^1_{b,x}$, it holds that $(H^1_{b,x})' \subset (H^1(0,1))'$. Furthermore, for any absolutely continuous curve $X : \mathbb{R}_+ \to [0,1]$ and $T > 0$, we set

$$\left[L^2((0,T),H^1_b)\right]_X := \{u \in L^2((0,T)\times(0,1)),\ u(t) \in H^1_{b,X(t)} \text{ for a.a. } t \in (0,T),$$
$$\int_0^T \|u(t)\|^2_{H^1_{b,X(t)}}\, dt < +\infty\}.$$

We also define

$$\left[L^2_{\text{loc}}(\mathbb{R}_+,H^1_b)\right]_X := \left\{u \in L^2_{\text{loc}}(\mathbb{R}_+\times(0,1)),\ u|_{(0,T)\times(0,1)} \in \left[L^2((0,T),H^1_b)\right]_X\ \forall T>0\right\}.$$

In addition, we define

$$\left[L^2_{\text{loc}}(\mathbb{R}_+,(H^1_b)')\right]_X := \{\phi \in L^2_{\text{loc}}(\mathbb{R}_+,(H^1(0,1))'),\ \phi(t) \in (H^1_{b,X(t)})' \text{ for a.a. } t \in \mathbb{R}_+,$$
$$\int_0^T \|\phi(t)\|^2_{(H^1_{b,X(t)})'}\, dt < +\infty\ \forall T>0\}.$$

Inspired from the analysis performed in [62, 61], we conjecture that a natural notion of weak solution for model (4.2.2) should be given by the following definition.

Definition 12 (Weak solution)**.** *Let $X^0 \in [0,1]$ and $\boldsymbol{c}^0 \in (H^1_{b,X^0})^n$ such that $\boldsymbol{c}^0(x) \in \mathcal{A}$ for almost every $x \in (0,1)$. A couple $(\boldsymbol{c}, X)$ is a weak solution of (4.2.2) if*

- *the function $X : \mathbb{R}_+ \to [0,1]$ is absolutely continuous;*
- *for any $T > 0$, $\boldsymbol{c}|_{(0,T)\times(0,1)} \in \left[L^2((0,T), H^1_b)\right]^n_X$;*
- *for almost any $(t,x) \in Q$, $\boldsymbol{c}(t,x) \in \mathcal{A}$;*
- *for almost any $t > 0$,*

$$X'(t) = \begin{cases} \sum_{i=1}^n F_i(t), & \text{if } X(t) \in (0,1), \\ 0, & \text{otherwise}, \end{cases} \tag{4.6.1}$$

  where

$$F_i(t) = \frac{1}{\sqrt{\beta_i^*}} c_i^g(t) - \sqrt{\beta_i^*} c_i^s(t), \ i \in \{1, \dots, n\};$$

- *for any $\boldsymbol{\varphi} \in \left[L^2_{\text{loc}}(\mathbb{R}_+, H^1_b)\right]^n_X$ such that $\partial_t \boldsymbol{\varphi} \in \left[L^2_{\text{loc}}(\mathbb{R}_+, (H^1_b)')\right]^n_X$ and such that there exists $T > 0$ such that $\boldsymbol{\varphi}(t) = 0$ for all $t \geq T$,*

$$\begin{aligned} &\int_0^\infty \langle \partial_t \boldsymbol{\varphi}, \boldsymbol{c} \rangle_{(H^1_{b,X(t)})', H^1_{b,X(t)}} \, dt + \int_0^1 \boldsymbol{c}^0(x) \cdot \boldsymbol{\varphi}(0,x) \, dt \\ &= \int_0^\infty \int_0^{X(s)} \partial_x \boldsymbol{\varphi}^T \boldsymbol{A}_s(\boldsymbol{c}) \partial_x \boldsymbol{c} \, dt + \int_0^\infty \int_{X(s)}^1 \partial_x \boldsymbol{\varphi}^T \boldsymbol{A}_g(\boldsymbol{c}) \partial_x \boldsymbol{c} \, dt \\ &- \int_0^\infty \boldsymbol{F}(t) \cdot [\![\boldsymbol{\varphi}(t)]\!] \, dt, \end{aligned} \tag{4.6.2}$$

  where $\boldsymbol{F}(t) = (F_i(t))_{i \in \{1,\dots,n\}}$ for almost all $t > 0$.

The study of the long-time asymptotic behaviour of such weak solutions is also on the scientific agenda. In particular, proving the conjecture inspired by the numerical results shown in Section 4.5 that the solution converges exponentially fast with respect to time to some stationary state of the model in the sense of Definition 11 is an interesting question. We intend to study these issues in a future work.

Résumé en français

Cette thèse traite de l'analyse, de la stabilisation et de l'approximation numérique de systèmes à diffusion croisée dans des domaines à frontière mobile. Ces systèmes apparaissent dans de nombreuses applications en sciences des matériaux et en biologie : croissance de cristaux et de biofilms, corrosion de l'acier, carbonatation du béton... Ce travail est spécialement motivé par la modélisation d'un procédé de dépôt vapeur utilisé pour la synthèse de couches minces semi-conductrices dans les cellules photovoltaïques.

Le procédé peut être décrit comme suit (voir Figure 1.2) : une plaquette est introduite dans une chambre chaude où des éléments chimiques sont injectés sous forme gazeuse. Au fur et à mesure que ces derniers se déposent sur le substrat, une couche solide hétérogène s'y développe. En raison des conditions de température, des effets de diffusion interviennent dans la couche solide jusqu'à ce que la plaquette soit retirée et le système figé.

Chapitre 1. Introduction

Pour fixer les idées, commençons par présenter le modèle de déposition introduit dans [24]. Il s'agit d'un système à diffusion croisée posé dans un domaine unidimensionnel dépendant du temps. Plus précisément, nous considérons une couche solide en expansion composée de $n+1$ différentes espèces chimiques. Le domaine considéré s'écrit $]0, e(t)[\subset \mathbb{R}_+$, où $e(t) > 0$ représente l'épaisseur de la couche. On travaille donc dans le domaine espace-temps non-cylindrique

$$U_e := \bigcup_{t\in\mathbb{R}_+^*} \{t\}\times]0, e(t)[.$$

Pour tout $i = 0, \dots, n$, on définit la fonction $F_i \in L^1_{\text{loc}}(\mathbb{R}_+^*)$ telle que $F_i(t)$ représente le flux d'atomes de l'espèce i absorbée à la surface de la couche mince au temps t. L'évolution de l'épaisseur du film est déterminée par les flux $(F_i)_{i=0,\dots,n}$ et est donnée par

$$e(t) = e_0 + \int_0^t \sum_{i=0}^n F_i(s)\, ds,\ t > 0, \tag{0.1}$$

où $e_0 > 0$ représente l'épaisseur initiale du film. Les fractions volumiques locales des différentes espèces $u_0, \dots, u_n$ sont censées satisfaire les contraintes

$$u_i(t,x) \geq 0 \text{ pour } i = 0, \dots, n \text{ et } \sum_{j=0}^n u_j(t,x) = 1,\ t > 0,\ x \in]0, e(t)[. \tag{0.2}$$

Ces contraintes permettent d'exprimer de manière équivalente u_0 comme $1 - \sum_{i=1}^n u_i$. Par conséquent, le système entier peut être réécrit en utilisant le vecteur inconnu $u := (u_1, \dots, u_n)^T$. En notant F la fonction à valeur vectorielle $(F_1, \dots, F_n)^T$, le système à diffusion croisée dans la couche solide est donné par :

$$\begin{cases} \partial_t u - \partial_x(A(u)\partial_x u) = 0, & (t,x) \in U_e, \\ (A(u)\partial_x u)(t,0) = 0, & t \in \mathbb{R}_+^*, \\ (A(u)\partial_x u)(t,e(t)) + e'(t)u(t,e(t)) = F(t), & t \in \mathbb{R}_+^*, \\ u(0,x) = u^0(x), & x \in]0, e_0[, \end{cases} \tag{0.3}$$

pour une application matricielle $A : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ appelée *matrice de diffusion* du système (voir par exemple (1.2.6)) et une condition initiale u^0 compatible avec les conditions (0.2). Les conditions aux limites indiquent que le système est isolé à $x = 0$ mais qu'il existe un flux vectoriel entrant $F(t)$ en $x = e(t)$, où le terme supplémentaire $e'(t)u(t, e(t))$ tient compte de la croissance de la couche.

Ce modèle présente les caractéristiques mathématiques qui nous intéressent dans cette thèse : premièrement, la description de la diffusion fortement couplée des constituants dans la couche conduit à un système à diffusion croisée, c'est-à-dire un système d'équations aux dérivées partielles paraboliques non linéaires. Je donne un aperçu de ces systèmes dans la Section 1.2. Deuxièmement, à cause de la croissance de la couche, les équations sont écrites dans un domaine à frontière mobile. Dans la Section 1.3, je présente quelques approches mathématiques pour ces problèmes et en particulier l'approche par interface diffuse qui me permet d'introduire l'équation de Cahn-Hilliard. Enfin, si l'on veut optimiser le procédé de dépôt vapeur, il est naturel de considérer les flux gazeux $(F_0, \dots, F_n)$ injectés comme *variables de contrôle au bord*. Je présente dans la Section 1.4 quelques idées de stabilisation, en me concentrant sur la méthode de backstepping pour les EDP.

Le travail original de cette thèse est divisé en trois chapitres. Le Chapitre 2 est adapté de l'article publié [68], avec Virginie Ehrlacher et Amaury Hayat. Le Chapitre 3 est adapté du travail soumis [69] en collaboration avec Virginie Ehrlacher, Greta Marino et Jan-Frederik Pietschmann. Le Chapitre 4 est une version étendue du travail publié [59], avec Clément Cancès, Claire Chainais-Hillairet et Virginie Ehrlacher.

Chapitre 2. Stabilisation par le bord

Dans ce chapitre, nous nous intéressons à la stabilisation par le bord du système (0.3). La principale motivation des auteurs de [24] pour l'étude d'un tel système était de contrôler les flux gazeux $(F_0, \dots, F_n)$ injectés pendant le processus de dépôt afin d'atteindre des profils de composition cibles. L'existence globale de solutions faibles au système en boucle ouverte (F dépend seulement du temps) a été démontrée en adaptant au cas d'une frontière mobile la *boundedness-by-entropy method*, présentée dans la Section 1.2.4. Les auteurs ont également obtenu un résultat de convergence en temps long des profils de fraction volumiques dans le cas de flux externes *constants*. Cependant, les profils

asymptotiques correspondants semblaient être stables avec seulement un très faible taux de convergence et nous nous sommes demandé s'il était possible d'améliorer ce taux en utilisant un meilleur contrôle du flux F. Nous renvoyons à la Section 2.2 pour une présentation complète des résultats de [24].

Nous nous intéressons à la stabilisation de la version linéarisée de (0.3) autour d'états de concentrations constantes. Le système linéarisé est donné par

$$\begin{cases} \partial_t \delta u - A(\overline{u})\partial_{xx}^2 \delta u = 0, & (t,x) \in U_{\overline{e}}, \\ A(\overline{u})\partial_x \delta u(t,\overline{e}(t)) + \overline{v}\delta u(t,\overline{e}(t)) = \delta\psi(t), & t \in \mathbb{R}_+^*, \\ A(\overline{u})\partial_x \delta u(t,0) = 0, & t \in \mathbb{R}_+^*, \\ \delta u(0,x) = \delta u^0(x), & x \in]0,\overline{e}_0[, \end{cases} \tag{0.4}$$

où $\delta u \in \mathbb{R}^n$ est l'état, $\delta\psi \in \mathbb{R}^n$ est le vecteur de contrôle, $\overline{v} > 0$ et $\overline{e}(t) = \overline{e}_0 + \overline{v}t$. Notons que le domaine "d'équilibre" $]0,\overline{e}(t)[$ est toujours en expansion mais croît à vitesse constante. Notre résultat est valide sous des hypothèses sur la matrice de diffusion croisée A qui s'appuient sur les conditions habituelles de structure entropique pour traiter le problème non linéaire (voir le Théorème 1), ainsi qu'une hypothèse de symétrie supplémentaire sur la *matrice de mobilité* (voir la définition (1.2.11)) du système à l'état considéré. En particulier, la matrice de diffusion croisée (1.2.6) satisfait ces conditions. Nous montrons que nous pouvons stabiliser le système linéarisé (0.4) en temps fini arbitrairement petit, avec une loi de rétro-action obtenue par la technique de backstepping inspirée de la méthode décrite dans la Section 1.4.3. En deux mots, il s'agit de trouver une transformation inversible du système vers un système stable, la loi de rétro-action étant alors directement déduite de la transformation.

Très peu de travaux ont abordé des questions de contrôle de systèmes à diffusion croisée [182, 220] et notre travail est, à ma connaissance, le premier à aborder la stabilisation par rétro-action de tels systèmes. Bien que notre résultat concerne le système linéarisé (0.4), il ouvre la voie à la stabilisation locale du système non linéaire (voir les perspectives dans la Section 1.6). Du point de vue du backstepping, nous étendons la méthode introduite dans [92] et décrite dans 1.4.3 à un contexte de frontière mobile. De nouvelles difficultés découlent de l'aspect "non-autonome" du système, en particulier la transformation de backstepping (voir (1.4.7)) doit dépendre du temps et il faut s'assurer que cela ne compromette pas la stabilité exponentielle (resp. la stabilité en temps fini). En effet, lorsqu'on applique la transformation inverse pour obtenir la stabilité exponentielle du système d'origine, le coût de l'estimation dépend de la norme de la transformation et de la norme de son inverse, qui dépendent elles-même du temps (voir (1.4.11)). Si cette norme croît exponentiellement vite en temps, le système d'origine pourrait ne pas être exponentiellement stable, et encore moins stable en temps fini, même si le système cible l'est. Nous montrons néanmoins que ce n'est pas une obstruction à la stabilisation de (0.4).

Nos contributions peuvent être résumées ainsi :

- Nous montrons que la structure entropique et l'hypothèse de symétrie sur la matrice de mobilité permettent de diagonaliser $A(\overline{u})$, réduisant la stabilisation de (0.4) à la stabilisation du problème scalaire, pour $\lambda, \sigma > 0$,

$$\begin{cases} \partial_t \zeta_\lambda^\sigma - \sigma \partial_{xx}^2 \zeta_\lambda^\sigma = 0, & (t,x) \in U_{\overline{e}}, \\ \sigma \partial_x \zeta_\lambda^\sigma(t, \overline{e}(t)) + \overline{v} \zeta_\lambda^\sigma(t, \overline{e}(t)) = \delta \psi_\lambda^\sigma(t), & t \in \mathbb{R}_+^*, \\ \sigma \partial_x \zeta_\lambda^\sigma(t, 0) = 0, & t \in \mathbb{R}_+^*. \end{cases} \tag{0.5}$$

  Le système cible est naturellement donné par

$$\begin{cases} \partial_t g_\lambda^\sigma - \sigma \partial_{xx}^2 g_\lambda^\sigma + \lambda g_\lambda^\sigma = 0, & (t,x) \in U_{\overline{e}}, \\ \sigma \partial_x g_\lambda^\sigma(t, \overline{e}(t)) + \overline{v} g_\lambda^\sigma(t, \overline{e}(t)) = 0, & t \in \mathbb{R}_+^*, \\ \sigma \partial_x g_\lambda^\sigma(t, 0) = 0, & t \in \mathbb{R}_+^*. \end{cases}$$

  Cette réduction est cruciale. Nous commentons les difficultés rencontrées dans le cas fortement couplé dans les conclusions du Chapitre 2.

- Nous dérivons formellement le problème du noyau scalaire dépendant du temps (2.6.9) et nous remarquons qu'il admet des solutions avec des variables séparées qui permettent de retrouver le problème du noyau classique posé dans un domaine en mouvement, voir (2.6.11). D'une certaine manière, cela signifie que la transformation de backstepping Volterra est "compatible" avec la frontière mobile. La loi de rétro-action scalaire est donnée par

$$\delta \psi_\lambda^\sigma(t) := \sigma k_\lambda^\sigma(\overline{e}(t), \overline{e}(t)) \zeta_\lambda^\sigma(t, \overline{e}(t)) + \int_0^{\overline{e}(t)} \left[\sigma \partial_x k_\lambda(\overline{e}(t), y) + \overline{v} k_\lambda(\overline{e}(t), y) \right] \zeta_\lambda^\sigma(t, y) dy.$$

  Le caractère bien posé de la transformation backstepping est ensuite rigoureusement vérifié dans un cadre de régularité L^2 (voir les résultats de la Section 2.4.5).

- Nous prouvons que le problème du noyau scalaire est bien posé et nous donnons des estimations quantitatives (voir Proposition 3). Les estimations sont données par, pour tout $x \in]0, \overline{e}(t)[$,

$$\int_0^x \left(|k_\lambda^\sigma(x,y)|^2 + |\nabla k_\lambda^\sigma(x,y)|^2 \right) dy \leq C e^{c\overline{e}(t)\sqrt{\lambda/\sigma}}, \tag{0.6}$$

$$\int_0^x \left(|l_\lambda^\sigma(x,y)|^2 + |\nabla l_\lambda^\sigma(x,y)|^2 \right) dy \leq C \left(\frac{\lambda}{\sigma} \right)^4 e^{c\overline{e}(t)}. \tag{0.7}$$

  Ceci permet de conclure à la stabilisation rapide de (0.5) (Corollaire 1) et donc du problème couplé (0.4) (Théorème 5).

- Enfin, nous utilisons les estimations (0.6)-(0.7) pour adapter la stratégie décrite dans la Section 1.4.3 afin d'obtenir une stabilisation en temps fini arbitraire (Théorème 6). Le point essentiel est que la constante de stabilité est de la forme $Ce^{c\sqrt{\lambda}}$ qui peut toujours être "battu" par le terme de décroissance $e^{-\lambda t}$ quand $\lambda \gg 1$.

Chapitre 3. Analyse d'un modèle Cahn-Hilliard avec diffusion croisée

Avant de détailler les contributions de ce chapitre, il est utile de présenter le modèle introduit dans [118]. Ce dernier décrit l'évolution d'un mélange où les effets de diffusion croisée entre les différentes espèces sont pris en compte et où une seule espèce tend à se séparer des autres. Le mélange occupe un domaine ouvert, lisse et borné $\Omega \subset \mathbb{R}^d$ avec $d = 1, 2, 3$ et est composé de $n+1$ espèces dont les fractions volumiques sont notées u_i, $i = 0, \dots, n$. En notant $u = (u_0, \dots, u_n)$, la dynamique du système est régie par la fonctionnelle d'énergie libre

$$E(u) := \int_\Omega \left[\sum_{i=0}^{n} (u_i \ln u_i - u_i + 1) + \frac{\varepsilon}{2} |\nabla u_0|^2 + \beta u_0 (1 - u_0) \right] dx, \tag{0.8}$$

où ε et β sont des constantes positives. Il s'agit d'une généralisation multi-espèces de l'énergie de Ginzburg-Landau classique avec potentiel logarithmique. Notant $\mu = D_u E(u)$ le potentiel chimique, le système d'évolution correspondant est donné formellement par

$$\partial_t u = \operatorname{div}(M(u) \nabla \mu) \text{ dans } \Omega \times (0, +\infty), \tag{0.9}$$

où $M : \mathbb{R}^{n+1} \to \mathbb{R}^{(n+1)\times(n+1)}$ est une matrice de mobilité dégénérée, voir (3.1.3) et la Section 3.1.2 pour une présentation complète du modèle. La matrice de mobilité est associée à la matrice de diffusion (1.2.6), déjà étudiée dans le chapitre précédent. En raison de leur interprétation en tant que fractions volumiques, les quantités u_i doivent satisfaire, pour $x \in \Omega$, $t \in (0, +\infty)$,

$$0 \le u_i(t, x) \le 1 \quad \text{pour tout } i = 0, \dots, n \quad \text{et} \quad \sum_{i=0}^{n} u_i(t, x) = 1. \tag{0.10}$$

Le système d'évolution est complété par des conditions aux limites de flux nul ainsi que des conditions initiales compatibles avec les contraintes. Le principal résultat de [118] est l'existence d'une solution à une formulation faible appropriée de ce problème.

Le but de notre travail est l'étude de l'énergie de Ginzburg-Landau dégénérée multi-espèces (0.8) et de sa relation avec le système d'équations de Cahn-Hilliard à diffusion croisée (0.9). Tout d'abord, nous étudions quelques solutions du problème stationnaire

$$0 = \operatorname{div}(M(u) \nabla \mu), \text{ dans } \Omega. \tag{0.11}$$

En général, l'analyse de ce type de système elliptique dégénéré est difficile. Dans ce travail, motivés par la structure de flot de gradient du système d'évolution mise en évidence ci-dessus (voir la Section 1.2.3), nous concentrons notre étude sur l'ensemble des minimiseurs locaux de la fonctionnelle d'énergie (0.8). Ces derniers sont des candidats naturels pour être solutions de (0.11) car l'on s'attend à ce que les solutions du système dépendant du temps convergent dans la limite en temps long vers l'un de ces minimiseurs locaux.

Nous obtenons des bornes uniformes *strictes* sur les minimiseurs locaux de (0.8) pour la topologie $L^\infty(\Omega)^{n+1}$. Ce résultat est basé sur un argument de compétiteur où la construction doit non seulement préserver les contraintes (0.10) mais aussi la masse de chaque espèce. Grâce à ces bornes strictes, nous pouvons dériver le système d'Euler Lagrange associé à l'énergie et obtenir de la régularité sur les minimiseurs, qui sont ainsi des solutions classiques du système stationnaire (0.11). Nous remarquons également que l'équation d'Euler-Lagrange pour l'espèce u_0 se découple, révélant un lien étroit avec l'énergie de Cahn-Hilliard à une espèce (3.2.22).

Lorsque les paramètres sont choisis de manière à ce que la fonctionnelle d'énergie soit strictement convexe (nous donnons des conditions explicites), l'unique minimiseur est constant et nous montrons par la méthode d'entropie que les solutions faibles du problème d'évolution (0.9) convergent vers cet état exponentiellement vite. Dans le cas non-convexe, la dynamique est plus complexe et nous l'étudions à l'aide d'un schéma volumes finis qui approche (0.9) en préservant les contraintes (0.10). Nous montrons que l'énergie libre discrète n'augmente pas en utilisant d'une part une règle de la chaîne logarithmique discrète et d'autre part une discrétisation semi-implicite convexe-concave en temps. Enfin nous présentons des simulations numériques en dimensions une et deux pour illustrer le comportement du schéma et étudier la variété des solutions stationnaires dans la limite en temps long (Section 3.5).

Chapitre 4. Couplage de systèmes à diffusion croisée par une interface mobile

Dans ce chapitre, nous proposons et étudions une extension du modèle (0.3). Dans ce dernier, les flux absorbés $F(t)$ étaient supposés connus alors qu'ils dépendent en réalité de l'interaction entre les phases gazeuse et solide dans la chambre chaude. Un modèle plus réaliste doit donc tenir compte de l'évolution de la phase gazeuse et de la façon dont le dépôt se produit à l'interface entre les deux phases. Nous proposons un premier modèle dans cette direction. Par souci de simplicité, nous ne considérons ici qu'un système isolé (pas de flux entrant dans la chambre chaude) afin de nous concentrer principalement sur le couplage par l'interface mobile.

Je présente ici brièvement le modèle et renvoie à la Section 4.2 pour plus de détails. Soit $\Omega = (0,1)$ le domaine physique contenant les phases solide et gazeuse. Pour tout $t \geq 0$, $e(t) \in [0,1]$ désigne la position à l'instant t de l'interface entre les deux phases. Plus précisément, à l'instant t, la phase solide occupe le domaine $(0, e(t))$ et la phase gazeuse occupe le domaine $(e(t), 1)$. Nous désignons par $Q := \mathbb{R}_+ \times \Omega$ le domaine espace-temps du problème.

Nous considérons n espèces chimiques différentes représentées par leurs densités de concentration molaire. Plus précisément, pour tout $i = 1, \ldots, n$, $u_i(t,x)$ représente la densité de concentration molaire de l'espèce i au temps $t \geq 0$ et au point $x \in \Omega$ et nous notons $u(t,x) := (u_i(t,x))_{i \in \{1,\ldots,n\}}$. Les contraintes *volume-filling* (0.10) doivent être satisfaites dans Q. Pour $(t,x) \in Q$ et $i = 1, \ldots, n$, nous notons $J_i(t,x) \in \mathbb{R}$ le flux molaire de l'espèce i au temps t et au point $x \in \Omega$ et notons $J(t,x) := (J_1(t,x), \ldots, J_n(t,x))^T$.

La conservation locale de la matière à l'intérieur de la phase solide et de la phase gazeuse implique

$$\partial_t c + \partial_x J = 0, \text{ dans }]0, e(t)[\cup(e(t), 1). \tag{0.12a}$$

Les phénomènes de diffusion croisée sont modélisés par les matrices de diffusion $A_s : \mathbb{R}^n \to \mathbb{R}^{n\times n}$ (resp. $A_g : \mathbb{R}^n \to \mathbb{R}^{n\times n}$) dans la phase solide (resp. gazeuse), via

$$\begin{aligned} J &= -A_s(c)\partial_x c, \ x \in]0, e(t)[\\ J &= -A_g(c)\partial_x c, \ x \in (e(t), 1). \end{aligned} \tag{0.12b}$$

Les matrices A_s et A_g doivent satisfaire certaines hypothèses liées à la structure entropique (voir la Section 1.2.4) et aux contraintes *volume-filling* (voir la Section 4.2.2). Sur la frontière du domaine complet Ω, nous imposons des conditions de flux nul

$$J(t, 0) = J(t, 1) = 0, \ t \geq 0. \tag{0.12c}$$

En outre, nous supposons que J et c sont suffisamment réguliers pour définir leur trace en $e(t)^{\pm}$: pour tout $t \geq 0$ tel que $e(t) \in (0, 1)$, nous définissons pour $i = 1, \ldots, n$,

$$\begin{aligned} J_i^s(t) &:= J_i(t, e(t)^-), \ J_i^g(t) := J_i(t, e(t)^+), \\ u_i^s(t) &:= u_i(t, e(t)^-), \ u_i^g(t) := u_i(t, e(t)^+). \end{aligned} \tag{0.12d}$$

Nous utilisons un vecteur de flux $F(t) = (F_i(t))_{i\in\{1,\ldots,n\}}$ qui rend compte des mécanismes de transition de phase situés au voisinage de l'interface mobile entre les phases solide et gazeuse. Nous nous concentrons dans ce travail sur des flux d'interface de type Butler-Volmer. Plus précisément, nous introduisons des potentiels chimiques de référence $\mu^{*,s} := (\mu_i^{*,s})_{i\in\{1,\ldots,n\}}, \mu^{*,g} := (\mu_i^{*,g})_{i\in\{1,\ldots,n\}} \in \mathbb{R}^n$ et définissons les constantes

$$\beta_i^* := \exp\left([\![\mu_i^*]\!]\right), \quad [\![\mu_i^*]\!] := \mu_i^{*,g} - \mu_i^{*,s} \quad i = 1, \ldots, n. \tag{0.12e}$$

Le vecteur $F(t)$ est alors défini pour tout $t \geq 0$ tel que $e(t) \in (0, 1)$ par

$$F_i(t) = \frac{1}{\sqrt{\beta_i^*}} u_i^g(t) - \sqrt{\beta_i^*} u_i^s(t), \ i = 1, \ldots, n. \tag{0.12f}$$

L'évolution de l'interface est définie, comme dans (0.1), par

$$e'(t) = \sum_{i=1}^{n} F_i(t), \ t \geq 0. \tag{0.12g}$$

Enfin, nous imposons les conditions aux limites suivantes sur l'interface mobile

$$-J^s(t) + e'(t)u^s(t) = -J^g(t) + e'(t)u^g(t) = F(t). \tag{0.12h}$$

Notre travail apporte les contributions suivantes :

- Nous introduisons un nouveau modèle de diffusion croisée avec interface mobile (0.12) et mettons en évidence sa structure entropique variationnelle. Cette dernière garantit la cohérence thermodynamique du modèle et jette les bases d'une analyse mathématique rigoureuse. Les états stationnaires sont identifiés (Proposition 6) et nous conjecturons le comportement en temps long.

- Un schéma volumes finis est introduit pour approcher le système. Contrairement au schéma conçu dans [72], nous ne redimensionnons pas le système dans un domaine fixe mais discrétisons plutôt l'interface mobile en suivant une approche de type *moving-mesh*. Aussi la principale nouveauté réside dans le traitement numérique de l'interface mobile.

- Nous prouvons par des arguments topologiques l'existence, à chaque pas temps, d'au moins une solution discrète au schéma qui préserve la structure complète du système continu (Proposition 7). En particulier, la mise à jour de l'interface et du maillage préserve la décroissance de l'entropie au niveau discret.

- Les résultats numériques illustrent les propriétés du modèle et le bon comportement du schéma (voir la Section 4.5). Ces résultats soutiennent également nos conjectures concernant le comportement en temps long.

Bibliography

[1] Helmut Abels and Mathias Wilke. "Convergence to Equilibrium for the Cahn Hilliard Equation with a Logarithmic Free Energy". In: *Nonlinear Analysis: Theory, Methods & Applications* 67.11 (2007), pp. 3176–3193. DOI: 10.1016/j.na.2006.10.002.

[2] Stefan Adams, Nicolas Dirr, Mark A. Peletier, and Johannes Zimmer. "From a Large-Deviations Principle to the Wasserstein Gradient Flow: A New Micro-Macro Passage". In: *Communications in Mathematical Physics* 307.3 (2011), pp. 791–815. DOI: 10.1007/s00220-011-1328-4.

[3] Stefan Adams, Nicolas Dirr, Mark A. Peletier, and Johannes Zimmer. "Large Deviations and Gradient Flows". In: *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 371.2005 (2013). DOI: 10.1098/rsta.2012.0341.

[4] Toyohiko Aiki and Adrian Muntean. "A Free-Boundary Problem for Concrete Carbonation: Front Nucleation and Rigorous Justification of the Square Root Law of Propagation". In: *Interfaces and Free Boundaries* 15.2 (2013), pp. 167–180. DOI: 10.4171/ifb/299.

[5] Toyohiko Aiki and Adrian Muntean. "Existence and Uniqueness of Solutions to a Mathematical Model Predicting Service Life of Concrete Structures". In: *Advances in Mathematical Sciences and Applications* 19.1 (2009), pp. 109–129.

[6] Toyohiko Aiki and Adrian Muntean. "Large Time Behavior of Solutions to a Moving-Interface Problem Modeling Concrete Carbonation". In: *Communications on Pure and Applied Analysis* 9.5 (2010), pp. 1117–1129. DOI: 10.3934/cpaa.2010.9.1117.

[7] Luca Alasio, Helene Ranetbauer, Markus Schmidtchen, and Marie-Therese Wolfram. "Trend to Equilibrium for Systems with Small Cross-Diffusion". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 54.5 (2020), pp. 1661–1688. DOI: 10.1051/m2an/2020008.

[8] Nicholas D. Alikakos, Peter W. Bates, and Xinfu Chen. "Convergence of the Cahn-Hilliard Equation to the Hele-Shaw Model". In: *Archive for Rational Mechanics and Analysis* 128.2 (1994), pp. 165–205. DOI: 10.1007/BF00375025.

[9] Samuel M. Allen and John W. Cahn. "A Microscopic Theory for Antiphase Boundary Motion and Its Application to Antiphase Domain Coarsening". In: *Acta Metallurgica* 27.6 (1979), pp. 1085–1095. DOI: 10.1016/0001-6160(79)90196-2.

[10] Fred Almgren, Jean E. Taylor, and Lihe Wang. "Curvature-Driven Flows: A Variational Approach". In: *SIAM Journal on Control and Optimization* 31.2 (1993), pp. 387–438. DOI: 10.1137/0331020.

[11] Herbert Amann. "Dynamic Theory of Quasilinear Parabolic Equations—I. Abstract Evolution Equations". In: *Nonlinear Analysis: Theory, Methods & Applications* 12.9 (1988), pp. 895–919. DOI: 10.1016/0362-546X(88)90073-9.

[12] Herbert Amann. "Dynamic Theory of Quasilinear Parabolic Equations. II. Reaction Diffusion Systems". In: *Differential and Integral Equations* 3.1 (1990). DOI: 10.57262/die/1371586185.

[13] Herbert Amann. "Dynamic Theory of Quasilinear Parabolic Systems. III. Global Existence". In: *Mathematische Zeitschrift* 202.2 (1989), pp. 219–250. DOI: 10.1007/BF01215256.

[14] Luigi Ambrosio. "Geometric Evolution Problems, Distance Function and Viscosity Solutions". In: *Calculus of Variations and Partial Differential Equations: Topics on Geometrical Evolution Problems and Degree Theory*. Ed. by Luigi Ambrosio, Norman Dancer, Giuseppe Buttazzo, Antonio Marino, and M. K. V. Murthy. Berlin, Heidelberg: Springer, 2000, pp. 5–93. DOI: 10.1007/978-3-642-57186-2_2.

[15] Luigi Ambrosio, Nicola Gigli, and Giuseppe Savaré. *Gradient Flows: In Metric Spaces and in the Space of Probability Measures*. Lectures in Mathematics ETH Zürich. Boston: Birkhäuser, 2005.

[16] Boris Andreianov, Clément Cancès, and Ayman Moussa. "A Nonlinear Time Compactness Result and Applications to Discretization of Degenerate Parabolic-Elliptic PDEs". In: *Journal of Functional Analysis* 273.12 (2017), pp. 3633–3670. DOI: 10.1016/j.jfa.2017.08.010.

[17] Anton Arnold, Peter Markowich, Giuseppe Toscani, and Andreas Unterreiter. "On Convex Sobolev Inequalities and the Rate of Convergence to Equilibrium for Fokker-Planck Type Equations". In: *Communications in Partial Differential Equations* 26.1-2 (2001), pp. 43–100. DOI: 10.1081/PDE-100002246.

[18] Jean Auriol, Federico Bribiesca-Argomedo, David Bou Saba, Michael Di Loreto, and Florent Di Meglio. "Delay-Robust Stabilization of a Hyperbolic PDE–ODE System". In: *Automatica* 95 (2018), pp. 494–502. DOI: 10.1016/j.automatica.2018.06.033.

[19] Jean Auriol and Florent Di Meglio. "Minimum Time Control of Heterodirectional Linear Coupled Hyperbolic PDEs". In: *Automatica* 71 (2016), pp. 300–307. DOI: 10.1016/j.automatica.2016.05.030.

[20] Jean Auriol and Florent Di Meglio. "Robust Output Feedback Stabilization for Two Heterodirectional Linear Coupled Hyperbolic PDEs". In: *Automatica* 115 (2020), p. 108896. DOI: 10.1016/j.automatica.2020.108896.

[21] Antonello Baccoli, Alessandro Pisano, and Yury Orlov. "Boundary Control of Coupled Reaction–Diffusion Processes with Constant Parameters". In: *Automatica* 54 (2015), pp. 80–90. DOI: 10.1016/j.automatica.2015.01.032.

[22] Rafael Bailo, José A. Carrillo, Serafim Kalliadasis, and Sergio P. Perez. *Unconditional Bound-Preserving and Energy-Dissipating Finite-Volume Schemes for the Cahn-Hilliard Equation*. 2021.

[23] Athmane Bakhta. "Mathematical Models and Numerical Simulation of Photovoltaic Devices". These. Université Paris-Est, 2017.

[24] Athmane Bakhta and Virginie Ehrlacher. "Cross-Diffusion Systems with Non-Zero Flux and Moving Boundary Conditions". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 52.4 (2018), pp. 1385–1415. DOI: 10.1051/m2an/2017053.

[25] Athmane Bakhta and Julien Vidal. "Modeling and Optimization of the Fabrication Process of Thin-Film Solar Cells by Multi-Source Physical Vapor Deposition". In: *Mathematics and Computers in Simulation* 185 (2021), pp. 115–133. DOI: 10.1016/j.matcom.2020.12.016.

[26] Dominique Bakry and Michel Émery. "Diffusions hypercontractives". In: *Séminaire de Probabilités XIX 1983/84*. Ed. by Jacques Azéma and Marc Yor. Vol. 1123. Berlin, Heidelberg: Springer Berlin Heidelberg, 1985, pp. 177–206. DOI: 10.1007/BFb0075847.

[27] John M. Ball. "The Calculus of Variations and Materials Science". In: *Quarterly of Applied Mathematics* 56.4 (1998), pp. 719–740. DOI: 10.1090/qam/1668735.

[28] Andras Balogh and Miroslav Krstic. "Infinite Dimensional Backstepping-Style Feedback Transformations for a Heat Equation with an Arbitrary Level of Instability". In: *European Journal of Control* 8.2 (2002), pp. 165–175. DOI: 10.3166/ejc.8.165-175.

[29] Georges Bastin, Jean-Michel Coron, and Amaury Hayat. "Diffusion and Robustness of Boundary Feedback Stabilization of Hyperbolic Systems". In: *Mathematics of Control, Signals, and Systems* 35.1 (2023), pp. 159–185. DOI: 10.1007/s00498-022-00335-0.

[30] William Beckner. "A Generalized Poincaré Inequality for Gaussian Measures". In: *Proceedings of the American Mathematical Society* 105.2 (1989), pp. 397–400.

[31] Peter Bella, Michael Goldman, and Barbara Zwicknagl. "Study of Island Formation in Epitaxially Strained Films on Unbounded Domains". In: *Archive for Rational Mechanics and Analysis* 218.1 (2015), pp. 163–217. DOI: 10.1007/s00205-015-0858-x.

[32] Judith Berendsen, Martin Burger, Virginie Ehrlacher, and Jan-Frederik Pietschmann. "Uniqueness of Strong Solutions and Weak–Strong Stability in a System of Cross-Diffusion Equations". In: *Journal of Evolution Equations* 20.2 (2020), pp. 459–483. DOI: 10.1007/s00028-019-00534-4.

[33] Michel Bertsch, Morton E. Gurtin, and Danielle Hilhorst. "On Interacting Populations That Disperse to Avoid Crowding: The Case of Equal Dispersal Velocities". In: *Nonlinear Analysis: Theory, Methods & Applications* 11.4 (1987), pp. 493–499. DOI: 10.1016/0362-546X(87)90067-8.

[34] Marianne Bessemoulin-Chatard, Claire Chainais-Hillairet, and Francis Filbet. "On Discrete Functional Inequalities for Some Finite Volume Schemes". In: *IMA Journal of Numerical Analysis* 35.3 (2015), pp. 1125–1149. DOI: 10.1093/imanum/dru032.

[35] Marianne Bessemoulin-Chatard and Francis Filbet. "A Finite Volume Scheme for Nonlinear Degenerate Parabolic Equations". In: *SIAM Journal on Scientific Computing* 34.5 (2012), B559–B583. DOI: 10.1137/110853807.

[36] James F. Blowey and Charles M. Elliott. "The Cahn–Hilliard Gradient Theory for Phase Separation with Non-Smooth Free Energy Part I: Mathematical Analysis". In: *European Journal of Applied Mathematics* 2.3 (1991), pp. 233–280. DOI: 10.1017/S095679250000053X.

[37] Dejan M. Bošković, Andras Balogh, and Miroslav Krstić. "Backstepping in Infinite Dimension for a Class of Parabolic Distributed Parameter Systems". In: *Mathematics of Control, Signals and Systems* 16.1 (2003), pp. 44–75. DOI: 10.1007/s00498-003-0128-6.

[38] Dieter Bothe. "On the Maxwell-Stefan Approach to Multicomponent Diffusion". In: *Parabolic Problems*. Ed. by Joachim Escher, Patrick Guidotti, Matthias Hieber, Piotr Mucha, Jan W. Prüss, Yoshihiro Shibata, Gieri Simonett, Christoph Walker, and Wojciech Zajaczkowski. Basel: Springer Basel, 2011, pp. 81–93. DOI: 10.1007/978-3-0348-0075-4_5.

[39] Dieter Bothe and Jan Prüss. "Modeling and Analysis of Reactive Multi-Component Two-Phase Flows with Mass Transfer and Phase Transition the Isothermal Incompressible Case". In: *Discrete and Continuous Dynamical Systems - S* 10.4 (2017), pp. 673–696. DOI: 10.3934/dcdss.2017034.

[40] Laurent Boudin, Bérénice Grec, and Vincent Pavan. "The Maxwell–Stefan Diffusion Limit for a Kinetic Model of Mixtures with General Cross Sections". In: *Nonlinear Analysis*. Advances in Reaction-Cross-Diffusion Systems 159 (2017), pp. 40–61. DOI: 10.1016/j.na.2017.01.010.

[41] Laurent Boudin, Bérénice Grec, and Francesco Salvarani. "A Mathematical and Numerical Analysis of the Maxwell-Stefan Diffusion Equations". In: *Discrete and Continuous Dynamical Systems - Series B* 17.5 (2012), pp. 1427–1440. DOI: 10.3934/dcdsb.2012.17.1427.

[42] Laurent Boudin, Bérénice Grec, and Francesco Salvarani. "The Maxwell-Stefan Diffusion Limit for a Kinetic Model of Mixtures". In: *Acta Applicandae Mathematicae* 136.1 (2015), pp. 79–90. DOI: 10.1007/s10440-014-9886-z.

[43] Franck Boyer and Sebastian Minjeaud. "Hierarchy of Consistent N-Component Cahn–Hilliard Systems". In: *Mathematical Models and Methods in Applied Sciences* 24.14 (2014), pp. 2885–2928.

[44] Matthieu Brachet, Philippe Parnaudeau, and Morgan Pierre. "Convergence to Equilibrium for Time and Space Discretizations of the Cahn-Hilliard Equation". In: *Discrete and Continuous Dynamical Systems - S* 15.8 (2022), p. 1987. DOI: 10.3934/dcdss.2022110.

[45] Andrea Braides. *Gamma-Convergence for Beginners*. Vol. 22. Clarendon Press, 2002.

[46] Andrea Braides. *Local Minimization, Variational Evolution and* Γ*-Convergence*. Vol. 2094. Lecture Notes in Mathematics. Cham: Springer International Publishing, 2014. DOI: 10.1007/978-3-319-01982-6.

[47] Kenneth A. Brakke. *The Motion of a Surface by Its Mean Curvature. (MN-20)*. Princeton University Press, 2015.

[48] Marcel Braukhoff, Claudia Raithel, and Nicola Zamponi. "Partial Hölder Regularity for Solutions of a Class of Cross-Diffusion Systems with Entropy Structure". In: *Journal de Mathématiques Pures et Appliquées* 166 (2022), pp. 30–69.

[49] Haïm Brezis. *Functional Analysis, Sobolev Spaces and Partial Differential Equations*. Springer International Publishing, 2011. DOI: 10.1007/978-0-387-70914-7.

[50] Lia Bronsard and Robert V Kohn. "Motion by Mean Curvature as the Singular Limit of Ginzburg-Landau Dynamics". In: *Journal of Differential Equations* 90.2 (1991), pp. 211–237. DOI: 10.1016/0022-0396(91)90147-2.

[51] Maria Bruna and S. Jonathan Chapman. "Diffusion of Multiple Species with Excluded-Volume Effects". In: *The Journal of Chemical Physics* 137.20 (2012), p. 204116. DOI: 10.1063/1.4767058.

[52] Aaron Brunk, Herbert Egger, Timileyin David Oyedeji, Yangyiwei Yang, and Bai-Xiang Xu. *On Existence, Uniqueness and Stability of Solutions to Cahn-Hilliard/Allen-Cahn Systems with Cross-Kinetic Coupling*. 2022. DOI: 10.48550/arXiv.2211.07153.

[53] Martin Burger, Marco Di Francesco, Jan-Frederik Pietschmann, and Bärbel Schlake. "Nonlinear Cross-Diffusion with Size Exclusion". In: *SIAM Journal on Mathematical Analysis* 42.6 (2010), pp. 2842–2871. DOI: 10.1137/100783674.

[54] Martin Burger, Sabine Hittmeir, Helene Ranetbauer, and Marie-Therese Wolfram. "Lane Formation by Side-Stepping". In: *SIAM Journal on Mathematical Analysis* 48.2 (2016), pp. 981–1005. DOI: 10.1137/15M1033174.

[55] Christopher I. Byrnes and Alberto Isidori. "New Results and Examples in Nonlinear Feedback Stabilization". In: *Systems & Control Letters* 12.5 (1989), pp. 437–442. DOI: 10.1016/0167-6911(89)90080-7.

[56] Luis A. Caffarelli and Nora E. Muler. "An L∞ Bound for Solutions of the Cahn-Hilliard Equation". In: *Archive for Rational Mechanics and Analysis* 133 (1995), pp. 129–144. DOI: 10.1007/BF00376814.

[57] John W. Cahn, Charles M. Elliott, and Amy Novick-Cohen. "The Cahn–Hilliard Equation with a Concentration Dependent Mobility: Motion by Minus the Laplacian of the Mean Curvature". In: *European Journal of Applied Mathematics* 7.3 (1996), pp. 287–301. DOI: 10.1017/S0956792500002369.

[58] John W. Cahn and John E. Hilliard. "Free Energy of a Nonuniform System. I. Interfacial Free Energy". In: *The Journal of Chemical Physics* 28.2 (1958), pp. 258–267. DOI: 10.1063/1.1744102.

[59] Clément Cancès, Jean Cauvin-Vila, Claire Chainais-Hillairet, and Virginie Ehrlacher. "Structure Preserving Finite Volume Approximation of Cross-Diffusion Systems Coupled by a Free Interface". In: *Finite Volumes for Complex Applications X*. Springer Proceedings in Mathematics & Statistics. 2023, pp. 205–213. DOI: 10.1007/978-3-031-40864-9_15.

[60] Clément Cancès, Claire Chainais-Hillairet, Anita Gerstenmayer, and Ansgar Jüngel. "Finite-Volume Scheme for a Degenerate Cross-Diffusion Model Motivated from Ion Transport". In: *Numerical Methods for Partial Differential Equations* 35.2 (2019), pp. 545–575. DOI: 10.1002/num.22313.

[61] Clément Cancès, Virginie Ehrlacher, and Laurent Monasse. *Finite Volumes for the Stefan-Maxwell Cross-Diffusion System*. 2020.

[62] Clément Cancès and Benoît Gaudeul. "A Convergent Entropy Diminishing Finite Volume Scheme for a Cross-Diffusion System". In: *SIAM Journal on Numerical Analysis* 58.5 (2020), pp. 2684–2710. DOI: 10.1137/20M1316093.

[63] Clément Cancès and Cindy Guichard. "Numerical Analysis of a Robust Free Energy Diminishing Finite Volume Scheme for Parabolic Equations with Gradient Structure". In: *Foundations of Computational Mathematics* 17.6 (2017), pp. 1525–1584. DOI: 10.1007/s10208-016-9328-6.

[64] Clément Cancès and Antoine Zurek. "A Convergent Finite Volume Scheme for Dissipation Driven Models with Volume Filling Constraint". In: *Numerische Mathematik* 151.1 (2022), pp. 279–328. DOI: 10.1007/s00211-022-01270-7.

[65] José A. Carrillo, Francis Filbet, and Markus Schmidtchen. "Convergence of a Finite Volume Scheme for a System of Interacting Species with Cross-Diffusion". In: *Numerische Mathematik* 145.3 (2020), pp. 473–511. DOI: 10.1007/s00211-020-01121-3.

[66] José A. Carrillo, Ansgar Jüngel, Peter A. Markowich, G. Toscani, and A. Unterreiter. "Entropy Dissipation Methods for Degenerate ParabolicProblems and Generalized Sobolev Inequalities". In: *Monatshefte fur Mathematik* 133.1 (2001), pp. 1–82. DOI: 10.1007/s006050170032.

[67] José A. Carrillo, Stefano Lisini, Giuseppe Savaré, and Dejan Slepčev. "Nonlinear Mobility Continuity Equations and Generalized Displacement Convexity". In: *Journal of Functional Analysis* 258.4 (2010), pp. 1273–1309. DOI: 10.1016/j.jfa.2009.10.016.

[68] Jean Cauvin-Vila, Virginie Ehrlacher, and Amaury Hayat. "Boundary Stabilization of One-Dimensional Cross-Diffusion Systems in a Moving Domain: Linearized System". In: *Journal of Differential Equations* 350 (2023), pp. 251–307. DOI: 10.1016/j.jde.2022.12.021.

[69] Jean Cauvin-Vila, Virginie Ehrlacher, Greta Marino, and Jan-Frederik Pietschmann. *Stationary Solutions and Large Time Asymptotics to a Cross-Diffusion-Cahn-Hilliard System*. 2023. DOI: 10.48550/arXiv.2307.05985.

[70] Claire Chainais-Hillairet. "Entropy Method and Asymptotic Behaviours of Finite Volume Schemes". In: *Finite Volumes for Complex Applications VII-Methods and Theoretical Aspects*. Ed. by Jürgen Fuhrmann, Mario Ohlberger, and Christian Rohde. Springer Proceedings in Mathematics & Statistics. Cham: Springer International Publishing, 2014, pp. 17–35. DOI: 10.1007/978-3-319-05684-5_2.

[71] Claire Chainais-Hillairet, Ansgar Jüngel, and Stefan Schuchnigg. "Entropy dissipative discretization of nonlinear diffusion equations and discrete Beckner inequalities". In: *ESAIM: Mathematical Modelling and Numerical Analysis - Modélisation Mathématique et Analyse Numérique* 50.1 (2016), pp. 135–162. DOI: 10.1051/m2an/2015031.

[72] Claire Chainais-Hillairet, Benoît Merlet, and Antoine Zurek. "Convergence of a Finite Volume Scheme for a Parabolic System with a Free Boundary Modeling Concrete Carbonation". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 52.2 (2018), pp. 457–480. DOI: 10.1051/m2an/2018002.

[73] Antonin Chambolle and Eric Bonnetier. "Computing the Equilibrium Configuration of Epitaxially Strained Crystalline Films". In: *SIAM Journal on Applied Mathematics* 62.4 (2002), pp. 1093–1121. DOI: 10.1137/S0036139900368571.

[74] Antonin Chambolle and Margherita Solci. "Interaction of a Bulk and a Surface Energy with a Geometrical Constraint". In: *SIAM Journal on Mathematical Analysis* 39.1 (2007), pp. 77–102. DOI: 10.1137/060649173.

[75] Li Chen, Esther S. Daus, Alexandra Holzinger, and Ansgar Jüngel. "Rigorous Derivation of Population Cross-Diffusion Systems from Moderately Interacting Particle Systems". In: *Journal of Nonlinear Science* 31.6 (2021), p. 94. DOI: 10.1007/s00332-021-09747-9.

[76] Li Chen and Ansgar Jüngel. "Analysis of a Multidimensional Parabolic Population Model with Strong Cross-Diffusion". In: *SIAM Journal on Mathematical Analysis* 36.1 (2004), pp. 301–322. DOI: 10.1137/S0036141003427798.

[77] Li Chen and Ansgar Jüngel. "Analysis of a Parabolic Cross-Diffusion Population Model without Self-Diffusion". In: *Journal of Differential Equations* 224.1 (2006), pp. 39–59. DOI: 10.1016/j.jde.2005.08.002.

[78] Wenbin Chen, Cheng Wang, Xiaoming Wang, and Steven M. Wise. "Positivity-Preserving, Energy Stable Numerical Schemes for the Cahn-Hilliard Equation with Logarithmic Potential". In: *Journal of Computational Physics: X* 3 (2019), p. 100031. DOI: 10.1016/j.jcpx.2019.100031.

[79] Xinfu Chen. "Generation and Propagation of Interfaces for Reaction-Diffusion Equations". In: *Journal of Differential Equations* 96.1 (1992), pp. 116–141. DOI: 10.1016/0022-0396(92)90146-E.

[80] Xiuqing Chen and Ansgar Jüngel. "A Note on the Uniqueness of Weak Solutions to a Class of Cross-Diffusion Systems". In: *Journal of Evolution Equations* 18.2 (2018), pp. 805–820. DOI: 10.1007/s00028-017-0420-4.

[81] Xiuqing Chen and Ansgar Jüngel. "Weak–Strong Uniqueness of Renormalized Solutions to Reaction–Cross-Diffusion Systems". In: *Mathematical Models and Methods in Applied Sciences* 29.02 (2019), pp. 237–270. DOI: 10.1142/S0218202519500088.

[82] Xiuqing Chen and Ansgar Jüngel. "When Do Cross-Diffusion Systems Have an Entropy Structure?" In: *Journal of Differential Equations* 278 (2021), pp. 60–72. DOI: 10.1016/j.jde.2020.12.037.

[83] Xiuqing Chen, Ansgar Jüngel, and Jian-Guo Liu. "A Note on Aubin-Lions-Dubinskii Lemmas". In: *Acta Applicandae Mathematicae* 133.1 (2014), pp. 33–43. DOI: 10.1007/s10440-013-9858-8.

[84] Yun-Gang Chen, Yoshikazu Giga, and Shun'ichi Goto. "Uniqueness and Existence of Viscosity Solutions of Generalized Mean Curvature Flow Equations". In: *Proceedings of the Japan Academy, Series A, Mathematical Sciences* 65.7 (1989), pp. 207–210. DOI: 10.3792/pjaa.65.207.

[85] Jean-Michel Coron. *Control and Nonlinearity*. Vol. 136. Mathematical Surveys and Monographs. Providence, Rhode Island: American Mathematical Society, 2009. DOI: 10.1090/surv/136.

[86] Jean-Michel Coron and B. d'Andrea-Novel. "Stabilization of a Rotating Body Beam without Damping". In: *IEEE Transactions on Automatic Control* 43.5 (1998), pp. 608–618. DOI: 10.1109/9.668828.

[87] Jean-Michel Coron, Ludovick Gagnon, and Morgan Morancey. "Rapid Stabilization of a Linearized Bilinear 1-D Schrödinger Equation". In: *Journal de Mathématiques Pures et Appliquées* 115 (2018), pp. 24–73. DOI: 10.1016/j.matpur.2017.10.006.

[88] Jean-Michel Coron, Amaury Hayat, Shengquan Xiang, and Christophe Zhang. "Stabilization of the Linearized Water Tank System". In: *Archive for Rational Mechanics and Analysis* 244.3 (2022), pp. 1019–1097. DOI: 10.1007/s00205-022-01778-0.

[89] Jean-Michel Coron, Long Hu, Guillaume Olive, and Peipei Shang. "Boundary Stabilization in Finite Time of One Dimensional Linear Hyperbolic Balance Laws with Coefficients Depending on Time and Space". In: *Journal of Differential Equations* 271 (2021), pp. 1109–1170. DOI: 10.1016/j.jde.2020.09.037.

[90] Jean-Michel Coron and Qi Lü. "Fredholm Transform and Local Rapid Stabilization for a Kuramoto–Sivashinsky Equation". In: *Journal of Differential Equations* 259.8 (2015), pp. 3683–3729. DOI: 10.1016/j.jde.2015.05.001.

[91] Jean-Michel Coron and Hoai-Minh Nguyen. "Dissipative Boundary Conditions for Nonlinear 1-D Hyperbolic Systems: Sharp Conditions Through an Approach via Time-Delay Systems". In: *SIAM Journal on Mathematical Analysis* 47.3 (2015), pp. 2220–2240. DOI: 10.1137/140976625.

[92] Jean-Michel Coron and Hoai-Minh Nguyen. "Null Controllability and Finite Time Stabilization for the Heat Equations with Variable Coefficients in Space in One Dimension via Backstepping Approach". In: *Archive for Rational Mechanics and Analysis* 225.3 (2017), pp. 993–1023. DOI: 10.1007/s00205-017-1119-y.

[93] Jean-Michel Coron and Hoai-Minh Nguyen. "Null-Controllability of Linear Hyperbolic Systems in One Dimensional Space". In: *Systems & Control Letters* 148 (2021), p. 104851. DOI: 10.1016/j.sysconle.2020.104851.

[94] Jean-Michel Coron and Hoai-Minh Nguyen. "Optimal Time for the Controllability of Linear Hyperbolic Systems in One-Dimensional Space". In: *SIAM Journal on Control and Optimization* 57.2 (2019), pp. 1127–1156. DOI: 10.1137/18M1185600.

[95] Jean-Michel Coron and Emmanuel Trélat. "Global Steady-State Controllability of One-Dimensional Semilinear Heat Equations". In: *SIAM Journal on Control and Optimization* 43.2 (2004), pp. 549–569. DOI: 10.1137/S036301290342471X.

[96] Yves Coudière, Thierry Gallouët, and Raphaèle Herbin. "Discrete Sobolev Inequalities and Lp Error Estimates for Finite Volume Solutions of Convection Diffusion Equations". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 35.4 (2001), pp. 767–778.

[97] Vito Crismale and Manuel Friedrich. "Equilibrium Configurations for Epitaxially Strained Films and Material Voids in Three-Dimensional Linear Elasticity". In: *Archive for Rational Mechanics and Analysis* 237.2 (2020), pp. 1041–1098. DOI: 10.1007/s00205-020-01525-3.

[98] Shibin Dai and Qiang Du. "Weak Solutions for the Cahn–Hilliard Equation with Degenerate Mobility". In: *Archive for Rational Mechanics and Analysis* 219.3 (2016), pp. 1161–1184. DOI: 10.1007/s00205-015-0918-2.

[99] Sara Daneri and Giuseppe Savaré. "Eulerian Calculus for the Displacement Convexity in the Wasserstein Distance". In: *SIAM Journal on Mathematical Analysis* 40.3 (2008), pp. 1104–1122. DOI: 10.1137/08071346X.

[100] Sara Daneri and Giuseppe Savaré. "Lecture Notes on Gradient Flows and Optimal Transport". In: *arXiv:1009.3737 [math]* (2010).

[101] Esther S. Daus, Ansgar Jüngel, and Antoine Zurek. "Convergence of a Finite-Volume Scheme for a Degenerate-Singular Cross-Diffusion System for Biofilms". In: *IMA Journal of Numerical Analysis* 41.2 (2021), pp. 935–973. DOI: 10.1093/imanum/draa040.

[102] Esther S. Daus, Pina Milišić, and Nicola Zamponi. "Analysis of a Degenerate and Singular Volume-Filling Cross-Diffusion System Modeling Biofilm Growth". In: *SIAM Journal on Mathematical Analysis* 51.4 (2019), pp. 3569–3605. DOI: 10.1137/18M1185806.

[103] Elisa Davoli and Paolo Piovano. "Analytical Validation of the Young–Dupré Law for Epitaxially-Strained Thin Films". In: *Mathematical Models and Methods in Applied Sciences* 29.12 (2019), pp. 2183–2223. DOI: 10.1142/S0218202519500441.

[104] Elisa Davoli and Paolo Piovano. "Derivation of a Heteroepitaxial Thin-Film Model". In: *Interfaces and Free Boundaries* 22.1 (2020), pp. 1–26. DOI: 10.4171/ifb/435.

[105] Piero De Mottoni and Michelle Schatzman. "Geometrical Evolution of Developed Interfaces". In: *Transactions of the American Mathematical Society* 347.5 (1995), pp. 1533–1589. DOI: 10.2307/2154960.

[106] Klaus Deckelnick, Gerhard Dziuk, and Charles M. Elliott. "Computation of Geometric Partial Differential Equations and Mean Curvature Flow". In: *Acta Numerica* 14 (2005), pp. 139–232. DOI: 10.1017/S0962492904000224.

[107] Klaus Deimling. *Nonlinear Functional Analysis*. Berlin, Heidelberg: Springer, 1985. DOI: 10.1007/978-3-662-00547-7.

[108] Laurent Desvillettes and Klemens Fellner. "Exponential Convergence to Equilibrium for Nonlinear Reaction-Diffusion Systems Arising in Reversible Chemistry". In: *System Modeling and Optimization: 26th IFIP TC 7 Conference, CSMO 2013, Klagenfurt, Austria, September 9-13, 2013, Revised Selected Papers 26*. Springer, 2014, pp. 96–104.

[109] Laurent Desvillettes, Thomas Lepoutre, and Ayman Moussa. "Entropy, Duality, and Cross Diffusion". In: *SIAM Journal on Mathematical Analysis* 46.1 (2014), pp. 820–853. DOI: 10.1137/130908701.

[110] Laurent Desvillettes, Thomas Lepoutre, Ayman Moussa, and Ariane Trescases. "On the Entropic Structure of Reaction-Cross Diffusion Systems". In: *Communications in Partial Differential Equations* 40.9 (2015), pp. 1705–1747. DOI: 10.1080/03605302.2014.998837.

[111] Helge Dietert and Ayman Moussa. *Persisting Entropy Structure for Nonlocal Cross-Diffusion Systems*. 2021.

[112] Karoline Disser. "Global Existence, Uniqueness and Stability for Nonlinear Dissipative Bulk-Interface Interaction Systems". In: *Journal of Differential Equations* 269.5 (2020), pp. 4023–4044. DOI: 10.1016/j.jde.2020.03.021.

[113] Jean Dolbeault, Bruno Nazaret, and Giuseppe Savaré. "A New Class of Transport Distances between Measures". In: *Calculus of Variations and Partial Differential Equations* 34.2 (2009), pp. 193–231. DOI: 10.1007/s00526-008-0182-5.

[114] Jérôme Droniou, Robert Eymard, Thierry Gallouet, and Raphaele Herbin. "Gradient Schemes: A Generic Framework for the Discretisation of Linear, Nonlinear and Nonlocal Elliptic and Parabolic Equations". In: *Mathematical Models and Methods in Applied Sciences* 23.13 (2013), pp. 2395–2432.

[115] Jérôme Droniou, Robert Eymard, Thierry Gallouët, Cindy Guichard, and Raphaèle Herbin. *The Gradient Discretisation Method*. Vol. 82. Mathématiques et Applications. Cham: Springer International Publishing, 2018. DOI: 10.1007/978-3-319-79042-8.

[116] Pierre-Étienne Druet, Katharina Hopf, and Ansgar Jüngel. *Hyperbolic-Parabolic Normal Form and Local Classical Solutions for Cross-Diffusion Systems with Incomplete Diffusion*. 2022. DOI: 10.48550/arXiv.2210.17244.

[117] Qiang Du and Xiaobing Feng. "Chapter 5 - The Phase Field Method for Geometric Moving Interfaces and Their Numerical Approximations". In: *Handbook of Numerical Analysis*. Ed. by Andrea Bonito and Ricardo H. Nochetto. Vol. 21. Geometric Partial Differential Equations - Part I. Elsevier, 2020, pp. 425–508. DOI: 10.1016/bs.hna.2019.05.001.

[118] Virginie Ehrlacher, Greta Marino, and Jan-Frederik Pietschmann. "Existence of Weak Solutions to a Cross-Diffusion Cahn-Hilliard Type System". In: *Journal of Differential Equations* 286 (2021), pp. 578–623. DOI: 10.1016/j.jde.2021.02.025.

[119] Charles M. Elliott and Harald Garcke. "Diffusional Phase Transitions in Multicomponent Systems with a Concentration Dependent Mobility Matrix". In: *Physica D: Nonlinear Phenomena* 109.3-4 (1997), pp. 242–256. DOI: 10.1016/S0167-2789(97)00066-3.

[120] Charles M. Elliott and Harald Garcke. "On the Cahn–Hilliard Equation with Degenerate Mobility". In: *SIAM Journal on Mathematical Analysis* 27.2 (1996), pp. 404–423. DOI: 10.1137/S0036141094267662.

[121] Charles M. Elliott and SA Luckhaus. "A Generalized Diffusion Equation for Phase Separation of a Multi-Component Mixture with Interfacial Free Energy. Inst". In: *Math. Appl* (1991).

[122] Charles M. Elliott and Zheng Songmu. "On the Cahn-Hilliard Equation". In: *Archive for Rational Mechanics and Analysis* 96.4 (1986), pp. 339–357. DOI: 10.1007/BF00251803.

[123] Nicolás Espitia, Andrey Polyakov, Denis Efimov, and Wilfrid Perruquetti. "Boundary Time-Varying Feedbacks for Fixed-Time Stabilization of Constant-Parameter Reaction–Diffusion Systems". In: *Automatica* 103 (2019), pp. 398–407. DOI: 10.1016/j.automatica.2019.02.013.

[124] Lawrence Evans. *Partial Differential Equations*. Second. Vol. 19. Graduate Studies in Mathematics. Providence, Rhode Island: American Mathematical Society, 2010. DOI: 10.1090/gsm/019.

[125] Lawrence C. Evans, Halil M. Soner, and Panagiotis E. Souganidis. "Phase Transitions and Generalized Motion by Mean Curvature". In: *Communications on Pure and Applied Mathematics* 45.9 (1992), pp. 1097–1123. DOI: 10.1002/cpa.3160450903.

[126] Lawrence C. Evans and Joel Spruck. "Motion of Level Sets by Mean Curvature. I". In: *Journal of Differential Geometry* 33.3 (1991), pp. 635–681. DOI: 10.4310/jdg/1214446559.

[127] Robert Eymard, Thierry Gallouët, Cindy Guichard, Raphaèle Herbin, and Roland Masson. "TP or Not TP, That Is the Question". In: *Computational Geosciences* 18.3 (2014), pp. 285–296. DOI: 10.1007/s10596-013-9392-9.

[128] Robert Eymard, Thierry Gallouët, and Raphaèle Herbin. "Finite Volume Methods". In: *Solution of Equation in $\mathbb{R}n$ (Part 3), Techniques of Scientific Computing (Part 3)*. Ed. by J. L. Lions and Philippe Ciarlet. Vol. 7. Handbook of Numerical Analysis. Elsevier, 2000, pp. 713–1020. DOI: 10.1016/S1570-8659(00)07005-8.

[129] Robert Eymard, Thierry Gallouït, Raphaèle Herbin, and Anthony Michel. "Convergence of a Finite Volume Scheme for Nonlinear Degenerate Parabolic Equations". In: *Numerische Mathematik* 92.1 (2002), pp. 41–82. DOI: 10.1007/s002110100342.

[130] David J Eyre. "An Unconditionally Stable One-Step Scheme for Gradient Systems". In: (1997), p. 15.

[131] David J. Eyre. "Systems of Cahn–Hilliard Equations". In: *SIAM Journal on Applied Mathematics* 53.6 (1993), pp. 1686–1712. DOI: 10.1137/0153078.

[132] David J. Eyre. "Unconditionally Gradient Stable Time Marching the Cahn-Hilliard Equation". In: *MRS Proceedings* 529 (1998), p. 39. DOI: 10.1557/PROC-529-39.

[133] Paul C. Fife. "Models for Phase Separation and Their Mathematics". In: (2000).

[134] Irene Fonseca, Nicola Fusco, Giovanni Leoni, and Massimiliano Morini. "Equilibrium Configurations of Epitaxially Strained Crystalline Films: Existence and Regularity Results". In: *Archive for Rational Mechanics and Analysis* 186.3 (2007), pp. 477–537. DOI: 10.1007/s00205-007-0082-4.

[135] Joaquin Fontbona and Sylvie Méléard. "Non Local Lotka-Volterra System with Cross-Diffusion in an Heterogeneous Medium". In: *Journal of Mathematical Biology* 70.4 (2015), pp. 829–854. DOI: 10.1007/s00285-014-0781-z.

[136] Ludovick Gagnon, Amaury Hayat, Shengquan Xiang, and Christophe Zhang. "Fredholm Transformation on Laplacian and Rapid Stabilization for the Heat Equation". In: *Journal of Functional Analysis* 283.12 (2022), p. 109664. DOI: 10.1016/j.jfa.2022.109664.

[137] Ludovick Gagnon, Pierre Lissy, and Swann Marx. "A Fredholm Transformation for the Rapid Stabilization of a Degenerate Parabolic Equation". In: *SIAM Journal on Control and Optimization* 59.5 (2021), pp. 3828–3859. DOI: 10.1137/20M1372603.

[138] Harald Garcke. "Curvature Driven Interface Evolution". In: *Jahresbericht der Deutschen Mathematiker-Vereinigung* 115.2 (2013), pp. 63–100. DOI: 10.1365/s13291-013-0066-2.

[139] Michael Gelantalis, Alfred Wagner, and Maria G. Westdickenberg. "Existence and Properties of Certain Critical Points of the Cahn-Hilliard Energy". In: *Indiana University Mathematics Journal* 66.5 (2017), pp. 1827–1877.

[140] Michael Gelantalis and Maria G. Westdickenberg. "Energy Barrier and Gamma Convergence in the D-Dimensional Cahn–Hilliard Equation". In: *Calculus of Variations and Partial Differential Equations* 54.1 (2015), pp. 791–829. DOI: 10.1007/s00526-014-0806-x.

[141] Yoshikazu Giga. *Surface Evolution Equations*. Monographs in Mathematics. Basel: Birkhäuser, 2006. DOI: 10.1007/3-7643-7391-1_2.

[142] Annegret Glitzky and Alexander Mielke. "A Gradient Structure for Systems Coupling Reaction–Diffusion Effects in Bulk and Interfaces". In: *Zeitschrift für angewandte Mathematik und Physik* 64.1 (2013), pp. 29–52. DOI: 10.1007/s00033-012-0207-y.

[143] Michael Goldman and Barbara Zwicknagl. "Scaling Law and Reduced Models for Epitaxially Strained Crystalline Films". In: *SIAM Journal on Mathematical Analysis* 46.1 (2014), pp. 1–24. DOI: 10.1137/120897250.

[144] Morton E. Gurtin and Allen C. Pipkin. "A Note on Interacting Populations That Disperse to Avoid Crowding". In: *Quarterly of Applied Mathematics* 42.1 (1984), pp. 87–94. DOI: 10.1090/qam/736508.

[145] Martin Herberg, Martin Meyries, Jan Prüss, and Mathias Wilke. "Reaction Diffusion Systems of Maxwell–Stefan Type with Reversible Mass-Action Kinetics". In: *Nonlinear Analysis*. Advances in Reaction-Cross-Diffusion Systems 159 (2017), pp. 264–284. DOI: 10.1016/j.na.2016.07.010.

[146] Maxime Herda and Antoine Zurek. "Study of an Entropy Dissipating Finite Volume Scheme for a Nonlocal Cross-Diffusion System". In: *ESAIM: Mathematical Modelling and Numerical Analysis* 57.3 (2023), pp. 1589–1617. DOI: 10.1051/m2an/2023032.

[147] Katharina Hopf and Martin Burger. "On Multi-Species Diffusion with Size Exclusion". In: *Nonlinear Analysis* 224 (2022), p. 113092. DOI: 10.1016/j.na.2022.113092.

[148] Long Hu, Florent Di Meglio, Rafael Vazquez, and Miroslav Krstic. "Control of Homodirectional and General Heterodirectional Linear Coupled Hyperbolic PDEs". In: *IEEE Transactions on Automatic Control* 61.11 (2016), pp. 3301–3314. DOI: 10.1109/TAC.2015.2512847.

[149] Long Hu, Rafael Vazquez, Florent Di Meglio, and Miroslav Krstic. "Boundary Exponential Stabilization of 1-Dimensional Inhomogeneous Quasi-Linear Hyperbolic Systems". In: *SIAM Journal on Control and Optimization* 57.2 (2019), pp. 963–998. DOI: 10.1137/15M1012712.

[150] Xiaokai Huo, Ansgar Jüngel, and Athanasios E. Tzavaras. "Weak-Strong Uniqueness for Maxwell–Stefan Systems". In: *SIAM Journal on Mathematical Analysis* 54.3 (2022), pp. 3215–3252. DOI: 10.1137/21M145210X.

[151] Tom Ilmanen. "Convergence of the Allen-Cahn Equation to Brakke's Motion by Mean Curvature". In: *Journal of Differential Geometry* 38.2 (1993), pp. 417–461. DOI: 10.4310/jdg/1214454300.

[152] Mojtaba Izadi, Javad Abdollahi, and Stevan S. Dubljevic. "PDE Backstepping Control of One-Dimensional Heat Equation with Time-Varying Domain". In: *Automatica* 54 (2015), pp. 41–48. DOI: 10.1016/j.automatica.2015.01.024.

[153] Mojtaba Izadi and Stevan Dubljevic. "Backstepping Output-Feedback Control of Moving Boundary Parabolic PDEs". In: *European Journal of Control* 21 (2015), pp. 27–35. DOI: 10.1016/j.ejcon.2014.11.002.

[154] Richard Jordan, David Kinderlehrer, and Felix Otto. "The Variational Formulation of the Fokker–Planck Equation". In: *SIAM Journal on Mathematical Analysis* 29.1 (1998), pp. 1–17. DOI: 10.1137/S0036141096303359.

[155] Ansgar Jüngel. *Entropy Methods for Diffusive Partial Differential Equations*. SpringerBriefs in Mathematics. Cham: Springer International Publishing, 2016. DOI: 10.1007/978-3-319-34219-1.

[156] Ansgar Jüngel. "The Boundedness-by-Entropy Principle for Cross-Diffusion Systems". In: *Nonlinearity* 28.6 (2015), pp. 1963–2001. DOI: 10.1088/0951-7715/28/6/1963.

[157] Ansgar Jüngel, Stefan Portisch, and Antoine Zurek. *A Convergent Finite-Volume Scheme for Nonlocal Cross-Diffusion Systems for Multi-Species Populations*. 2023. DOI: 10.48550/arXiv.2302.10993.

[158] Ansgar Jüngel, Stefan Portisch, and Antoine Zurek. "Nonlocal Cross-Diffusion Systems for Multi-Species Populations and Networks". In: *Nonlinear Analysis* 219 (2022), p. 112800. DOI: 10.1016/j.na.2022.112800.

[159] Ansgar Jüngel and Ines Viktoria Stelzer. "Entropy Structure of a Cross-Diffusion Tumor-Growth Model". In: *Mathematical Models and Methods in Applied Sciences* 22.07 (2012), p. 1250009. DOI: 10.1142/S0218202512500091.

[160] Ansgar Jüngel and Ines Viktoria Stelzer. "Existence Analysis of Maxwell–Stefan Systems for Multicomponent Mixtures". In: *SIAM Journal on Mathematical Analysis* 45.4 (2013), pp. 2421–2440. DOI: 10.1137/120898164.

[161] Ansgar Jüngel and Martin Vetter. *A Convergent Entropy-Dissipating BDF2 Finite-Volume Scheme for a Population Cross-Diffusion System*. 2023. DOI: 10.48550/arXiv.2301.03200.

[162] Ansgar Jüngel and Antoine Zurek. "A Convergent Structure-Preserving Finite-Volume Scheme for the Shigesada–Kawasaki–Teramoto Population System". In: *SIAM Journal on Numerical Analysis* 59.4 (2021), pp. 2286–2309. DOI: 10.1137/20M1381058.

[163] Ansgar Jüngel and Antoine Zurek. "A Discrete Boundedness-by-Entropy Method for Finite-Volume Approximations of Cross-Diffusion Systems". In: *IMA Journal of Numerical Analysis* 43.1 (2023), pp. 560–589. DOI: 10.1093/imanum/drab101.

[164] Ansgar Jüngel and Antoine Zurek. "A Finite-Volume Scheme for a Cross-Diffusion Model Arising from Interacting Many-Particle Population Systems". In: *Finite Volumes for Complex Applications IX - Methods, Theoretical Aspects, Examples*. Ed. by Robert Klöfkorn, Eirik Keilegavlen, Florin A. Radu, and Jürgen Fuhrmann. Vol. 323. Cham: Springer International Publishing, 2020, pp. 223–231. DOI: 10.1007/978-3-030-43651-3_19.

[165] Simon Kerschbaum and Joachim Deutscher. "Backstepping Control of Coupled Linear Parabolic PDEs With Space and Time Dependent Coefficients". In: *IEEE Transactions on Automatic Control* 65.7 (2020), pp. 3060–3067. DOI: 10.1109/TAC.2019.2944918.

[166] Torben Klinkert. "Comprehension and Optimisation of the Co-Evaporation Deposition of Cu(In,Ga)Se2 Absorber Layers for Very High Efficiency Thin Film Solar Cells". PhD thesis. Université Pierre et Marie Curie - Paris VI, 2015.

[167] Daniel Koditschek. "Adaptive Techniques for Mechanical Systems". In: *Departmental Papers (ESE)* (1987).

[168] Rajamani Krishna and J. A. Wesselingh. "The Maxwell-Stefan Approach to Mass Transfer". In: *Chemical Engineering Science* 52.6 (1997), pp. 861–911. DOI: 10.1016/S0009-2509(96)00458-7.

[169] Miroslav Krstic and Andrey Smyshlyaev. "Backstepping Boundary Control for First-Order Hyperbolic PDEs and Application to Systems with Actuator and Sensor Delays". In: *Systems & Control Letters* 57.9 (2008), pp. 750–758. DOI: 10.1016/j.sysconle.2008.02.005.

[170] Miroslav Krstić and Andrey Smyshlyaev. *Boundary Control of PDEs: A Course on Backstepping Designs*. Advances in Design and Control 16. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2008.

[171] Konrad Horst Wilhelm Küfner. "Invariant Regions for Quasilinear Reaction Diffusion Systems and Applications to a Two Population Model". In: *Nonlinear Differential Equations and Applications NoDEA* 3.4 (1996), pp. 421–444. DOI: 10.1007/BF01193829.

[172] Philippe Laurençot and Bogdan-Vasile Matioc. "Weak-Strong Uniqueness for a Class of Degenerate Parabolic Cross-Diffusion Systems". In: (2022). DOI: 10.48550/ARXIV.2207.00361.

[173] Tim Laux and Kerrek Stinson. "Sharp Interface Limit of the Cahn-Hilliard Reaction Model for Lithium-ion Batteries". In: (2022). DOI: 10.48550/ARXIV.2209.07380.

[174] Alpha Albert Lee, Andreas Münch, and Endre Süli. "Sharp-Interface Limits of the Cahn–Hilliard Equation with Degenerate Mobility". In: *SIAM Journal on Applied Mathematics* 76.2 (2016), pp. 433–456. DOI: 10.1137/140960189.

[175] Leoni and Mora. *Topics in the Calculus of Variations: Recent Advances and New Trends*. Tech. rep. 2018.

[176] Thomas Lepoutre. "Contributions En Dynamique de Populations". 2017.

[177] Thomas Lepoutre, Michel Pierre, and Guillaume Rolland. "Global Well-Posedness of a Conservative Relaxed Cross Diffusion System". In: *SIAM Journal on Mathematical Analysis* 44.3 (2012), pp. 1674–1693. DOI: 10.1137/110848839.

[178] Matthias Liero and Alexander Mielke. "Gradient Structures and Geodesic Convexity for Reaction–Diffusion Systems". In: *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences* 371.2005 (2013), p. 20120346. DOI: 10.1098/rsta.2012.0346.

[179] Weijiu Liu. "Boundary Feedback Stabilization of an Unstable Heat Equation". In: *SIAM Journal on Control and Optimization* 42.3 (2003), pp. 1033–1043. DOI: 10.1137/S0363012902402414.

[180] Stephan Luckhaus and Thomas Sturzenhecker. "Implicit Time Discretization for the Mean Curvature Flow Equation". In: *Calculus of Variations and Partial Differential Equations* 3.2 (1995), pp. 253–271. DOI: 10.1007/BF01205007.

[181] Jan Maas and Alexander Mielke. "Modeling of Chemical Reaction Systems with Detailed Balance Using Gradient Structures". In: *Journal of Statistical Physics* 181.6 (2020), pp. 2257–2303. DOI: 10.1007/s10955-020-02663-4.

[182] Gabriela Marinoschi. "A Control Problem for a Cross-Diffusion System in a Nonhomogeneous Medium". In: *Journal of Biological Dynamics* 7 Suppl 1 (2013), pp. 88–107. DOI: 10.1080/17513758.2013.836574.

[183] Peter A Markowich and Cédric Villani. "On the Trend to Equilibrium for the Fokker-Planck Equation: An Interplay between Physics and Functional Analysis". In: *Mat. Contemp* 19 (2000), pp. 1–29.

[184] Donald M. Mattox. *Handbook of Physical Vapor Deposition (PVD) Processing*. William Andrew, 2010.

[185] Benoît Merlet, Juliette Venel, and Antoine Zurek. *Analysis of a One Dimensional Energy Dissipating Free Boundary Model with Nonlinear Boundary Conditions. Existence of Global Weak Solutions*. 2022. DOI: 10.48550/arXiv.2212.03642.

[186] Alexander Mielke. "A Gradient Structure for Reaction–Diffusion Systems and for Energy-Drift-Diffusion Systems". In: *Nonlinearity* 24.4 (2011), pp. 1329–1346. DOI: 10.1088/0951-7715/24/4/016.

[187] Alexander Mielke. "Geodesic Convexity of the Relative Entropy in Reversible Markov Chains". In: *Calculus of Variations and Partial Differential Equations* 48.1 (2013), pp. 1–31. DOI: 10.1007/s00526-012-0538-8.

[188] Alexander Mielke, Jan Haskovec, and Peter A. Markowich. "On Uniform Decay of the Entropy for Reaction–Diffusion Systems". In: *Journal of Dynamics and Differential Equations* 27.3 (2015), pp. 897–928. DOI: 10.1007/s10884-014-9394-x.

[189] Alexander Mielke, Mark A. Peletier, and D. R. Michiel Renger. "On the Relation between Gradient Flows and the Large-Deviation Principle, with Applications to Markov Chains and Diffusion". In: *Potential Analysis* 41.4 (2014), pp. 1293–1327. DOI: 10.1007/s11118-014-9418-5.

[190] Alain Miranville. *The Cahn–Hilliard Equation: Recent Advances and Applications*. Philadelphia, PA: Society for Industrial and Applied Mathematics, 2019. DOI: 10.1137/1.9781611975925.

[191] Luciano Modica. "The Gradient Theory of Phase Transitions and the Minimal Interface Criterion". In: *Archive for Rational Mechanics and Analysis* 98.2 (1987), pp. 123–142. DOI: 10.1007/BF00251230.

[192] Jeff Morgan and Bao Quoc Tang. "Global Well-Posedness for Volume–Surface Reaction–Diffusion Systems". In: *Communications in Contemporary Mathematics* 25.04 (2023). DOI: 10.1142/S021919972250002X.

[193] A. Moussa. "Some Variants of the Classical Aubin–Lions Lemma". In: *Journal of Evolution Equations* 16.1 (2016), pp. 65–93. DOI: 10.1007/s00028-015-0293-3.

[194] Basil Nicolaenko, Bruno Scheurer, and Roger Temam. "Some Global Dynamical Properties of a Class of Pattern Formation Equations". In: *Communications in Partial Differential Equations* 14.2 (1989), pp. 245–297. DOI: 10.1080/03605308908820597.

[195] Amy Novick-Cohen. "Chapter 4 The Cahn–Hilliard Equation". In: *Handbook of Differential Equations: Evolutionary Equations*. Vol. 4. Elsevier, 2008, pp. 201–228. DOI: 10.1016/S1874-5717(08)00004-2.

[196] Milton Ohring. *Materials Science of Thin Films: Depositon and Structure*. Elsevier, 2001.

[197] Felix Otto. "The Geometry of Dissipative Evolution Equations: The Porous Medium Equation". In: *Communications in Partial Differential Equations* 26.1-2 (2001), pp. 101–174. DOI: 10.1081/PDE-100002243.

[198] Felix Otto and Weinan E. "Thermodynamically Driven Incompressible Fluid Mixtures". In: *The Journal of Chemical Physics* 107.23 (1997), pp. 10177–10184. DOI: 10.1063/1.474153.

[199] Felix Otto, Sebastian Scholtes, and Maria G. Westdickenberg. "Optimal L1-type Relaxation Rates for the Cahn–Hilliard Equation on the Line". In: *SIAM Journal on Mathematical Analysis* 51.6 (2019), pp. 4645–4682. DOI: 10.1137/18M1192640.

[200] Felix Otto and Maria G. Westdickenberg. "Relaxation to Equilibrium in the One-Dimensional Cahn–Hilliard Equation". In: *SIAM Journal on Mathematical Analysis* 46.1 (2014), pp. 720–756. DOI: 10.1137/130925517.

[201] Felix Otto and Michael Westdickenberg. "Eulerian Calculus for the Contraction in the Wasserstein Distance". In: *SIAM Journal on Mathematical Analysis* 37.4 (2005), pp. 1227–1255. DOI: 10.1137/050622420.

[202] Kevin J. Painter. "Continuous Models for Cell Migration in Tissues and Applications to Cell Sorting via Differential Chemotaxis". In: *Bulletin of Mathematical Biology* 71.5 (2009), pp. 1117–1147. DOI: 10.1007/s11538-009-9396-8.

[203] Kevin J. Painter and Thomas Hillen. "Volume-Filling and Quorum-Sensing in Models for Chemosensitive Movement". In: *Canadian Applied Mathematics Quarterly* 10.4 (2002), pp. 501–544.

[204] Robert L. Pego and Oliver Penrose. "Front Migration in the Nonlinear Cahn-Hilliard Equation". In: *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* 422.1863 (1989), pp. 261–278. DOI: 10.1098/rspa.1989.0027.

[205] Mark A. Peletier. *Variational Modelling: Energies, Gradient Flows, and Large Deviations*. 2014.

[206] Michel Pierre and Didier Schmitt. "Blowup in Reaction-Diffusion Systems with Dissipation of Mass". In: *SIAM Review* 42.1 (2000), pp. 93–106. DOI: 10.1137/S0036144599359735.

[207] Hugh O. Pierson. *Handbook of Chemical Vapor Deposition: Principles, Technology and Applications*. William Andrew, 1999.

[208] Jacobus Portegies and Mark A. Peletier. "Well-Posedness of a Parabolic Moving-Boundary Problem in the Setting of Wasserstein Gradient Flows". In: *Interfaces and Free Boundaries* (2010), pp. 121–150. DOI: 10.4171/IFB/229.

[209] Jan Prüss and Gieri Simonett. *Moving Interfaces and Quasilinear Parabolic Evolution Equations*. Vol. 105. Monographs in Mathematics. Cham: Springer International Publishing, 2016. DOI: 10.1007/978-3-319-27698-4.

[210] Jeremy Quastel. "Diffusion of Color in the Simple Exclusion Process". In: *Communications on Pure and Applied Mathematics* 45.6 (1992), pp. 623–679. DOI: 10.1002/cpa.3160450602.

[211] Etienne Sandier and Sylvia Serfaty. "Gamma-Convergence of Gradient Flows with Applications to Ginzburg-Landau". In: *Communications on Pure and Applied Mathematics* 57.12 (2004), pp. 1627–1672. DOI: 10.1002/cpa.20046.

[212] Filippo Santambrogio. *Optimal Transport for Applied Mathematicians: Calculus of Variations, PDEs, and Modeling*. Vol. 87. Progress in Nonlinear Differential Equations and Their Applications. Cham: Springer International Publishing, 2015. DOI: 10.1007/978-3-319-20828-2.

[213] Giulio Schimperna. "Global Attractors for Cahn–Hilliard Equations with Nonconstant Mobility". In: *Nonlinearity* 20.10 (2007), p. 2365. DOI: 10.1088/0951-7715/20/10/006.

[214] Giulio Schimperna and Sergey Zelik. "Existence of Solutions and Separation from Singularities for a Class of Fourth Order Degenerate Parabolic Equations". In: *Transactions of the American Mathematical Society* 365.7 (2013), pp. 3799–3829. DOI: 10.1090/S0002-9947-2012-05824-7.

[215] Sylvia Serfaty. "Gamma-Convergence of Gradient Flows on Hilbert and Metric Spaces and Applications". In: *Discrete & Continuous Dynamical Systems - A* 31.4 (2011), pp. 1427–1451. DOI: 10.3934/dcds.2011.31.1427.

[216] Nanako Shigesada, Kohkichi Kawasaki, and Ei Teramoto. "Spatial Segregation of Interacting Species". In: *Journal of Theoretical Biology* 79.1 (1979), pp. 83–99. DOI: 10.1016/0022-5193(79)90258-3.

[217] Matthew J. Simpson, Kerry A. Landman, and Barry D. Hughes. "Multi-Species Simple Exclusion Processes". In: *Physica A: Statistical Mechanics and its Applications* 388.4 (2009), pp. 399–406. DOI: 10.1016/j.physa.2008.10.038.

[218] Andrey Smyshlyaev and Miroslav Krstic. "Closed-Form Boundary State Feedbacks for a Class of 1-D Partial Integro-Differential Equations". In: *IEEE Transactions on Automatic Control* 49.12 (2004), pp. 2185–2202. DOI: 10.1109/TAC.2004.838495.

[219] Andrey Smyshlyaev and Miroslav Krstic. "On Control Design for PDEs with Space-Dependent Diffusivity or Time-Dependent Reactivity". In: *Automatica* 41.9 (2005), pp. 1601–1608. DOI: 10.1016/j.automatica.2005.04.006.

[220] P. T. Sowndarrajan, Jeyaraj Manimaran, Amar Debbouche, and Lingeshwaran Shangerganesh. "Distributed Optimal Control of a Tumor Growth Treatment Model with Cross-Diffusion Effect". In: *The European Physical Journal Plus* 134.9 (2019), p. 463. DOI: 10.1140/epjp/i2019-12866-8.

[221] Jana Stará and Oldřich John. "Some (New) Counterexamples of Parabolic Systems". In: *Commentationes Mathematicae Universitatis Carolinae* 36.3 (1995), pp. 503–510.

[222] Barbara E. E. Stoth. "Convergence of the Cahn–Hilliard Equation to the Mullins Sekerka Problem in Spherical Symmetry". In: *Journal of Differential Equations* 125.1 (1996), pp. 154–183. DOI: 10.1006/jdeq.1996.0028.

[223] Jean E. Taylor and John W. Cahn. "Linking Anisotropic Sharp and Diffuse Surface Motion Laws via Gradient Flows". In: *Journal of Statistical Physics* 77.1 (1994), pp. 183–197. DOI: 10.1007/BF02186838.

[224] Giovanni Maria Troianiello. *Elliptic Differential Equations and Obstacle Problems*. Springer Science & Business Media, 2013.

[225] John Tsinias. "Sufficient Lyapunov-like Conditions for Stabilization". In: *Mathematics of Control, Signals and Systems* 2.4 (1989), pp. 343–357. DOI: 10.1007/BF02551276.

[226] Andreas Unterreiter, Anton Arnold, Peter Markowich, and Giuseppe Toscani. "On Generalized Csiszár-Kullback Inequalities". In: *Monatshefte für Mathematik* 131 (2000), pp. 235–253.

[227] Juan Luis Vazquez. *The Porous Medium Equation: Mathematical Theory*. Oxford Mathematical Monographs. Oxford: Clarendon, 2007.

[228] Rafael Vazquez, Miroslav Krstic, and Jean-Michel Coron. "Backstepping Boundary Stabilization and State Estimation of a 2× 2 Linear Hyperbolic System". In: *2011 50th IEEE Conference on Decision and Control and European Control Conference*. IEEE, 2011, pp. 4937–4942.

[229] Cédric Villani. *Optimal Transport: Old and New*. Grundlehren Der Mathematischen Wissenschaften 338. Berlin Heidelberg: Springer, 2009.

[230] Shuonan Wu and Jinchao Xu. "Multiphase Allen–Cahn and Cahn–Hilliard Models and Their Discretizations with the Effect of Pairwise Surface Tensions". In: *Journal of Computational Physics* 343 (2017), pp. 10–32. DOI: 10.1016/j.jcp.2017.04.039.

[231] Peter Würfel and Uli Würfel. *Physics of Solar Cells: From Basic Principles to Advanced Concepts*. John Wiley & Sons, 2016.

[232] Shengquan Xiang. *Quantitative Rapid and Finite Time Stabilization of the Heat Equation*. 2020.

[233] Nicola Zamponi and Ansgar Jüngel. "Analysis of Degenerate Cross-Diffusion Population Models with Volume Filling". In: *Annales de l'Institut Henri Poincaré C, Analyse non linéaire* 34.1 (2017), pp. 1–29. DOI: 10.1016/j.anihpc.2015.08.003.

[234] Christophe Zhang. "Finite-Time Internal Stabilization of a Linear 1-D Transport Equation". In: *Systems & Control Letters* 133 (2019), p. 104529. DOI: 10.1016/j.sysconle.2019.104529.

[235] Christophe Zhang. "Internal Rapid Stabilization of a 1-D Linear Transport Equation with a Scalar Feedback". In: *Mathematical Control & Related Fields* 12.1 (2022), p. 169. DOI: 10.3934/mcrf.2021006.

[236] Jonathan Zinsl and Daniel Matthes. "Transport Distances and Geodesic Convexity for Systems of Degenerate Diffusion Equations". In: *Calculus of Variations and Partial Differential Equations* 54.4 (2015), pp. 3397–3438. DOI: 10.1007/s00526-015-0909-z.

[237] Antoine Zurek. "Numerical Approximation of a Concrete Carbonation Model: Study of the Square Root Law of Propagation". In: *Numerical Methods for Partial Differential Equations* 35.5 (2019), pp. 1801–1820. DOI: 10.1002/num.22377.

[238] Antoine Zurek. "Problèmes à interface mobile pour la dégradation de matériaux et la croissance de biofilms : analyse numérique et modélisation". PhD thesis. 2019.