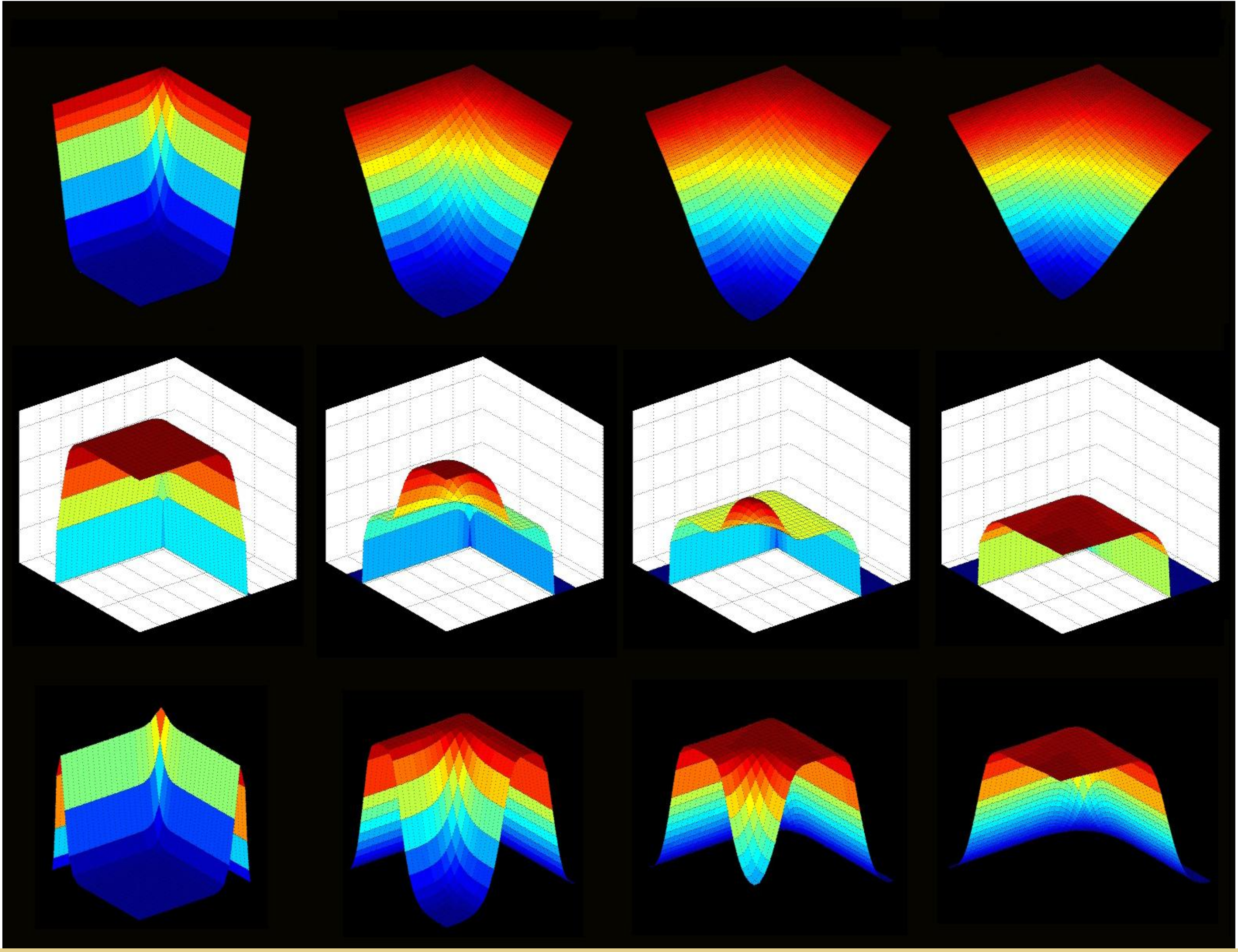

Elías Alfredo Gudiño Rojas

RECENT DEVELOPMENTS IN NON-FICKIAN DIFFUSION: A NEW LOOK AT VISCOELASTIC MATERIALS

Tese de Doutoramento em Matemática orientada pelos Professores Doutores José A. Ferreira e Paula de Oliveira e apresentada ao Departamento de Matemática da Faculdade de Ciências e Tecnologia da Universidade de Coimbra

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Recent developments in non-Fickian diffusion: a new look at viscoelastic materials

Author:
Elías A. Gudiño R.

Supervisors:
Professor Doutor José A. Ferreira
Professora Doutora Paula de Oliveira

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Abstract

The aim of this dissertation is to fully understand from a mathematical point of view the two coupled processes of sorption of a fluid by a viscoelastic material and the successive or simultaneous desorption of the fluid with solved molecules of a chemical compound which is dispersed in the material. These two coupled processes have a central role in several areas of Life Sciences and Material Sciences namely in Controlled Drug Delivery.

When a penetrant fluid diffuses into a viscoelastic material, such as a polymer, it is well known that the process cannot be completely described by Fick's classical law of diffusion. The reason lies in the fact that as the fluid diffuses into the material, it causes a deformation which induces a stress driven diffusion that act as a barrier to the fluid penetration. Thus a modified flux must be considered, resulting from the sum of the Fickian flux and a non-Fickian flux. We propose a new interpretation of this non-Fickian mass flux as being related to a convective field which represents an opposition of the polymer to the incoming penetrant fluid.

To study the complete problem of sorption coupled with desorption, we progressively address more complex models. We begin by studying the process of sorption in Chapter 1, we generalize the model to a more abstract formulation in Chapter 2, and we study a numerical method for the abstract formulation in Chapter 3. The complete problem of sorption coupled with desorption is addressed in Chapter 4.

The first sorption model studied is based on an integro-differential equation, coupled with initial and boundary conditions. The non-linear dependence between strain and the incoming fluid concentration is considered and introduced in a Boltzmann integral with a kernel computed from a Maxwell-Wiechert model. To illustrate the behavior of the model we solve it numerically on a general nonuniform grid in space and a uniform grid in time. We exhibit numerical simulations that give some insight of the dependence of the solution on the different parameters that describe the viscoelastic properties of the polymer.

This lead us to a generalization of this model by considering a class of integro-differential equations of Volterra type. We establish the well posedness, in the Hadamard sense, of the initial boundary value problem. The stability analysis is separated in two cases, non-singular kernels and weakly singular kernels.

An implicit explicit difference scheme, which can be seen as a fully discrete piecewise linear finite element method, is proposed to discretize the general model. Stability and convergence results for the method are established showing that it is second order convergent in space and first order convergent in time. The numerical analysis of the method does not follow the usual splitting of the global error using the solution of an elliptic equation induced by the integro-differential equation. A new approach, that enable us to reduce the smoothness required for the theoretical solution, is used. The results are established for both non-singular and weakly singular kernels.

A tridimensional model of the whole process of sorption and desorption is presented in Chapter 4. A viscoelastic matrix with a dispersed drug, or a chemical compound, is considered. The model is based on a system of partial differential equations coupled with boundary conditions over a moving boundary. We combine non-Fickian sorption of a penetrant fluid , non-Fickian desorption of the fluid with dispersed drug, with non-linear dissolution of a drug agent and polymer swelling. An Implicit-Explicit numerical scheme is used to numerically solve the model and some plots are presented to illustrate the behavior of the approximations.

Experimental rheological information of the polymer-solvent matrix system can be easily introduced in the models studied in this dissertation because all the parameters can be measured or estimated according to well-known theories of viscoelastic materials. This makes the models suitable for both data fitting and quantitative prediction of drug release kinetics, opening new routes of research in Material Science.

Keywords: non-Fickian diffusion, non-linear viscoelasticity, drug delivery systems, viscoelastic diffusion coefficient.

Resumo

O principal objetivo da presente dissertação é o estudo matemático de dois processos que ocorrem acoplados : a absorção de um fluido por um material viscoelástico em que existem moléculas dispersas de um composto químico no estado sólido e a sucessiva, ou simultânea, libertação do fluido com moléculas já dissolvidas. Estes dois processos acoplados desempenham um papel central em muitas áreas das Ciências da Vida e da Ciência dos Materiais com particular destaque para a Libertação Controlada de Fármacos.

Quando um fluido se difunde num material viscoelástico, como por exemplo um polímero, o processo não pode ser corretamente descrito pela lei de difusão clássica de Fick. A razão reside no facto de, ao difundir-se, o fluido causar uma deformação que induz uma resposta mecânica do material, sob a forma de uma tensão, que atua como uma barreira, dificultando a penetração do fluido. Torna-se portanto necessário definir um fluxo modificado, que resulta da soma de um fluxo Fickiano com um fluxo não Fickiano. Nesta dissertação propomos uma nova interpretação do conceito de fluxo não Fickiano, como sendo resultante de um campo convectivo, e representando uma oposição do material à entrada do fluido.

No sentido de estudar o problema completo, absorção acoplado com a libertação, apresentamos nesta dissertação modelos progressivamente mais complexos. Começamos por estudar no Capítulo 1 o processo de absorção, generalizamos o modelo para um quadro funcional mais abstrato no Capítulo 2 e procedemos a uma análise de um método numérico, para este último modelo, no Capítulo 3. O problema completo, absorção conjugado com libertação, é estudado no Capítulo 4.

O primeiro modelo de absorção que estudamos baseia-se numa equação integro-diferencial acoplada com condições iniciais e de fronteira. Baseando-nos em argumentos físicos, estabelecemos uma forma para a relação funcional não linear entre a deformação causada pelo fluido e a sua concentração. Esta relação é introduzida num integral de Boltzman com um núcleo calculado a partir do modelo de Maxwell-Wiechert. Para ilustrar o comportamento do modelo e analisar a dependência da solução relativamente aos parâmetros, todos eles com um significado físico, o problema é resolvido numericamente com um método Implícito-Explícito numa malha não uniforme no espaço e uniforme no tempo.

O modelo precedente motivou o estudo de um modelo generalizado, que se baseia numa classe de equações integro-diferenciais de tipo Volterra. Apresentamos uma análise de estabilidade, para o caso de núcleos regulares e fracamente singulares. Provamos também que o problema está bem posto no sentido de Hadamard.

A discretização do modelo generalizado é feita com um esquema de diferenças finitas Implícito-Explícito, que pode ser considerado como um modelo completamente discreto de elementos finitos

lineares. São estabelecidos resultados de estabilidade e convergência que provam que o método é de segunda ordem no espaço e de primeira ordem no tempo. A técnica de análise utilizada não segue a clássica divisão [1] do erro global, com auxílio de uma equação elíptica induzida pela equação integro-diferencial. Uma nova abordagem proposta permite reduzir as hipóteses de regularidade sobre a solução teórica. Os resultados são estabelecidos para núcleos regulares e fracamente singulares.

Um modelo tridimensional do processo completo de absorção e libertação é apresentado no Capítulo 4. Considera-se uma matriz viscoelástica com um fármaco, ou qualquer outro composto químico, disperso. O modelo baseia-se num sistema de equações de derivadas parciais estabelecido num domínio móvel completado com condições iniciais e de fronteira . O sistema diferencial combina a absorção não Fickiana do fluido, a libertação não Fickiana do fluido com fármaco dissolvido, o processo não linear de dissolução do fármaco e ainda o aumento de volume da matriz [2]. O problema é resolvido numericamente e analisada a dependência da solução relativamente aos parâmetros que caracterizam as propriedades da matriz, do fluido e do fármaco.

Os modelos apresentados na dissertação são modelos fenomenológicos estabelecidos a partir de considerações de carácter físico. Todos os parâmetros podem ser diretamente medidos a partir de experiências laboratoriais ou calculados com base em teorias de viscoelasticidade. Esta característica dos modelos torna-os particularmente atrativos, permitindo fazer previsões de comportamento dos fenómenos e abrindo novas perspetivas de investigação no âmbito da Ciência dos Materiais.

Palavras chave: difusão não-Fickiana, viscoelasticidade não linear, sistemas de libertação controlada de fármacos, coeficiente de difusão viscoelástica.

[1] Splitting em língua inglesa.
[2] Swelling em língua inglesa.

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Contents

Introduction

Polymers, both synthetic and natural, are present in our everyday life as they possess many different unique physical properties that make them very versatile and suitable for a wide range of applications. Those unique properties have become more important recently in pharmaceutical applications, more precisely, in controlled drug delivery systems. The pharmaceutical industry and biomedical device developers have taken a keen interest in the design of such systems, as it has become a rapidly evolving and lucrative market.

Traditional drug delivery systems such as intravenous injections, topical creams and oral medications do not allow the control of the drug delivery kinetics as they follow the release profile shown in Figure 0.1, in which after each administration, the drug concentration increases in the blood and then decreases until the next administration. These delivery systems are not efficient in maintaining therapeutic levels of drug concentration over long periods of time as they rely on systemic blood circulation and biological membrane absorption to distribute the medication. In some cases, like for example eye drops for topical ocular administration, the delivery is extremely inefficient since only 1% to 5% penetrates the cornea reaching intraocular tissues [25].

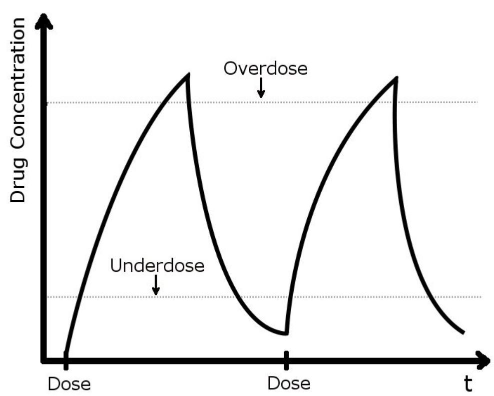

Fig. 0.1: Release profile of traditional delivery systems

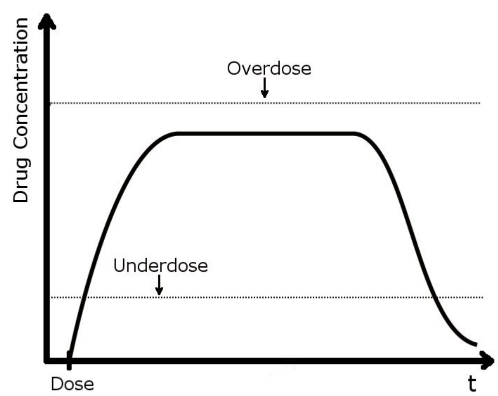

Fig. 0.2: Release profile of controlled delivery systems

A controlled drug delivery takes place by carefully combining a polymeric carrier with a drug or other active agent in such a way that the active agent is released from the carrier in a predesigned manner, in order to obtain an adequate and more efficient delivery profile suitable for a particular situation or treatment. Due to significant advances in polymer science, nowadays technologies allow the enhancement of the properties of polymers, which are known to have an important influence in the drug delivery rates [46]. Thus it is possible to maintain therapeutic levels of drug concentration over long periods of time, the reduction of the dosing frequency and the elimination of the possibility of both under and overdosing (Figure 0.2).

Among the most recent uses that can be found these days in the pharmaceutical industry for controlled drug delivery systems are:

- Slow release of contraceptive chemicals for both men and women;
- Slow release of insulin for diabetics;
- Transdermal patches for pain relief;
- Intraocular implants for diseases associated with high ocular pressure;
- Therapeutic lenses coated with antibiotics, anti-inflammatory and/or anti allergy drugs;
- Sustained release of estrogen and progesterone for menopausal women.

One of the most important problems in controlled drug release technology is the prediction of drug release kinetics. By understanding the physical aspects of the process, it is possible to formulate mathematical models to describe it. Thus the mathematical modeling of drug delivery, is a field that keeps increasing its importance in the academic and industrial context. Since these models have proven to be reliable tools in the design of new and/or the optimization of existing drug delivery systems without the need of animal testing in laboratories and costly in vitro experiments.

As the drug release from a polymeric matrix is mainly controlled by penetrant uptake, drug dissolution and drug diffusion through the swelling polymeric network [9, 10, 33], the establishment of mathematical models for drug release is not an easy task since there are many complexities that arise as a consequence of the physical properties of polymeric materials, i.e. its viscoelastic behavior. Many different models have been proposed in the literature [6, 32, 33, 36, 37, 46] but none of them accurately and completely describe the delivery phenomena.

The more successful models in terms of realistic quantitative prediction are based on physical interpretation of real phenomena such as diffusion, dissolution, swelling, erosion, precipitation and/or degradation. By taking into consideration many of these phenomena, the model can become more realistic and accurate. Nonetheless if a model is too complex, it can be difficult to use because it requires the knowledge of many parameters, whose determination in many cases is not straightforward.

The first process we have to understand is sorption, that is fluid uptake. If we want to describe the diffusion process of a liquid agent into a polymer, two main phenomena must be considered: the rate of diffusion of the fluid and the change in the internal structure of the material. If the rate of penetrant diffusion is much smaller or much bigger than the rate of relaxation of the polymer-solvent system, the transport is properly described by Fick's law, defined by the following conservation law

$$\frac{\partial C}{\partial t} = -\nabla \cdot J_F \ .$$

In this equation $C = C(x,t)$ is the fluid concentration, $J_F = J_F(x,t)$ represents the Fickian flux defined by

$$J_F = -D(C)\nabla C \ ,$$

and the function $D(C)$ represents the Fickian diffusion coefficient of the solvent.

If the rate of penetrant diffusion is of the same order of the relaxation process, Fick's law does not represent an accurate description of the phenomenon [48, 49, 50]. The reason for this is that the classical Fick's law does not take into consideration the viscoelastic nature of polymers. As the diffusing penetrant enters the polymer, it causes a deformation which induces a stress driven diffusion. Thus several authors [6, 11, 12, 32] have proposed diffusion models based on a modified flux resulting from the sum of the Fickian flux J_F and a non Fickian flux J_{NF}, the traditional mass conservation law is replaced by

$$\frac{\partial C}{\partial t} = -\nabla \cdot (J_F(C) + J_{NF}(\sigma)) \ , \tag{0.1}$$

with $J_{NF} = J_{NF}(x,t)$ defined by

$$J_{NF} = -Dv(C)\nabla\sigma \ ,$$

where the function $D_v(C)$ represents the viscoelastic diffusion coefficient of the polymer and $\sigma = \sigma(x,t)$ represents the stress.

The main purpose of this work is to describe the non-Fickian diffusion process by proposing an accurate and physically sound mathematical model that takes into consideration the viscoelastic character of polymers. This model has the important feature of easily and directly incorporate experimental rheological information about polymer-solvent matrix systems. This aspect opens the possibility of using the model for both data fitting and quantitative prediction of the effects of formulation and processing parameters over drug release kinetics.

Additional applications involving the diffusional release of a dispersed or dissolved agent from a polymeric carrier, i.e. removal of solvent from polymer solutions during dry spinning, diffusional release of pollutants or additives from polymers into the environment and controlled release of agriculture chemicals, further extend the interest of the results we present in this thesis.

In Chapter 1 we will begin with the formal mathematical formulation of the model. We introduce a initial boundary value problem to model solvent sorption by a viscoelastic material. In order to complete (0.1), we have to consider a stress evolution equation which introduces in the problem the strain ε as a third variable. Several constitutive relationships between stress and strain have been considered in the literature. We mention, without being exhaustive, the works [8, 13, 14, 22, 40, 41]. In these works, equations of type

$$\frac{\partial \sigma}{\partial t} + \beta\sigma = \alpha\varepsilon + \gamma\frac{\partial \varepsilon}{\partial t} \ , \tag{0.2}$$

have been used, where β, α and γ are positive constants with a precise physical meaning associated to the mechanistic arrays considered to model the viscoelastic behavior of polymers [5].

In order to solve problem (0.1), (0.2), coupled with adequate boundary and initial conditions, the strain must be eliminated. In the previously mentioned papers, the strain is considered proportional to the concentration of the penetrant fluid, that is $\varepsilon = \kappa C$, where $\kappa > 0$ is a constant. Then

(0.2) can be rewritten (assuming $\sigma(x,0)=0$) as

$$\sigma = \kappa \int_0^t e^{-(t-s)\beta}(\alpha C(s) + \gamma \frac{\partial C}{\partial s}(s))ds \ .$$

The previous approaches present some serious drawbacks. Firstly because a typical response of a polymeric material to a stress cannot be represented by one single relaxation time ($\frac{1}{\beta}$). Secondly as the Young's modulus of polymers are relatively low when compared to other structural materials, strains and deformations can be relatively large and laboratorial experiments indicate that the deformation ε of a polymer obeys a more complex relation than simple proportionality to the penetrant concentration. To overcome these drawbacks we propose a different approach based on:

(i) The use of a Boltzmann integral of type

$$\sigma(t) = -\int_0^t E(t-s)\frac{\partial \varepsilon}{\partial s}(s)ds \ , \tag{0.3}$$

where $E(t)$ is the relaxation modulus corresponding to a generalized Maxwell-Wiechert mechanical model [5]. We note that the minus sign in (0.3) means that as the penetrant solvent strains the polymeric matrix, a stress of opposite sign is developed. This means that the non-Fickian part of (0.1) acts as a barrier to the diffusion.

(ii) The use of a non-linear relation between the strain and the penetrant concentration, $\frac{\partial \varepsilon}{\partial t} = f(C, \frac{\partial C}{\partial t})$.

(iii) The use of a functional relation for the viscoelastic diffusion coefficient D_v in function of the concentration C.

We will present a mathematical deduction of the functional relation between the strain and the penetrant concentration taking into consideration the viscoelastic properties of polymers. To the best of our knowledge, the philosophy underlying our model, which results from a combination of the previous points, has not been proposed in the literature till now.

A major issue in the field of non-Fickian diffusion modeling is a proper interpretation of the viscoelastic diffusion coefficient D_v. For example Camera-Roda et al., 1990 and Cohen et al., 1991 consider that D_v should be a positive parameter with the only restriction that when $C=0$, then $D_v=0$, to account for the fact that no stress gradient contributes to the mass flux when there is no concentration. While Liu et al., 2005 argue that D_v should be negative to account for the existence of a convective negative flux related to the viscoelastic properties of polymers.

We will present two mathematical deductions for a concentration dependent functional relation for D_v. The first one based on Darcy's law and the second one on the Hagen-Poiseuille equation. These relations lead to novel interpretations of the non-Fickian flux, namely by establishing that D_v is positive and increasing function of C.

In order to numerically solve the initial boundary value problem associated to the model, we will propose an Implicit-Explicit piecewise linear finite element method. We will exhibit several plots to illustrate the behavior of the numerical solution.

The original results presented in Chapter 1 correspond to the work:

- J.A. Ferreira , M. Grassi, E. Gudiño, P. de Oliveira , A new look to non-Fickian diffusion, Preprint of the Department of Mathematics, Universidade de Coimbra, No. 13-05, 2013,

which is submitted for publication.

In Chapter 2 we study the well posedness in the Hadamard sense of the initial boundary value problem introduced in Chapter 1. We rewrite the integro-differential equation associated to the model in a more general way, namely, as a class of quasilinear integro-differential equations of Volterra type. We consider this generalization, in order to include initial boundary value problems that arise in other scientific domains like material science [35, 42, 44] as well as in life sciences [17, 18, 28, 38, 43]. Thus the stability and convergence results that we establish for the numerical approximation of the initial boundary value problem obtained using a piecewise linear finite element method, can be applied in a wide range of contexts.

We use the results presented by Grazelli et al., 1991 to establish the conditions for existence and uniqueness of the solution of a weak formulation of the initial boundary value problem. Then we use energy estimate techniques to obtain stability results for two classes of problems. The first class arises when we consider in the integro-differential equation of our generalized model non-singular kernels. The second one, when we consider in the integro-differential equation of our generalized model weakly singular kernels. We show in both cases that the problem is stable under initial perturbations in bounded time intervals.

In Chapter 3 we propose a piecewise linear finite element method to solve numerically the initial boundary value problem studied before. We refer that the finite element scheme can be seen as a fully discrete finite difference method. The stability and convergence analysis of such method will be considered. First we consider a semi-discretization in space of the initial boundary value problem of the generalized model. Then we establish a semi-discrete version of the stability results presented in Chapter 2, for both non-singular and singular kernels. In order to estimate the error induced by the spatial discretization, we use an approach based in the work of Ferreira et al., 2012 that does not follow the usual split of the error introduced by Wheeler 1973, which is largely followed in the literature. This new approach enables us to reduce the smoothness required from the theoretical solution, when the usual split technique is used. We show second order convergence in space with respect to the space step size for the cases of non-singular and singular kernels.

We introduce a fully discretization of the initial boundary problem of the generalized model and present the fully discrete version of the stability results deduced in Chapter 2, once again for both non-singular and singular kernels. We also present the fully discrete versions of the convergence results obtained for the semi-discrete case.

The original results presented in Chapter 2 and Chapter 3 are a generalization of the published works:

- J.A. Ferreira, E. Gudiño, P. de Oliveira, Analytical and Numerical Study of Memory Formalisms in Diffusion Processes, Modelling and Simulation in Fluid Dynamics in Porous Media, Springer Proceedings in Mathematics & Statistics. 28, 67-85, 2013.

- J.A. Ferreira , E. Gudiño, P. de Oliveira , A second order approximation for quasilinear non-Fickian diffusion models, Computational Methods in Applied Mathematics, No. 13 (4), 471–493, 2013.

In Chapter 4 we present a tridimensional mathematical model to describe the sorption of a solvent by a polymeric cylinder, followed by polymer swelling and drug release. For solvent sorption we use the model introduced in Chapter 1. For drug release, we assume that as the solvent penetrates into the polymer, the drug is present in two states dissolved and undissolved, thus the drug release is controlled by both non-Fickian diffusion and a non-linear dissolution. As the amount of dissolved drug does not induce, locally, any kind of re-arrangement of the polymeric chains, the non-Fickian character of the diffusion equation that describes the drug release is due to solvent uptake.

We track the moving front resulting from the swelling of the polymer by considering a volume conservation equation [45]. As we assume the swelling to be independent in the radial and axial directions we use this volume conservation equation to track separately both of the moving fronts [29]. We propose an Implicit-Explicit finite difference method to numerically solve the system of partial differential equations of the model and show some plots to illustrate the behavior of the numerical solutions.

The original results presented in Chapter 4 were first published for the one dimensional case in:

- J.A. Ferreira , M. Grassi, E. Gudiño, P. de Oliveira , A mathematical model for controlled drug delivery in swelling polymers, CMMSE 2013: Proceedings of the 13th International Conference on Mathematical Methods in Science and Engineering, Volume 2, 630-641, 2013,

then generalized for the tridimensional case in:

- J.A. Ferreira , M. Grassi, E. Gudiño, P. de Oliveira , A 3D model for mechanistic control of drug release, Preprint of the Department of Mathematics, Universidade de Coimbra, No. 13-42, September 25, 2013. To appear in SIAM Journal on Applied Mathematics

which is accepted for publication.

Chapter 1

A mathematical model for solvent sorption by a viscoelastic material

In this chapter we introduce a mathematical model to study the non-Fickian diffusion of a liquid agent into a polymeric sample. We consider a modified law for the flux where diffusive and mechanical properties are coupled. By assuming that the non-Fickian part of the flux acts as a barrier to the diffusion, we will deduce physically sound mathematical expressions for the strain and the viscoelastic diffusion coefficient of the polymer.

Let us consider a polymeric sample $\Omega \subset \mathbb{R}^3$, with boundary $\partial\Omega$. In what follows we introduce a initial boundary value problem to describe the sorption and the transport of a solvent with concentration C into Ω.

Let us recall that the Fickian diffusion of a penetrant is described by the conservation law

$$\frac{\partial C}{\partial t} = -\nabla \cdot J_F \ , \tag{1.1}$$

where $C = C(x,t)$ is the fluid concentration and $J_F = J_F(t,x)$ represents the flux and is defined by

$$J_F(t,x) = -D\nabla C(x,t) \ , \tag{1.2}$$

where D is the diffusion coefficient for the penetrant fluid.

To take into account viscoelastic effects we consider a modified flux expressed as the sum of a Fickian flux J_F and a non-Fickian contribution J_{NF} defined by

$$J_{NF}(x,t) = -D_v \nabla \sigma(t,x) \ , \tag{1.3}$$

where $\sigma = \sigma(x,t)$ represents the stress and D_v stands for the viscoelastic diffusion coefficient. The balance equation describing the behavior of the penetrant fluid is represented by (1.1) with J_F replaced by $J = J_F + J_{NF}$.

From (1.1), (1.2) and (1.3) we have

$$\frac{\partial C}{\partial t} = \nabla \cdot (D(C)\nabla C) + \nabla \cdot (D_v(C)\nabla \sigma) \ \text{ in } \ \Omega \times (0,T] \ . \tag{1.4}$$

To represent the stress σ, we consider a Boltzman integral which represents the response of a material to a time depending strain input ε, defined by

$$\sigma(t) = -\int_0^t E(t-s)\frac{\partial \varepsilon}{\partial s}(s)ds\ , \tag{1.5}$$

where the relaxation modulus $E(t)$ is assumed regular enough for the purposes of the mathematical analysis in Chapter 2.

To relate the strain ε with the concentration C of the penetrant, we assume

$$\varepsilon = f(C)\ ,$$

where f is assumed regular enough for the mathematical analysis of Chapter 2.

Replacing (1.5) in (1.4) and assuming that $\nabla f(C(0)) = 0$, we obtain after integrating by parts

$$\frac{\partial C}{\partial t} = \nabla\cdot(D(C)\nabla C - D_v(C)E(0)\nabla f(C)) + \nabla\cdot\left(D_v(C)\int_0^t \frac{\partial E(t-s)}{\partial s}\nabla f(C(s))ds\right)\ . \tag{1.6}$$

Equation (1.6) is completed with the initial condition

$$C(x,0) = C_0,\ x\in\Omega\ , \tag{1.7}$$

and the Dirichlet boundary conditions

$$C \ = \ C_{eq} \ \text{ on } \ \partial\Omega\times(0,T]\ . \tag{1.8}$$

The flux J associated with (1.6) is defined by

$$J(C) = -(D(C)\nabla C - D_v(C)E(0)\nabla f(C)) - D_v(C)\int_0^t \frac{\partial E(t-s)}{\partial s}\nabla f(C(s))ds\ . \tag{1.9}$$

In what follows, taking into account a phenomenological description of the sorption and diffusion of the solvent into a viscoelastic polymeric matrix, we specify expressions for the relaxation modulus $E(t)$ in Section 1.1, the relation between strain and concentration f in Section 1.2 and the viscoelastic diffusion coefficient D_v in Section 1.3. Then, in Section 1.4 we combine those expressions with the integro-differential equation 1.6 to complete the model for solvent sorption by a viscoelastic material. The qualitative behavior of the solution will be illustrated in Section 1.5 with some numerical simulations.

1.1 Mechanical model for viscoelastic behavior

We use simple mechanical models to represent solid and fluids, that are put together to describe viscoelastic effects. These models consider different combinations of springs and dampers to model the viscoelastic properties of polymers. The springs model the elastic behavior and the dampers the viscous behavior. For any of these arrays an equation that relates strain and stress can be

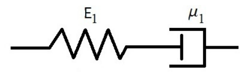

Fig. 1.1: Maxwell fluid model

established by considering equilibrium and kinematic equations for the system and constitutive equations for the elements.

The simplest mechanical array that can be considered to study the viscoelastic behavior of a polymer is the Maxwell fluid model, which consist of a spring and a damper in series as shown in Figure 1.1. To develop a mathematical relation between stress and strain we begin by considering the following equilibrium equation

$$\sigma = \sigma_s = \sigma_d \ , \tag{1.10}$$

where σ is the total stress, σ_s is the stress in the spring and σ_d is the stress in the damper. The kinematic equation is given by

$$\varepsilon = \varepsilon_s + \varepsilon_d \ , \tag{1.11}$$

where ε is the total strain, ε_s the strain in the spring and ε_d the strain in the damper. The constitutive equations are

$$\sigma_s = E_1 \varepsilon_s \ \text{ and } \ \sigma_d = \mu_1 \frac{\partial \varepsilon_d}{\partial t} \ , \tag{1.12}$$

where E_1 is the Young modulus of the spring and μ_1 is the viscosity of the liquid inside of the damper.

Taking time derivatives in (1.11) and using (1.10) and (1.12) we get

$$\frac{\partial \sigma}{\partial t} + \frac{E_1}{\mu_1}\sigma = E_1 \frac{\partial \varepsilon}{\partial t} \ , \tag{1.13}$$

where the inverse of the coefficient of the stress is defined as the relaxation time, $\tau_1 = \frac{\mu_1}{E_1}$. Assuming that $\sigma(0) = 0$, the solution of (1.13) is given by

$$\sigma(t) = E_1 \int_0^t e^{-\frac{t-s}{\tau_1}} \frac{\partial \varepsilon}{\partial s}(s) \, ds \ . \tag{1.14}$$

The Maxwell fluid model is useful to understand some basic aspects of the viscoelastic behavior of some polymers, but it cannot represent the behavior of real polymers over their complete history of use. In fact it is well known [5] that a polymer possesses a distribution of many relaxation times and that an individual polymeric chain can be thought of as having various relaxation times. Therefore to model the viscoelastic properties of polymers we consider a generalized Maxwell-Wiechert model [5] with $m+1$ arms in parallel, where m of them are Maxwell fluid elements and one of them is a free spring as in Figure 1.2. From an experimental point of view, the generalized Maxwell-Wiechert model is well adapted to be used in laboratory to simulate realistic polymer behavior by selecting adequately the parameters to fit the experimental values obtained from laboratorial tests.

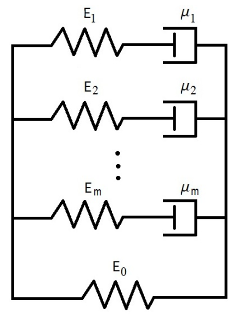

Fig. 1.2: Maxwell-Wiechert model

Let σ_i for $i = 1, \ldots, m$ represent the stress of each Maxwell fluid arm and σ_0 the stress of the free spring. Equilibrium gives

$$\sigma = \sigma_0 + \sum_{i=1}^{m} \sigma_i \ ,$$

and then from (1.14), if follows that

$$\sigma(t) = \int_0^t \left(\sum_{i=1}^{m} E_i e^{-\frac{t-s}{\tau_i}} + E_0 \right) \frac{\partial \varepsilon}{\partial s}(s)\, ds \ . \tag{1.15}$$

where the $E_i's$ are the Young modulus of the spring elements, the $\mu_i's$ the viscosity of the dampers, $\tau_i = \frac{\mu_i}{E_i}$ are the relaxation times associated to each of the m Maxwell fluid arms and E_0 stands for the Young modulus of the free spring. We note that the relaxation modulus $E(t)$ of the Maxwell-Wiechert model is then represented by

$$E(t) = \sum_{i=1}^{m} E_i e^{-\frac{t}{\tau_i}} + E_0 \ . \tag{1.16}$$

There are many different ways to classify polymers according to their molecular structure. However, most polymers can be broadly classified as either thermoplastics or thermosets [5]. The fundamental difference between the two is that thermoplastic polymers can be melted or molded while thermosetting polymers cannot be melted or molded in the general sense of the term. One of the most used methods to characterize these behaviors is the relaxation test, where a constant strain is applied to a uniaxial tensile bar. The stress needed to keep a constant strain will decrease with time. The stress will decay to zero for a thermoplastic polymer and to a limiting constant for thermosetting polymers as shown in Figure 1.3. Thermoplastic and thermosetting polymers are sometimes identified by other names such as linear and cross-linked respectively.

Note that in (1.16) when $E_0 = 0$ the stress will go to zero as t tends to infinity. On the other hand when $E_0 \neq 0$ the stress will decay to a limiting constant. Thus the Maxwell-Wiechert model is well suited to model both thermoplastic and thermosetting polymers by carefully choosing E_0.

We will assume that the non-Fickian flux J_{NF} act as a barrier to the diffusion process, thus as

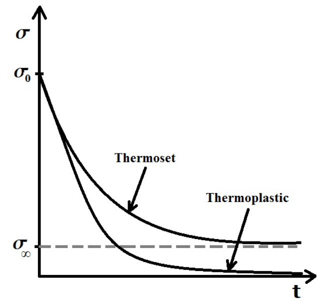

Fig. 1.3: Relaxation test

the solvent diffuses into the polymer a stress of opposite sign develops. Then we rewrite (1.15) as

$$\sigma(t) = -\int_0^t \left(\sum_{i=1}^{m} E_i e^{-\frac{t-s}{\tau_i}} + E_0 \right) \frac{\partial f(C)}{\partial s}(s)\, ds \;, \tag{1.17}$$

where $f(C)$ is a non linear relation between strain and concentration. Such relation will be established in the following section.

1.2 Functional relation between deformation and concentration

In what follows we deduce a physically sound non linear relation between the strain ε and the concentration C. Let us begin by considering, for the sake of simplicity, that we have a cylindrical dry polymeric sample with cross section S and volume V_0 as shown in Figure 1.4. We also assume that the deformation ε occurs only in a direction orthogonal to S.

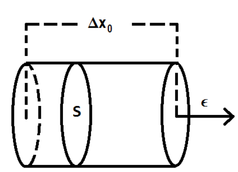

Fig. 1.4: Cylindrical dry polymeric sample

By Δx_0 we represent its thickness in the dry state, defined as

$$\Delta x_0 = \frac{V_0}{S} \;. \tag{1.18}$$

After swelling the thickness of the sample can be calculated as

$$\Delta x = \frac{V_0 + V_S}{S} \;, \tag{1.19}$$

where V_S is the volume of solvent absorbed by the sample up to time t. As the deformation occurs orthogonally to S, then it can be calculated with the following expression

$$\varepsilon = \frac{\Delta x - \Delta x_0}{\Delta x_0} \, . \tag{1.20}$$

Combining (1.18) and (1.19) in (1.20) we obtain

$$\varepsilon = \frac{\frac{V_0+V_S}{S} - \frac{V_0}{S}}{\frac{V_0}{S}} \, ,$$

which after rearranging terms can be rewriten as

$$\varepsilon = \frac{V_S}{V_0} \, . \tag{1.21}$$

Let m_S and ρ_S represent the solvent mass and density respectively. As m_S can be defined as

$$m_S = \rho_S V_S \, ,$$

then from (1.21) we get that

$$\varepsilon = \frac{m_S}{\rho_S V_0} \, . \tag{1.22}$$

We note that equation (1.22) holds under the reasonable hypothesis that the mixing of the polymer and the solvent occurs in an ideal manner that is the final volume of the swelling element is $V_0 + V_S$. Considering that the concentration C is defined by

$$C = \frac{m_S}{V_0 + V_S} \, ,$$

we get that

$$V_0 = V_S \left(\frac{\rho_S - C}{C} \right) \, , \tag{1.23}$$

From (1.22) and (1.23) we deduce that $\varepsilon = f(C)$ with

$$f(C) = \frac{C}{\rho_S - C} \, . \tag{1.24}$$

We have from (1.24) that $f(C)$ is an increasing positive function of the concentration as shown in Figure 1.5 (for $\rho_S = 1000 \; Kg/m^3$).

We note that from the definition of m_S and C, we obtain

$$C = \rho_S \frac{V_S}{V_0 + V_S} \, ,$$

therefore $\rho_S > C$. Thus, in the context of physically meaningful values of C the function f is smooth.

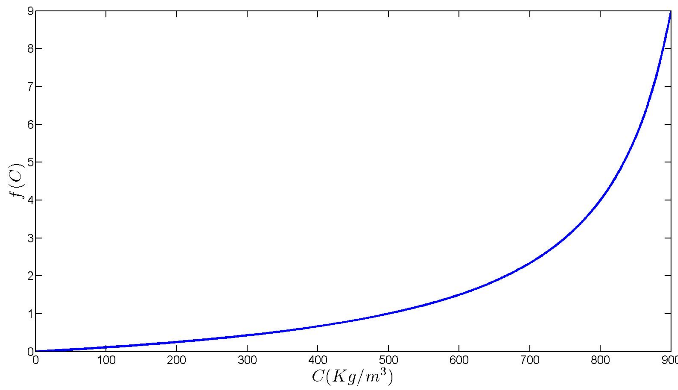

Fig. 1.5: Behavior of $f(C)$

1.3 Viscoelastic diffusion coefficient

The physical meaning of the diffusion coefficient D is very well know and there are many different functional relations that describe its behavior. For the viscoelastic diffusion coefficient D_v there is not too much information, even its sign is not clear throughout the literature. Some authors [24, 40, 41] consider D_v constant and negative while in the works [6, 8, 13, 14, 15, 32] D_v is considered to be a positive parameter. In what follows we present two different approaches to compute D_v. The first one is based on Darcy's law and the second one on the Hagen-Poiseuille equation.

As we assume the existence of a stress gradient $\nabla\sigma$, this implies the existence of a velocity field v. Then the non-Fickian flux J_{NF} can be interpreted as a convective field of form

$$J_{NF} = vC \, . \tag{1.25}$$

Let us consider that the polymeric sample is a porous media. Then by Darcy's law [51] we have

$$v = -K\nabla p \, , \tag{1.26}$$

where p is the hydrostatic pressure and K is the hydraulic conductivity. The parameter K can be computed using the Kozeny-Carman equation

$$K = \frac{r_f^2\alpha^3}{4G\mu(1-\alpha)^2} \, , \tag{1.27}$$

where r_f is the fiber radius, α is the concentration dependent porosity, μ is the pure solvent shear viscosity and G is the Kozeny constant. The porosity α is defined by $\alpha = C/\rho_S$ where ρ_S represents the pure penetrant density.

As the convective field is induced by the stress we have

$$-D_v(C)\nabla\sigma = vC \, ,$$

and by identifying the stress σ with the pressure p, we conclude that

$$D_v(C) = KC \; . \tag{1.28}$$

We present now a second functional relation for $D_v(C)$. The main difference of this approach is that the velocity is now computed using the Hagen-Poiseuille equation. We have

$$v = -\frac{R^2}{8\mu}\nabla p \; , \tag{1.29}$$

where R stands for the radius of a virtual cross section of the polymeric sample available for the convective flux, p is the pressure and μ represents the viscosity of a polymer-solvent solution characterized by a liquid (or solvent) concentration equal to C (local solvent concentration). Thus from (1.25), (1.29) and identifying again the pressure p with the viscoelastic stress σ, we deduce

$$D_v(C) = \frac{R^2 C}{8\mu} \; . \tag{1.30}$$

Let us study now the evolution in time of R. Let m_S and V_S represent the mass and volume of the solvent respectively. If ρ_S represents its density then $m_S = \rho_S V_S$ and $C = \frac{m_S}{V_0+V_S}$, where V_0 is the volume of the polymeric matrix in the dry state. We conclude then

$$V_s = \frac{C}{\rho_S - C} V_0 \; ,$$

and from (1.18), we have

$$\frac{V_S}{\Delta x_0} = \frac{C}{\rho_S - C} S \; . \tag{1.31}$$

The first member in (1.31) can be interpreted as a virtual cross section S_v available for convective flow. As $S_v = \pi R^2$ and $S = \pi R_0^2$, where R_0 is the radius of the dry sample, we deduce

$$R^2 = \frac{C}{\rho_S - C} R_0^2 \; . \tag{1.32}$$

From (1.30) and (1.32), we finally have

$$D_v(C) = \frac{C^2}{\rho_S - C}\frac{R_0^2}{8\mu} \; . \tag{1.33}$$

We note that from both approaches, (1.28) and (1.33), we can conclude that:

- $D_v(C)$ is positive, thus the non-Fickian flux J_{NF} represents a contribution to the mass flux which develops from high stress to low stress;

- $D_v(C)$ is an increasing function of C;

- $D_v(0) = 0$ which accounts for the fact that no stress gradient contributes to the mass flux when $C = 0$.

Even though the Darcy approach is originated from the study of fluid motion in a porous medium while the Hagen-Poiseuille approach is strictly connected to the flux of a fluid flowing through a long cylindrical pipe, both of them lead to qualitatively similar behaviors for D_v as function of local solvent concentration C, as shown in Figure 1.6 where we plotted $\log_{10}(D_v)$ as a function of C for the two approaches. The main difference is that the Darcy approach leads to smaller values for D_v which reflects a smaller influence of the polymer-solvent viscoelastic properties on penetrant uptake. In the Darcy case the shear viscosity considered is that of the pure solvent (0.001 *Pas* for water). In the Hagen-Poiseuille case the shear viscosity considered is that of the polymer-solvent system (10^5 *Pas*).

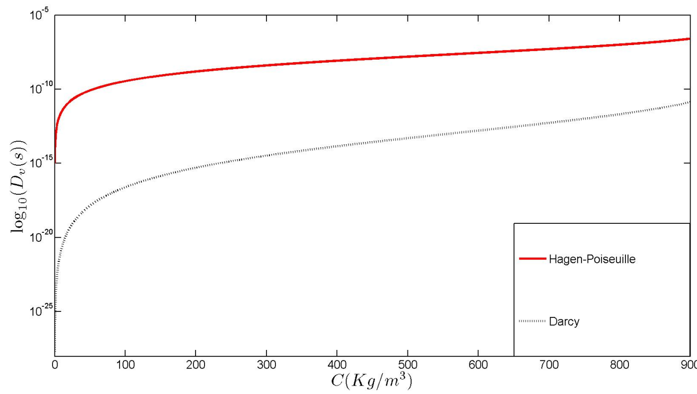

Fig. 1.6: Quantitative comparison of the two approaches for $\log_{10}(D_v)$

We note that when D_v is defined as in (1.33), in the context of physically meaningful values of C the function D_v is smooth, since $\rho_S > C$.

1.4 Complete model for solvent uptake

In this Section we rewrite the IBVP (1.6)-(1.8) taking into consideration the previously introduced functional relations.

We begin by assuming that the relaxation modulus E is defined as in (1.16), the functional relation f between strain and concentration is defined by (1.24), the viscoelastic diffusion coefficient D_v can be defined by (1.28) or (1.33) and that the diffusion coefficient $D(C)$ has a Fujita-type exponential dependence [30] with

$$D(C) = D_{eq} exp(-\beta(1 - \frac{C}{C_{eq}})) \ , \tag{1.34}$$

where D_{eq} is the diffusion coefficient of the liquid agent in the fully swollen sample and β a dimensionless positive constants.

We have then from (1.6) that the IBVP is given by the equation

$$\begin{aligned}\frac{\partial C}{\partial t} &= \nabla\cdot\Bigg(\Bigg(D(C)-D_v(C)\left(\sum_{i=0}^{m}E_i\right)\frac{\rho_S}{(\rho_S-C)^2}\Bigg)\nabla C\\ &\quad +D_v(C)\sum_{i=1}^{m}\frac{E_i}{\tau_i}\int_0^t e^{\frac{(s-t)}{\tau_i}}\frac{\rho_S\nabla C(r)}{(\rho_S-C(r))^2}dr\Bigg)\ ,\end{aligned}\tag{1.35}$$

coupled with initial condition

$$C(x,0)=C_0,\ x\in\Omega\ ,\tag{1.36}$$

and the Dirichlet boundary conditions

$$C\ =\ C_{eq}\ \text{ on }\ \partial\Omega\times(0,T]\ .\tag{1.37}$$

The flux is defined as

$$\begin{aligned}J(C) &= -\Bigg(\Bigg(D(C)-D_v(C)\left(\sum_{i=0}^{m}E_i\right)\frac{\rho_S}{(\rho_S-C)^2}\Bigg)\nabla C\\ &\quad +D_v(C)\sum_{i=1}^{m}\frac{E_i}{\tau_i}\int_0^t e^{\frac{(s-t)}{\tau_i}}\frac{\rho_S\nabla C(r)}{(\rho_S-C(r))^2}dr\Bigg)\ .\end{aligned}\tag{1.38}$$

The well posedness in the Hadamard sense of the IBVP (1.35)-(1.45) will be studied in Chapter 2.

1.5 Qualitative behavior of the mathematical model

In order to illustrate the behavior of the solution we solve numerically the IBVP (1.35)-(1.37) with an IMEX (implicit-explicit) method that will be studied in Chapter 3. We assume that the polymeric matrix is homogeneous and consequently we can assume that $\Omega=[-L,L]$. We also assume a symmetric condition at $x=0$.

Let $h=(h_1,h_2,...,h_N)$ be such that $\sum_{j=1}^{N}h_j=L$. Let us consider a nonuniform space grid $I_h=\left\{x_j,\ j=0,1,..,N\right\}$, with $x_0=0$, $x_N=L$ and $x_j-x_{j-1}=h_j$. By D_{-x} we represent the usual backward finite difference operator. Let u_h be a function defined over I_h and $\mathbb{W}_h$ the space of grid functions defined in I_h. For $u_h\in\mathbb{W}_h$ we introduce the following finite-difference operator

$$D_x^{\frac{1}{2}}u_h(x_j)\ =\ \frac{u_h(x_{j+1})-u_h(x_j)}{h_{j+\frac{1}{2}}}\ ,\tag{1.39}$$

where $h_{j+\frac{1}{2}}=\frac{h_{j+1}+h_j}{2}$. We also introduce the following notation:

$$M_hu_h(x_j)\ =\ \frac{1}{2}(u_h(x_{j-1})+u_h(x_j)),\quad j=1,\dots,N\ ,\tag{1.40}$$

$$M_hu_h(x_0)\ =\ 0,\quad u_h\in\mathbb{W}_{h,0}\ ,\tag{1.41}$$

where $\mathbb{W}_{h,0}$ denotes the subspace of $\mathbb{W}_h$ of functions null on the boundary points.

In $[0,T]$ we consider a uniform time grid $J_{\Delta t} = \{t_n,\ n = 0,1,2,...,M\}$, with $t_0 = 0,\ t_M = T$ and $t_n - t_{n-1} = \Delta t$. We use the rectangular rule to approximate the integral in (1.35) and the backward finite-difference operator D_{-t} to approximate the first partial derivative with respect to t.

The fully discrete approximation for C at (x_j,t_n), $C_h^n(x_j)$, is defined by

$$\begin{aligned} & D_{-t}C_h^n(x_j) \\ & = D_x^{\frac{1}{2}}\left(\left(D(M_hC_h^{n-1}(x_j)) - D_v(M_hC_h^{n-1}(x_j))\left(\sum_{i=0}^{m} E_i\right)\frac{\rho_S}{(\rho_S - M_hC_h^{n-1}(x_j))^2}\right)D_{-x}C_h^n(x_j)\right) \\ & +\Delta t\sum_{s=0}^{n-1}\left(\sum_{i=1}^{m}\frac{E_i}{\tau_i}e^{\frac{(t_s-t_n)}{\tau_i}}\right)D_x^{\frac{1}{2}}\left(D_v(M_hC_h^{n-1}(x_j)\frac{\rho_S}{(\rho_S - M_hC_h^s(x_j))^2}D_{-x}C_h^s(x_j)\right)\ , \end{aligned} \tag{1.42}$$

for $j = 1,\ldots,\ N-1$, with boundary conditions

$$C_h^n(x_0) = C_h^n(x_1), \quad \text{for } n = 1,\ldots,\ M\ , \tag{1.43}$$

$$C_h^n(x_N) = C_{eq}, \quad \text{for } n = 1,\ldots,\ M\ , \tag{1.44}$$

and the initial condition

$$C_h^0(x_j) = R_hC_0(x_j), \quad \text{for } j = 1,\ldots,\ N-1\ . \tag{1.45}$$

To illustrate the behavior of the fluid concentration during the sorption step we consider the IBVP (1.35)-(1.37) and we use the previous IMEX method to numerically solve the problem. In Chapter 3 we will establish stability and convergence results for the IMEX method (1.42)-(1.45). We show that the method is stable under initial perturbation in bounded time intervals, second order convergent in space and first order convergent in time, provided that some smoothness conditions are satisfied by the solution C and its approximation C_h.

We consider $m = 1$, that is, a Maxwell fluid arm in parallel with a free spring. The following values for the parameters have been considered,

$$\begin{aligned} L &= 1\times10^{-3}\ m,\ h_{max} = 1.25\times10^{-5}\ m,\ D_{eq_l} = 3.74\times10^{-9}\ m^2/s,\ D_{eq_d} = 2.72\times10^{-10}\ m^2/s, \\ \beta &= 2.5,\ \hat{\mu} = 1\times10^5\ Pas,\ E_1 = 9\times10^3\ Pa,\ E_0 = 1\times10^3\ Pa,\ \mu_1 = 225\times10^4\ Pas, \\ \rho_S &= 1000\ kg/m^3,\ C_{eq} = 755\ Kg/m^3,\ C_0 = 0\ Kg/m^3, \Delta t = 0.01\ s. \end{aligned}$$

In Figure 1.7 we plot a comparison of the non-Fickian part of the flux J_{NF} as defined in (1.3), considering the definition of D_v established from Darcy's law (1.28) versus the definition of D_v deduced from the Hagen-Poiseuille equation (1.33). We observe that in agreement with Figure 1.6, when D_v is given by (1.33) a higher opposition to the diffusion is present.

In Figure 1.8 we have a plot of the complete flux J when D_v is given by (1.28) versus when it is given by (1.33). In accordance with the behavior observed in Figure 1.7 when D_v is given by (1.33) the model predicts a slower sorption of the solvent into the polymeric sample.

In Figure 1.9 we present a plot of the evolution in time of the concentration C for different values of x. In $x = 0$ we considered symmetry conditions and in $x = 1\times10^{-3}$ we considered

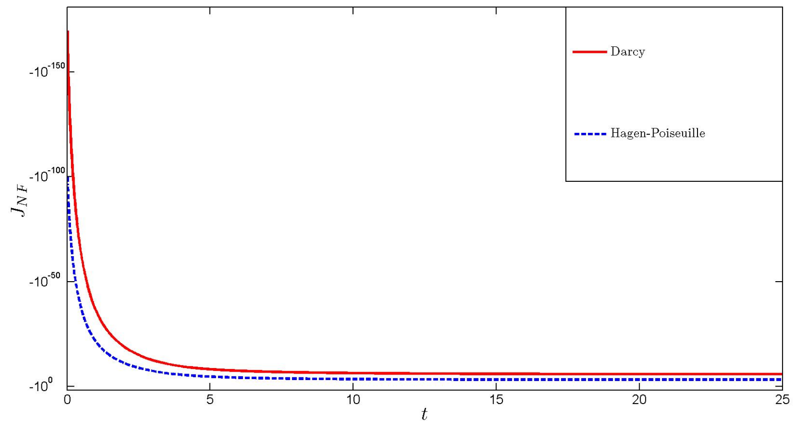

Fig. 1.7: Non-Fickian flux J_{NF} for $x = 5 \times 10^{-4}$

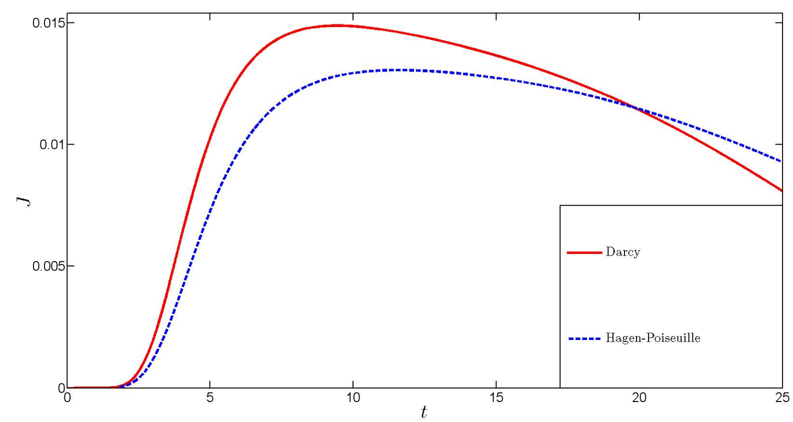

Fig. 1.8: Total flux J for $x = 5 \times 10^{-4}$

the constant source of concentration C_{eq}. Therefore higher values of x correspond to points in space that are closer to where the constant source of concentration is allocated. We observe that as expected, as x increases , the solvent uptake is faster.

In Figure 1.10 we plotted the concentration profile inside of the polymer for different values of t. We observe that the solutions develop from low levels of concentration to high levels of concentration as expected, since the transport occurs from right to left in the plot. Also the amount of solvent inside the polymer increases with time.

In Figure 1.11 we plotted the concentration C as a function of the parameter E_1. We observe that C is a decreasing function of E_1.

In Figure 1.12 we have a plot of the concentration C as a function of the parameter μ_1. We observe that C is a decreasing function of μ_1.

According to Flory theory [27] there is a link between E_0 and C_{eq}, more precisely, at equilib-

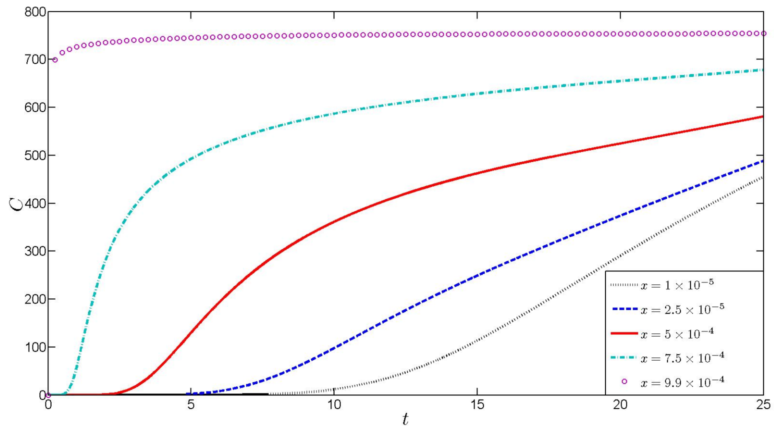

Fig. 1.9: Concentration for different x

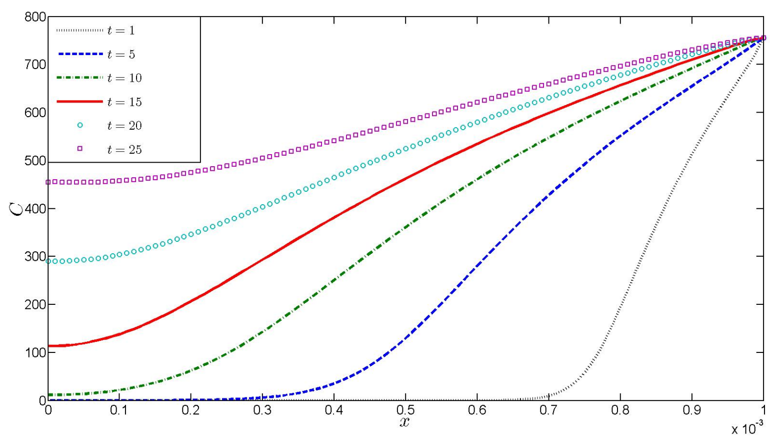

Fig. 1.10: Concentration for different t

rium we have

$$ln(1-\phi_p)+\phi_p+\chi\phi_p^2+\rho_x V_1\left(\phi_p^{\frac{1}{3}}-0.5\phi_p\right)=0\ , \tag{1.46}$$

where ϕ_p represent the polymer volume fraction, V_1 the solvent molar volume, ρ_x is the cross-link density [1] and χ is the Flory interaction parameter. As ρ_x can be computed by

$$\rho_x=\frac{E_0}{3R_gA_T}\ , \tag{1.47}$$

where R_g is the universal gas constant and A_T the absolute temperature, assuming that $\chi=0.6$, $A_T=298.15\ K$ and $V_1=18.064\times10^{-6}\ m^3/mol$, then once E_0 is fixed, ϕ_p can be calculated with

[1] Number of bonds that link one polymer chain to another per unit of volume

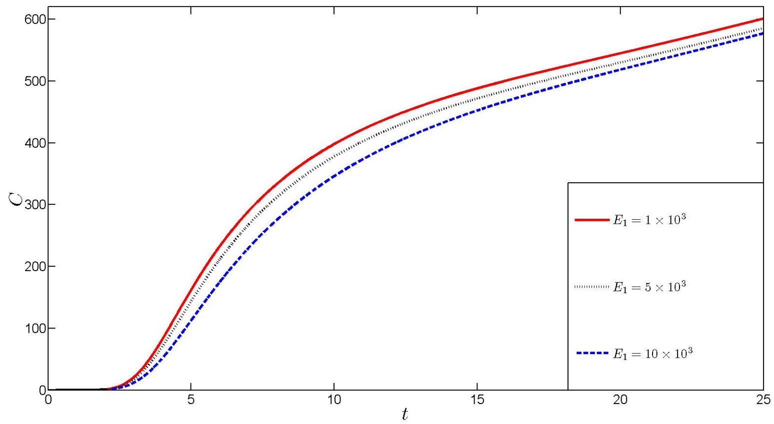

Fig. 1.11: Concentration as a function of E_1

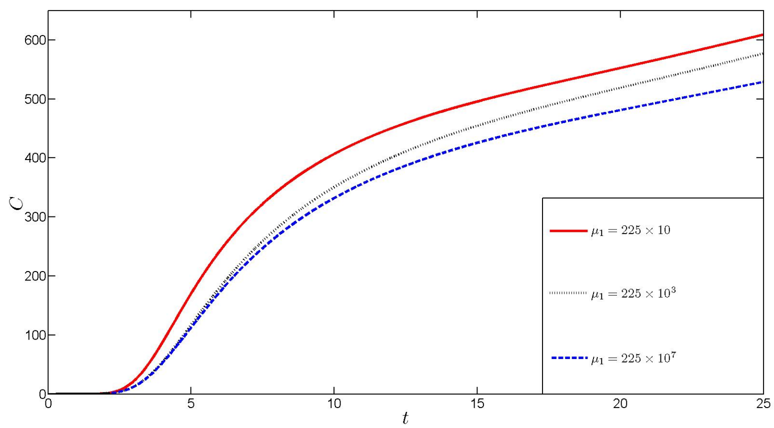

Fig. 1.12: Concentration as a function of μ_1

(1.46) and the corresponding C_{eq} can be obtained from

$$C = \rho_S(1 - \phi_p) \ . \tag{1.48}$$

In Figure 1.13 we plotted the concentration C as a function of the parameter E_0 and its corresponding C_{eq}. We observe that as expected C is a decreasing function of E_0. In fact, as E_0 increases the cross-link density increases, less mobility has the polymer, and a stronger opposition develops to the incoming fluid.

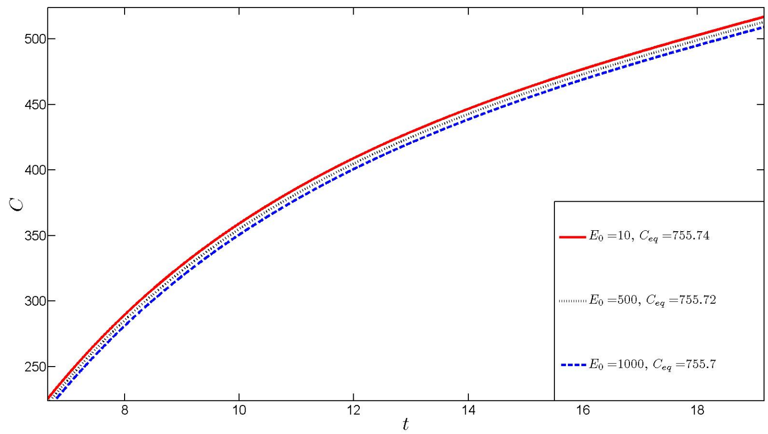

Fig. 1.13: Concentration as a function of E_0

We have proposed a new non-linear non-Fickian model for sorption of a solvent into a polymeric matrix. The model is based on a new interpretation of the non-Fickian flux and the establishment of non-linear functional relations for the strain ε and the diffusion coefficient D_v. The great advantage of this model consists in the possibility of easily and directly incorporating experimental rheological information about the polymer-solvent system (knowledge of E_i and μ_i). This makes the model appropriate for both data fitting and quantitative prediction. As the model needs to be numerically solved, we proposed an IMEX finite difference method (which will be studied in Chapter 3) and presented some numerical simulations to illustrate the behavior of the solution and the effect that some of the parameters that describe the viscoelastic properties of the polymer have on the model.

Chapter 2

Well posedness of an abstract model

The main objective of chapter 2 is the study of the well posedness, in the Hadamard sense, of a class of quasi-linear integro-differential equations that generalize equation (1.6). The non-linear function f, presented in (1.6), is unbounded as well as its successive derivatives. However, from a phenomenological perspective, we always have $C < \rho_S$, which means that from a physical point of view f is a bounded function. This comments allow us to consider in what follows a class of quasi-linear integro-differential equations where the nonlinear function f satisfy some smoothness assumptions that will be specified later. Existence and uniqueness conditions will be addressed in Section 2.3 using the results presented by M. Grazelli and A. Lorenzi in [31]. In Section 2.4 stability is studied. Some notations and preliminary results are introduced in Section 2.1.

2.1 Notation and preliminary results

Let $L^2(\Omega)$ and $H_0^1(\Omega)$ be the usual spaces. In $L^2(\Omega)$ and $H_0^1(\Omega)$ we consider respectively the inner products $(.,.)$ and $(.,.)_1$. By $\|.\|$ and $\|.\|_1$ we represent respectively the norms in $L^2(\Omega)$ and $H_0^1(\Omega)$. The usual semi-norm in $H_0^1(\Omega)$ is denoted by $|.|_1$. Let V be a Banach space. We denote by $L^2(0,T;V)$ the space of Bochner-measurable functions $v: \ (0,T) \mapsto V$ such that

$$\|v\|^2_{L^2(0,T;V)} = \int_0^T \|v(t)\|_V^2 dt < \infty \, .$$

We denote by $H^s(0,T;V)$ the space of functions v in $L^2(0,T;V)$ whose distributional time derivatives up to order s are also in $L^2(0,T;V)$. In this space we consider the following norm

$$\|v\|^2_{H^s(0,T;V)} = \sum_{i=0}^{s} \int_0^T \left\| \frac{d^i v}{dt^i} \right\|_V^2 < \infty \, .$$

By $L^\infty(0,T;V)$ we denote the space of essentially bounded Bochner measurable functions $v: [0,T] \to V$. In this space we consider the following norm

$$\|v\|_{L^\infty(0,T;V)} = \underset{[0,T]}{ess\ sup} \|v(t)\|_V < \infty \, .$$

We denote by $\mathscr{C}^p(0,T;V)$ the space of continuous functions $v:[0,T]\to V$ such that its derivatives up to order p are continuous with respect to the norm $\|.\|_V$. By $\mathscr{C}_B^p(\mathbb{R}^n)$ we represent the space of bounded continuous functions in $\mathbb{R}^n$ with bounded derivatives up to order p.

By $W^{1,\infty}(\Omega)$, we denote the space of Bochner measurable functions $v:\Omega\to\mathbb{R}$ such that

$$\|v\|_{W^{1,\infty}(\Omega)} = \sum_{j=0}^{1} \underset{\Omega}{ess\ sup}|v^{(j)}| < \infty \, .$$

We consider the following space $\mathscr{W}(0,T) = \{v\in L^2(0,T;H_0^1(\Omega)) : \frac{\partial v}{\partial t}\in L^2(0,T;H^{-1}(\Omega))\}$, where $H^{-1}(\Omega)$ denotes the dual space of $H_0^1(\Omega)$. In $H^{-1}(\Omega)$ we consider the norm

$$\|\mathbb{F}\|_{H^{-1}(\Omega)} = sup\{|\langle\mathbb{F},v\rangle| \, : \, v\in H_0^1(\Omega),\ \|v\|_1\leq 1\} \, ,$$

where $\langle\cdot,\cdot\rangle$ denotes the duality pairing in $H_0^1(\Omega)\times H^{-1}(\Omega)$.

By $L^1(0,T)$ we denote the space of functions $v:\ (0,T)\mapsto\mathbb{R}$ such that

$$\|v\|_{L^1(0,T)} = \int_0^T |v(t)|dt < \infty \, .$$

The next Lemma, known as the Gronwall Lemma, will be use in the proof of the stability results that we present in this chapter.

Lemma (Gronwall's Lemma, [34])**.** *Let $y(t)$ and $f(t)$ be non-negative functions on $[0,T]$ having one-sided limits at every $t\in[0,T]$, and c a non-negative constant. If for every $0\leq t\leq T$ we have*

$$y(t)\leq c+\int_0^t f(s)y(s)ds \, ,$$

then

$$y(t)\leq c\ exp\left(\int_0^t f(s)ds\right) \, ,$$

for all $0\leq t\leq T$.

The Poincaré-Friedrich's inequality

$$\|v\|\leq a_\Omega|v|_1,\ v\in H_0^1(\Omega) \, , \tag{2.1}$$

where a_Ω is a positive constant depending on Ω, will also be used in what follows.

2.2 Weak formulation

Without loss of generality we will replace the Dirichlet boundary conditions (1.8) by homogeneous Dirichlet boundary conditions, that is

$$C \;=\; 0 \text{ on } \partial\Omega\times(0,T] \, . \tag{2.2}$$

To define a general weak formulation of the IBVP (1.6), (1.7), (2.2) we begin by rewriting (1.6) as

$$\frac{\partial C}{\partial t} = \nabla\cdot(G(C)\nabla C) + \nabla\cdot\left(\int_0^t K(t-s)F(C(t),C(s))\nabla C(s)ds\right) + Z\,. \tag{2.3}$$

The IBVP (2.3), (1.7) and (2.2), is then replaced by the variational problem (**VP**): Find $C \in \mathscr{W}(0,T)$ such that the initial condition (1.7) hold almost everywhere and

$$(\frac{\partial C}{\partial t}(t),v) + (G(C(t))\nabla C(t),\nabla v) + \int_0^t K(t-s)(F(C(t),C(s))\nabla C(s),\nabla v)ds = (Z(t),v)\,, \tag{2.4}$$

a. e. in $(0,T)$, for all $v \in H_0^1(\Omega)$.

We note that if we consider

$$\begin{aligned} G(C(t)) &= D(C(t)) - E(0)D_v(C(t))f'(C(t))\,, & (2.5)\\ F(C(t),C(s)) &= D_v(C(t))f'(C(s))\,, & (2.6)\\ K(t-s) &= \frac{\partial E(t-s)}{\partial s}\,, & (2.7)\\ Z(t) &= 0\,, & (2.8) \end{aligned}$$

then the weak formulation of (1.6) is represented by (2.4).

We also have that the weak formulation of (1.35) is represented by (2.4) when

$$\begin{aligned} G(C(t)) &= D(C(t)) - D_v(C(t))\left(\sum_{i=0}^m E_i\right)\frac{\rho_S}{(\rho_S - C(t))^2}\,, & (2.9)\\ F(C(t),C(s)) &= D_v(C(t))\frac{\rho_S}{(\rho_S - C(s))^2}\,, & (2.10)\\ K(t-s) &= \sum_{i=1}^m \frac{E_i}{\tau_i}e^{-\frac{t-s}{\tau_i}}\,, & (2.11)\\ Z(t) &= 0\,, & (2.12) \end{aligned}$$

with D defined as in (1.34) and D_v as in (1.28) or (1.33).

2.3 Existence and uniqueness

In [31] M. Grazelli and A. Lorenzi studied the nonlinear Cauchy problem

$$\begin{aligned} \frac{\partial u}{\partial t}(t) + \mathbb{A}(u(t)) &= \int_0^t \mathbb{K}(t,s,u(s),\frac{\partial u}{\partial t}(s))ds + g(t) \quad \text{a.e.} \quad t \in (0,T] & (2.13)\\ u(0) &= u_0\,, & (2.14) \end{aligned}$$

where $\mathbb{A}$, $\mathbb{K}$ are nonlinear operators, g is a given function and u_0 is a given element. They proved that if the nonlinear operators $\mathbb{A} : H_0^1(\Omega) \to H^{-1}(\Omega)$, $\mathbb{K} : Q_T \times H_0^1(\Omega) \times H^{-1}(\Omega) \to H^{-1}(\Omega)$, where $Q_T = \{(t,s) \in \mathbb{R}^2 : 0 < s < t < T\}$ satisfy the following assumptions:

(i) there exists a constant M such that $\|\mathbb{A}(v)\|_{H^{-1}(\Omega)} \leq M\|v\|_1, \ \forall v \in H_0^1(\Omega)$;

(ii) there exists a constant $\tilde{M}$ such that $\|\mathbb{A}(v) - \mathbb{A}(w)\|_{H^{-1}(\Omega)} \leq \tilde{M}\|v-w\|_1, \ \forall v, w \in H_0^1(\Omega)$;

(iii) there exist a positive constant α such that

$$\langle \mathbb{A}(v) - \mathbb{A}(w), v - w \rangle \geq \alpha \|v-w\|_1^2, \ \forall v, w \in H_0^1(\Omega) \ ;$$

(iv) there exist a function $\mathscr{K} : Q_T \to \mathbb{R}$ such that $\mathscr{K} \in L^1(0,T)$ and

$$\|\mathbb{K}(t,s,v,w) - \mathbb{K}(t,s,\tilde{v},\tilde{w})\|_{H^{-1}(\Omega)} \leq \mathscr{K}(t-s)\left(\|v-\tilde{v}\|_1 + \|w-\tilde{w}\|_{H^{-1}(\Omega)}\right) \ ,$$

a.e. $(t,s) \in Q_T$, for any $v, \ \tilde{v} \in H_0^1(\Omega)$ and $w, \ \tilde{w} \in H^{-1}(\Omega)$,

then for the Cauchy problem (2.13)-(2.14), there exists a unique solution that satisfy the condition $u \in L^\infty(0,T;L^2(\Omega)) \bigcap L^2(0,T;H_0^1(\Omega))$ with $\frac{\partial u}{\partial t} \in L^2(0,T;H^{-1}(\Omega))$, provided that

$$\mathbb{K}(t,s,0,0) = 0 \quad \text{a.e. } (t,s) \in Q_T \ , \tag{2.15}$$
$$g \in L^2(0,T;H^{-1}(\Omega)) \ , \tag{2.16}$$
$$u_0 \in L^2(\Omega) \ . \tag{2.17}$$

Let us set now

$$\mathbb{A}(u)v = \int_\Omega G(u)\nabla u \cdot \nabla v \, dx \ , \quad \forall v \in H_0^1(\Omega) \ ,$$

for any $u \in H_0^1(\Omega)$,

$$\mathbb{K}(t,s,u,w)v = \int_\Omega \mathscr{K}(t-s)F(u(t),u(s))\nabla u(s) \cdot \nabla v \, dx \ , \quad \text{a.e. } t,s \in [0,T], \ \forall v \in H_0^1(\Omega) \ ,$$

for any $u \in H_0^1(\Omega)$ and $w \in H^{-1}(\Omega)$, $g = Z$ and

$$\mathscr{K}(t-s) = K(t-s) \ .$$

If we consider that the following conditions hold

$$|G| \leq \alpha_0 \ , \tag{2.18}$$
$$|G(p_1)\xi_1 - G(p_2)\xi_2| \leq \alpha_1 |\xi_1 - \xi_2| \quad \forall \ \xi_1, \xi_2 \in \mathbb{R}^3 \ , \tag{2.19}$$
$$(G(p_1)\xi_1 - G(p_2)\xi_2)(\xi_1 - \xi_2) \geq \alpha_2 (\xi_1 - \xi_2)^2 \quad \forall \ \xi_1, \xi_2 \in \mathbb{R}^3 \ , \tag{2.20}$$
$$|F(p_1,q_1)\xi_1 - F(p_2,q_2)\xi_2| \leq \alpha_3 |\xi_1 - \xi_2| \quad \forall \ \xi_1, \xi_2 \in \mathbb{R}^3 \ , \tag{2.21}$$
$$K \in L^1(0,T) \ , \tag{2.22}$$

then conditions $(i) - (iv)$ are satisfied. Thus, the existence and uniqueness of the variational problem (**VP**) is established, provided that $Z \in L^2(0,T;H^{-1}(\Omega))$.

We note that when K is defined as in (2.11), the condition $K \in L^1(0,T)$ is clearly satisfied.

2.4 Stability

Even though for the existence and uniqueness of the solution of the variational problem (**VP**), it is enough to assume that $K \in L^1(0,T)$, in the stability analysis that follows, the smoothness of K has an important role. In fact depending on such smoothness we get estimates that hold for different classes of problems. Thus we will present two results, a first one where we assume that $K \in L^2(0,T)$ and a second one where we assume that $K \in L^1(0,T)$. When $K \in L^2(0,T)$ no especial conditions need to be imposed on the coefficient functions G and F other than the smoothness conditions necessary for the existence and uniqueness of the solution. On the other hand when we reduce the smoothness conditions over K and we assume that $K \in L^1(0,T)$, it is necessary to impose stronger conditions on G and F.

In order to establish the following stability result, for the variational initial value problem defined in (1.6), we fix a solution C and we will analyze the behavior of $w = C - \tilde{C}$, where $\tilde{C}$ is another solution of the variational problem corresponding to a perturbed initial condition.

Theorem 2.1. *Let us suppose that $K \in L^2(0,T)$, $G \in \mathscr{C}_B^1(\mathbb{R})$, $F \in \mathscr{C}_B^1(\mathbb{R}^2)$ and that $0 < G_0 \le G$. If C and $\tilde{C}$ are solutions of (**VP**) such that $C, \tilde{C} \in \mathscr{C}^1(0,T;L^2(\Omega)) \bigcap \mathscr{C}(0,T;W^{1,\infty}(\Omega))$, then for $w = C - \tilde{C}$, with $w(0) = w_0$, there exists a constant c_1 depending on the coefficient functions G, F and on the kernel K such that*

$$\|w(t)\|^2 + \int_0^t |w(s)|_1^2 ds \le \|w_0\|^2 e^{c_1(\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))}+1)t} \; . \tag{2.23}$$

Proof. From (2.4) we have

$$\begin{aligned}
&(\frac{\partial w}{\partial t}(t), w(t)) + (G(C(t))\nabla C(t) - G(\tilde{C}(t))\nabla \tilde{C}(t), \nabla w(t)) \\
&+ \int_0^t K(t-s)(F(C(t),C(s))\nabla C(s) - F(\tilde{C}(t),\tilde{C}(s))\nabla \tilde{C}(s)), \nabla w(t))ds = 0 \; .
\end{aligned} \tag{2.24}$$

Summing and subtracting in (2.24) the terms

$$(G(\tilde{C}(t))\nabla C(t), \nabla w(t)) \; , \; \int_0^t K(t-s)(F(\tilde{C}(t),\tilde{C}(s))\nabla C(s), \nabla w(t))ds \; ,$$

we obtain

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2 + (G(\tilde{C}(t))\nabla w(t), \nabla w(t)) = P_1 + P_2 + P_3 \; ,$$

where

$$\begin{aligned}
P_1 &= ((G(C(t)) - G(\tilde{C}(t)))\nabla C(t), \nabla w(t)) \; , && (2.25)\\
P_2 &= \int_0^t K(t-s)(F(\tilde{C(t)}, \tilde{C(s)})\nabla w(s), \nabla w(t))\, ds \; , && (2.26)\\
P_3 &= \int_0^t K(t-s)((F(C(t),C(s)) - F(\tilde{C}(t),\tilde{C}(s)))\nabla C(s), \nabla w(t))\, ds \; . && (2.27)
\end{aligned}$$

As $|G| \geq G_0 > 0$, we get

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2 + G_0|w(t)|_1^2 \leq P_1 + P_2 + P_3 \ . \tag{2.28}$$

To estimate P_1 we begin by considering the mean value theorem to obtain

$$P_1 \leq \|C(t)\|_{W^{1,\infty}(\Omega)} G_b' \|w(t)\| |w(t)|_1 \ ,$$

where $|G'| \leq G_b'$ in $\mathbb{R}$. Then, applying Cauchy's inequality we conclude

$$P_1 \leq \frac{\|C(t)\|^2_{W^{1,\infty}(\Omega)}}{4\xi_1}(G_b')^2\|w(t)\|^2 + \xi_1|w(t)|_1^2 \ , \tag{2.29}$$

where $\xi_1 > 0$ is an arbitrary constant.

For P_2 if follows that

$$P_2 \leq F_b \int_0^t K(t-s)|w(s)|_1 ds |w(t)|_1 \ ,$$

where $|F| \leq F_b$ in $\mathbb{R}^2$. Then by Cauchy's inequality and since $K \in L^2(0,T)$, we conclude

$$P_2 \leq \frac{F_b^2}{4\xi_2}\|K\|^2_{L^2(0,T)} \int_0^t |w(s)|_1^2 ds + \xi_2|w(t)|_1^2 \ , \tag{2.30}$$

where $\xi_2 > 0$ is an arbitrary constant.

For P_3 using the Mean Value Theorem we obtain

$$\begin{aligned} P_3 \ \leq \ & F_{x,b}\|C\|_{L^\infty(0,T;W^{1,\infty}(\Omega))} \int_0^t K(t-s)ds \|w(t)\| |w(t)|_1 \\ & + F_{y,b}\|C\|_{L^\infty(0,T;W^{1,\infty}(\Omega))} \int_0^t K(t-s)\|w(s)\| ds |w(t)|_1 \end{aligned}$$

where $|\partial_x F| \leq F_{x,b}$ and $\left|\partial_y F\right| \leq F_{y,b}$ in $\mathbb{R}^2$. Then by Cauchy's and Poincaré-Friedrich's inequalities we deduce

$$\begin{aligned} P_3 \ \leq \ & \frac{\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))}}{4\xi_3}\left((F_{x,b})^2\|K\|^4_{L^1(0,T)}\|w(t)\| + a_\Omega(F_{y,b})^2\|K\|^2_{L^2(0,T)}\int_0^t |w(s)|_1^2 ds\right) \\ & + 2\xi_3|w(t)|_1^2 \ , \end{aligned} \tag{2.31}$$

where $\xi_3 > 0$ is an arbitrary constant.

Applying inequalities (2.29), (2.30) and (2.31) to (2.28) and considering $\xi = \xi_i$ for $i = 1,2,3$, we obtain

$$\frac{d}{dt}\left(\|w(t)\|^2 + \int_0^t |w(s)|_1^2 ds\right) \leq \Theta\left(\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))} + 1\right)\left(\|w(t)\|^2 + \int_0^t |w(s)|_1^2 ds\right) \ ,$$

where

$$\Theta = \frac{\frac{1}{2\xi}\max\{(G_b')^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)},\, F_b^2\|K\|^2_{L^2(0,T)},\, a_\Omega(F_{y,b})^2\|K\|^2_{L^2(0,T)}\}}{\min\{1,2(G_0-4\xi)\}}\ ,$$

when ξ is fixed by

$$G_0-4\xi>0\ .$$

Therefore there exists a constant c_1 depending on the coefficients functions G, F and the kernel K such that

$$\|w(t)\|^2+\int_0^t|w(s)|_1^2ds \le \|w_0\|^2+c_1\left(\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))}+1\right)\int_0^t\left(\|w(s)\|^2+\int_0^s|w(r)|_1^2dr\right)ds\ .$$

Finally applying Gronwall lemma we conclude (2.23). □

If we consider two solutions C and $\tilde{C}$ of (**VP**), smooth enough in the sense that the conditions of Theorem 2.1 are satisfied, with initial concentrations $C(0)$ and $\tilde{C}(0)$ respectively, then inequality (2.23) means that (**VP**) is stable under initial perturbations for bounded time intervals.

As we have mentioned before, it is possible to reduce the smoothness conditions over the kernel function K, by imposing stronger conditions on the coefficient functions G and F. Moreover we note that in the upper bound (2.23), we have an amplification factor $e^{\Theta t}$. In the following result we also show that this amplification factor can be reduced to the unity.

Corollary 2.1. *Let $K\in L^1(0,T)$ and G, F, C, $\tilde{C}$ satisfy the assumptions of Theorem 2.1, if $\xi>0$ is such that*

$$\begin{aligned} d_1 &= G_0-3\xi-\frac{a_\Omega}{4\xi}\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))}\left((G_b')^2+(F_{y,b})^2\|K\|^4_{L^1(0,T)}\right)\\ &\quad -a_\Omega\|C\|_{L^\infty(0,T;W^{1,\infty}(\Omega))}F_{x,b}\|K\|^2_{L^1(0,T)}-\frac{1}{4\xi}F_b^2\|K\|^4_{L^1(0,T)}>0\ , \end{aligned} \tag{2.32}$$

then

$$\|w(t)\|^2+\int_0^t|w(s)|_1^2ds\le\frac{1}{\min\{1,2d_1\}}\|w_0\|^2\ . \tag{2.33}$$

Proof. From the proof of Theorem (2.1), we have from (2.28) and the estimate (2.29) that

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2+(G_0-\xi_1)|w(t)|_1^2\le\frac{\|C(t)\|^2_{W^{1,\infty}(\Omega)}}{4\xi_1}(G_b')^2\|w(t)\|^2+P_2+P_3\ , \tag{2.34}$$

where P_2 and P_3 are defined respectively by (2.26) and (2.27), the constant $\xi_1>0$ is arbitrary. In what follows we estimate P_2 and P_3.

For P_2 we have that

$$P_2 \le \frac{F_b^2\|K\|^2_{L^1(0,T)}}{4\xi_2}\int_0^t|K(t-s)||w(s)|_1^2ds+\xi_2|w(t)|_1^2\ , \tag{2.35}$$

where $\xi_2 > 0$ is an arbitrary constant.

For P_3 we obtain

$$
\begin{aligned}
P_3 \;\leq\;& \left(a_\Omega \|C\|_{L^\infty(0,T;W^{1,\infty}(\Omega))} F_{x,b} \|K\|^2_{L^1(0,T)} + \xi_3\right) |w(t)|_1^2 \\
&+ \frac{a_\Omega}{4\xi_3} \|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))} (F_{y,b})^2 \|K\|^2_{L^1(0,T)} \int_0^t |K(t-s)|\; |w(s)|_1^2 ds\,, \qquad (2.36)
\end{aligned}
$$

where $\xi_3 > 0$ is an arbitrary constant.

Then applying the estimates (2.35) and (2.36) to (2.34) (with $\xi = \xi_i$, for $i = 1,2,3$) and integrating with respect to t, we deduce

$$
\begin{aligned}
&\|w(t)\|^2 + 2\left(G_0 - 3\xi - \frac{a_\Omega}{4\xi}\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))} (G_b')^2\right. \\
&\left.+ a_\Omega \|C\|_{L^\infty(0,T;W^{1,\infty}(\Omega))} F_{x,b} \|K\|^2_{L^1(0,T)}\right) \int_0^t |w(s)|_1^2 ds \\
&\leq \|w_0\|^2 + \frac{1}{2\xi}\left(\|C\|^2_{L^\infty(0,T;W^{1,\infty}(\Omega))} a_\Omega (F_{y,b})^2 \|K\|^2_{L^1(0,T)}\right. \\
&\left.- F_b^2 \|K\|^2_{L^1(0,T)}\right) \int_0^t \int_0^s |K(s-r)|\; |w(r)|_1^2 dr\, ds\,. \qquad (2.37)
\end{aligned}
$$

Note that by changing the order of integration we have

$$
\int_0^t \int_0^s K(s-r)|w(r)|_1^2 dr\, ds = \int_0^t \left(\int_r^t K(s-r) ds\right) |w(r)|_1^2 dr \leq \|K\|^2_{L^1(0,T)} \int_0^t |w(s)|_1^2 ds\,.
$$

Thus we deduce from (2.37) that

$$
\|w(t)\|^2 + \int_0^t |w(s)|_1^2 ds \leq \frac{1}{\min\{1, 2d_1\}} \|w_0\|^2\,,
$$

where d_1 is defined as in (2.32). Finally, we conclude (2.33) provided that $d_1 > 0$. □

When F is defined by (2.6) the smoothness conditions of Theorem 2.1 over F can be satisfied provided that D_v and f are smooth enough. Namely, $D_v \in \mathscr{C}_B^1(\mathbb{R})$ and $f \in \mathscr{C}_B^2(\mathbb{R})$. Note that when f is defined as in (1.24) and D_v is given by (1.33) in the context of physically meaningful values of C the previous smoothness conditions are satisfied.

When G is defined by (2.5), in addition to assuming that $D_v \in \mathscr{C}_B^1(\mathbb{R})$ and $f \in \mathscr{C}_B^2(\mathbb{R})$, if we consider that $D \in \mathscr{C}_B^1((R))$, then the smoothness conditions of Theorem 2.1 over G can be satisfied. Note that when D is defined as in (1.34), the condition $D \in \mathscr{C}_B^1((R))$ is clearly satisfied.

As we also need for G to be bounded from below, the inequality

$$
D(C(t)) > E(0) D_v(C(t)) f'(C(t)),\ \forall t \in [0,T]\,, \qquad (2.38)
$$

must be satisfied. Hence we need to impose the following condition on the coefficients

$$
D_0 - E(0) D_{v,b} f_b' > 0\,, \qquad (2.39)
$$

where $D \geq D_0 > 0$, $|D_v| \leq D_{v,b}$ and $|f'| \leq f'_b$.

We note that (2.39) is a reasonable assumption. Indeed, from the mathematical point of view it means that the parabolic part of (1.6) has to dominate over the hyperbolic part of the equation. From the physical point of view it means that the non-Fickian part of (1.6) cannot dominate the equation because it would lead to a negative total flux.

Notice that when K is defined as in (2.11), the condition $K \in L^2(0,T)$ is clearly satisfied.

Chapter 3

Stability and convergence of the discrete model

In this chapter we study the piecewise linear finite element method used in the first chapter to illustrate the qualitative behavior of the new non-fickian model introduced in this work. For the ease of presentation the problem is studied for the one dimensional case with $\Omega = [0, b]$.

We start by introducing a semi-discrete approximation of the IBVP (2.3), (1.7) and (2.2). For the semi-discrete approximation we establish a version of Theorem 2.1 and Corollary 2.1. Moreover, we establish error estimates that show that the error introduced by the semi-discretization is second order convergent in space. Then, we introduce the full discretization of the problem and deduce the fully discrete method to compute an approximation for the solution of the IBVP under consideration.

Following an implicit-explicit approach: the semi-discrete problem is integrated in time using an implicit-explicit method and we discretize the integral term using a rectangular rule. The implicit-explicit approach allows the reduction of the computational cost maintaining good stability properties. For the fully discrete approximation we deduce fully discrete versions of the results established for the semi-discrete approximation.

3.1 Notation and preliminary results

Let $h = (h_1, h_2, ..., h_N)$ be such that $\sum_{j=1}^{N} h_j = b$. We consider a sequence of vectors of step-sizes $h = (h_1, \ldots, h_N)$ such that, as $N \to \infty$, $h_{max} = \max_{j=1,\ldots,N} h_j \to 0$. Each vector $h = (h_1, \ldots, h_N)$ induces in $\overline{\Omega}$ the nonuniform grid $I_h = \left\{x_j,\ j = 0, 1, .., N\right\}$ with $x_0 = 0$, $x_N = b$ and $x_j - x_{j-1} = h_j$. We denote by $\mathbb{W}_h$ the space of grid functions defined in I_h. By D_{-x} we denote the usual backward finite difference operator and by $D_x^{\frac{1}{2}}$ the finite difference operator defined as in (1.39).

We also introduce the following notation:

$$
\begin{aligned}
g_h(x_j) &= \frac{1}{h_{j+\frac{1}{2}}}\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} g(x)\,dx, \quad j=1,\dots,N-1\ , && (3.1)\\
g_h(x_0) &= \frac{2}{h_1}\int_0^{x_{1-\frac{1}{2}}} g(x)dx\ , && (3.2)\\
g_h(x_N) &= \frac{2}{h_N}\int_{x_{N-\frac{1}{2}}}^{b} g(x)\,dx\ . && (3.3)
\end{aligned}
$$

By $\mathbb{W}_{h,0}$ we represent the subspace of $\mathbb{W}_h$ of functions null on the boundary points. For $u_h,\ v_h \in \mathbb{W}_{h,0}$ we introduce the inner product

$$
(u_h, v_h)_h = \sum_{j=1}^{N-1} h_{j+\frac{1}{2}} u_h(x_j) v_h(x_j)\ .
$$

We denote by $\|.\|_h$ the norm induced by the above inner product. For $u_h,\ v_h \in \mathbb{W}_h$ we introduce the notations

$$
(u_h, v_h)_+ = \sum_{j=1}^{N} h_j u_h(x_j) v_h(x_j)\ ,
$$

and

$$
\|u_h\|_+^2 = \sum_{j=1}^{N} h_j (u_h(x_j))^2\ .
$$

In $\mathbb{W}_h$ we introduce the norm $\|.\|_{1,h}$ defined by

$$
\|u_h\|_{1,h}^2 = \|u_h\|_h^2 + \|D_{-x}u_h\|_+^2\ ,\ u_h \in \mathbb{W}_h\ .
$$

Note that for all $u_h \in \mathbb{W}_h$ and $v_h \in \mathbb{W}_{h,0}$ we have that

$$
\begin{aligned}
(D_x^{\frac{1}{2}} u_h, v_h)_h &= \sum_{j=1}^{N-1} u_h(x_{j+1}) v_h(x_j) - \sum_{j=1}^{N-1} u_h(x_j) v_h(x_j)\\
&= \sum_{j=1}^{N} u_h(x_j) v_h(x_{j-1}) - \sum_{j=1}^{N} u_h(x_j) v_h(x_j)\\
&= -\sum_{j=1}^{N} h_j u_h(x_j) \left(\frac{v_h(x_j) - v_h(x_{j-1})}{h_j}\right)\\
&= -(u_h, D_{-x}v_h)_+\ .
\end{aligned}
$$

Let $\mathscr{W}_h(0,T)$ be defined by $\mathscr{W}_h(0,T) = \{v \in L^2(0,T;\mathbb{W}_{h,0}) : v' \in L^2(0,T;\mathbb{W}_h^{-1})\}$, where $\mathbb{W}_h^{-1}$ denotes the dual space of $\mathbb{W}_h$.

As some smoothness on the numerical approximation C_h is needed, we denote by $\mathscr{C}^1(0,T;\mathbb{W}_h)$ the space of functions $u_h : [0,T] \mapsto \mathbb{W}_h$ which have first order continuous derivative with respect to the norm $\|.\|_{1,h}$.

By $\mathbb{W}_h^{1,\infty}$ we denote the space of functions $v_h : \mathbb{W}_h \to \mathbb{R}$ such that

$$\|v_h\|_{\mathbb{W}_h^{1,\infty}} = \max_{j=1,\dots,\,N-1} |v_h(x_j)| + \max_{j=1,\dots,\,N} |D_{-x}v_h(x_j)| < \infty \,, \tag{3.4}$$

and by $L^\infty(0,T;\mathbb{W}_h^{1,\infty})$ the space of functions $v : [0,T] \to \mathbb{W}_h^{1,\infty}$ such that

$$\|v_h\|_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})} = \underset{[0,T]}{ess\ sup}\, \|v_h(t)\|_{\mathbb{W}_h^{1,\infty}} < \infty \,.$$

We denote by $W^{k,p}(\Omega)$ the Sobolev space of functions v in $L^p(\Omega)$ such that for every multi-index α with $|\alpha| \le k$, the α^{th}-weak partial derivative of v, denoted as $D^\alpha v$, is also in $L^p(\Omega)$. In this space we consider the following norm

$$\|v\|_{W^{k,p}(\Omega)}^p = \sum_{|\alpha|\le k} \|v\|_{L^p(\Omega)}^p \,.$$

The discrete Poincaré-Friedrich's inequality

$$\|v_h\|_h^2 \le a_b \|D_{-x}v_h\|_+^2,\ v \in \mathbb{W}_{h,0}, \tag{3.5}$$

where a_b is a positive constant, will be used in the proof of the results that we present in this chapter.

In order to estimate the truncation error induced by the spatial discretization the following lemma, known as the Bramble-Hilbert Lemma, will be used extensively in this work.

Lemma (Bramble-Hilbert Lemma, [3])**.** *Let Ω be an open subset of $\mathbb{R}^n$ with a Lipschitz-continuous boundary. For some integer $k \ge 0$ and some number $p \in [0,\infty]$, let λ be a continuous linear form on the space $W^{k+1,p}(\Omega)$ with the property that*

$$\forall u \in P_k(\Omega), \quad \lambda(u) = 0 \,,$$

where P_k represents the space of polynomials of degree k. Then there exists a constant $c(\Omega)$ such that

$$\forall v \in W^{k+1,p}(\Omega), \quad |\lambda(v)| \le c(\Omega) \|\lambda\|_{W^{k+1,p}(\Omega)}^\star |v|_{W^{k+1,p}(\Omega)} \,,$$

where $\|.\|_{W^{k+1,p}(\Omega)}^\star$ denotes the norm in the dual space of $W^{k+1,p}(\Omega)$.

Let V be a Banach space. For $s = 0,1$, by $\mathscr{C}^s(0,T;V)$ we denote the space of functions $v : [0,T] \to V$ such that $v^{(s)} : [0,T] \to V$ is continuous and

$$\|v\|_{\mathscr{C}^s(0,T;V)} = \max_{[0,T]} \|v^{(s)}(t)\|_V < \infty \,.$$

In the proof of the convergence result for the fully-discrete case, the following discrete Gronwall lemma will be used:

Lemma 3.1. *(Discrete Gronwall Lemma -Lemma 4.3 of [7]) Let y_n, $n \in \mathbb{N}$, be a sequence of nonnegative real numbers satisfying*

$$y_n \leq \beta_n + \sum_{l=0}^{n-1} f_l y_l, \in \mathbb{N} ,$$

where $f_l \geq 0$ and β_n, $n \in \mathbb{N}$, is a nondecreasing sequence of nonnegative numbers. Then

$$y_n \leq \beta_n exp\left(\sum_{l=0}^{n-1} f_l\right), \quad n \in \mathbb{N} .$$

3.2 Semi-discrete problem

In order to introduce the semi-discrete formulation of (**VP**), we begin by introducing the semi-discrete approximation $C_h(t)$ for the solution $C(t)$ of the IBVP (2.3), (1.7) and (2.2), defined as

$$\begin{aligned} \frac{dC_h}{dt}(x_j,t) &= D_x^{\frac{1}{2}}\left(G(M_hC_h(x_j,t))D_{-x}C_h(x_j,t)\right) \\ &+D_x^{\frac{1}{2}}\left(\int_0^t K(t-s)F(M_hC_h(x_j,t),M_hC_h(x_j,s))D_{-x}C_h(x_j,s)ds\right) \\ &+Z_h(x_j,t) , \end{aligned} \tag{3.6}$$

for $j = 1,2,..,N-1$ and $t \in (0,T]$.

Equation (3.6) is coupled with the initial condition

$$C_h(x_j,0) = C_0, \text{ for } j = 1,2,.., N-1 , \tag{3.7}$$

and we assume for simplicity the homogeneous boundary conditions

$$C(0,t) = 0 \text{ for } t \in (0,T] , \tag{3.8}$$
$$C(b,t) = 0 \text{ for } t \in (0,T] . \tag{3.9}$$

The semi-discrete variational problem is defined by (**SDVP**): Find $C_h \in \mathscr{W}_h(0,T)$ such that (3.7) holds and

$$\begin{aligned} &(\frac{dC_h}{dt}(t),v_h)_h + (G(M_hC_h(t))D_{-x}C_h(t),D_{-x}v_h)_+ \\ &+\int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}C_h(s),D_{-x}v_h)_+ds \\ &= (Z_h(t),v_h)_h , \quad \text{a.e. in (0,T)}, \ \forall\, v_h \in \mathbb{W}_{h,0} . \end{aligned} \tag{3.10}$$

3.2.1 Semi-discrete stability

In what follows we establish a semi-discrete version of Theorem 2.1 and Corollary 2.1. Analogously as in the continuous case, we will fix a solution C_h and we analyze the behavior of $w_h = C_h - \tilde{C}_h$, where $\tilde{C}$ is another solution of (**SDVP**), corresponding to a perturbed initial condition.

Theorem 3.1. *Let us suppose that $K \in L^2(0,T)$, $G \in \mathscr{C}^1_B(\mathbb{R})$, $F \in \mathscr{C}^1_B(\mathbb{R}^2)$ and $0 < G_0 \leq G$. If C_h and $\tilde{C}_h$ are solutions of (**SDVP**) such that $C_h, \tilde{C}_h \in \mathscr{C}^1(0,T;\mathbb{W}_h) \bigcap \mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})$, then for $w_h(t) = C_h(t) - \tilde{C}_h(t)$, with $w_h(0) = w_{h,0}$, there exists a positive constant c_1 depending on the coefficients functions G, F and on the kernel K such that*

$$\|w_h(t)\|_h^2 + \int_0^t \|D_{-x}w_h(s)\|_+^2 ds \leq \|w_{h,0}\|_h^2 e^{c_1(\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}+1)t} . \tag{3.11}$$

Proof. Following the proof of Theorem 2.1, from (3.10) we obtain

$$\frac{1}{2}\frac{d}{dt}\|w_h(t)\|_h^2 + G_0\|D_{-x}w_h(t)\|_+^2 \leq P_{h,1} + P_{h,2} + P_{h,3} , \tag{3.12}$$

where

$$P_{h,1} = ((G(M_hC_h(t)) - G(M_h\tilde{C}_h(t)))D_{-x}C_h(t), D_{-x}w_h(t))_+ , \tag{3.13}$$

$$P_{h,2} = \int_0^t K(t-s)(F(M_h\tilde{C}_h(t), M_h\tilde{C}_h(s))D_{-x}w_h(s), D_{-x}w_h(t))_+ ds , \tag{3.14}$$

$$P_{h,3} = \int_0^t K(t-s)((F(M_hC_h(t), M_hC_h(s)) - F(\tilde{C}_h(t), \tilde{C}_h(s)))D_{-x}C_h(s), D_{-x}w_h(t))_+ ds . \tag{3.15}$$

In what follows, we estimate separately the terms $P_{h,1}$, $P_{h,2}$ and $P_{h,3}$.

To estimate $P_{h,1}$ by the Mean Value Theorem and Cauchy's inequality we obtain

$$|P_{h,1}| \leq \frac{\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}(G_b')^2\|w_h(t)\|_h^2 + \xi\|D_{-x}w_h(t)\|_+^2 , \tag{3.16}$$

where $\xi > 0$ is an arbitrary constant.

For $P_{h,2}$, from Cauchy's inequality, it follows that

$$|P_{h,2}| \leq \frac{F_b^2}{4\xi}\|K\|^2_{L^2(0,T)}\int_0^t \|D_{-x}w_h(s)\|_+^2 ds + \xi\|D_{-x}w_h(t)\|_+^2 . \tag{3.17}$$

For $P_{h,3}$ using the Mean Value Theorem, Cauchy's inequality and the discrete Poincaré-Friedrich's inequality, we deduce

$$\begin{aligned} |P_{h,3}| \leq\ & \frac{\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}\Big((F_{x,b})^2\|K\|^4_{L^1(0,T)}\|w_h(t)\|_h^2 \\ & + a_b(F_{y,b})^2\|K\|^2_{L^2(0,T)}\int_0^t \|D_{-x}w_h(s)\|_+^2 ds\Big) + 2\xi\|D_{-x}w_h(t)\|_+^2 . \end{aligned} \tag{3.18}$$

Applying inequalities (3.16), (3.17) and (3.18) to (3.12) we obtain

$$\begin{aligned}&\frac{d}{dt}\left(\|w_h(t)\|_h^2+\int_0^t\|D_{-x}w_h(s)\|_+^2ds\right)\\&\leq\Theta\left(\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}+1\right)\left(\|w_h(t)\|_h^2+\int_0^t|D_{-x}w_h(s)|_+^2ds\right)\ ,\end{aligned}$$

where

$$\Theta\ =\ \frac{\frac{1}{2\xi}\max\{(G_b')^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)},F_b^2\|K\|^2_{L^2(0,T)},a_b(F_{y,b})^2\|K\|^2_{L^2(0,T)}\}}{\min\{1,2(G_0-4\xi)\}}\ ,$$

and ξ is fixed by

$$G_0-4\xi>0\ .$$

Therefore there exists a constant c_1 depending on the coefficients functions G, F and the kernel K such that

$$\begin{aligned}&\|w_h(t)\|^2+\int_0^t\|D_{-x}w_h(s)\|_+^2ds\\&\leq c_1\left(\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}+1\right)\int_0^t\left(\|w_h(s)\|_h^2+\int_0^s\|D_{-x}w_h(r)\|_+^2dr\right)ds+\|w_{h,0}\|^2\ .\end{aligned}$$

Finally the application of Gronwall lemma leads to (3.11).

□

We note that inequality (3.11) means that (**SDVP**) is stable under initial perturbations for bounded time intervals. Once again, it is possible to consider less smoothness conditions over the kernel function K and reduce to the unity the amplification factor $e^{\Theta t}$, provided that we impose stronger restrictions on the coefficient functions G and F.

Corollary 3.1. *If $K\in L^1(0,T)$, under the assumptions of Theorem 3.1 for G, F, C_h and $\tilde{C}_h$, provided that $\xi>0$ is such that*

$$\begin{aligned}d_2\ =\ &G_0-3\xi-\frac{a_b}{4\xi}\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}\left((G_b')^2+(F_{y,b})^2\|K\|^4_{L^1(0,T)}\right)-\frac{F_b^2}{4\xi}\|K\|^4_{L^1(0,T)}\\&-a_b\|C_h\|_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}F_{x,b}\|K\|^2_{L^1(0,T)}>0\ ,\end{aligned}\tag{3.19}$$

then

$$\|w_h(t)\|_h^2+\int_0^t\|D_{-x}w_h(s)\|_+^2ds\leq\frac{1}{\min\{1,2d_2\}}\|w_{h,0}\|_h^2\ .\tag{3.20}$$

Proof. Following the proof of Theorem (3.1) we obtain that

$$\frac{1}{2}\frac{d}{dt}\|w_h(t)\|_h^2+(G_0-\xi)\|D_{-x}w_h(t)\|_+^2\leq\frac{\|C_h\|^2_{L^\infty(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}(G_b')^2\|w_h(t)\|_h^2+P_{h,2}+P_{h,3}\ ,\tag{3.21}$$

where $P_{h,2}$ and $P_{h,3}$ are defined respectively by (3.14) and (3.15).

We estimate now the terms $\hat{P}_{h,2}$ and $\hat{P}_{h,2}$.

For $\hat{P}_{h,2}$ we have that the next inequality holds

$$|P_{h,2}| \leq \frac{F_b^2}{4\xi}\|K\|^2_{L^1(0,T)}\int_0^t |K(t-s)|\ \|D_{-x}w_h(s)|^2_+ ds + \xi\|D_{-x}w_h(t)\|^2_+ \ . \tag{3.22}$$

For $P_{h,3}$ we obtain the following estimate

$$\begin{aligned} |P_{h,3}| \ &\leq \ \frac{a_b}{4\xi}\|C_h\|^2_{L^\infty(0,T;\mathbb{W}^{1,\infty}_h)}(F_{y,b})^2\|K\|^2_{L^1(0,T)}\int_0^t |K(t-s)|\ \|D_{-x}w_h(s)\|^2_+ ds \\ &+\Big(a_b\|C_h\|_{L^\infty(0,T;\mathbb{W}^{1,\infty}_h)}F_{x,b}\|K\|^2_{L^1(0,T)}+\xi\Big)\|D_{-x}w_h(t)\|^2_+ \ . \end{aligned} \tag{3.23}$$

Then applying inequalities (3.22) and (3.23) to (3.21), integrating with respect to t and changing the order of integration, we deduce

$$\|w_h(t)\|^2_h + 2d_2\int_0^t \|D_{-x}w_h(s)\|^2_+ ds \leq \|w_{h,0}\|^2_h \ ,$$

where d_2 is defined as in (3.19). Then provided that $d_2 > 0$ we conclude (3.20). □

3.2.2 Convergence analysis

Let $C(t)$ and $C_h(t)$ be the solutions of (**VP**) and (**SDVP**) respectively, we represent by $E_h(t)$ the error induced by the spatial discretization introduced in (3.6), with $E_h(t) = R_hC(t) - C_h(t)$, where $R_h : \mathscr{C}([0,b]) \mapsto \mathbb{R}$ denotes the pointwise restriction operator

$$R_hu(x_j) = u(x_j) \ \text{ for } \ j = 0,1,.., N \ .$$

The convergence analysis that follows is not the one usually used in the literature and which was introduced by Wheeler in [52]. Wheeler's approach is based on the following splitting of the error

$$E_h(t) = \rho_h(t) + \theta(t) \ ,$$

where $\rho_h(t) = R_hC(t) - \tilde{C}_h(t)$ and $\theta(t) = \tilde{C}_h(t) - C_h(t)$ being $\tilde{C}_h(t)$ the solution of an elliptic problem that depends on t. In [2], a one dimensional linear version of (2.3) was considered and the authors proved, following the previous approach, that $\|E_h(t)\|_h = O(h^2_{max})$ and $\|D_{-x}E_h(t)\|_+ = O(h^2_{max})$ under the following smoothness assumption:

$$C \in H^1(0,T,H^3(0,b)) \cap L^2(0,T,H^3(0,b) \cap H^1_0(0,b)) \ . \tag{3.24}$$

We will follow the approach introduced in [26] for a two dimensional linear version of (2.3). The authors showed that by using their approach, it is possible to weaken the smoothness conditions that are required when Wheeler's splitting technic is used. Thus (3.24) can be replaced by

$$C \in H^1(0,T;H^2(0,b)) \bigcap L^2(0,T;H^3(0,b) \cap H^1_0(0,b)) \ . \tag{3.25}$$

In order to simplify the presentation of the proof of the convergence result that follows we introduce the following auxiliary lemmas.

Lemma 3.2. *Let g be a function defined over an interval $[0,b]$ such that $g \in H^2(0,b)$. If we consider a nonuniform grid $I_h = \{x_j,\ j = 0,1,..,N\}$ with $x_0 = 0$, $x_N = b$ and $x_j - x_{j-1} = h_j$, then for the functional*

$$\lambda(g) = \frac{h_j}{2}(g(x_j) + g(x_{j-1})) - \int_{x_{j-1}}^{x_j} g(x)dx \,,$$

there exists a constant c such that

$$|\lambda(g)| \le c h_j^2 \|g''\|_{L^1(x_{j-1},\, x_j)} \,. \tag{3.26}$$

Proof. Let v be a function defined by $v(\delta) = g(x_{j-1} + h_j\delta)$ for $\delta \in [0,1]$. Then we have that

$$\lambda(g) = h_j \left(\frac{1}{2}(v(1) + v(0)) - \int_0^1 v(\delta)d\delta \right) \,.$$

The functional

$$\hat{\lambda}(v) = \frac{1}{2}(v(1) + v(0)) - \int_0^1 v(\delta)d\delta \,,$$

is bounded in $H^2(0,1)$ and vanishes for $v = 1$ and $v = \delta$. Therefore by the Bramble-Hilbert Lemma there exists a constant c such that

$$\left|\hat{\lambda}(v)\right| \le c\|v''\|_{L^1(0,1)} \,.$$

As $\|v''\|_{L^1(0,1)} = h_j\|g''\|_{L^1(x_{j-1},\, x_j)}$ we conclude (3.26). □

Lemma 3.3. *Let g be a function defined over an interval $[0,b]$ such that $g \in H^1(0,b)$. If we consider a nonuniform grid $I_h = \{x_j,\ j = 0,1,..,N\}$ with $x_0 = 0$, $x_N = b$ and $x_j - x_{j-1} = h_j$, then for the functional*

$$\lambda(g) = \frac{h_j}{2}(g(x_j) - g(x_{j-1})) + \int_{x_{j-1}}^{x_{j-\frac{1}{2}}} g(x)dx - \int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx \,,$$

there exists a constant c such that

$$|\lambda(g)| \le c h_j \|g'\|_{L^1(x_{j-1},\, x_j)} \,. \tag{3.27}$$

Proof. Let v be a function defined by $v(\delta) = g(x_{j-1} + h_j\delta)$ for $\delta \in [0,1]$. Then we have that

$$\lambda(g) = h_j \left(\frac{1}{2}(v(1) - v(0)) + \int_0^{\frac{1}{2}} v(\delta)d\delta - \int_{\frac{1}{2}}^1 v(\delta)d\delta \right) \,.$$

The functional

$$\hat{\lambda}(v) = \frac{1}{2}(v(1) - v(0)) + \int_0^{\frac{1}{2}} v(\delta)d\delta - \int_{\frac{1}{2}}^1 v(\delta)d\delta \,,$$

is bounded in $H^1(0,1)$ and vanishes for $v = 1$. Therefore by the Bramble-Hilbert Lemma there exists a constant c such that

$$\left|\hat{\lambda}(v)\right| \le c\|v'\|_{L^1(0,1)} \,.$$

As $\|v'\|_{L^1(0,1)} = \|g'\|_{L^1(x_{j-1},\, x_j)}$ we conclude (3.27). □

Lemma 3.4. *Let g be a function defined over an interval $[0,b]$ such that $g \in H^3(0,b)$. If we consider a nonuniform grid $I_h = \{x_j,\ j = 0,1,..,N\}$ with $x_0 = 0$, $x_N = b$ and $x_j - x_{j-1} = h_j$, then for the functional*

$$\lambda(g) = D_{-x}g(x_j) - \frac{\partial g}{\partial x}(x_{j-\frac{1}{2}}) \ ,$$

there exists a constant c such that

$$|\lambda(g)| \leq ch_j \|g'''\|_{L^1(x_{j-1},\, x_j)} \ . \tag{3.28}$$

Proof. Let v be a function defined by $v(\delta) = g(x_{j-1} + h_j\delta)$ for $\delta \in [0,1]$. Then we have that

$$\lambda(g) = \frac{1}{h_j}\left(v(1) - v(0) - v'(\frac{1}{2})\right) \ .$$

The functional

$$\hat{\lambda}(v) = v(1) - v(0) - v'(\frac{1}{2}) \ ,$$

is bounded in $H^3(0,1)$ and vanishes for $v = 1$, $v = \delta$ and $v = \delta^2$. Therefore by the Bramble-Hilbert Lemma there exists a constant c such that

$$\left|\hat{\lambda}(v)\right| \leq c\|v'''\|_{L^1(0,1)} \ .$$

As $\|v'''\|_{L^1(0,1)} = h_j^2\|g'''\|_{L^1(x_{j-1},\, x_j)}$ we conclude (3.28). □

Lemma 3.5. *Let g be a function defined over an interval $[0,b]$ such that $g \in H^2(0,b)$. If we consider a nonuniform grid $I_h = \{x_j,\ j = 0,1,..,N\}$ with $x_0 = 0$, $x_N = b$ and $x_j - x_{j-1} = h_j$, then for the functional*

$$\lambda(g) = \frac{1}{2}\left(g(x_j) + g(x_{j-1})\right) - g(x_{j-\frac{1}{2}}) \ ,$$

there exists a constant c such that

$$|\lambda(g)| \leq ch_j \|g''\|_{L^1(x_{j-1},\, x_j)} \ . \tag{3.29}$$

Proof. Let v be a function defined by $v(\delta) = g(x_{j-1} + h_j\delta)$ for $\delta \in [0,1]$. Then we have that the functional

$$\lambda(g) = \frac{1}{2}(v(1) + v(0)) - v(\frac{1}{2}) \ .$$

is bounded in $H^2(0,1)$ and vanishes for $v = 1$ and $v = \delta$. Therefore by the Bramble-Hilbert Lemma there exists a constant c such that

$$|\lambda(v)| \leq c\|v''\|_{L^1(0,1)} \ .$$

As $\|v''\|_{L^1(0,1)} = h_j\|g''\|_{L^1(x_{j-1},\, x_j)}$ we conclude (3.29). □

In the stability analysis, the smoothness of K had an influence on the estimates that can be obtained. In the convergence analysis that follows, we will also consider two cases depending on the smoothness of K. We begin by assuming that $K \in L^2(0,T)$ to obtain a second order convergence result. Then we assume that $K \in L^1(0,T)$ to obtain another second order convergence result with stronger conditions on the coefficient functions G and F.

Theorem 3.2. *Let us suppose that $K \in L^2(0,T)$, $G \in \mathscr{C}_B^1(\mathbb{R})$, $F \in \mathscr{C}_B^1(\mathbb{R}^2)$ and $0 < G_0 \leq G$. If C and C_h are solutions of (**VP**) and (**SDVP**) respectively, such that C satisfies* (3.25)*, then there exist constants $\hat{c}_1$ and $\hat{c}_2$ depending on the coefficient functions G, F and on the kernel K such that*

$$\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds \leq \hat{c}_2 h_{max}^4 e^{\hat{c}_1(\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}+1)t} \int_0^t T_r(s)ds\ , \tag{3.30}$$

where

$$T_r(t) = \left\|\frac{\partial C}{\partial t}(t)\right\|^2_{H^2(0,b)} + (\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}+1)\left(\|C(t)\|^2_{H^3(0,b)} + \int_0^t \|C(s)\|^2_{H^3(0,b)}ds\right) \tag{3.31}$$

Proof. As we have

$$\frac{dE_h}{dt}(t) \ \ = \ \ R_h\frac{\partial C}{\partial t}(t) - \frac{dC_h}{dt}(t)\ ,$$

multiplying by $E_h(t)$ with respect to $(,)_h$ and considering (3.6), we deduce

$$\begin{aligned}(\frac{dE_h}{dt}(t),E_h(t))_h \ \ = \ \ & (R_h\frac{\partial C}{\partial t}(t),E_h(t))_h + (G(M_hC_h(t))D_{-x}C_h(t),D_{-x}E_h(t))_+ \\ & + \int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}C_h(s),D_{-x}E_h(t))_+ ds \\ & -(Z_h(t),E_h(t))_h\ .\end{aligned} \tag{3.32}$$

As we have that

$$\begin{aligned}&\sum_{j=1}^{N-1}\left(\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} \frac{\partial^2 C}{\partial x^2}(x,t)dx\right)E_h(x_j,t) \\ &= \sum_{j=1}^{N}\frac{\partial C}{\partial x}(x_{j-\frac{1}{2}},t)dx\, E_h(x_{j-1},t) - \sum_{j=1}^{N}\frac{\partial C}{\partial x}(x_{j-\frac{1}{2}},t)dx\, E_h(x_j,t) \\ &= -\sum_{j=1}^{N} h_j\hat{M}_h\frac{\partial C}{\partial x}(x_j,t)D_{-x}E_h(x_j,t)\ ,\end{aligned}$$

where $\hat{M}_h$ is defined by $\hat{M}_h v(x_j) = R_h v(x_{j-\frac{1}{2}})$, then we obtain

$$\begin{aligned}(Z_h(t),E_h(t))_h \ \ = \ \ & (\left(\frac{\partial C}{\partial t}\right)_h(t),E_h(t))_h + (G(\hat{M}_hC(t))\hat{M}_h\frac{\partial C}{\partial x}(t),D_{-x}E_h(t))_+ \\ & + \int_0^t K(t-s)(F(\hat{M}_hC(t),\hat{M}_hC(s))\hat{M}_h\frac{\partial C}{\partial x}(s),D_{-x}E_h(t))_+ ds\ ,\end{aligned} \tag{3.33}$$

where $\left(\frac{\partial C}{\partial t}\right)_h(t)$ is defined by (3.1)-(3.3) with g replaced by $\frac{\partial C}{\partial t}(t)$

Summing and subtracting the terms

$$(G(M_hC(t))D_{-x}R_hC(t),D_{-x}E_h(t))_+\ ,\ \int_0^t K(t-s)(F(M_hC(t),M_hC(s))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds\ ,$$

in (3.33), we get that

$$\begin{aligned}
&(Z_h(t),E_h(t))_h\\
&= -(G(M_hC(t))D_{-x}R_hC(t)-G(\hat{M}_hC(t))\hat{M}_h\frac{\partial C}{\partial x}(t),D_{-x}E_h(t))_+\\
&\quad +(G(M_hC(t))D_{-x}R_hC(t),D_{-x}E_h(t))_+\\
&\quad -\int_0^t K(t-s)(F(M_hC(t),M_hC(s))D_{-x}R_hC(s)-F(\hat{M}_hC(t),\hat{M}_hC(s))\hat{M}_h\frac{\partial C}{\partial x}(s),D_{-x}E_h(t))_+ds\\
&\quad +\int_0^t K(t-s)(F(M_hC(t),M_hC(s))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds+(\left(\frac{\partial C}{\partial t}\right)_h,E_h(t))_h\ . \qquad (3.34)
\end{aligned}$$

From (3.32) and (3.34) we deduce

$$\frac{1}{2}\frac{d}{dt}\|E_h(t)\|_h^2 = T_1+T_2+T_{h,1}+T_{h,2}+T_{h,3}\ , \qquad (3.35)$$

where

$$\begin{aligned}
T_1 &= (G(M_hC_h(t))D_{-x}C_h(t)-G(M_hC(t))D_{-x}R_hC(t),D_{-x}E_h(t))_+\ , &(3.36)\\
T_2 &= \int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}C_h(s)\\
&\quad -F(M_hC(t),M_hC(s))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds\ , &(3.37)\\
T_{h,1} &= (R_h\frac{\partial C}{\partial t}(t)-\left(\frac{\partial C}{\partial t}\right)_h(t),E_h(t))_h\ , &(3.38)\\
T_{h,2} &= (G(M_hC(t))D_{-x}R_hC(t)-G(\hat{M}_hC(t))\hat{M}_h\frac{\partial C}{\partial x}(t),D_{-x}E_h(t))_+\ , &(3.39)\\
T_{h,3} &= \int_0^t K(t-s)(F(M_hC(t),M_hC(s))D_{-x}R_hC(s)\\
&\quad -F(\hat{M}_hC(t),\hat{M}_hC(s))\hat{M}_h\frac{\partial C}{\partial x}(s),D_{-x}E_h(t))_+ds\ . &(3.40)
\end{aligned}$$

In what follows we estimate each of the above terms separately. We begin with T_1. By summing and subtracting the term

$$(G(M_hC_h(t))D_{-x}R_hC(t),D_{-x}E_h(t))_+\ ,$$

we obtain

$$\begin{aligned}
T_1 &= ((G(M_hC_h(t))-G(M_hC(t)))D_{-x}R_hC(t),D_{-x}E_h(t))_+\\
&\quad -(G(M_hC_h(t))D_{-x}E_h(t),D_{-x}E_h(t))_+\ .
\end{aligned}$$

As we have that

$$
\begin{aligned}
&|(((G(M_hC_h(t))-G(M_hC(t)))D_{-x}R_hC(t),D_{-x}E_h(t))_+| \\
&\leq G_b' \sum_{j=1}^{N} D_{-x}R_hC(x_j,t)M_hE(x_j,t)D_{-x}E_h(x_j,t) \\
&\leq G_b' \|C(t)\|_{W^{1,\infty}(0,b)}\|E_h(t)\|_h\|D_{-x}E_h(t)\|_+ \\
&\leq \frac{(G_b')^2}{4\xi_1}\|C(t)\|^2_{W^{1,\infty}(0,b)}\|E_h(t)\|_h^2+\xi_1\|D_{-x}E_h(t)\|_+^2 \ ,
\end{aligned}
$$

where $\xi_1>0$ is arbitrary, then it follows that

$$
|T_1| \leq \frac{(G_b')^2}{4\xi_1}\|C(t)\|^2_{W^{1,\infty}(0,b)}\|E_h(t)\|_h^2+(\xi_1-G_0)\|D_{-x}E_h(t)\|_+^2 \ . \tag{3.41}
$$

To obtain an estimate for T_2 we start by adding and subtracting

$$
\int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds \ ,
$$

to obtain

$$
\begin{aligned}
T_2 \ = \ & -\int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}E_h(s),D_{-x}E_h(t))_+ds \\
&+\int_0^t K(t-s)((F(M_hC_h(t),M_hC_h(s))-F(M_hC(t),M_hC(s)))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds \ .
\end{aligned}
$$

We have successively

$$
\begin{aligned}
&\left|\int_0^t K(t-s)(F(M_hC_h(t),M_hC_h(s))D_{-x}E_h(s),D_{-x}E_h(t))_+ds\right| \\
&\quad\leq \ \|K\|_{L^2(0,T)}F_b\left(\int_0^t \|D_{-x}E_h(s)\|_h^2ds\right)^{\frac{1}{2}}\|D_{-x}E_h(t)\|_+ \\
&\quad\leq \ \frac{F_b^2}{4\xi_2}\|K\|^2_{L^2(0,T)}\int_0^t \|D_{-x}E_h(s)\|_h^2ds+\xi_2\|D_{-x}E_h(t)\|_+ \ ,
\end{aligned}
$$

where $\xi_2>0$ is arbitrary, and

$$
\begin{aligned}
&\left|\int_0^t K(t-s)((F(M_hC_h(t),M_hC_h(s))-F(M_hC(t),M_hC(s)))D_{-x}R_hC(s),D_{-x}E_h(t))_+ds\right| \\
&\leq \ \|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))}\Bigg((a_b)^{\frac{1}{2}}(F_{y,b})\|K\|_{L^2(0,T)}\left(\int_0^t \|D_{-x}E_h(s)\|_h^2ds\right)^{\frac{1}{2}}\|D_{-x}E_h(t)\|_+ \\
&\qquad +(F_{x,b})\|K\|^2_{L^1(0,T)}\|E_h(t)\|_h\|D_{-x}E_h(t)\|_+\Bigg) \\
&\leq \ \frac{\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}}{4\xi_2}\left(a_b(F_{y,b})^2\|K\|^2_{L^2(0,T)}\int_0^t \|D_{-x}E_h(s)\|_h^2ds+(F_{x,b})^2\|K\|^4_{L^1(0,T)}\|E_h(t)\|_h^2\right) \\
&\qquad +2\xi_2\|D_{-x}E_h(t)\|_+^2 \ .
\end{aligned}
$$

Then taking into account the previous estimates we deduce for T_2, the following upper bound holds

$$\begin{aligned}|T_2| \leq\ & \frac{\|K\|^2_{L^2(0,T)}}{4\xi_2}(F_b^2+\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}a_b(F_{y,b})^2)\int_0^t \|D_{-x}E_h(s)\|_h^2 ds \\ & +\frac{\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}}{4\xi_2}(F_{x,b})^2\|K\|^4_{L^1(0,T)}\|E_h(t)\|_h^2+3\xi_2\|D_{-x}E_h(t)\|_+^2 \ . \end{aligned} \tag{3.42}$$

We obtain now an estimate for $T_{h,1}$. In order to simplify the calculations, we use the notation $R_h\frac{\partial C}{\partial t}(x_j,t)=g(x_j)$, for all $j=1,\dots,N$. We have

$$\begin{aligned} T_{h,1} &= \sum_{j=1}^{N-1}\left(h_{j+\frac{1}{2}}g(x_j)-\int_{x_{j-\frac{1}{2}}}^{x_{j+\frac{1}{2}}} g(x)dx\right)E_h(x_j,t) \\ &= \sum_{j=1}^{N-1}\left(\frac{h_j}{2}g(x_j)-\int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx\right)E_h(x_j,t)+\sum_{j=1}^{N-1}\left(\frac{h_{j+1}}{2}g(x_j)-\int_{x_j}^{x_{j+\frac{1}{2}}} g(x)dx\right)E_h(x_j,t) \\ &= \sum_{j=1}^{N}\left(\frac{h_j}{2}g(x_j)-\int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx\right)E_h(x_j,t)+\sum_{j=1}^{N}\left(\frac{h_j}{2}g(x_{j-1})-\int_{x_{j-1}}^{x_{j-\frac{1}{2}}} g(x)dx\right)E_h(x_{j-1},t), \end{aligned}$$

and summing and subtracting the terms

$$\sum_{j=1}^{N}\frac{h_j}{4}g(x_j)E_h(x_{j-1},t) \ \text{ and } \ \sum_{j=1}^{N}\frac{h_j}{4}g(x_{j-1})E_h(x_j,t)\ ,$$

we deduce

$$\begin{aligned} T_{h,1} =\ & \sum_{j=1}^{N}\frac{h_j}{4}(g(x_j)+g(x_{j-1}))(E_h(x_j,t)+E_h(x_{j-1},t)) \\ & +\sum_{j=1}^{N}\frac{h_j}{4}(g(x_j)-g(x_{j-1}))(E_h(x_j,t)-E_h(x_{j-1},t)) \\ & -\sum_{j=1}^{N}\left(\int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx\right)E_h(x_j,t)-\sum_{j=1}^{N}\left(\int_{x_{j-1}}^{x_{j-\frac{1}{2}}} g(x)dx\right)E_h(x_{j-1},t)\ . \end{aligned}$$

Adding and subtracting the terms

$$\sum_{j=1}^{N}\left(\int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx\right)E_h(x_{j-1},t) \ \text{ and } \ \sum_{j=1}^{N}\left(\int_{x_{j-1}}^{x_{j-\frac{1}{2}}} g(x)dx\right)E_h(x_j,t)\ ,$$

we rewrite $T_{h,1}$ as

$$T_{h,1}=T^a_{h,1}+T^b_{h,1}\ , \tag{3.43}$$

where

$$
\begin{aligned}
T_{h,1}^{a} &= \frac{1}{2}\sum_{j=1}^{N}\left(\frac{h_j}{2}(g(x_j)+g(x_{j-1}))-\int_{x_{j-1}}^{x_j} g(x)dx\right)(E_h(x_j,t)+E_h(x_{j-1},t))\ ,\\
T_{h,1}^{b} &= \frac{1}{2}\sum_{j=1}^{N}\left(\frac{h_j}{2}(g(x_j)-g(x_{j-1}))+\int_{x_{j-1}}^{x_{j-\frac{1}{2}}} g(x)dx-\int_{x_{j-\frac{1}{2}}}^{x_j} g(x)dx\right)(E_h(x_j,t)-E_h(x_{j-1},t))\ .
\end{aligned}
$$

To estimate $T_{h,1}^{a}$ we apply Lemma 3.2 and we conclude that there exists a constant c_a satisfying he following

$$
\begin{aligned}
|T_{h,1}^{a}| &\leq \frac{c_a}{2}\sum_{j=1}^{N} h_j^2\|g''\|_{L^1(x_{j-1},\,x_j)}(E_h(x_j,t)+E_h(x_{j-1},t))\\
&\leq \frac{c_a h_{max}^2}{2}\sum_{j=1}^{N}\|g''\|_{L^2(x_{j-1},\,x_j)}h_j^{\frac{1}{2}}E_h(x_j,t)+\frac{c_a h_{max}^2}{2}\sum_{j=1}^{N}\|g''\|_{L^2(x_{j-1},\,x_j)}h_j^{\frac{1}{2}}E_h(x_{j-1},t)\\
&\leq \frac{c_a h_{max}^2}{2}|g|_{H^2(0,b)}\left(\sum_{j=1}^{N-1}h_jE_h^2(x_j,t)\right)^{\frac{1}{2}}+\frac{c_a h_{max}^2}{2}|g|_{H^2(0,b)}\left(\sum_{j=1}^{N-1}h_{j+1}E_h^2(x_j,t)\right)^{\frac{1}{2}}\\
&\leq \frac{a_b c_a^2 h_{max}^4}{2\xi_3}|g|_{H^2(0,b)}^2+\frac{\xi_3}{2}\|D_{-x}E_h(t)\|_{+}^2\ ,
\end{aligned}
\tag{3.44}
$$

where $\xi_3>0$ is arbitrary.

An estimate for $T_{h,1}^{b}$ is obtained applying Lemma 3.3 which guarantee the existence of a positive constant c_b, such that

$$
\begin{aligned}
|T_{h,1}^{b}| &\leq \frac{c_b}{2}\sum_{j=1}^{N}h_j\|g'\|_{L^2(x_{j-1},\,x_j)}(h_j)^{\frac{1}{2}}(E_h(x_j,t)-E_h(x_{j-1},t))\\
&\leq \frac{c_b h_{max}^2}{2}\sum_{j=1}^{N}|g|_{H^1(0,b)}\|D_{-x}E_h(t)\|_{+}\\
&\leq \frac{c_b^2 h_{max}^4}{8\xi_3}|g|_{H^1(0,b)}^2+\frac{\xi_3}{2}\|D_{-x}E_h(t)\|_{+}^2\ .
\end{aligned}
\tag{3.45}
$$

Then from (3.43), (3.44) and (3.45) we obtain

$$
|T_{h,1}| \leq \frac{c_1^2 h_{max}^4}{4\xi_3}\left\|\frac{\partial C}{\partial t}(t)\right\|_{H^2(0,b)}^2+\xi_3\|D_{-x}E_h(t)\|_{+}^2\ ,
\tag{3.46}
$$

where $c_1=\max\{2a_bc_a,\frac{c_b}{2}\}$.

To estimate $T_{h,2}$ we begin by summing and subtracting the term

$$
(G(\hat{M}_hC(t))D_{-x}R_hC(t),D_{-x}E_h(t))_{+}\ ,
$$

obtaining

$$T_{h,2} = T^a_{h,2} + T^b_{h,2} \ , \tag{3.47}$$

where

$$\begin{aligned} T^a_{h,2} &= (G(\hat{M}_h C(t))(D_{-x} R_h C(t) - \hat{M}_h \frac{\partial C}{\partial x}(t)), D_{-x} E_h(t))_+ \ , \\ T^a_{h,2} &= ((G(M_h C(t)) - G(\hat{M}_h C(t))) D_{-x} R_h C(t), D_{-x} E_h(t))_+ \ . \end{aligned}$$

Lemma 3.4 allow us to obtain an estimate for $T^a_{h,2}$. In fact, from this lemma there exists a constant c_2, such that

$$\begin{aligned} |T^a_{h,2}| &\leq h^2_{max} c_2 G_b \, |C(t)|^2_{H^3(0,b)} \, \|D_{-x} E_h(t)\|_+ \\ &\leq \frac{h^4_{max}}{4\xi} c_2^2 G_b^2 \, |C(t)|^2_{H^3(0,b)} + \xi_4 \|D_{-x} E_h(t)\|^2_+ \ , \end{aligned} \tag{3.48}$$

where $\xi_4 > 0$ is arbitrary.

Applying Mean Value Theorem to $T^b_{h,2}$ we deduce

$$|T^b_{h,2}| \leq G'_b \|C(t)\|_{W^{1,\infty}(0,b)} \sum_{j=1}^{N} h_j \left| \frac{1}{2}(C(x_j,t) + C(x_{j-1},t)) - C(x_{j-\frac{1}{2}},t) \right| \, \left| D_{-x} E_h(x_j,t) \right| \ ,$$

and by Lemma 3.5 there exists a constant c_3, such that

$$\begin{aligned} |T^b_{h,2}| &\leq h^2_{max} c_3 G'_b \|C(t)\|_{W^{1,\infty}(0,b)} \, |C(t)|_{H^2(0,b)} \, \|D_{-x} E_h(t)\|_+ \\ &\leq \frac{h^4_{max}}{4\xi_4} c_3^2 (G'_b)^2 \|C(t)\|^2_{W^{1,\infty}(0,b)} \, |C(t)|^2_{H^2(0,b)} + \xi_4 \|D_{-x} E_h(t)\|^2_+ \ . \end{aligned} \tag{3.49}$$

Then from (3.47), (3.48) and (3.49) we deduce

$$|T_{h,2}| \leq \frac{h^4_{max}}{4\xi_4} (c_2^2 G_b^2 + c_3^2 (G'_b)^2 \|C(t)\|^2_{W^{1,\infty}(0,b)}) \|C(t)\|^2_{H^3(0,b)} + 2\xi_4 \|D_{-x} E_h(t)\|^2_+ \ , \tag{3.50}$$

where $c_2 > 0$ and $c_3 > 0$ are constants.

For $T_{h,3}$ we add and subtract the term

$$\int_0^t K(t-s)(F(\hat{M}_h C(t), \hat{M}_h C(s))) D_{-x} R_h C(s), D_{-x} E_h(t))_+ ds$$

to obtain

$$T_{h,3} = T^a_{h,3} + T^b_{h,3} \ , \tag{3.51}$$

where

$$
\begin{aligned}
T_{h,3}^{a} &= \int_0^t K(t-s)(F(M_hC(t),M_hC(s))(D_{-x}R_hC(s)-\hat{M}_h\frac{\partial C}{\partial x}(s)),D_{-x}E_h(t))_+ ds \, , \\
T_{h,3}^{b} &= +\int_0^t K(t-s)((F(M_hC(t),M_hC(s))-F(\hat{M}_hC(t),\hat{M}_hC(s)))D_{-x}R_hC(s),D_{-x}E_h(t))_+ ds
\end{aligned}
$$

Applying Lemma 3.4 to $T_{h,3}^{a}$ we conclude that there exists a constant c_4, such that

$$
\begin{aligned}
|T_{h,3}^{a}| &\le h_{max}^2 c_4 F_b \|K\|_{L^2(0,T)} \left(\int_0^t |C(s)|^2_{H^3(0,b)}\, ds\right)^{\frac{1}{2}} \|D_{-x}E_h(t)\|_+ \\
&\le \frac{h_{max}^4}{4\xi_5} c_4^2 F_b^2 \|K\|^2_{L^2(0,T)} \int_0^t |C(s)|^2_{H^3(0,b)}\, ds + \xi_5 \|D_{-x}E_h(t)\|_+^2 \, , \qquad (3.52)
\end{aligned}
$$

where $\xi_5 > 0$ is arbitrary.

Applying Mean Value Theorem to $T_{h,3}^{b}$ we get

$$
\begin{aligned}
&|T_{h,3}^{b}| \\
&\le F_{x,b}\|C\|_{L^\infty(W^{1,\infty}(0,b))}\|K\|^2_{L^1(0,T)} \sum_{j=1}^{N} h_j \left|\frac{1}{2}(C(x_j,t)+C(x_{j-1},t))-C(x_{j-\frac{1}{2}},t)\right| \left|D_{-x}E_h(x_j,t)\right| \\
&+F_{y,b}\|C\|_{L^\infty(W^{1,\infty}(0,b))}\int_0^t |K(t-s)| \sum_{j=1}^{N} h_j \left|\frac{1}{2}(C(x_j,s)+C(x_{j-1},s))-C(x_{j-\frac{1}{2}},s)\right| \left|D_{-x}E_h(x_j,t)\right| ds \, ,
\end{aligned}
$$

and by Lemma 3.5 there exists constants c_5 and c_6 such that

$$
\begin{aligned}
|T_{h,3}^{b}| &\le h_{max}^2 c_5 F_{x,b}\|C\|_{L^\infty(W^{1,\infty}(0,b))}\|K\|^2_{L^1(0,T)} |C(t)|_{H^2(0,b)} \|D_{-x}E_h(t)\|_+ \\
&\quad + h_{max}^2 c_6 F_{y,b}\|C\|_{L^\infty(W^{1,\infty}(0,b))}\|K\|_{L^2(0,T)} \left(\int_0^t |C(s)|^2_{H^2(0,b)}\, ds\right)^{\frac{1}{2}} \|D_{-x}E_h(t)\|_+ \\
&\le \frac{h_{max}^4}{4\xi_5} c_5^2 (F_{x,b})^2 \|C\|^2_{L^\infty(W^{1,\infty}(0,b))}\|K\|^4_{L^1(0,T)} |C(t)|^2_{H^2(0,b)} \\
&\quad + \frac{h_{max}^4}{4\xi_5} c_6^2 (F_{y,b})^2 \|C\|^2_{L^\infty(W^{1,\infty}(0,b))}\|K\|^2_{L^2(0,T)} \int_0^t |C(s)|^2_{H^2(0,b)}\, ds \\
&\quad + 2\xi_5 \|D_{-x}E_h(t)\|_+ \, , \qquad (3.53)
\end{aligned}
$$

Then we obtain from (3.51), (3.52) and (3.53) that

$$
\begin{aligned}
|T_{h,3}| &\le \frac{h_{max}^4}{4\xi_5} \|K\|^2_{L^2(0,T)} (c_4^2 F_b^2 + c_6^2 \|C\|^2_{L^\infty(W^{1,\infty}(0,b))}(F_{y,b})^2) \int_0^t \|C(s)\|^2_{H^3(0,b)} ds \\
&\quad + \frac{h_{max}^4}{4\xi_5} c_5^2 \|C\|^2_{L^\infty(W^{1,\infty}(0,b))}(F_{x,b})^2 \|K\|^4_{L^1(0,T)} |C(t)|^2_{H^2(0,b)} + 3\xi_5 \|D_{-x}E_h(t)\|_+^2 \, . \qquad (3.54)
\end{aligned}
$$

Applying inequalities (3.41), (3.42), (3.46), (3.50) and (3.54) (considering $\xi_i = \xi$, for $i = 1,\dots,5$) to (3.35) we deduce

$$\frac{d}{dt}\left(\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds\right)$$
$$\le \Theta_1\left(\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}+1\right)\left(\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds\right) + h_{max}^4 \Theta_2 T_r(t)\ , \quad (3.55)$$

where $T_r(t)$ is defined as in (3.31) and

$$\Theta_1 = \frac{\frac{1}{2\xi}\max\{(G_b')^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)}, F_b^2\|K\|^2_{L^2(0,T)}, a_b(F_{y,b})^2\|K\|^2_{L^2(0,T)}\}}{\min\{1,2(G_0-10\xi)\}}\ ,$$
$$\Theta_2 = \frac{\frac{1}{2\xi}\gamma}{\min\{1,2(G_0-10\xi)\}}\ ,$$

with

$$\gamma = \max\{c_1^2, c_2^2G_b^2 + c_3^2(G_b')^2, c_5^2(F_{x,b})^2\|K\|^4_{L^1(0,T)}, c_4^2F_b^2\|K\|^2_{L^2(0,T)}, c_6^2(F_{y,b})^2\|K\|^2_{L^2(0,T)}\}\ ,$$

when ξ is fixed by

$$G_0 - 10\xi > 0\ .$$

Therefore we conclude from (3.55) that there exist positive constants $\hat{c}_1$ and $\hat{c}_2$ depending on G, F and K such that

$$\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds$$
$$\le \hat{c}_1(\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}+1)\int_0^t\left(\|E_h(s)\|_h^2 + \int_0^s \|D_{-x}E_h(r)\|^2_{1,h}dr\right)ds + \hat{c}_2 h_{max}^4\int_0^t T(s)ds\ .$$

Finally applying Gronwall lemma we deduce (3.30).

□

As a corollary of Theorem 3.2 we have the following convergence result.

Corollary 3.2. *Under the assumptions of Theorem 3.2, there exists a positive constant c_T that does not depend on h such that*

$$\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds \le c_T h_{max}^4\ . \quad (3.56)$$

Proof. From the proof of Theorem 3.2, it follows that there exist positive constants $\hat{c_1}$ and $\hat{c}_2$ such that the next inequality holds

$$\hat{c}_2 e^{\hat{c}_1(\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}+1)t}\int_0^t T_r(s)ds \le c_T\ ,$$

where

$$c_T = \hat{c}_2 e^{\hat{c}_1(\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}+1)T}\Big(\|C\|^2_{H^1(0,T;H^2(0,b))} + (\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}+1)\,\|C\|^2_{L^2(0,T;H^3(0,b))}\,(1+T)\Big)\,,$$

then from (3.30) the result follows.

□

As in the stability analysis, in what follows we establish a new error estimate considering weaker conditions on K, namely $K \in L^1(0,T)$. Again, we are also able to reduce the amplification factor $e^{\Theta t}$, but we must consider stronger conditions on the coefficient functions.

Corollary 3.3. *Let $K \in L^1(0,T)$, under the assumptions of Theorem 3.2 for G, F, C and C_h. If there exists a positive constant ξ such that*

$$\begin{aligned} d_3 &= G_0 - 9\xi - \frac{a_b}{4\xi}\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}\Big((G_b')^2 + (F_{y,b})^2\|K\|^4_{L^1(0,T)}\Big) - \frac{F_b^2}{4\xi}\|K\|^4_{L^1(0,T)} \\ &\quad - \|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))} a_b F_{x,b}\|K\|^2_{L^1(0,T)} > 0\,, \end{aligned} \tag{3.57}$$

then there exists a constant $\hat{c}_T$ depending on the coefficient functions G, F and on the kernel K such that

$$\|E_h(t)\|_h^2 + \int_0^t \|D_{-x}E_h(s)\|_+^2 ds \le \hat{c}_T h^4_{max}\,. \tag{3.58}$$

Proof. Following the proof of Theorem 3.2 we deduce

$$\begin{aligned} &\frac{1}{2}\frac{d}{dt}\|E_h(t)\|_h^2 + \left(G_0 - 4\xi - \frac{(G_b')^2 a_b}{4\xi}\|C\|^2_{L^\infty(W^{1,\infty}(0,b))}\right)\|D_{-x}E_h(t)\|_+^2 \\ &\le T_2 + T_{h,3} + \frac{h^4_{max}}{4\xi}(c_2^2 G_b^2 + c_3^2 (G_b')^2\|C(t)\|^2_{W^{1,\infty}(0,b)})\|C(t)\|^2_{H^3(0,b)} \\ &+ \frac{c_1^2 h^4_{max}}{4\xi}\left\|\frac{\partial C}{\partial t}(t)\right\|^2_{H^2(0,b)}\,, \end{aligned} \tag{3.59}$$

where T_2 and $T_{h,3}$ are defined respectively by (3.37) and (3.40). In what follows we estimate the terms T_2 and $T_{h,3}$ separately.

For T_2, we deduce the following inequality

$$\begin{aligned} |T_2| &\le \frac{F_b^2}{4\xi}\|K\|^2_{L^1(0,T)}\int_0^t K(t-s)\|D_{-x}E_h(s)\|_h^2 ds \\ &\quad + \frac{a_b(F_{y,b})^2}{4\xi}\|C\|^2_{L^\infty(0,T;W^{1,\infty}(0,b))}\|K\|^2_{L^1(0,T)}\int_0^t K(t-s)\|D_{-x}E_h(s)\|_h^2 ds \\ &\quad + \Big(\|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))} a_b F_{x,b}\|K\|^2_{L^1(0,T)} + 2\xi\Big)\|D_{-x}E_h(t)\|_+^2 \end{aligned} \tag{3.60}$$

For $T_{h,3}$, the following upper bound can be established

$$\begin{aligned} |T_{h,3}| &\leq \frac{h_{max}^4}{4\xi}\|K\|_{L^1(0,T)}^2\left(c_4^2F_b^2+c_6^2\|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))}^2(F_{y,b})^2\right)\int_0^t K(t-s)\|C(s)\|_{H^3(0,b)}^2 ds \\ &\quad +\frac{h_{max}^4}{4\xi}c_5^2\|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))}^2(F_{x,b})^2\|K\|_{L^1(0,T)}^4\,|C(t)|_{H^2(0,b)}^2+3\xi\,\|D_{-x}E_h(t)\|_+^2 \,. \end{aligned} \tag{3.61}$$

Applying inequalities (3.60) and (3.61) to (3.59), integrating with respect to t and changing the order of integration we deduce

$$\|E_h(t)\|_h^2+2d_3\int_0^t\|D_{-x}E_h(s)\|_+^2 ds \quad \leq \quad h_{max}^4\frac{\Theta_1}{2\xi}\int_0^t T_r(s)\,ds\;,$$

where d_3 is defined as in (3.57), $T_r(t)$ as in (3.31) and

$$\Theta_1=\max\{c_1^2,c_2^2G_b^2+c_3^2(G_b')^2,c_5^2(F_{x,b})^2\|K\|_{L^1(0,T)}^4,c_4^2F_b^2\|K\|_{L^1(0,T)}^4,c_6^2(F_{y,b})^2\|K\|_{L^1(0,T)}^4\}\;.$$

Then, provided that $d_3>0$ and taking

$$\hat{c}_T=\frac{\Theta_1}{\min\{1,2d_3\}}\left(\|C\|_{H^1(0,T;H^2(0,b))}^2+(\|C\|_{L^\infty(0,T;W^{1,\infty}(0,b))}^2+1)\,\|C\|_{L^2(0,T;H^3(0,b))}^2\,(1+T)\right)\;,$$

we conclude (3.58).

$\square$

3.3 Fully discrete method

To integrate in time an IMEX (implicit-explicit) method will be used. In $[0,T]$ we consider a uniform time grid $J_{\Delta t}=\{t_n,\ n=0,1,2,...,M\}$, with $t_0=0$, $t_M=T$ and $t_n-t_{n-1}=\Delta t$. We use the rectangular rule to approximate the integral in (3.6) and the backward finite-difference operator D_{-t} to approximate the first partial derivative with respect to t. Then the fully discrete approximation for C at (x_j,t_n), $C_h^n(x_j)$, is defined by the following set of equations

$$\begin{aligned} D_{-t}C_h^n(x_j) &= D_x^{\frac{1}{2}}\left(G(M_hC_h^{n-1}(x_j))D_{-x}C_h^n(x_j)\right)+Z(x_j,t_n) \\ &\quad +\Delta t\sum_{s=0}^{n-1}K(t_n-t_s)D_x^{\frac{1}{2}}\left(F(M_hC_h^{n-1},M_hC_h^s(x_j))D_{-x}C_h^s(x_j)\right)\;, \end{aligned} \tag{3.62}$$

for $j=1,\dots,\ N-1$, with boundary conditions

$$C_h^n(x_0)=C_h^n(x_N)=0,\quad \text{for } n=1,\dots,\ M\;, \tag{3.63}$$

and the initial condition

$$C_h^0(x_j)=R_hC_0(x_j),\quad \text{for } j=1,\dots,\ N-1\;. \tag{3.64}$$

We remark that the previous fully discrete in time and space scheme can be written in the following equivalent form

$$\begin{aligned}(D_{-t}C_h^n, v_h)_h &= -(G(M_hC_h^{n-1})D_{-x}C_h^n, D_{-x}v_h)_+ + (Z_h(t_n), v_h)_h \\ &\quad -\Delta t\sum_{s=0}^{n-1} K(t_n-t_s)(F(M_hC_h^{n-1}, M_hC_h^s)D_{-x}C_h^s, D_{-x}v_h)_+ \ ,\end{aligned} \tag{3.65}$$

for all $v_n \in \mathbb{W}_{h,0}$ and for $n = 1,\dots,\ M$.

3.3.1 Fully-discrete Stability

In what follows we establish a fully-discrete version of Theorem 2.1 and Corollary 2.1. As in the previous cases we will fix a solution C_h and we analyze the behavior of $w_h^n = C_h^n - \tilde{C}_h^n$ (for $n = 0,1,\dots,M$), where $\tilde{C}_h$ is another solution of the IBVP (3.62)-(3.64), corresponding to a perturbed initial condition.

Once again the smoothness of the kernel function K has an important role in the estimates. As the integral term was discretized using the rectangular rule, we will consider the following assumption over K:

$$\Delta t\sum_{s=0}^{n-1} |K(t_n-t_s)|^i \le k\ , \quad \text{for } i = 1,2\ . \tag{3.66}$$

We note that when K is defined as in (2.11), the condition (3.66) is clearly satisfied.

We will obtain a first stability estimate assuming (3.66). Then, in order to reduce the smoothness we require over K, we will introduce an alternative discretization over time to replace the equation(3.62) in the IMEX method. This will allow us to replace the condition (3.66) by $K \in L^1(0,T)$.

Theorem 3.3. *Let us suppose that K satisfies* (3.66)*, $G \in \mathscr{C}_B^1(\mathbb{R})$, $F \in \mathscr{C}_B^1(\mathbb{R}^2)$ and $0 < G_0 \le G$. If C_h and $\tilde{C}_h$ are solutions of* (3.62)-(3.64) *such that $C_h, \tilde{C}_h \in \mathscr{C}^1(0,T;\mathbb{W}_h)\bigcap\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})$, then for $w_h^n = C_h^n - \tilde{C}_h{}^n$, with $w_h^0 = w_{h,0}$, there exist positive constants c_1 and c_2 depending on the coefficients functions G, F and on the kernel K such that*

$$\|w_h^n\|_h^2 + \Delta t\sum_{s=0}^{n}\|D_{-x}w_h^s\|_+^2 ds \le c_2\left(\|w_{h,0}\|^2 + \Delta t\|D_{-x}w_h^0\|_+^2\right) e^{\left(c_1(1+\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})})T\right)}\ . \tag{3.67}$$

Proof. Following the proof of Theorem 3.1, we deduce from (3.65) that

$$(D_{-t}w_h^n, w_h^n)_h + G_0\|D_{-x}w_h^n\|_+^2 \le P_{h,1}^n + P_{h,2}^n + P_{h,3}^n\ , \tag{3.68}$$

where

$$\begin{aligned}P_{h,1}^n &= ((G(M_hC_h^{n-1}) - G(M_h\tilde{C}_h^{n-1}))D_{-x}C_h^n, D_{-x}w_h^n)_+\ ,\\ P_{h,2}^n &= \Delta t\sum_{s=0}^{n-1} K(t_n-t_s)(F(M_h\tilde{C}_h^{n-1}, M_h\tilde{C}_h^s)D_{-x}w_h^s, D_{-x}w_h^n)_+\ ,\\ P_{h,3}^n &= \Delta t\sum_{s=0}^{n-1} K(t_n-t_s)((F(M_hC_h^{n-1}, M_hC_h^s) - F(\tilde{C}_h^{n-1}, \tilde{C}_h^s))D_{-x}C_h^s, D_{-x}w_h^n)_+\ .\end{aligned}$$

Following the ideas of the proofs of the continuous case and the semi-discrete case, we will estimate each of the above terms separately.

An estimate for $P^n_{h,1}$ follows from the estimate (3.16) for $P_{h,1}$

$$|P^n_{h,1}| \leq \frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}^{1,\infty}_h)}}{4\xi}(G'_b)^2\|w^{n-1}_h\|^2_h + \xi\|D_{-x}w^n_h\|^2_+ \ , \tag{3.69}$$

where $\xi > 0$ is an arbitrary constant.

It can be shown from the estimate (3.17) for $P_{h,2}$ that for $P^n_{h,2}$ holds the following

$$|P^n_{h,2}| \leq \frac{F_b^2}{4\xi}k\Delta t\sum_{s=0}^{n-1}\|D_{-x}w^s_h\|^2_+ + \xi\|D_{-x}w^n_h\|^2_+ \ . \tag{3.70}$$

Following the deduction of the estimate (3.18) for $P_{h,3}$, we easily get for $P^n_{h,3}$ the following upper bound

$$\begin{aligned} |P^n_{h,3}| \ &\leq \ \frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}^{1,\infty}_h)}}{4\xi}\left((F_{x,b})^2k^2\|w^{n-1}_h\|^2_h + a_b(F_{y,b})^2k\Delta t\sum_{s=0}^{n-1}\|D_{-x}w^s_h\|^2_+\right) \\ &\quad +2\xi\|D_{-x}w^n_h\|^2_+ \ . \end{aligned} \tag{3.71}$$

Applying inequalities (3.69), (3.70) and (3.71) to (3.68), we obtain

$$\|w^n_h\|^2_h + 2(G_0 - 4\xi)\Delta t\|D_{-x}w^n_h\|^2_+ \leq (1+\Theta_1\Delta t)\|w^{n-1}_h\|^2_h + \Theta_2(\Delta t)^2\sum_{s=0}^{n-1}\|D_{-x}w^s_h\|^2_+ \ ,$$

where

$$\begin{aligned} \Theta_1 \ &= \ \frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}^{1,\infty}_h)}}{2\xi}\left((G'_b)^2 + (F_{x,b})^2k^2\right) \ , \\ \Theta_2 \ &= \ \frac{k}{2\xi}\left(F_b^2 + a_b(F_{y,b})^2\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}^{1,\infty}_h)}\right) \ . \end{aligned}$$

Summing from $s = 1, \ldots, n$, we deduce

$$\begin{aligned} \|w^n_h\|^2 + \Delta t\sum_{s=0}^{n}\|D_{-x}w^s_h\|^2_+ ds \ &\leq \ c_1(1+\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}^{1,\infty}_h)})\Delta t\sum_{s=0}^{n-1}\left(\|w^s_h\|^2_h + \Delta t\sum_{r=0}^{s}\|D_{-x}w^r_h\|^2_+\right) \\ &\quad + \frac{1}{\min\{1, 2(G_0-4\xi)\}}\left(\|w_{h,0}\|^2 + 2(G_0-4\xi)\Delta t\|D_{-x}w^0_h\|^2_+\right) \ , \end{aligned}$$

where c_1 is a constant depending on the coefficients functions G, F and the kernel K when ξ is fixed by

$$G_0 - 4\xi > 0 \ .$$

Finally the application of the discrete Gronwall lemma leads to (3.67).

□

We note that inequality (3.67) means that the IVBP (3.62)-(3.64) is unconditionally stable under initial perturbations for bounded time intervals.

In order to establish a new stability estimate considering weaker conditions over K, we replace (3.62) by

$$\begin{aligned} D_{-t}C_h^n(x_j) &= D_x^{\frac{1}{2}}\left(G(M_hC_h^{n-1}(x_j))D_{-x}C_h^n(x_j)\right)+Z(x_j,t_n) \\ &\quad +\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}K(t_n-r)dr D_x^{\frac{1}{2}}\left(F(M_hC_h^{n-1},M_hC_h^s(x_j))D_{-x}C_h^s(x_j)\right)\,, \end{aligned} \tag{3.72}$$

which can be written in the following equivalent form

$$\begin{aligned} (D_{-t}C_h^n,v_h)_h &= -(G(M_hC_h^{n-1})D_{-x}C_h^n,D_{-x}v_h)_+ +(Z_h(t_n),v_h)_h \\ &\quad -\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}K(t_n-r)dr(F(M_hC_h^{n-1},M_hC_h^s)D_{-x}C_h^s,D_{-x}v_h)_+\,, \end{aligned} \tag{3.73}$$

for all $v_h\in\mathbb{W}_{h,0}$ and for $n=1,\ldots,\ M$.

As in the previous cases, in the following result we reduce the exponential factor $e^{\Theta T}$ to the unity and consider less smoothness over K by imposing stronger restrictions of the coefficient functions. However we need to impose a stability condition.

Corollary 3.4. *Let us suppose that $K\in L^1(0,T)$, $G\in\mathscr{C}_B^1(\mathbb{R})$, $F\in\mathscr{C}_B^1(\mathbb{R}^2)$ and $0<G_0\le G$. If C_h and $\tilde{C}_h$ are solutions of* (3.72), (3.63), (3.64) *such that $C_h,\tilde{C}_h\in\mathscr{C}^1(0,T;\mathbb{W}_h)\bigcap\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})$, for $w_h^n=C_h^n-\tilde{C}_h{}^n$, with $w_h^0=w_{h,0}$ and there exists a positive constant ξ such that*

$$\begin{aligned} d_4 &= G_0-4\xi-\frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}a_b\left((G_b')^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)}\right)\Delta t \\ &\quad -\frac{\|K\|^4_{L^1(0,T)}}{4\xi}\left(F_b^2+a_b(F_{y,b})^2\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}\right)\Delta t>0\,, \end{aligned} \tag{3.74}$$

then

$$\|w_h^n\|_h^2+\Delta t\sum_{s=0}^n\|D_{-x}w_h^s\|_+^2\le\frac{\max\{1,2(G_0-4\xi)\}}{\min\{1,2d_4\}}\left(\|w_{h,0}\|^2+\Delta t\|D_{-x}w_h^0\|_+^2\right)\,. \tag{3.75}$$

Proof. Following the proof of Theorem 3.3 we deduce

$$\begin{aligned} &\|w_h^n\|_h^2+2(G_0-\xi)\Delta t\|D_{-x}w_h^n\|_+^2 \\ &\le 2\Delta t|\hat{P}_{h,1}^n|+2\Delta t|\hat{P}_{h,2}^n|+\left(\Delta t\frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}}{2\xi}(G_b')^2+1\right)\|w_h^{n-1}\|_h^2\,, \end{aligned} \tag{3.76}$$

where $\hat{P}^n_{h,1}$ and $\hat{P}^n_{h,2}$ are defined by

$$
\begin{aligned}
\hat{P}^n_{h,1} &= \sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}} K(t_n-r)dr(F(M_h\tilde{C}_h^{n-1},M_h\tilde{C}_h^s)D_{-x}w_h^s,D_{-x}w_h^n)_+ \ ,\\
\hat{P}^n_{h,2} &= \sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}} K(t_n-r)dr((F(M_hC_h^{n-1},M_hC_h^s)-F(\tilde{C}_h^{n-1},\tilde{C}_h^s))D_{-x}C_h^s,D_{-x}w_h^n)_+ \ .
\end{aligned}
$$

In what follows we estimate the terms $\hat{P}^n_{h,1}$, $\hat{P}^n_{h,2}$ and then combine those estimates with the inequality (3.76).

For $\hat{P}^n_{h,1}$, we have that the following inequality holds

$$
\begin{aligned}
|\hat{P}^n_{h,1}| &\leq F_b\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|D_{-x}w_h^s\|_+\|D_{-x}w_h^n\|_+\\
&\leq \frac{F_b^2}{4\xi}\|K\|^2_{L^1(0,T)}\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|D_{-x}w_h^s\|_+^2+\xi\|D_{-x}w_h^n\|_+^2 \ . \qquad (3.77)
\end{aligned}
$$

For $\hat{P}^n_{h,2}$, it can be shown the following

$$
\begin{aligned}
|\hat{P}^n_{h,2}| &\leq \|C_h\|_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}\Big(F_{x,b}\|K\|^2_{L^1(0,T)}\|w_h^{n-1}\|_h\\
&\quad +F_{y,b}\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|w_h^s\|_h\Big)\|D_{-x}w_h^n\|_+\\
&\leq \frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}\Big((F_{x,b})^2\|K\|^4_{L^1(0,T)}\|w_h^{n-1}\|_h^2\\
&\quad +a_b(F_{y,b})^2\|K\|^2_{L^1(0,T)}\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|D_{-x}w_h^s\|_+^2\Big)\\
&\quad +2\xi\|D_{-x}w_h^n\|_+^2 \ . \qquad (3.78)
\end{aligned}
$$

Applying inequalities (3.77) and (3.78) to (3.76) we get that

$$
\begin{aligned}
&\|w_h^n\|_h^2+2(G_0-4\xi)\Delta t\|D_{-x}w_h^n\|_+^2\\
&\leq (1+\Theta_1\Delta t)\|w_h^{n-1}\|_h^2+\Theta_2(\Delta t)^2\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|D_{-x}w_h^s\|_+^2 \ ,
\end{aligned}
$$

where

$$
\begin{aligned}
\Theta_1 &= \frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}}{2\xi}\left((G_b')^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)}\right) \ ,\\
\Theta_2 &= \frac{\|K\|^2_{L^1(0,T)}}{2\xi}\left(F_b^2+a_b(F_{y,b})^2\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}\right) \ .
\end{aligned}
$$

Summing from $s=1,\dots,\ n$, we deduce

$$
\begin{aligned}
&\|w_h^n\|^2+2(G_0-4\xi)\Delta t\sum_{s=0}^{n}\|D_{-x}w_h^s\|_+^2 ds\\
&\leq \Theta_1\Delta t\sum_{s=0}^{n-1}\|w_h^s\|_h^2+\Theta_2(\Delta t)^2\sum_{s=1}^{n}\sum_{\ell=0}^{s-1}\int_{t_\ell}^{t_{\ell+1}}|K(t_s-r)|dr\|D_{-x}w_h^\ell\|_+^2\\
&+\|w_{h,0}\|^2+2(G_0-4\xi)\Delta t\|D_{-x}w_h^0\|_+^2\ ,
\end{aligned}
\tag{3.79}
$$

Note that by changing the order of summation we obtain

$$
\begin{aligned}
\sum_{s=1}^{n}\sum_{\ell=0}^{s-1}\int_{t_\ell}^{t_{\ell+1}}|K(t_s-r)|dr\|D_{-x}w_h^\ell\|_+^2 &= \sum_{\ell=0}^{n-1}\sum_{s=\ell+1}^{n}\int_{t_\ell}^{t_{\ell+1}}|K(t_s-r)|dr\|D_{-x}w_h^\ell\|_+^2\\
&= \sum_{\ell=0}^{n-1}\sum_{s=\ell+1}^{n}\int_{(s-\ell-1)\Delta t}^{(s-\ell)\Delta t}|K(r)|dr\|D_{-x}w_h^\ell\|_+^2\\
&\leq \|K\|_{L^1(0,T)}^2\sum_{s=0}^{n}\|D_{-x}w_h^s\|_+^2\ ,
\end{aligned}
$$

then from (3.80) we get

$$
\|w_h^n\|^2+2d_4\Delta t\sum_{s=0}^{n}\|D_{-x}w_h^s\|_+^2 ds\leq \max\{1,2(G_0-4\xi)\}\left(\|w_{h,0}\|^2+\Delta t\|D_{-x}w_h^0\|_+^2\right)\ ,
$$

where d_4 is defined by (3.74). Then provided that $d_4>0$ we conclude (3.75). □

Let ξ be such that $G_0-4\xi>0$. Then if we assume that Δt satisfies the following stability condition

$$
\Delta t\leq\frac{G_0-4\xi}{\gamma}\ ,
\tag{3.80}
$$

where γ is defined as

$$
\begin{aligned}
\min\{&\frac{\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}}{4\xi}a_b\left((G_b')^2+(F_{x,b})^2\|K\|_{L^1(0,T)}^4\right),\\
&\frac{\|K\|^4_{L^1(0,T)}}{4\xi}\left(F_b^2+a_b(F_{y,b})^2\|C_h\|^2_{\mathscr{C}(0,T;\mathbb{W}_h^{1,\infty})}\right)\}\ ,
\end{aligned}
$$

then (3.75) holds. Inequality (3.80) establish a condition that allow us to conclude the last stability result.

3.3.2 Convergence analysis

Let C be solution of the IBVP (2.3), (1.7), (2.2) and let $E_h^n=R_hC(t_n)-C_h^n$, $n=0,\dots,\ M$, be the global error. In what follows we establish the completely discrete versions of Theorem 3.2 and Corollary 3.3.

As the integral term was discretized using the rectangular grid rule, in order to obtain an estimate for E_h^n we need to replace the assumption $K \in L^2(0,T)$ by the following one:

$$K \in H^1(0,T)\ . \tag{3.81}$$

Later we will show, that condition (3.81) can be relaxed by imposing stronger restrictions on G and F. In this case, it would be enough that K satisfy the condition $K \in L^1(0,T)$.

In order to simplify the presentation of the proof of the convergence result that follows, we introduce the next auxiliary lemma.

Lemma 3.6. *Let g be a function defined over an interval $[0,T]$ such that $g \in H^2(0,T)$. If we consider a uniform grid $J_{\Delta t} = \{t_n,\ n = 0,1,..,M\}$ with $t_0 = 0$, $t_M = T$ and $t_n - t_{n-1} = \Delta t$, then for the functional*

$$\lambda(g) = D_{-t}g(t_n) - \frac{\partial g}{\partial t}(t_n)$$

there exists a constant c such that

$$|\lambda(g)| \leq c\|g''\|_{L^1(t_{n-1},\,t_n)}\ , \tag{3.82}$$

Proof. Let v be a function defined by $v(\delta) = g(t_{n-1} + \Delta t\delta)$ for $\delta \in [0,1]$. Then we have that

$$\lambda(g) = \frac{1}{\Delta t}\left(v(1) - v(0) - v'(1)\right)\ .$$

The functional

$$\hat{\lambda}(v) = v(1) - v(0) - v'(1)\ ,$$

is bounded in $H^2(0,1)$ and vanishes for $v = 1$ and $v = \delta$. Therefore by the Bramble-Hilbert Lemma there exists a constant c such that

$$\left|\hat{\lambda}(v)\right| \leq c\|v''\|_{L^1(0,1)}\ .$$

Since $\|v''\|_{L^1(0,1)} = \Delta t\|g''\|_{L^1(t_{n-1},\,t_n)}$ we conclude (3.82). □

Theorem 3.4. *Let $C \in \mathscr{C}(0,T,H^3(0,1)\cap H_0^1(0,1)) \cap \mathscr{C}^1(0,T,H^2(0,1))$ be the solution of (**VP**) and let C_h^n be its approximation defined by (3.62). If $K \in H^1(0,T)$ and satisfies (3.66), $G \in \mathscr{C}_B^1(\mathbb{R})$, $F \in \mathscr{C}_B^1(\mathbb{R}^2)$ and $0 < G_0 \leq G$, then there exist positive constants $\hat{c}_1$ and $\hat{c}_2$ depending on the coefficients functions G, F and on the kernel K such that, for the fully discrete error, holds the following*

$$\|E_h^n\|_h^2 + \Delta t\sum_{s=0}^{n}\|D_{-x}e_h^s\|_+^2 \ \leq\ \frac{exp\left(T\frac{\hat{c}_1(1+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))})}{\min\{1-2\xi\Delta t,2(G_0-15\xi)\}}\right)}{\min\{1-2\xi\Delta t,2(G_0-15\xi)\}}\left(\Delta t\sum_{s=1}^{n}T_h^s\right), \tag{3.83}$$

where T_h^s is given by

$$\begin{aligned}
T_h^s &= \hat{c}_2\Big[h_{max}^4\Big(\|C\|^2_{\mathscr{C}^1(0,T,H^2(0,b))}+(1+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T,H^3(0,b))}\Big)\\
&\quad +h_{max}^4\Big(\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|C\|^2_{\mathscr{C}(0,T,H^2(0,b))}+(1+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))})\|C\|^2_{L^2(0,T,H^3(0,b))}\Big)\\
&\quad +\Delta t\Big(\|R_hC\|^2_{H^2(t_{s-1},t_s,\mathbb{W}_h)}+2\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|R_hC\|_{H^1(t_{s-1},t_s;\mathbb{W}_h)}\Big)\\
&\quad +\Delta t^2\Big(\|C\|^2_{L^2(0,T,W^{1,\infty}(0,b))}+\|C\|^2_{H^1(0,T,W^{1,\infty}(0,b))}+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|C\|^2_{H^1(0,T,\mathbb{W}_h)}\Big)\Big]\ ,
\end{aligned} \tag{3.84}$$

ξ is such that

$$G_0-15\xi>0\ , \tag{3.85}$$

and Δt is fixed by

$$1-2\xi\Delta t>0\ . \tag{3.86}$$

Proof. Following the proof of Theorem 3.2, we deduce that

$$(D_{-t}E_h^n,E_h^n)_h=T_1^n+T_2^n+T_{h,1}^n+T_{h,2}^n+T_{h,3}^n\ , \tag{3.87}$$

where

$$\begin{aligned}
T_1^n &= (G(M_hC_h^{n-1})D_{-x}C_h^n-G(M_hC(t_{n-1}))D_{-x}R_hC(t_n),D_{-x}E_h^n)_+\ ,\\
T_2^n &= \Delta t\sum_{s=0}^{n-1}K(t_n-t_s)(F(M_hC_h^{n-1},M_hC_h^s)D_{-x}C_h^s\\
&\quad -F(M_hC(t_{n-1}),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+\ ,\\
T_{h,1}^n &= (D_{-t}R_hC(t_n)-\left(\frac{\partial C}{\partial t}\right)_h(t_n),E_h^n)_h\ ,\\
T_{h,2}^n &= (G(M_hC(t_{n-1}))D_{-x}R_hC(t_n)-G(\hat{M}_hC(t_n))\hat{M}_h\frac{\partial C}{\partial x}(t_n),D_{-x}E_h^n)_+\ ,\\
T_{h,3}^n &= \Delta t\sum_{s=0}^{n-1}K(t_n-t_s)F(M_hC(t_{n-1}),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+\\
&\quad -\int_0^{t_n}K(t_n-r)(F(\hat{M}_hC(t_n),\hat{M}_hC(r))\hat{M}_h\frac{\partial C}{\partial x}(r),D_{-x}E_h^n)_+dr\ .
\end{aligned}$$

As in the proof of Theorem 3.2, in what follows we estimate separately the terms defined above. From the estimation of T_1 (3.41) we obtain that

$$|T_1^n|\leq\frac{(G_b')^2}{4\xi_1}\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|E_h^{n-1}\|_h^2+(\xi_1-G_0)\|D_{-x}E_h^n\|_+^2\ , \tag{3.88}$$

where $\xi_1>0$ is an arbitrary constant.

For T_2^n, if follows from the estimation of T_2 (3.42) that

$$
\begin{aligned}
|T_2^n| \;\leq\; & \frac{k}{4\xi_2}(F_b^2+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}a_b(F_{y,b})^2)\Delta t\sum_{s=0}^{n-1}\|D_{-x}E_h^s\|_h^2 \\
& +\frac{\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}}{4\xi_2}k^2(F_{x,b})^2\|E_h^{n-1}\|_h^2+3\xi_2\|D_{-x}E_h^n\|_+^2\;, \qquad (3.89)
\end{aligned}
$$

where $\xi_2>0$ is an arbitrary constant.

For $T_{h,1}^n$ we begin by adding and subtracting the term

$$
(R_h\frac{\partial C}{\partial t}(t_n),E_h^n)_+\;,
$$

to obtain

$$
T_{h,1}^n=T_{h,1}^n(a)+T_{h,1}^n(b)\;,
$$

where

$$
T_{h,1}^n(a)=(D_{-t}R_hC(t_n)-R_h\frac{\partial C}{\partial t}(t_n),E_h^n)_h\;,
$$

and

$$
T_{h,1}^n(b)=(R_h\frac{\partial C}{\partial t}(t_n)-\left(\frac{\partial C}{\partial t}\right)_h(t_n),E_h^n)_h\;.
$$

From the estimation of $T_{h,1}$ (3.46) we have that

$$
|T_{h,1}^n(a)| \;\leq\; \frac{c_1^2h_{max}^4}{4\xi_3}\left\|\frac{\partial C}{\partial t}(t_n)\right\|^2_{H^2(0,b)}+\xi_3\|D_{-x}E_h^n\|_+^2\;,
$$

where $\xi_3>0$ is an arbitrary constant.

For $T_{h,1}^n(b)$, by the Lemma 3.6 there exists a constant c_2 such that

$$
\begin{aligned}
T_{h,1}^n(b) \;&\leq\; c_2(\Delta t)^{\frac{1}{2}}\|R_hC\|_{H^2(t_{n-1},t_n;\mathbb{W}_h)}\|E_h^n\|_h \\
&\leq\; \frac{c_2^2}{4\xi_3}\Delta t\|R_hC\|^2_{H^2(t_{n-1},t_n;\mathbb{W}_h)}+\xi_3\|E_h^n\|_h^2\;.
\end{aligned}
$$

Then we deduce

$$
\begin{aligned}
|T_{h,1}^n| \;\leq\; & \frac{c_1^2h_{max}^4}{4\xi_3}\|C\|^2_{\mathscr{C}^1(0,T;H^2(0,b))}+\frac{c_2^2}{4\xi_3}\Delta t\|R_hC\|^2_{H^2(t_{n-1},t_n;\mathbb{W}_h)}+\xi_3\|E_h^n\|_h^2 \\
& +\xi_3\|D_{-x}E_h^n\|_+^2\;. \qquad (3.90)
\end{aligned}
$$

To estimate $T_{h,2}^n$ we add and subtract the term

$$
(G(M_hC(t_n))D_{-x}R_hC(t_n),D_{-x}E_h^n)_+\;,
$$

to obtain

$$T^n_{h,2} = T^n_{h,2}(a) + T^n_{h,2}(b) \ ,$$

where

$$T^n_{h,2}(a) = (G(M_hC(t_n))D_{-x}R_hC(t_n) - G(\hat{M}_hC(t_n))\hat{M}_h\frac{\partial C}{\partial x}(t_n), D_{-x}E^n_h)_+ \ ,$$

and

$$T^n_{h,2}(b) = ((G(M_hC(t_{n-1})) - G(M_hC(t_n)))D_{-x}R_hC(t_n), D_{-x}E^n_h)_+ \ .$$

From the estimation of $T_{h,2}$ (3.50) we have

$$|T^n_{h,2}(a)| \leq \frac{h^4_{max}}{4\xi_4}c_3^2(G_b^2 + (G'_b)^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))})\|C(t_n)\|^2_{H^3(0,b)} + 2\xi_4\|D_{-x}E^n_h\|^2_+ \ ,$$

where $c_3 > 0$ is a constant and $\xi_4 > 0$ is arbitrary.

For $T^n_{h,2}(b)$ we have

$$\begin{aligned} |T^n_{h,2}(b)| &\leq (G'_b)\|C(t_n)\|_{W^{1,\infty}(0,b)}\sum_{j=1}^N h_j\left|\int_{t_{n-1}}^{t_n} M_h\frac{\partial C}{\partial t}(x_j,t)\,dt\right|\left|D_{-x}E^n_h(x_j)\right| \\ &\leq (G'_b)\|C(t_n)\|_{W^{1,\infty}(0,b)}(\Delta t)^{\frac{1}{2}}\|R_hC\|_{H^1(t_{n-1},t_n;\mathbb{W}_h)}\|D_{-x}E^n_h\|_+ \\ &\leq \frac{(G'_b)^2}{4\xi_4}\Delta t\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(t_{n-1},t_n;\mathbb{W}_h)} + \xi_4\|D_{-x}E^n_h\|^2_+ \ , \end{aligned}$$

then we obtain that

$$\begin{aligned} |T^n_{h,2}| \ \leq\ & \frac{h^4_{max}}{4\xi_4}c_3^2(G_b^2 + (G'_b)^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T;H^3(0,b))} \\ & + \frac{(G'_b)^2}{4\xi_4}\Delta t\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(t_{n-1},t_n;\mathbb{W}_h)} + 3\xi_4\|D_{-x}E^n_h\|^2_+ \ , \end{aligned} \tag{3.91}$$

To estimate $T^n_{h,3}$ we begin by adding and subtracting the term

$$\int_0^{t_n} K(t_n - r)(F(M_hC(t_n), M_hC(r))D_{-x}R_hC(r), D_{-x}E^n_h)_+ dr \ ,$$

to obtain

$$T^n_{h,3} = T^n_{h,3}(a) + T^n_{h,3}(b) \ ,$$

where

$$\begin{aligned} T^n_{h,3}(a) \ =\ & \int_0^{t_n} K(t_n - r)(F(M_hC(t_n), M_hC(r))D_{-x}R_hC(r) \\ & -F(\hat{M}_hC(t_n), \hat{M}_hC(r))M_h\frac{\partial C}{\partial x}(r), D_{-x}E^n_h)_+ dr \ , \end{aligned}$$

and

$$
\begin{aligned}
T^n_{h,3}(b) &= \Delta t \sum_{s=0}^{n-1} K(t_n - t_s) F(M_h C(t_{n-1}), M_h C(t_s)) D_{-x} R_h C(t_s), D_{-x} E^n_h)_+ \\
&\quad - \int_0^{t_n} K(t_n - r)(F(M_h C(t_n), M_h C(r)) D_{-x} R_h C(r), D_{-x} E^n_h)_+ dr \ .
\end{aligned}
$$

For $T^n_{h,3}(a)$ we have from the estimation of $T_{h,3}$ (3.54) the inequality

$$
\begin{aligned}
|T^n_{h,3}(a)| &\leq \frac{h^4_{max}}{4\xi_5} \|K\|^2_{L^2(0,T)} \left(c_4^2 F_b^2 + c_6^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} (F_{y,b})^2 \right) \int_0^{t_n} \|C(r)\|^2_{H^3(0,b)} dr \\
&\quad \frac{h^4_{max}}{4\xi_5} c_5^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} (F_{x,b})^2 \|K\|^4_{L^1(0,T)} |C(t_n)|^2_{H^2(0,b)} + 3\xi_5 \|D_{-x} E_h(t)\|^2_+ \ .
\end{aligned}
$$

In order to estimate $T^n_{h,3}(b)$ first we add and subtract the term

$$
\Delta t \sum_{s=0}^{n-1} K(t_n - t_s)(F(M_h C(t_n), M_h C(t_s)) D_{-x} R_h C(t_s), D_{-x} E^n_h)_+ \ ,
$$

to deduce

$$
T^n_{h,3}(b) = T^n_{h,3}(b,1) + T^n_{h,3}(b,2) \ ,
$$

where

$$
\begin{aligned}
T^n_{h,3}(b,1) &= \Delta t \sum_{s=0}^{n-1} K(t_n - t_s)(F(M_h C(t_n), M_h C(t_s)) D_{-x} R_h C(t_s), D_{-x} E^n_h)_+ \\
&\quad - \int_0^{t_n} K(t_n - r)(F(M_h C(t_n), M_h C(r)) D_{-x} R_h C(r), D_{-x} E^n_h)_+ dr \ ,
\end{aligned}
$$

and

$$
T^n_{h,3}(b,2) = \Delta t \sum_{s=0}^{n-1} K(t_n - t_s)((F(M_h C(t_{n-1}), M_h C(t_s)) - F(M_h C(t_n), M_h C(t_s))) D_{-x} R_h C(t_s), D_{-x} E^n_h)_+ .
$$

By estimating the error of the rectangular rule we have that

$$
\begin{aligned}
|T^n_{h,3}(b,1)| &\leq \Delta t F_b \int_0^{t_n} |K'(t_n - r)| \|C(s)\|_{W^{1,\infty}(0,b)} dr \|D_{-x} E^n_h\|_+ \\
&\quad + \Delta t F_{y,b} \int_0^{t_n} |K(t_n - r)| \left\| R_h \frac{\partial C}{\partial t}(r) \right\|_h \|C(r)\|_{W^{1,\infty}(0,b)} dr \|D_{-x} E^n_h\|_+ \\
&\quad + \Delta t F_b \int_0^{t_n} |K(t_n - r)| \left\| \frac{\partial C}{\partial t}(r) \right\|_{W^{1,\infty}(0,b)} dr \|D_{-x} E^n_h\|_+ \ .
\end{aligned}
$$

Therefore the following inequality holds

$$
\begin{aligned}
|T^n_{h,3}(b,1)| &\leq (\Delta t)^2 \frac{1}{4\xi_6} \|K\|^2_{H^1(0,t_n)} \Big(F_b^2 (\|C\|^2_{L^2(0,T;W^{1,\infty}(0,b))} + \|C\|^2_{H^1(0,t_n;W^{1,\infty}(0,b))}) \\
&\quad + (F_{y,b})^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} \|R_h C\|^2_{H^1(0,t_n;\mathbb{W}_h)} \Big) + 3\xi_6 \|D_{-x} E^n_h\|^2_+ \ ,
\end{aligned}
$$

where $\xi_6 > 0$ is an arbitrary constant.

We have that for $T^n_{h,3}(b,2)$ it follows the estimate

$$
\begin{aligned}
|T^n_{h,3}(b,2)| &\leq k(\Delta t)^{\frac{1}{2}} F_{x,b} \|C(t_n)\|_{W^{1,\infty}(0,b)} \|R_h C\|_{H^1(t_{n-1},t_n;\mathbb{W}_h)} \|D_{-x} E^n_h\|_+ \\
&\leq \frac{k^2 (F_{x,b})^2}{\xi_6} \Delta t \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} \|R_h C\|^2_{H^1(t_{n-1},t_n;\mathbb{W}_h)} + \xi_6 \|D_{-x} E^n_h\|^2_+ \ .
\end{aligned}
$$

Then for $T^n_{h,3}$ it holds that

$$
\begin{aligned}
|T^n_{h,3}| &\leq \frac{h^4_{max}}{4\xi_5} \|K\|^2_{L^2(0,T)} (c_4^2 F_b^2 + c_6^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} (F_{y,b})^2) \|C\|^2_{L^2(0,T;H^3(0,b))} \\
&\quad + \frac{h^4_{max}}{4\xi_5} c_5^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} (F_{x,b})^2 \|K\|^4_{L^1(0,T)} \|C\|^2_{\mathscr{C}(0,T;H^2(0,b))} \\
&\quad + (\Delta t)^2 \|K\|^2_{H^1(0,T)} \frac{1}{4\xi_6^2} \Big(F_b^2 (\|C\|^2_{L^2(0,T;W^{1,\infty}(0,b))} + \|C\|^2_{H^1(0,T;W^{1,\infty}(0,b))}) \\
&\quad + (F_{y,b})^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} \|R_h C\|^2_{H^1(0,T;\mathbb{W}_h)} \Big) \\
&\quad + \frac{k^2 (F_{x,b})^2}{\xi_6} \Delta t \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))} \|R_h C\|^2_{H^1(t_{n-1},t_n;\mathbb{W}_h)} + (3\xi_5 + 4\xi_6) \|D_{-x} E^n_h\|^2_+ \qquad (3.92)
\end{aligned}
$$

Considering in (3.87) the estimates (3.88), (3.89), (3.90), (3.91) and (3.92) with $\xi_i = \xi$, for $i = 1, \ldots,\ 6$, we deduce

$$
\begin{aligned}
\|E^s_h\|^2_h + 2(G_0 - 15\xi)\Delta t \|D_{-x} E^s_h\|^2_+ &\leq (1 + \Delta t \Phi) \|E^{s-1}_h\|^2_h + 2\xi \Delta t \|E^s_h\|^2_h \\
&\quad + \Delta t^2 \Psi \sum_{r=0}^{s-1} \|D_{-x} E^r_h\|^2_+ + \Delta t T^s_h \ , \qquad (3.93)
\end{aligned}
$$

where T^s_h is given by (3.84), with $\hat{c}_2$ defined by

$$
\begin{aligned}
\hat{c}_2 &= \frac{1}{2\xi} \max\{c_1^2,\ c_2^2,\ c_3^2 G_b^2,\ (G'_b)^2,\ c_4^2 F_b^2 \|K\|^2_{L^2(0,T)},\ c_6^2 (F_{y,b})^2 \|K\|^2_{L^2(0,T)}, \\
&\quad c_5^2 (F_{x,b})^2 \|K\|^4_{L^1(0,T)},\ F_b^2 \|K\|^2_{H^1(0,T)},\ (F_{y,b})^2 \|K\|^2_{H^1(0,T)},\ k^2 (F_{x,b})^2\} \ ,
\end{aligned}
$$

and

$$
\begin{aligned}
\Phi &= \frac{\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}}{2\xi} \left((G'_b)^2 + k^2 (F_{x,b})^2 \right) \ , \\
\Psi &= \frac{k}{2\xi} (F_b^2 + a_b (F_{y,b})^2 \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}) \ .
\end{aligned}
$$

Summing for $s=1,\ldots,\ n$ in (3.93) then we deduce

$$(1-2\xi\Delta t)\|E_h^n\|_h^2+2(G_0-15\xi)\Delta t\sum_{s=1}^{n}\|D_{-x}E_h^s\|_+^2\leq$$
$$(\Phi+2\xi)\Delta t\sum_{s=0}^{n-1}\|E_h^s\|_h^2+\Delta t^2\Psi\sum_{s=1}^{n}\sum_{r=0}^{s-1}\|D_{-x}E_h^r\|_+^2+\Delta t\sum_{s=1}^{n}T_h^s\ ,$$

which gives

$$\begin{aligned}\|E_h^n\|_h^2+\Delta t\sum_{s=0}^{n}\|D_{-x}e_h^s\|_+^2\ &\leq\ \frac{\max\{\Phi+2\xi,\Psi\}\Delta t}{\min\{1-2\xi\Delta t,2(G_0-15\xi)\}}\sum_{s=0}^{n-1}\left(\|E_h^s\|_h^2+\Delta t\sum_{r=0}^{s}\|D_{-x}E_h^r\|_+^2\right)\\ &\quad+\frac{1}{\min\{1-2\xi\Delta t,2(G_0-15\xi)\}}\left(\Delta t\sum_{s=1}^{n}T_h^s\right),\end{aligned}$$

for $n=1,\ldots,\ M$, provided that (3.85) and (3.86) hold.

Finally applying the discrete Gronwall lemma, we conclude (3.83), where

$$\hat{c}_1=\frac{1}{2\xi}\max\{(G_b')^2+k^2(F_{x,b})^2+2\xi,kF_b^2,ka_b(F_{y,b})^2\}\ .$$

□

As a corollary of Theorem 3.4 we have the next convergence result.

Corollary 3.5. *Let $C\in\mathscr{C}(0,T,H^3(0,b)\cap H_0^1(0,b))\cap\mathscr{C}^1(0,T,H^2(0,b))$ be the solution of (**VP**) and let C_h^n be its approximation defined by* (3.62). *Under the conditions of Theorem 3.4, there exists a positive constant c_c that does not depend on h nor Δt such that $E_h^n=R_hC(t_n)-C_h^n$, $n=0,\ldots,\ M$, satisfies*

$$\|E_h^n\|_h^2+\Delta t\sum_{s=0}^{n}\|D_{-x}E_h^s\|_+^2\leq c_c(h_{max}^4+\Delta t^2)\ , \tag{3.94}$$

for $\Delta t\in(0,\Delta t_0)$ provided that Δt_0 satisfies (3.86).

Proof. It follows easily from the fact that

$$\Delta t\sum_{s=1}^{n}T_h^s\ \ \leq\ \ \hat{c}_2(a_1h_{max}^4+a_2\Delta t^2)$$

where

$$\begin{aligned}a_1\ &=\ T\Big[\Big(\|C\|^2_{\mathscr{C}^1(0,T,H^2(0,b))}+(1+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T,H^3(0,b))}\Big)\\ &\quad+\Big(\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|C\|^2_{\mathscr{C}(0,T,H^2(0,b))}+(1+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))})\|C\|^2_{L^2(0,T,H^3(0,b))}\Big)\\ &\quad+\Big(\|C\|^2_{L^2(0,T,W^{1,\infty}(0,b))}+\|C\|^2_{H^1(0,T,W^{1,\infty}(0,b))}+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|C\|^2_{H^1(0,T,\mathbb{W}_h)}\Big)\Big]\\ a_2\ &=\ \|R_hC\|^2_{H^2(0,T,\mathbb{W}_h)}+2\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|R_hC\|_{H^1(0,T;\mathbb{W}_h)}\ .\end{aligned}$$

□

In the next result we consider less smoothness over K in order to obtain a new convergence estimate. To do so, it is necessary to consider that the approximation C_h is calculated using (3.72).

Corollary 3.6. *Let $C \in \mathscr{C}(0,T,H^3(0,1) \cap H_0^1(0,1)) \cap \mathscr{C}^1(0,T,H^2(0,1))$ be the solution of (**VP**) and let C_h^n be its approximation defined by* (3.72). *If $K \in L^1(0,T)$, $G \in \mathscr{C}_B^1(\mathbb{R})$, $F \in \mathscr{C}_B^1(\mathbb{R}^2)$, $0 < G_0 \leq G$ and there exists a positive constant ξ such that*

$$G_0 - 14\xi - \|K\|^2_{L^1(0,T)}\Psi - a_b(\Phi + 2\xi) > 0 \,, \tag{3.95}$$

where

$$\begin{aligned}
\Phi &= \frac{\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}}{4\xi}\left((G_b')^2 + (F_{x,b})^2\|K\|^4_{L^1(0,T)}\right) \,, && (3.96)\\
\Psi &= \frac{\|K\|^2_{L^1(0,T)}}{4\xi}(F_b^2 + \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}a_b(F_{y,b})^2) \,, && (3.97)
\end{aligned}$$

then there exist a positive constant c_r such that

$$\begin{aligned}
&\|E_h^n\|_h^2 + \Delta t \sum_{s=0}^{n} \|D_{-x}e_h^s\|_+^2 \\
&\leq \frac{c_r(h_{max}^4 + \Delta t^2)}{\min\{1 - 2\xi\Delta t, 2(G_0 - 14\xi - \|K\|^2_{L^1(0,T)}\Psi - a_b(\Phi + 2\xi))\}} \,,
\end{aligned} \tag{3.98}$$

when Δt satisfies

$$1 - 2\xi\Delta t > 0 \,. \tag{3.99}$$

Proof. From the proof of Theorem 3.4 we have

$$\begin{aligned}
&\|E_h^n\|_h^2 + 2(G_0 - 5\xi)\Delta t\|D_{-x}E_h^n\|_+^2 \\
&\leq \left(\frac{(G_b')^2}{2\xi}\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\Delta t + 1\right)\|E_h^{n-1}\|_h^2 + 2\xi\Delta t\|E_h^n\|_h^2 \\
&+ \frac{c_1^2 h_{max}^4}{2\xi}\Delta t\,\|C\|^2_{\mathscr{C}^1(0,T;H^2(0,b))} + \frac{c_2^2}{2\xi}(\Delta t)^2\|R_hC\|^2_{H^2(t_{n-1},t_n;\mathbb{W}_h)} \\
&+ \frac{h_{max}^4}{2\xi}c_3^2\Delta t(G_b^2 + (G_b')^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T;H^3(0,b))} \\
&+ \frac{(G_b')^2}{2\xi}(\Delta t)^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(t_{n-1},t_n;\mathbb{W}_h)} \\
&+ 2\Delta t\hat{T}_1^n + 2\Delta t\hat{T}_{h,1}^n \,,
\end{aligned} \tag{3.100}$$

where

$$
\begin{aligned}
\hat{T}_1^n &= \sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)(F(M_hC_h^{n-1},M_hC_h^s)D_{-x}C_h^s \\
&\quad -F(M_hC(t_{n-1}),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+ \ , \\
\hat{T}_{h,1}^n &= \sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)F(M_hC(t_{n-1}),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+ \\
&\quad -\int_0^{t_n} K(t_n-r)(F(\hat{M}_hC(t_n),\hat{M}_hC(r))\hat{M}_h\frac{\partial C}{\partial x}(r),D_{-x}E_h^n)_+dr \ .
\end{aligned}
$$

For $\hat{T}_1^n$, we have that the following estimate holds

$$
\begin{aligned}
|\hat{T}_1^n| &\le \frac{\|K\|_{L^1(0,T)}^2}{4\xi}(F_b^2+\|C\|_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}^2 a_b(F_{y,b})^2)\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\right)\|D_{-x}E_h^s\|_+^2 \\
&\quad +\frac{\|C\|_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}^2}{4\xi}(F_{x,b})^2\|K\|_{L^1(0,T)}^4\|E_h^{n-1}\|_h^2+3\xi\|D_{-x}E_h^n\|_+^2 \ . \qquad (3.101)
\end{aligned}
$$

To estimate $\hat{T}_{h,1}^n$, we begin by adding and subtracting the term

$$\int_0^{t_n} K(t_n-r)(F(M_hC(t_n),M_hC(r))D_{-x}R_hC(r),D_{-x}E_h^n)_+dr \ ,$$

to obtain

$$\hat{T}_{h,1}^n = \hat{T}_{h,1}^n(a)+\hat{T}_{h,1}^n(b) \ ,$$

where

$$
\begin{aligned}
\hat{T}_{h,1}^n(a) &= \int_0^{t_n} K(t_n-r)(F(M_hC(t_n),M_hC(r))D_{-x}R_hC(r) \\
&\quad -F(\hat{M}_hC(t_n),\hat{M}_hC(r))M_h\frac{\partial C}{\partial x}(r),D_{-x}E_h^n)_+dr \ ,
\end{aligned}
$$

and

$$
\begin{aligned}
\hat{T}_{h,1}^n(b) &= \sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)F(M_hC(t_{n-1}),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+ \\
&\quad -\int_0^{t_n} K(t_n-r)(F(M_hC(t_n),M_hC(r))D_{-x}R_hC(r),D_{-x}E_h^n)_+dr \ .
\end{aligned}
$$

The term $\hat{T}_{h,1}^n(a)$ can be estimated as follows

$$
\begin{aligned}
&|\hat{T}_{h,1}^n(a)| \\
&\le \frac{h_{max}^4}{4\xi}\|K\|_{L^1(0,T)}^2\left(c_4^2F_b^2+c_6^2\|C\|_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}^2(F_{y,b})^2\right)\int_0^{t_n}|K(t_n-r)|\|C(r)\|_{H^3(0,b)}^2dr \\
&+\frac{h_{max}^4}{4\xi}c_5^2\|C\|_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}^2(F_{x,b})^2\|K\|_{L^1(0,T)}^4\|C(t_n)\|_{H^2(0,b)}^2+3\xi\|D_{-x}E_h(t)\|_+^2 \ .
\end{aligned}
$$

In order to estimate $\hat{T}^n_{h,1}(b)$ we add and subtract the term

$$\sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)(F(M_hC(t_n),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+ \ ,$$

then we deduce

$$\hat{T}^n_{h,1}(b)=\hat{T}^n_{h,1}(b,1)+\hat{T}^n_{h,1}(b,2) \ ,$$

where

$$\begin{aligned}\hat{T}^n_{h,1}(b,1) \ &= \ \sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)(F(M_hC(t_n),M_hC(t_s))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+ \\ &\quad -\int_0^{t_n} K(t_n-r)(F(M_hC(t_n),M_hC(r))D_{-x}R_hC(r),D_{-x}E_h^n)_+dr \ ,\end{aligned}$$

and

$$\begin{aligned}\hat{T}^n_{h,1}(b,2) \ &= \ \sum_{s=0}^{n-1}\left(\int_{t_s}^{t_{s+1}} K(t_n-r)dr\right)((F(M_hC(t_{n-1}),M_hC(t_s)) \\ &\quad -F(M_hC(t_n),M_hC(t_s)))D_{-x}R_hC(t_s),D_{-x}E_h^n)_+.\end{aligned}$$

The term $\hat{T}^n_{h,1}(b,1)$ satisfy the following inequality

$$\begin{aligned}|\hat{T}^n_{h,1}(b,1)| \ &\leq \ \Delta t F_{y,b}\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|\left\|R_h\frac{\partial C}{\partial t}(r)\right\|_h\|C(r)\|_{W^{1,\infty}(0,b)}dr\|D_{-x}E_h^n\|_+ \\ &\quad +\Delta t F_b\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|\left\|\frac{\partial C}{\partial t}(r)\right\|_{W^{1,\infty}(0,b)}dr\|D_{-x}E_h^n\|_+ \ ,\end{aligned}$$

therefore we obtain

$$\begin{aligned}|\hat{T}^n_{h,1}(b,1)| \ &\leq \ \Delta t\frac{1}{4\xi}\|K\|^2_{L^1(0,T)}\left(F_b^2\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\|C\|^2_{H^1(t_s,t_{s+1};W^{1,\infty}(0,b))}\right. \\ &\quad \left.+(F_{y,b})^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\|R_hC\|^2_{H^1(t_s,t_{s+1};\mathbb{W}_h)}\right) \\ &\quad +2\xi\|D_{-x}E_h^n\|_+^2 \ .\end{aligned}$$

For the estimation of $\hat{T}^n_{h,1}(b,2)$ we have that the next inequality holds

$$|\hat{T}^n_{h,1}(b,2)|\leq\frac{(F_{x,b})^2}{4\xi}\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\Delta t\|K\|^4_{L^1(0,T)}\|R_hC\|_{H^1(t_{n-1},t_n;\mathbb{W}_h)}+\xi\|D_{-x}E_h^n\|_+^2 \ .$$

Then

$$
\begin{aligned}
&|\hat{T}^n_{h,1}| \\
&\leq \frac{h^4_{max}}{4\xi}\|K\|^2_{L^1(0,T)}\left(c_4^2F_b^2+c_6^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}(F_{y,b})^2\right)\int_0^{t_n}|K(t_n-r)|dr\|C\|^2_{\mathscr{C}(0,T;H^3(0,b))} \\
&+\frac{h^4_{max}}{4\xi}c_5^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}(F_{x,b})^2\|K\|^4_{L^1(0,T)}\|C\|^2_{\mathscr{C}(0,T;H^2(0,b))} \\
&+\Delta t\frac{1}{4\xi}\|K\|^2_{L^1(0,T)}\left(\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\left(F_b^2\|C\|^2_{H^1(t_s,t_{s+1};W^{1,\infty}(0,b))}\right.\right. \\
&\left.\left.+(F_{y,b})^2\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(t_s,t_{s+1};\mathbb{W}_h)}\right)\right) \\
&+\frac{(F_{x,b})^2}{4\xi}\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\Delta t\|K\|^4_{L^1(0,T)}\|R_hC\|_{H^1(t_{n-1},t_n;\mathbb{W}_h)}+6\xi\|D_{-x}E_h(t)\|^2_+ \ . \qquad (3.102)
\end{aligned}
$$

Applying inequalities (3.101) and (3.102) to (3.100), we deduce

$$
\begin{aligned}
&\|E^n_h\|^2_h+2(G_0-14\xi)\Delta t\|D_{-x}E^n_h\|^2_+ \\
&\leq(1+2\Phi\Delta t)\|E^{n-1}_h\|^2_h+2\xi\Delta t\|E^n_h\|^2_h+2\Psi\Delta t\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\|D_{-x}E^s_h\|^2_+ \\
&+\Delta\hat{T}^n_r \ , \qquad (3.103)
\end{aligned}
$$

where Φ, Ψ are defined respectively by (3.96), (3.97) and

$$
\begin{aligned}
&\hat{T}^n_r \\
&=c_{r_1}h^4_{max}\left[\|C\|^2_{\mathscr{C}^1(0,T;H^2(0,b))}+(1+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T;H^3(0,b))}\right. \\
&\left.+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|C\|^2_{\mathscr{C}(0,T;H^2(0,b))}\right] \\
&+c_{r_2}\Delta t\left[+\|R_hC\|^2_{H^2(t_{n-1},t_n;\mathbb{W}_h)}+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|_{H^1(t_{n-1},t_n;\mathbb{W}_h)}\right. \\
&\left.+\sum_{s=0}^{n-1}\int_{t_s}^{t_{s+1}}|K(t_n-r)|dr\left(\|C\|^2_{H^1(t_s,t_{s+1};W^{1,\infty}(0,b))}+\|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(t_s,t_{s+1};\mathbb{W}_h)}\right)\right] \ ,
\end{aligned}
$$

with

$$
\begin{aligned}
c_{r_1} &= \frac{1}{2\xi}\max\{c_1^2,\ c_3^2G_b^2+c_4^2F_b^2\|K\|^4_{L^1(0,T)},\ c_3^2(G'_b)^2 \\
&\qquad +c_6^2(F_{y,b})^2\|K\|^4_{L^1(0,T)},\ c_5^2(F_{x,b})^2\|K\|^4_{L^1(0,T)}\} \ , \\
c_{r_2} &= \frac{1}{2\xi}\max\{c_2^2,\ \ F_b^2\|K\|^2_{L^1(0,T)},\ (F_{y,b})^2\|K\|^2_{L^1(0,T)},\ (G'_b)^2+(F_{x,b})^2\|K\|^4_{L^1(0,T)}\} \ .
\end{aligned}
$$

Summing for $s = 1,\dots,n$ in (3.103) and changing the order of summation we deduce

$$(1-2\xi\Delta t)\|E_h^n\|_h^2 + 2(G_0 - 14\xi - \|K\|^2_{L^1(0,T)}\Psi)\Delta t \sum_{s=0}^{n} \|D_{-x}E_h^s\|_+^2$$
$$\leq 2(\Phi+\xi)\Delta t \sum_{s=0}^{n-1} \|E_h^s\|_h^2 + \Delta t \sum_{s=1}^{n} \hat{T}_r^s \,. \tag{3.104}$$

Finally, as we have that

$$\Delta t \sum_{s=1}^{n} \hat{T}_r^s \;\leq\; a_1 h_{max}^4 + a_2 \Delta t^2 \,,$$

where

$$\begin{aligned} a_1 &= c_{r_1} T \Big[\|C\|^2_{\mathscr{C}^1(0,T,H^2(0,b))} + (1+\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))})\|C\|^2_{\mathscr{C}(0,T,H^3(0,b))} \\ &\quad + \|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|C\|^2_{\mathscr{C}(0,T,H^2(0,b))}\Big] \\ a_2 &= c_{r_2} \Big[\|R_hC\|^2_{H^2(0,T,\mathbb{W}_h)} + (1+\|K\|^2_{L^1(0,T)})\|C\|^2_{\mathscr{C}(0,T,W^{1,\infty}(0,b))}\|R_hC\|_{H^1(0,T;\mathbb{W}_h)} \\ &\quad + \|C\|^2_{\mathscr{C}(0,T;W^{1,\infty}(0,b))}\|R_hC\|^2_{H^1(0,T;\mathbb{W}_h)}\Big] \,, \end{aligned}$$

we deduce from (3.104) the inequality

$$(1-2\xi\Delta t)\|E_h^n\|_h^2 + 2(G_0 - 14\xi - \|K\|^2_{L^1(0,T)}\Psi - a_b(\Phi+\xi))\Delta t \sum_{s=0}^{n} \|D_{-x}E_h^s\|_+^2$$
$$\leq \max\{a_1,a_2\}(h_{max}^4 + \Delta t^2) \,,$$

which leads to (3.98) provided that (3.95) and (3.99) holds. □

3.4 Numerical simulations

In what follows, we illustrate the convergence estimates presented in the previous sections.

In the first numerical simulation we consider a linear problem with a smooth kernel. We consider the IBVP (2.3), (1.7), (2.2)

$$G(C(t)) = 1 + C(t),\; F(C(t),C(s)) = 10C(s),\; K = e^{-\frac{1}{2}t} \,, \tag{3.105}$$

and select Z as well as the initial and boundary conditions such that this IBVP has the following solution

$$C(x,t) = e^{-t}(1-x)(arctan(\alpha(x-\frac{1}{2})) + arctan(\frac{\alpha}{2})),\; x\in[0,1],\; t\in[0,T] \,, \tag{3.106}$$

where $\alpha = 80$. If α is large, the solution C has an interior layer in the neighborhood of $x = \frac{1}{2}$. This fact motivates this first example where the solution is non-smooth.

The numerical approximation C_h was obtained with the method (3.62)-(3.64), with nonuniform grids in the spatial domain and with an uniform grid in the time domain with $T = 0.1$ and $\Delta t = 1\times 10^{-7}$. The initial spatial grid I_h was arbitrary and the following grids were obtained introducing in $[x_j, x_{j+1}]$ the midpoint.

In Table 3.1 we present the error

$$\mathbb{E}_p = \max_n \left(\|E_h(t_n)\|^2_{h_p} + \Delta t \sum_{s=0}^{n} \|E_h(s)\|^2_{1,h_p} \right)^{\frac{1}{2}}, \tag{3.107}$$

and the rate R_p defined by

$$R_p = \frac{\ln(\mathbb{E}_p/\mathbb{E}_{p+1})}{\ln(h_{p_{max}}/h_{p+1_{max}})}. \tag{3.108}$$

N_p	$\mathbb{E}_p$	$h_{p_{max}}$	R_p
34	2.4837×10^{-2}	4.2514×10^{-2}	-
68	6.5927×10^{-3}	2.1257×10^{-2}	1.9136
136	1.6906×10^{-3}	1.0628×10^{-2}	1.9633
272	4.2602×10^{-4}	5.3142×10^{-3}	1.9886
544	1.0610×10^{-4}	2.6571×10^{-3}	2.0055
1088	2.6492×10^{-5}	1.3286×10^{-3}	2.0017
2176	6.6132×10^{-6}	6.6428×10^{-4}	2.0021
4352	1.6449×10^{-6}	3.3214×10^{-4}	2.0074

Tab. 3.1: Convergence order in space for non singular kernels

We note that the numerical results presented in Table 3.1 agree with the theoretical results presented in Theorem 3.4 and Corollary 3.5 that is $\mathbb{E}_p = O(h^2_{max})$.

Let us consider now the IMEX method (3.72) studied when $K \in L^1(0,T)$. In (2.3), (1.7), (2.2) we consider again a linear situation with

$$G(C(t)) = 10 + C(t),\ F(C(t),C(s)) = 2,\ K(t) = \frac{1}{\sqrt{t}}, \tag{3.109}$$

where Z, the initial and boundary conditions are selected such that this IBVP has the following solution

$$C(x,t) = t^2(1-x)(arctan(\alpha(x-\frac{1}{2})) + arctan(\frac{\alpha}{2})),\ x\in[0,1],\ t\in[0,T], \tag{3.110}$$

where $\alpha = 80$.

N_p	$h_{p_{max}}$	$\mathbb{E}_p$	R_p
48	3.2407×10^{-2}	1.6811×10^{-2}	-
96	1.6204×10^{-2}	4.8871×10^{-3}	1.7823
192	8.1019×10^{-3}	1.2970×10^{-3}	1.9138
384	4.0509×10^{-3}	3.3723×10^{-4}	1.9434
768	2.0255×10^{-3}	8.4680×10^{-5}	1.9936
1536	1.0127×10^{-3}	2.1257×10^{-5}	1.9941
3072	5.0637×10^{-4}	5.2172×10^{-6}	2.0266

Tab. 3.2: Convergence order in space for singular kernels

In Table 3.2 we present the error $\mathbb{E}_p$ and the convergence rate R_p defined respectively by (3.113) and (3.114). We observe that in agreement with Corollary 3.6 we have that $\mathbb{E}_p = O(h_{max}^2)$.

Tables 3.1 and 3.2 were obtained by fixing Δt and calculating the convergence order in space. In what follows we fix the spatial grid and study the convergence order in time.

Let us consider in the IVBP (2.3), (1.7), (2.2) with

$$G(C) = 1 + C,\ F(C) = 10C,\ K = e^{-\frac{1}{2}t}, \tag{3.111}$$

where Z as well as the initial and boundary conditions are such that this IBVP has the following solution

$$C(x,t) = e^{-t}(1-x)(arctan(\alpha(x-\frac{1}{2}) + arctan(\frac{\alpha}{2})),\ x\in[0,1],\ t\in[0,T]\ , \tag{3.112}$$

where $\alpha = 20$.

The numerical approximation C_h was obtained with the method (3.62)-(3.64) with nonuniform grids in the spatial domain $\Omega = [0,1]$ with $h_{max} = 9.3622\times 10^{-3}$ and with an uniform grid in the time domain $[0, 0.1]$.

In Table 3.3 we present the error

$$\hat{\mathbb{E}}_p = \max_{n=1,\ldots,M_p}\left(\|e_h(t_n)\|_h^2 + \Delta t_p\sum_{s=1}^{n}\|D_{-x}e_h(s)\|_+^2\right)^{\frac{1}{2}}\ , \tag{3.113}$$

and the rate R_p defined by

$$\hat{R}_p = \frac{\ln(\hat{\mathbb{E}}_p/\hat{\mathbb{E}}_{p+1})}{\ln(\Delta t_p/\Delta t_{p+1})}\ . \tag{3.114}$$

We note that the numerical results presented in Table 3.3 coincide with the theoretical results presented in Theorem 3.4 and Corollary 3.5, that is $\hat{\mathbb{E}}_p = O(\Delta t)$.

M_p	$\hat{\mathbb{E}}_p$	Δt	$\hat{R}_p$
35	6.7198×10^{-3}	2.8571×10^{-3}	-
40	5.8417×10^{-3}	2.5000×10^{-3}	1.0487
45	5.1607×10^{-3}	2.2222×10^{-3}	1.0524
50	4.6171×10^{-3}	2.0000×10^{-3}	1.0564
55	4.1746×10^{-3}	1.8182×10^{-3}	1.0571
60	3.8070×10^{-3}	1.6667×10^{-3}	1.0595
65	3.4974×10^{-3}	1.5385×10^{-3}	1.0597
70	3.2334×10^{-3}	1.4286×10^{-3}	1.0589

Tab. 3.3: Convergence order in time

By using a different approach, first introduced in [26] for a linear version of (3.6), that differs from the one usually followed in the literature introduced by Wheeler in [52], we where able to prove for the semi-discrete and fully discrete approximations that the discrete L^2 norm of the spatial discretization error and of its discrete gradient are second order convergent with respect to the space step size. In each case we presented different results depending on the smoothness of the kernel function K. Our approach not only allowed the weakening of the smoothness conditions usually required when Wheeler's technique is used, but also let us consider the case of weakly singular kernels, which to the best of our knowledge, has not been considered before in this type of convergence estimates.

In what concerns the numerical simulations presented, they illustrate the theoretical results proved at least for linear coefficients. Some efforts need to be invest in the future to illustrate these results for quasi-linear problems.

Chapter 4

A tridimensional model for drug release

In this chapter, we propose a tridimensional mathematical model to describe the drug release from a cylindrical polymeric matrix. We assume that the fluid diffuses into the matrix creating a stress driven diffusion, thus a non-Fickian mass flux. To describe this phenomenon, we consider the model presented in Chapter 1 for solvent sorption. For the drug release, as we assume that the drug is present in two states dissolved and undissolved, the process will be described by non-Fickian diffusion associated to solvent uptake, coupled with non-linear dissolution. To describe the swelling of the polymeric cylinder, we will consider a volume conservation equation to track the movement of the fronts, in both radial and axial directions.

In Section 4.1 we introduce the system of partial differential equations that define the model, coupled with initial and boundary conditions. In Section 4.2 we consider a volume conservation equation to describe the swelling of the polymeric matrix, this equation will allow us to track the movement of the spatial boundary. In Section 4.3 we propose an IMEX numerical scheme to solve the model and in Section 4.4 some plots are presented to illustrate the behavior of the numerical simulations.

4.1 Mathematical model

Let us consider a cylindrical polymeric matrix, with initial solid drug loading C_s^0. As the solvent penetrates the polymeric matrix, solid drug dissolves and then the dissolved drug diffuses out. The following assumptions are made in the model:

(a) Swelling is homogeneous and independent in the radial and axial directions;

(b) The transport of liquid within the polymer occurs by non-Fickian diffusion;

(c) The transport of drug out of the polymer occurs by non-Fickian diffusion associated with solvent uptake and non-linear dissolution;

(d) The positions of the polymer swelling front and dissolution front coincide;

(e) A perfect sink condition is maintained for the drug and equilibrium concentrations are maintained for the liquid.

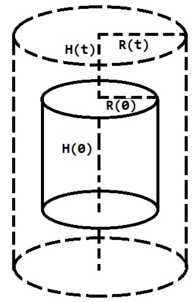

Fig. 4.1: Cylindrical domain

Let C_l denote the concentration of the liquid solvent, the functional relation between C_l and the strain ε, is defined from (1.24) by

$$f_l(C_l) = \frac{C_l}{\rho_l - C_l} \,, \tag{4.1}$$

where ρ_l denotes the density of the liquid. Assuming that the polymer behavior is describe by the generalized Maxwell-Wiechert model with $m+1$ arms, then from (1.17) and (4.1) we have that the stress associated to solvent uptake and exerted by the polymer is defined as

$$\sigma_l = -\left(\sum_{k=0}^{m} E_k\right) f_l + \int_0^t \left(\sum_{k=1}^{m} \frac{E_k}{\tau_k} e^{-\frac{t-s}{\tau_k}}\right) f_l(s)ds \,. \tag{4.2}$$

The evolution of solvent penetration, drug diffusion and dissolution are described by the following equations on the domain $\Omega \subset \mathbb{R}^3$ and for $t > 0$,

$$\frac{\partial C_l}{\partial t} = \nabla \cdot (D_l(C_l)\nabla C_l + D_v(C_l)\nabla \sigma_l) \,, \tag{4.3}$$

$$\frac{\partial C_d}{\partial t} = \nabla \cdot (D_d(C_l)\nabla C_d + \upsilon(C_l)C_d) + K_d \left(\frac{C_s - C_d}{C_s}\right) C_l S(C_s) \,, \tag{4.4}$$

$$\frac{\partial C_s}{\partial t} = -K_d \left(\frac{C_s - C_d}{C_s}\right) C_l S(C_s) \,, \tag{4.5}$$

where C_d, C_s denote the concentration of dissolved and solid drug respectively, D_l, D_d the diffusion coefficients of the liquid solvent and the dissolved drug respectively, K_d denotes the constant dissolution rate of the drug, υ is defined as

$$\upsilon(C_l) = D_v(C_l)\frac{\nabla \sigma_l}{C_l} \,,$$

and S is the Heaviside step function defined by

$$S(x) = \begin{cases} 0, & x \leq 0 \\ 1, & x > 0 \,. \end{cases}$$

Equation (4.3) states that liquid transport is due to Fickian (J_F) and non-Fickian (J_{NF}) diffusion, defined respectively in (1.2) and (1.3). At the same time, equation (4.4) states that the local concentration of dissolved drug depends on Fickian diffusion ($D_d(C_l)\nabla C_d$), convection ($\upsilon(C_l)$) and on solid drug dissolution. While solid drug dissolution can take place provided that $C_l > 0$, the velocity field υ is due to the stress induced by the solvent income. Indeed, we have that $\upsilon = J_{NF}/C_l$.

A Fujita-type [30] exponential dependence for $D_l(C_l)$ and $D_d(C_l)$ is assumed with

$$\begin{aligned} D_l(C_l) &= D_{eq_l} exp(-\beta_l(1-\frac{C_l}{C_l^e})) , & (4.6)\\ D_d(C_l) &= D_{eq_d} exp(-\beta_d(1-\frac{C_l}{C_l^e})) , & (4.7) \end{aligned}$$

where D_{eq_l}, D_{eq_d} denote respectively the diffusion coefficients of the liquid solvent and the dissolved drug in the fully swollen sample and β_l, β_d dimensionless positive constants.

We consider a cylindrical domain $\Omega \subset \mathbb{R}^3$ with initial radius R_0 and height H_0 (Figure 4.1). The domain presents a moving boundary defined by the functions $H(t)$ and $R(t)$ that represent respectively the height and the radius of the cylinder at time t. Due to the symmetry in θ direction, the three dimensional problem is reduced to a two dimensional case. Therefore equations (4.3)-(4.5) can be rewritten in cylindrical coordinates as

$$\begin{aligned} \frac{\partial C_l}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left(rD_l(C_l)\frac{\partial C_l}{\partial r} + rD_v(C_l)\frac{\partial \sigma_l}{\partial r}\right) + \frac{\partial}{\partial z}\left(D_l(C_l)\frac{\partial C_l}{\partial z} + D_v(C_l)\frac{\partial \sigma_l}{\partial z}\right) , & (4.8)\\ \frac{\partial C_d}{\partial t} &= \frac{1}{r}\frac{\partial}{\partial r}\left(rD_d(C_l)\frac{\partial C_d}{\partial r} + r\upsilon(C_l)C_d\right) + \frac{\partial}{\partial z}\left(D_d(C_l)\frac{\partial C_d}{\partial z} + \upsilon(C_l)C_d\right) & \\ &\quad + K_d\left(\frac{C_s - C_d}{C_s}\right)C_l S(C_s) , & (4.9)\\ \frac{\partial C_s}{\partial t} &= -K_d\left(\frac{C_s - C_d}{C_s}\right)C_l S(C_s) , & (4.10) \end{aligned}$$

where $0 < r < R(t)$, $0 < z < H(t)$ and $t > 0$. Equations (4.8)-(4.10) are completed with initial conditions

$$C_l = C_l^0,\ C_d = 0,\ C_s = C_s^0 \ :\ \text{for } t = 0,\ 0 \le r \le R_0,\ 0 \le z \le H_0 , \qquad (4.11)$$

where C_l^0, $C_s^0 \in \mathbb{R}$ are positive constants. At the cylinder surface, the boundary conditions are

$$C_l = C_l^e,\ C_d = 0 :\ \text{for } t > 0,\ r = R(t),\ 0 \le z \le H(t) \text{ and } z = H(t),\ 0 \le r \le R(t) , \qquad (4.12)$$

where $C_l^e \in \mathbb{R}$ is a positive constant representing the concentration of the liquid agent in the exterior of the cylinder. Symmetry conditions are applied at the center of the matrix, hence we also have that

$$\begin{aligned} \frac{\partial C_l}{\partial z} = \frac{\partial C_d}{\partial z} = 0 \quad &: \quad \text{for } t > 0,\ r = 0,\ 0 \le z \le H(t) , & \\ \frac{\partial C_l}{\partial r} = \frac{\partial C_d}{\partial r} = 0 \quad &: \quad \text{for } t > 0,\ z = 0,\ 0 \le r \le R(t) . & (4.13) \end{aligned}$$

4.2 Tracking of the swelling fronts

In order to track the moving fronts due to swelling, we consider the following conservation equation, where the total volume of the matrix is the sum of water, dissolved and undissolved drug volumes. We have

$$\pi R^2(t)H(t) = \int_0^{H(t)}\int_0^{R(t)} 2\pi r\left[\frac{1}{\rho_l}C_l(r,z,t) + \frac{1}{\rho_d}\left(C_d(r,z,t)+C_s(r,z,t)\right)\right] dr\, dz + \frac{m_0}{\rho_p}\ , \quad (4.14)$$

where ρ_p and ρ_d denote the density of the polymer and the drug respectively, m_0 represent the initial mass of the dry polymeric matrix.

Since we assume the swelling to be independent in the two directions, by taking time derivatives in (4.14), the moving fronts in the radial and axial direction can be separately tracked.

To track the moving front in the radial direction we begin by fixing $H(t) = H$ and taking time derivative in (4.14) to obtain

$$\begin{aligned} R(t)H\frac{dR(t)}{dt} &= \int_0^{H}\int_0^{R(t)} r\left[\frac{1}{\rho_l}\frac{\partial C_l}{\partial t}(r,z,t) + \frac{1}{\rho_d}\frac{\partial}{\partial t}\left(C_d(r,z,t)+C_s(r,z,t)\right)\right] dr\, dz \\ &\quad + \int_0^H R(t)\frac{\partial R(t)}{\partial t}\left(\frac{C_l^e}{\rho_l} + \frac{C_s|_{R(t)}}{\rho_d}\right) dz\ . \end{aligned} \quad (4.15)$$

As we have

$$\begin{aligned} &\int_0^{H}\int_0^{R(t)} \frac{r}{\rho_l}\frac{\partial C_l}{\partial t}(r,z,t) dr\, dz \\ = &\int_0^H \frac{R(t)}{\rho_l}\left(D_l(C_l(R(t),z,t))\frac{\partial C_l}{\partial r}(R(t),z,t) + D_v(C_l(R(t),z,t))\frac{\partial \sigma_l}{\partial r}(R(t),z,t)\right) \end{aligned} \quad (4.16)$$

and

$$\begin{aligned} &\int_0^{H}\int_0^{R(t)} r\frac{1}{\rho_d}\frac{\partial}{\partial t}\left(C_d(r,z,t)+C_s(r,z,t)\right) dr\, dz \\ &= \int_0^H \frac{R(t)}{\rho_d}D_d(C_l(R(t),z,t))\frac{\partial C_d}{\partial r}(R(t),z,t) dz\ , \end{aligned} \quad (4.17)$$

it follows from (4.15)-(4.17) that

$$\begin{aligned} \left(1 - \frac{C_l^e}{\rho_l} - \frac{C_s|_{R(t)}}{\rho_d}\right) H\frac{dR(t)}{dt} &= \int_0^H \left[\frac{1}{\rho_l}\left(D_l(C_l^e)\frac{\partial C_l}{\partial r}(R(t),z,t) + D_v(C_l^e)\frac{\partial \sigma_l}{\partial r}(R(t),z,t)\right)\right. \\ &\quad \left. + \frac{1}{\rho_d}D_d(C_l^e)\frac{\partial C_d}{\partial r}(R(t),z,t)\right] dz\ . \end{aligned} \quad (4.18)$$

To track the moving front in the axial direction, we fix $R(t) = R$ and proceeding as before we deduce

$$\begin{aligned} \left(1 - \frac{C_l^e}{\rho_l} - \frac{C_s|_{H(t)}}{\rho_d}\right) R^2\frac{dH(t)}{dt} &= 2\int_0^R \left[\frac{1}{\rho_l}\left(D_l(C_l^e)\frac{\partial C_l}{\partial z}(r,H(t),t) + D_v(C_l^e)\frac{\partial \sigma_l}{\partial z}(r,H(t),t)\right)\right. \\ &\quad \left. + \frac{1}{\rho_d}D_d(C_l^e)\frac{\partial C_d}{\partial z}(r,H(t),t)\right] r\, dr\ . \end{aligned} \quad (4.19)$$

We note that if no mechanistic effects are taken into account and the drug is considered to exist only in the dissolved state then (4.18) and (4.19) reduce to the moving boundary conditions in [29].

4.3 Numerical scheme

We propose a coupled Implicit-Explicit (IMEX) method to solve the initial-boundary value problem (4.8)-(4.13) and (4.18), (4.19).

In $[0,T]$ we consider a grid $P=\{t_n, n=0,1,...,M\}$, with $t_0=0$, $t_M=T$ and $t_n-t_{n-1}=\Delta t$. We denote by D_{-t} the usual backward finite difference operator with respect to the time variable.

As the spatial boundary is changing in time, we consider in the initial interval $[0,R_0]$ a uniform grid $I(t_0)=\{r_i,\ i=0,1,..,N(t_0)\}$, with $r_0=0$, $r_{N(t_0)}=R_0$ and $r_i-r_{i-1}=\Delta r$. Then in each interval $[0,R(t_n)]$ we consider a non-uniform grid $I(t_n)=\{r_i,\ i=0,1,..,N(t_n)\}$, with $r_0=0$, $r_{N(t_n)}=R(t_n)$ and $r_i-r_{i-1}=\Delta r_i$. We denote by D_{-r} and D_r the usual backward and forward finite difference operator with respect to the space variable r.

Analogously in the initial interval $[0,H_0]$, we consider a uniform grid $J(t_0)=\left\{z_j,\ j=0,1,..,N(t_0)\right\}$, with $z_0=0$, $z_{K(t_0)}=H_0$ and $z_j-z_{j-1}=\Delta z$. Then in each interval $[0,H(t_n)]$ we consider a non-uniform grid $J(t_n)=\left\{z_j,\ j=0,1,..,K(t_n)\right\}$, with $z_0=0$, $z_{K(t_n)}=H(t_n)$ and $z_j-z_{j-1}=\Delta z_j$. We denote by D_{-z} and D_z the usual backward and forward finite difference operator with respect to the space variable z.

Let M_{h_r} and M_{h_z} be average operators defined as

$$\begin{aligned}
M_{h_r}u_h(r_i,z_j) &= \frac{1}{2}(u_h(r_{i-1},z_j)+u_h(r_i,z_j))\ ,\\
M_{h_z}u_h(r_i,z_j) &= \frac{1}{2}(u_h(r_i,z_{j-1})+u_h(r_i,z_j))\ .
\end{aligned}$$

We introduce the following notations

$$\begin{aligned}
IM_{l,r}(r_i,z_j,t_n) &= D_l(M_{h_r}C_{l_h}^{n-1}(r_i,z_j))D_{-r}C_{l_h}^{n}(r_i,z_j)\ ,\\
IM_{l,z}(r_i,z_j,t_n) &= D_l(M_{h_z}C_{l_h}^{n-1}(r_i,z_j))D_{-z}C_{l_h}^{n}(r_i,z_j)\ ,\\
EX_{l,r}(r_i,z_j,t_{n-1}) &= D_v(M_{h_r}C_{l_h}^{n-1}(r_i,z_j))D_{-r}\sigma_{l_h}^{n-1}(r_i,z_j)\ ,\\
EX_{l,z}(r_i,z_j,t_{n-1}) &= D_v(M_{h_z}C_{l_h}^{n-1}(r_i,z_j))D_{-z}\sigma_{l_h}^{n-1}(r_i,z_j)\ ,
\end{aligned}$$

and

$$\begin{aligned}
IM_{d,r}(r_i,z_j,t_n) &= D_d(M_{h_r}C_{l_h}^{n}(r_i,z_j))D_{-r}C_{d_h}^{n}(r_i,z_j)\ ,\\
IM_{d,z}(r_i,z_j,t_n) &= D_d(M_{h_z}C_{l_h}^{n}(r_i,z_j))D_{-z}C_{d_h}^{n}(r_i,z_j)\ ,\\
EX_{d,r}(r_i,z_j,t_{n-1}) &= D_v(M_{h_r}C_{l_h}^{n}(r_i,z_j))\frac{M_{h_r}C_{d_h}^{n}(r_i,z_j)}{M_{h_r}C_{l_h}^{n}(r_i,z_j)}D_{-r}\sigma_{l_h}(C_{l_h}^{n}(r_i,z_j))\ ,\\
EX_{d,z}(r_i,z_j,t_{n-1}) &= D_v(M_{h_z}C_{l_h}^{n}(r_i,z_j))\frac{M_{h_z}C_{d_h}^{n}(r_i,z_j)}{M_{h_z}C_{l_h}^{n}(r_i,z_j)}D_{-z}\sigma_{l_h}(C_{l_h}^{n}(r_i,z_j))\ ,
\end{aligned}$$

where we have used IM and EX to underline the implicit and the explicit character of the discretization respectively.

The IMEX method for (4.8)-(4.10) is defined by

$$\begin{aligned} D_{-t}C_{l_h}^n(r_i,z_j) &= \frac{1}{r_i}D_r\left((M_{h_r}r_i)IM_{l,r}(r_i,z_j,t_n)+(M_{h_r}r_i)EX_{l,r}(r_i,z_j,t_{n-1})\right) \\ &\quad +D_z\left(IM_{l,z}(r_i,z_j,t_n)+EX_{l,z}(r_i,z_j,t_{n-1})\right)\ , \qquad (4.20) \\ D_{-t}C_{d_h}^n(r_i,z_j) &= \frac{1}{r_i}D_r\left((M_{h_r}r_i)IM_{d,r}(r_i,z_j,t_n)+(M_{h_r}r_i)EX_{d,r}(r_i,z_j,t_{n-1})\right) \\ &\quad +D_z\left(IM_{d,z}(r_i,z_j,t_n)+EX_{d,z}(r_i,z_j,t_{n-1})\right) \\ &\quad +K_d\left(\frac{C_{s_h}^{n-1}(r_i,z_j)-C_{d_h}^{n-1}(r_i,z_j)}{C_{s_h}^{n-1}(r_i,z_j)}\right)C_{l_h}^n(r_i,z_j)S(C_{s_h}^{n-1}(r_i,z_j))\ , \qquad (4.21) \\ D_{-t}C_{s_h}^n(r_i,z_j) &= -K_d\left(\frac{C_{s_h}^{n-1}(r_i,z_j)-C_{d_h}^{n}(r_i,z_j)}{C_{s_h}^{n-1}(r_i,z_j)}\right)C_{l_h}^n(r_i,z_j)S(C_{s_h}^{n-1}(r_i,z_j))\ , \qquad (4.22) \end{aligned}$$

with initial conditions

$$C_{l_h}^0=C_l^0,\ C_{d_h}^0=0,\ C_{s_h}=C_s^0\ :\ \text{for } t=0,\ 0\le r_i\le R_0,\ 0\le z_j\le H_0\ , \qquad (4.23)$$

boundary conditions on the cylinder surface

$$\begin{aligned} C_{l_h}=C_l^e,\ C_{d_h}=0 \quad &: \quad \text{for } n>0,\ r_i=R(t_n),\ 0\le z_j\le H(t_n) \\ &\quad\ \text{and } z_j=H(t_n),\ 0\le r_i\le R(t_n)\ , \qquad (4.24) \end{aligned}$$

and symmetric conditions at the axes

$$\begin{aligned} D_{-z}C_{l_h}=D_{-z}C_{d_h}=0 \quad &: \quad \text{for } n>0,\ r_i=0,\ 0\le z_j\le H(t_n)\ , \\ D_{-r}C_{l_h}=D_{-r}C_{d_h}=0 \quad &: \quad \text{for } n>0,\ z_j=0,\ 0\le r_i\le R(t_n)\ . \qquad (4.25) \end{aligned}$$

The moving front defined by (4.18) and (4.19) is tracked with the following equations

$$\begin{aligned} \left(1-\frac{C_l^e}{\rho_l}-\frac{C_s|_{R(t_n)}}{\rho_d}\right)H(t_n)D_{-t}R(t_{n+1}) &= \Delta z\sum_{j=1}^{K(t_n)}\frac{1}{\rho_l}\Big(D_l(C_l^e)D_{-r}C_{l_h}^n(R(t_n),z_j) \\ &\quad +D_v(C_l^e)D_{-r}\sigma_{l_h}^n(R(t_n),z_j)\Big) \\ &\quad +\frac{1}{\rho_d}D_d(C_l^e)D_{-r}C_{d_h}^n(R(t_n),z_j\ , \qquad (4.26) \end{aligned}$$

and

$$\begin{aligned} \left(1-\frac{C_l^e}{\rho_l}-\frac{C_s|_{H(t_n)}}{\rho_d}\right)R^2(t_n)D_{-t}H(t_{n+1}) &= 2\Delta r\sum_{i=1}^{N(t_n)}\frac{r_i}{\rho_l}\Big(D_l(C_l^e)D_{-r}C_{l_h}^n(r_i,H(t_n)) \\ &\quad +D_v(C_l^e)D_{-r}\sigma_{l_h}^n(r_i,H(t_n))\Big) \\ &\quad +\frac{r_i}{\rho_d}D_d(C_l^e)D_{-r}C_{d_h}^n(r_i,H(t_n))\ . \qquad (4.27) \end{aligned}$$

We compute the concentration profiles at time step t_n using the known concentration profiles at t_{n-1} with boundary conditions (4.24) and (4.25). Then we use (4.26) and (4.27) to obtain the new front position for the next time step.

4.4 Numerical simulations

In what follows we exhibit some numerical results for the initial-boundary value problem (4.8)-(4.13) and (4.18), (4.19) using the method (4.20)-(4.27). In (4.2) we consider $m = 1$, that is a Maxwell fluid arm in parallel with a free spring. The following values for the parameters have been considered,

$$\begin{aligned}
R_0 &= 1\times 10^{-3}\ m,\ \Delta r_{max} = 5\times 10^{-5}\ m,\ H_0 = 1\times 10^{-3}\ m,\ \Delta z_{max} = 5\times 10^{-5}\ m,\\
D_{eq_l} &= 3.74\times 10^{-9}\ m^2/s,\ D_{eq_d} = 2.72\times 10^{-10}\ m^2/s,\ \beta_l = 0.8,\ \beta_d = 0.5,\ \hat{\mu} = 20\times 10^5\ Pas,\\
\rho_l &= 1000\ kg/m^3,\ \rho_p = 1175\ kg/m^3,\ \rho_d = 1400\ kg/m^3,\ E_1 = 9\times 10^3\ Pa,\ E_0 = 1\times 10^3\ Pa,\\
\mu_1 &= 225\times 10^4\ Pas,\ C_l^e = 755\ Kg/m^3,\ C_l^0 = 0\ Kg/m^3,\ C_s^0 = 4.5\ Kg/m^3,\\
K_d &= 1\times 10^{-2}\ s^{-1} \text{ and } \Delta t = 0.01\ s.
\end{aligned}$$

In Figures 4.2 we plot the behavior of the concentration of the liquid solvent as it diffuses into the polymeric cylinder at $t = 1s$, $t = 8s$, $t = 15s$ and $t = 25s$. A quarter of the cylinder cross section was modeled due to symmetries. The axes z and r correspond to the inner part of the cylinder where symmetry conditions (4.13) were considered. The outer parts correspond to the expansion fronts where the constant source of concentration C_l^e is assumed. We observe a smooth solution that develops from low levels of concentration to high levels of concentration as expected, since the liquid penetration occurs from the outermost regions of the plot toward the axes.

In Figures 4.3 we present plots of the concentration of dissolved drug at $t = 1s$, $t = 8s$, $t = 15s$ and $t = 25s$. As before, the axes z and r correspond to the inner part of the cylinder where symmetry conditions (4.13) were considered. The outermost part of the plots correspond to the expansion fronts where a perfect sink condition is assumed. We observe that regions where the concentration of the liquid solvent is high, correspond to regions where the concentration of dissolved drug is also high.

In Figures 4.4 we show plots of the concentration of solid drug at $t = 1s$, $t = 8s$, $t = 15s$ and $t = 25s$. We observe that as the concentration of dissolved drug increases, the concentration of solid drug decreases smoothly towards the moving fronts. On the contrary to what is observed in the plots of dissolved drug, the regions of highest solid drug concentration correspond to regions of lowest liquid agent concentration.

In Figures 4.5 and 4.6 we plot the movement in time of the dimensionless swelling fronts in both axial and radial directions. We observe that in both cases, the initial uptake of the solvent produces an initial rapid growth of the swelling followed by an equilibrium state of the fronts.

In Figures 4.7 and 4.8 we present the dimensionless swelling fronts as functions of the parameter E_0 and its corresponding C_l^e. In both cases we observe that the fronts are decreasing functions of E_0. We note that this behavior is physically sound, since an increase in E_0 corresponds to an increase in the resistance of the polymer to swelling.

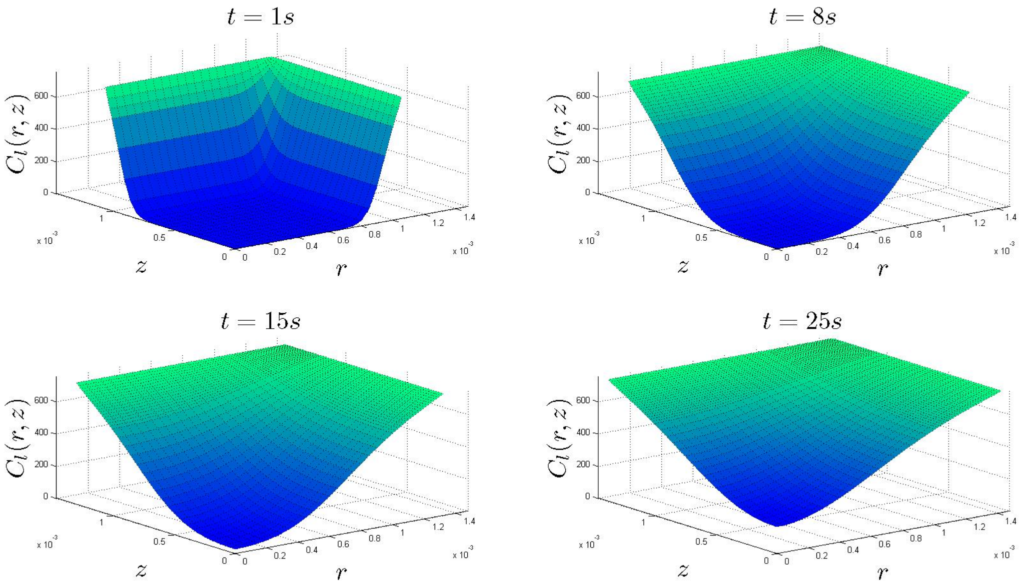

Fig. 4.2: Concentration of solvent C_l, for different t

By $M_d/M_{d_0}(t)$, where M_d is the total mass of drug released at time t and M_{d_0} is the initial mass loaded in the polymeric matrix, we represent the dimensionless total mass of drug released at time t defined as

$$M_d/M_{d_0}(t) = 1 - \frac{2}{R_0^2 H_0 C_s^0} \int_0^{H(t)} \int_0^{R(t)} r\,(C_s(r,z,t) + C_d(r,z,t))\,dr\,dz\,, \tag{4.28}$$

and by $M_s/M_\infty(t)$ the mass of the liquid solvent inside of the matrix at time t, defined as

$$M_s/M_\infty(t) = \frac{2}{R_{eq}^2 H_{eq} C_l^e} \int_0^{H(t)} \int_0^{R(t)} r C_l(r,z,t) dr\,dz\,, \tag{4.29}$$

where R_{eq} and H_{eq} are the values of $R(t)$ and $H(t)$ at equilibrium, respectively.

In order the study the effects of swelling in drug release we plot M_d/M_{d_0} as a function of E_0 in Figures 4.9 and 4.10. In Figure 4.9 we assume that the polymer does not swell and in Figure 4.10 a moving boundary due to swelling is considered. When we say that no swelling is present we mean that $L(t) = L_0$ for all t. We observe in Figure 4.9 that M_d/M_{d_0} is a decreasing function of E_0. Conversely in Figure 4.10 we observe that M_d/M_{d_0} is an increasing function of E_0. As shown in Figures 4.7 and 4.8, an E_0 decrease implies a swelling increase and, therefore, the dissolved drug has to travel a larger distance to the moving front. Consequently, less dissolved drug accumulates at the front where the perfect sink condition is assumed and the mass of drug released decreases as the swelling increases.

In Figures 4.11 and 4.12 we present plots of M_s/M_∞ and M_d/M_{d_0} respectively as a function of μ_1. Figure 4.11 shows that M_s/M_∞ is a decreasing function of μ_1 and Figure 4.12 that M_d/M_{d_0} is

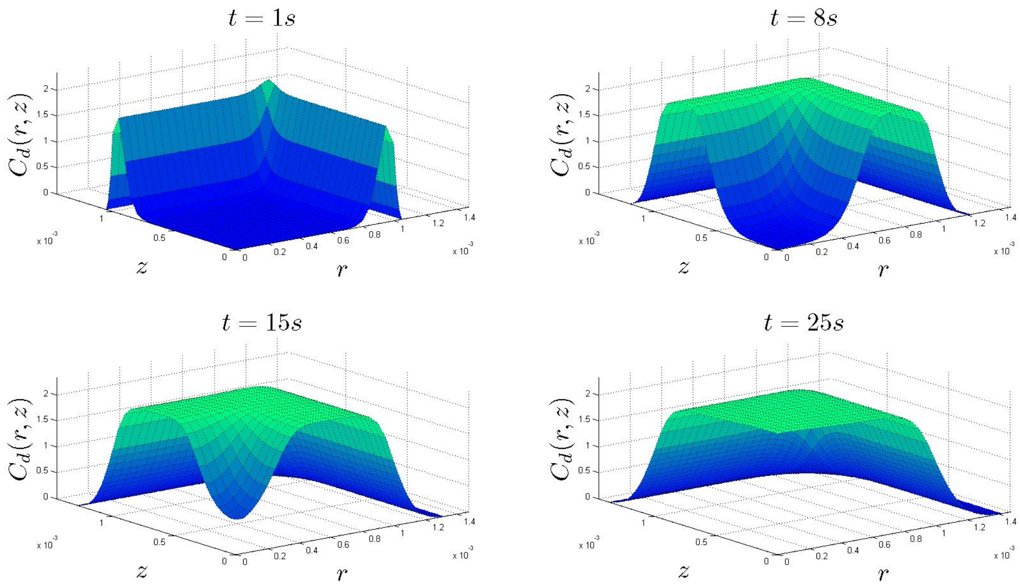

Fig. 4.3: Concentration of dissolved drug C_d, for different t

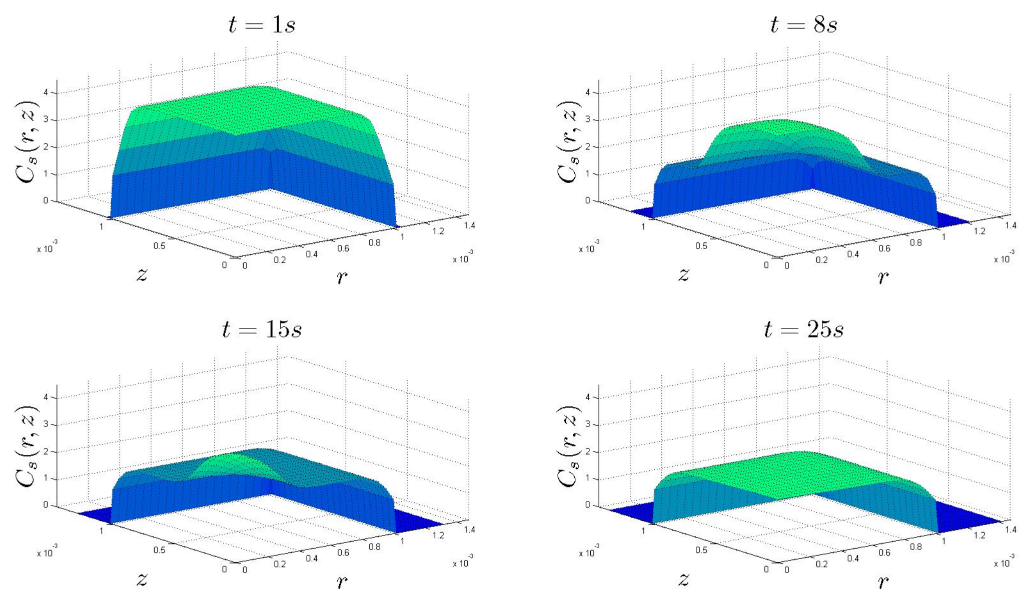

Fig. 4.4: Concentration of undissolved drug C_s, for different t

an increasing function of μ_1. To obtain the results presented in Figure 4.11 we did a $5th$ degree polynomial fitting in order to avoid the jumps that appear as a consequence of the moving of the boundary.

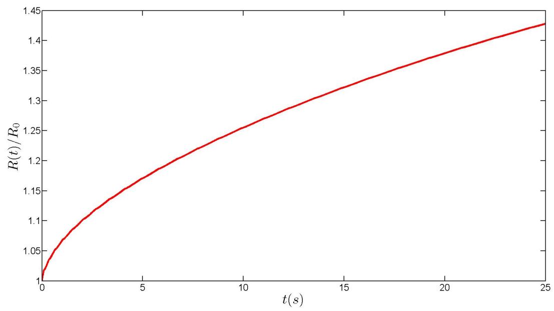

Fig. 4.5: Swelling in the radial direction

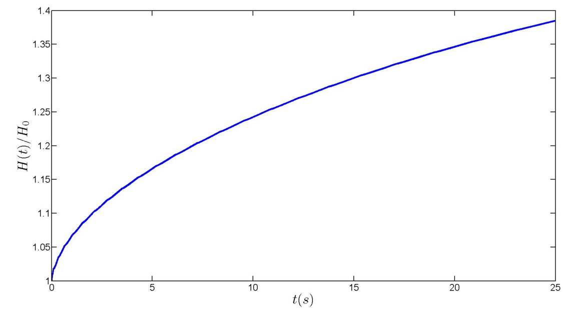

Fig. 4.6: Swelling in the axial direction

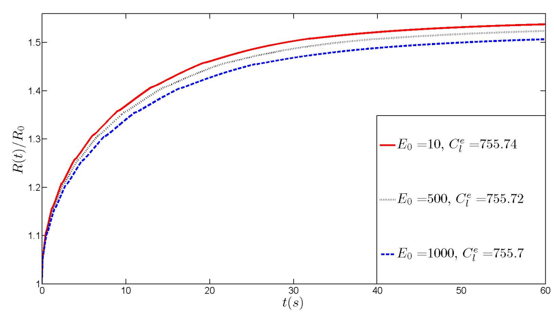

Fig. 4.7: Radial swelling, $R(t)/R_0$ as a function of E_0

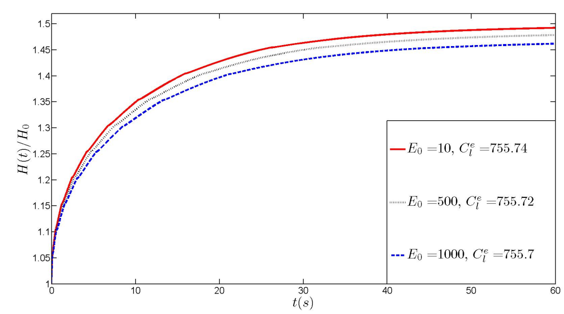

Fig. 4.8: Axial swelling, $H(t)/H_0$ as a function of E_0

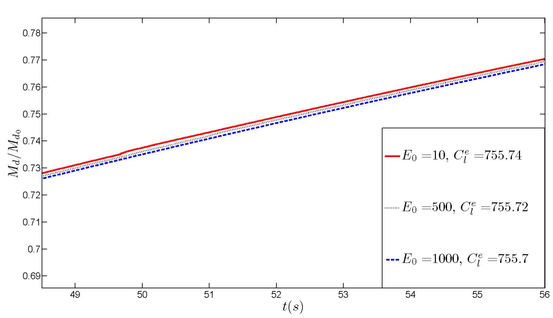

Fig. 4.9: Mass of drug released, M_d/M_{d_0} as a function of E_0 with $L(t) = L_0$

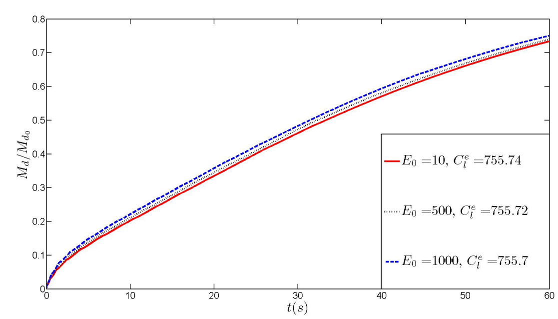

Fig. 4.10: Mass of drug released, M_d/M_{d_0} as a function of the parameter E_0

Finally in Figure 4.13 we plot $R(t)/H(t)$ for different initial values of R_0/H_0. As proved by Tanaka in [39], we observe that upon swelling, $R(t)/H(t)$ is constant and approximately equal to R_0/H_0.

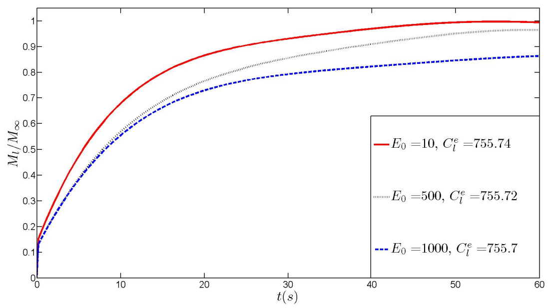

Fig. 4.11: Mass of solvent, M_s/M_∞ as a function of the viscosity μ_1

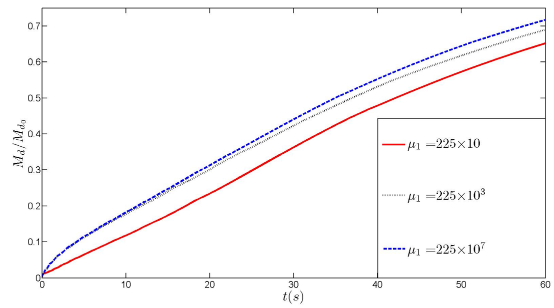

Fig. 4.12: Mass of drug released, M_d/M_{d_0} as a function of the viscosity μ_1

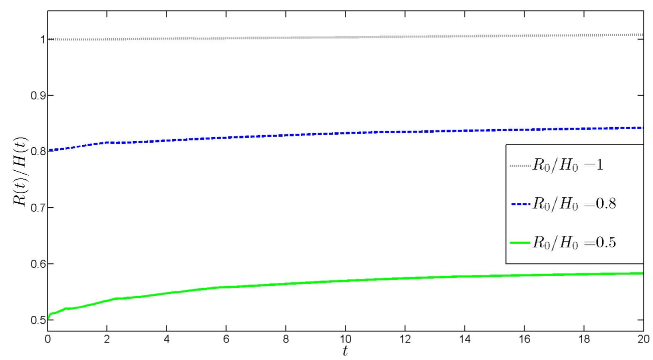

Fig. 4.13: $R(t)/H(t)$ as a function of R_0/H_0

To finalize this chapter it should be stressed that the model considered here depends on a set of physical parameters that can be measured or estimated. This property makes the mathematical model very attractive in what concerns real applications.

The qualitative behavior of the mathematical model was illustrated considering a significant set of numerical results presented in several plots. Moreover, the sensitivity of the model on the set of physical parameters was also illustrated. All the numerical results were obtained using an IMEX method defined in a moving boundary domain where the spatial grids are changing in time. Considering that we developed a realistic model and a comprehensive analysis of the dependence of the solution on the parameters, we believe that some of our findings can open new routes of research in Material Science and namely in Drug Delivery.

In this chapter we do not present the stability and convergence analysis of the numerical method used. The fact that the spatial grids change in time makes these studies a very challenging problem that we intend to address in the future.

Conclusions and future work

A non-linear non-Fickian model for sorption of a fluid by a viscoelastic material and the successive or simultaneous desorption of the fluid with solved molecules of a chemical compound which is dispersed in the material is proposed. A new interpretation of the non-Fickian flux lead us to the establishment of non-linear functional relations for the strain ε and the viscoelastic diffusion coefficient D_v. The numerical simulations of the model showed solutions with behaviors which are physically sound. Even though our numerical results have been validated, from a qualitative point of view, by leading experts in viscoelastic materials and controlled Drug Delivery, it would be interesting in the near future to compare the model with experimental results. Also as the mathematical deduction for D_v was based in two different approaches, the Darcy approach which is established in the framework of fluid motion in a porous medium and the Hagen-Poiseuille approach which is strictly connected to the flux of an homogeneous fluid in a pipe, an interesting question naturally arises: can each one of the approaches be identified with specific families of polymers?.

In order to expand the scope of our work to other applications involving the diffusional release of a dispersed agent from a polymeric carrier or situations where the transport phenomena cannot be described by the classical diffusion equation, we made an abstract formulation of the model. We proposed a finite difference method to numerically solve the IBVP defined by the integro-differential equation of Volterra type (2.3) and we presented several stability and convergence results that can be applied for different classes of problems depending on the smoothness of the kernel function K and the restrictions that can be imposed on the coefficient functions G and F. These restrictions have for the moment a mathematical character in the sense they have been imposed for technical reasons. An interesting interdisciplinary open question is to look for the existence of physical arguments underlying the mathematical assumptions used in the theorems.

A tridimensional mathematical model for drug release from a cylindrical viscoelastic matrix was proposed. To solve the initial-boundary value problem associated to the system of equations of the model, we introduced an IMEX finite difference method. As we considered that the spatial boundary was moving in time, we worked in the discretization with a time dependent non-uniform spatial grid. The implementation of the IMEX over this grid, poses very challenging computational problems mainly related to the computational cost of solving the model for large intervals of time, which raises different questions regarding the optimization of the implementation of the model. From the numerical analysis point of view, it would be interesting to study the stability and convergence of the approximations. We hope to address these questions in a future research work.

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