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COUPLING HYPERBOLIC AND PARABOLIC IBVP: APPLICATIONS TO DRUG DELIVERY

Tese no âmbito do Programa Interuniversitário de Doutoramento em Matemática, orientada pelo Professor Doutor José Augusto Mendes Ferreira e apresentada ao Departamento de Matemática da Faculdade de Ciências e Tecnologia da Universidade de Coimbra.

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POCH
PROGRAMA OPERACIONAL CAPITAL HUMANO

Abstract

In this thesis, we study a system of partial differential equations defined by a hyperbolic equation - a wave equation, and two parabolic equations - a quasilinear diffusion-reaction equation and a convection-diffusion-reaction equation. In this system, the reaction term of the first parabolic equation depends on the solution of the wave equation, the convective velocity of the second parabolic equation depends on the solution of the wave equation and its gradient, and the diffusion coefficient of the convection-diffusion-reaction equation depends on the solutions of the other two equations. This system arises in the mathematical modeling of several multiphysics processes, as for instance in ultrasound enhanced drug delivery. In this case, the propagation of the acoustic pressure wave, which is described by the hyperbolic equation, induces an increase in the temperature of the target tissue, an increase of the convective drug transport, and the increase of the temperature induces an increase of the diffusion drug transport.

Here we propose an algorithm to solve this coupled problem defined in a two-dimensional spatial domain. Our numerical method can be seen, simultaneously, as a fully discrete in space, piecewise linear finite element method, where special quadrature rules are considered, and as a finite difference method defined in nonuniform rectangular grids. We provide the theoretical convergence support where we show that the numerical approximations for the solution of the hyperbolic equation are second order convergent with respect to a discrete H^1- norm. This result allows us to conclude that the numerical approximations for the gradient do not deteriorate the quality of the numerical approximations for the solution of the last parabolic equation. For the numerical approximations for the two parabolic equations, we also establish second order convergence but with respect to a discrete L^2- norm. These convergence results are proved assuming lower regularity conditions than those usually imposed.

In the scope of the finite difference methods, our results can be seen as supraconvergence results because the method uses nonuniform rectangular grids where the correspondent truncation errors are only first order convergent with respect to the norm $\|\cdot\|_\infty$. As the method can be constructed considering piecewise linear finite element method, in the language of the finite element methods our results can be seen as superconvergence results. In fact, it is well known that piecewise linear finite element methods for elliptic equations lead to first order convergent approximations with respect to the usual H^1- norm.

Numerical results illustrating the theoretical support are also included, highlighting the sharpness of the smoothness assumption on the solutions of the multiphysics problem. It is reported in the literature the use of ultrasound to increase the drug transport and its absorption within the target tissue in different contexts, as for instance in cancer treatment. A simple version of the mathematical

problem studied in this work is considered to illustrate the effectiveness of the use of ultrasound to enhance the drug transport.

Keywords: hyperbolic equation, parabolic equation, piecewise linear finite element method, finite difference method, convergence analysis, supra-superconvergence, drug transport enhanced by ultrasound.

Resumo

Nesta tese estudamos um sistema de equações diferenciais de derivadas parciais definido por uma equação hiperbólica – uma equação de onda, e duas equações parabólicas – uma equação de difusão-reação quase linear e uma equação de convecção-difusão-reação. Neste sistema, o termo reativo da primeira equação parabólica depende da solução da equação da onda, e a velocidade convectiva da segunda equação parabólica depende da solução da primeira equação e do seu gradiente. O coeficiente de difusão da última equação depende também das soluções das duas primeiras equações. O problema matemático que motivou esta dissertação surge no contexto de diversos problemas físicos, como por exemplo, no contexto da libertação controlada de fármacos estimulada por ultrassons. Neste caso, a propagação da onda de pressão acústica descrita pela equação hiperbólica, induz um aumento da temperatura no tecido alvo, um aumento no transporte do fármaco, e o aumento da temperatura induz um aumento do transporte difusivo do fármaco.

Neste trabalho, propomos um método numérico para o sistema diferencial definido num domínio espacial de duas dimensões. O nosso método pode ser visto, simultaneamente, como um método de elementos finitos segmentado linear discreto no espaço, e como um método de diferenças finitas definido em malhas retangulares não uniformes. Para este método provamos a segunda ordem de convergência, relativamente a uma norma que pode ser vista como uma versão discreta da norma usual de H^1, para a discretização da equação hiperbólica. Este resultado permite concluir que a aproximação para o gradiente não deteriora a qualidade da aproximação para a concentração. Estabelecemos que as aproximações para a temperatura e para a concentração também são de segunda ordem, mas relativamente a uma norma que pode ser vista como uma discretização da norma usual de L^2. Os resultados de convergência são demonstrados utilizando condições de regularidade mais fracas do que as usadas usualmente.

No contexto dos métodos de diferenças finitas, uma vez que consideramos malhas não uniformes onde os erros de truncatura associados são de primeira ordem relativamente à norma $\|\cdot\|_\infty$, os nossos resultados podem ser vistos como resultados de supraconvergência. Visto que o método proposto pode ser visto como um método de elementos finitos segmentado linear, no contexto dos métodos de elementos finitos os nossos resultados podem ser vistos como resultados de superconvergência. De facto, é bem conhecido que os métodos de elementos finitos segmentados lineares para equações elípticas levam a aproximações convergentes de primeira ordem, relativamente à norma usual de H^1.

Os resultados teóricos obtidos são ilustrados numericamente. A precisão das condições de regularidade impostas às soluções do sistema diferencial contínuo é também analisada numericamente. Podemos encontrar na literatura que o uso de ultrassons leva a um aumento do transporte do fármaco e da sua absorção pelo tecido alvo em diferentes contextos, como por exemplo em tratamentos de

cancro. Uma versão simples do sistema estudado neste trabalho é considerada para ilustrar a eficiência do uso dos ultrassons como estímulo ao transporte de fármacos.

Palavras-Chave: equação hiperbólica, equação parabólica, método de elementos finitos segmentado linear, método de diferenças finitas, análise de convergência, supra-superconvergência, transporte de fármacos estimulado por ultrassons.

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Chapter 1

Introduction

In this thesis, we consider a multiphysics problem where a wave propagation phenomenon is coupled with two diffusion processes. Our main aim is to propose an adequate numerical method for the following system of partial differential equations

$$a\frac{\partial^2 p}{\partial t^2}+b\frac{\partial p}{\partial t}=\nabla\cdot(E\nabla p)+f_3, \tag{1.1}$$

$$\frac{\partial T}{\partial t}=\nabla\cdot(D_T(T)\nabla T)+kT+f_2(p), \tag{1.2}$$

$$\frac{\partial c}{\partial t}+\nabla\cdot(v(p,\nabla p)c)-\nabla\cdot(D_c(p,T)\nabla c)=f_1, \tag{1.3}$$

defined in $\Omega\times(0,T_f]$, where $\Omega\in\mathbb{R}^2$ is a bounded domain with boundary $\partial\Omega$ and $T_f>0$ is a time duration. The differential system (1.1), (1.2) and (1.3) is complemented with the initial conditions

$$p(0)=p_0,\frac{\partial p}{\partial t}(0)=p_{v,0} \text{ in } \Omega, \tag{1.4}$$

$$T(0)=T_0 \text{ in } \Omega, \tag{1.5}$$

$$c(0)=c_0 \text{ in } \Omega, \tag{1.6}$$

and to simplify, we impose the following homogeneous Dirichlet boundary conditions

$$p(t)=0 \text{ on } \partial\Omega\times(0,T_f], \tag{1.7}$$

$$T(t)=0 \text{ on } \partial\Omega\times(0,T_f], \tag{1.8}$$

$$c(t)=0 \text{ on } \partial\Omega\times(0,T_f]. \tag{1.9}$$

By simplicity, in this work, we assume that $\Omega = (0,1)^2$. The coupled initial boundary value problem (IBVP) (1.1)-(1.9) arises, for instance, in the modeling of ultrasound enhanced drug transport. For this reason, we will refer p, T and c as acoustic pressure, temperature and concentration, respectively. Basically, from the physical point of view, ultrasound enhanced drug transport involves the propagation of acoustic waves through a biological tissue. The propagation of these waves generates heat that dissipates through the tissue. The drug transport is enhanced by both: temperature rise and propagation of acoustic waves. The acoustic waves propagation can be modeled by the wave-type equation (1.1), while bioheat transfer and drug transport can be modeled by the parabolic-type equations (1.2) and (1.3), respectively.

To avoid drug side effects and to increase the drug available in the target tissue, nanocarriers have been studied to transport the drug. Liposomes, micelles, dendrimers, nanotubes, gold particles, are some examples that have been used to avoid the side effects induced by chemotherapy systemically administered. In these cases, to control and to increase the drug released in the target tissue as well as to increase the drug absorption, the nanocarriers are combined with activation processes. Stimuli responsive drug delivery systems (SRDDS) are drug delivery systems where the characteristic of the carriers and the properties of specific stimuli play a central role. They were developed as an answer to the need to reduce drug side effects, to break the barriers to the drug transport and to increase the drug available in the target tissue.

The enhancers used in SRDDS can be split into three main classes: physical, chemical and biological ([28]). Some examples of each class are

(i) Physical enhancers: temperature, electric and magnetic fields, ultrasound, light;

(ii) Chemical enhancers: pH, glucose, ionic strength;

(iii) Biological enhancers: enzymes, endogenous receptors.

From here onwards, we focus on ultrasound enhanced drug delivery.

The application of ultrasound to enhance drug transport through biological tissues has been used in different medical contexts like, for instance, transdermal drug delivery, cancer treatment, blood-brain barrier disruption, hyperthermia triggered drug delivery. Ultrasound is particularly useful for drug delivery into impermeable biological barriers, as cell membranes, and on the delivery of large weight or low diffusivity molecules (see [8], [9], [18], [21], [31], [32], [33], [34], [36], [37], [39], [40], [41], [43], [47]). In cancer treatment, reports on the use of ultrasounds to increase the drug release from polymeric micelles, liposomes, or microbubbles are presented in the literature. In this case, ultrasound generates pressure waves that propagate through the target tissue inducing the drug release from the carriers as well as increasing the drug absorption ([9], [20], [46]).

The exact mechanisms induced by the propagation of acoustic waves are not completely elucidated. However, it is known that the ultrasound propagation induces compression and expansion of the microbubbles dispersed in the medium leading to an oscillatory behavior in the medium pressure. It is accepted that acoustic wave propagation involves thermal and mechanical processes or a combination of both. In the first case, acoustic waves lead to a temperature increase due to the absorption of acoustic energy. Consequently, ultrasound has been used to control the drug delivery from temperature-sensitive drug nanocarriers. Furthermore, due to the increase of blood flow and permeability in the target tissue, they have been used to increase drug transport (see, e.g. [38] and its references). The mechanical effects can originate acoustic radiation forces ([4]) which induce the acoustic streaming - a convective flow in the fluid phase of the medium. This convective field can also be taken into account for increasing the drug delivery rate to specific sites ([10]). However, the main mechanical effect induced by ultrasound propagation is the so-called cavitation. Cavitation is characterized by the expansion and compression of endogeneous or exogeneous gas microbubbles that oscillate and induce a fluid flow with velocity proportional to the amplitude of the oscillations. If violent changes in the acoustic wave amplitude occur, the microbubbles collapse (inertial cavitation) generating shock waves that can lead to pore formation in the cellular membranes (see [12] and [41] and its references). Stable cavitation occurs when the bubbles oscillate without collapsing. The increase of tissue permeability due to cavitation is not completely understood (see [37] and its references). Nevertheless, it is established that the micro-scale phenomena associated with cavitation induces a convective and diffusive transport at a macro-scale (see, for instance, [22], [26], [27], [29]).

The previous consideration on the phenomena associating the acoustic pressure propagation with the increasing on the temperature, the increasing on the convective drug transport as well as the increasing on the drug diffusion transport, are the basis for the functional relations between the parameters of the differential system (1.1)-(1.3) and the correspondent unknowns p, T and c. In fact, we assumed in this system that the temperature source f_2 in (1.2) depends on the acoustic pressure p; the convective velocity v in (1.3) depends on p and on its gradient ∇p; the drug diffusion coefficient D_c in (1.3) depends on T and on p.

Modeling and numerical simulation of ultrasound enhanced drug transport has been subject of research in the last years. For example, in [24] the following linear acoustic pressure wave equation

$$\frac{1}{v_s^2}\frac{\partial^2 p}{\partial t^2}+\frac{\tilde{a}}{v_s^2}\frac{\partial p}{\partial t}=\rho\nabla\cdot\left(\frac{1}{\rho}\nabla p\right), \tag{1.10}$$

and the nonlinear Westervelt-Lighthill equation

$$\frac{1}{v_s^2}\frac{\partial^2 p}{\partial t^2}-\frac{\delta}{v_s^4}\frac{\partial^3 p}{\partial t^3}-\frac{\beta}{2\rho v_s^4}\frac{\partial^2 p}{\partial t^2}=\rho\nabla\cdot\left(\frac{1}{\rho}\nabla p\right), \tag{1.11}$$

were considered. In (1.10), ρ is the tissue density, v_s is the sound speed, $\tilde{a}=a\sqrt{\frac{a^4v_s^4}{4\pi^2 f^2}+v_s^2}$, being a the material attenuation coefficient, f the wave frequency. In (1.11), δ is the acoustic diffusivity in a thermoviscous fluid and β is a nonlinear coefficient of the medium. In biomedical applications as the ones that we would like to consider later, the acoustic wave propagation given by equation (1.10), or (1.11), is coupled with the Pennes's bioheat equation

$$\rho K\frac{\partial T}{\partial t}=\nabla\cdot(\hat{K}\nabla T)+\rho Q+\rho S-\rho_b c_b\rho\omega(T-T_b), \tag{1.12}$$

where T is the temperature, K is the specific heat capacity, $\hat{K}$ is the thermal conductivity, Q is the metabolic heat generation rate, ω is the perfusion rate, ρ_b, c_b and T_b are the density, specific heat capacity and temperature of the blood, and $S=a\dfrac{p^2}{\rho v_s}$. In this paper the drug concentration equation was not considered because the authors were only interested in the mathematical description of ultrasound and temperature dynamics. In [34], it is also constructed a model to simulate the influence of the ultrasound absorption in the temperature, in the skull. The ultrasound propagation in fluids and soft tissues is described by a hyperbolic equation similar to (1.10). However, to study the ultrasound in the skull, it is considered the visco-elastic wave equation of solids

$$\rho \frac{\partial^2 u}{\partial t^2} = \Big(\mu + \eta \frac{\partial}{\partial t}\Big)\Delta u + \Big(\lambda + \mu + \xi \frac{\partial}{\partial t} + \frac{\mu}{3}\frac{\partial}{\partial t}\Big)\nabla(\nabla \cdot u), \tag{1.13}$$

where Δ denotes the Laplacian operator, u denotes the particle displacement, λ and μ are the first and second Lamé coefficients and η and ξ are the first and second viscosity parameters. These two wave equations are coupled with a partial differential equation similar to (1.12) for the temperature behavior.

A multiphysics approach to describe ultrasound enhanced drug transport is introduced in [48]. In this paper the authors consider the drug release from thermosensitive nanocarriers-liposomes, the drug transport and the drug absorption by a solid tumor. Pennes's bioheat equations, similar to equation (1.12), are used to describe the temperature evolution in the tumor, normal tissue and in the blood (depending on the acoustic pressure). It is also considered the drug transport in the intersticial fluid and the drug effects on the tumor cells dynamics. It should be noticed that the diffusion coefficients are assumed constant which means, temperature and acoustic pressure independent.

A multiphysics and multidomain approach is considered in [35] to mathematically describe the drug release from thermosensitive liposomes loaded with doxorubicin (a drug used to treat cancer). The Penne's bioheat equation (1.12) is coupled with a nonlinear acoustic equation of the type (1.11). The drug concentration in the nanocarriers is governed by a convection-diffusion-reaction equation where the reaction term describes the drug released by the liposomes enhanced by the temperature, and the diffusion coefficient is assumed constant. The released drug admits three states: free, bound and internalized, being the concentration of the first type described by a convection-diffusion-reaction equation with a constant diffusion coefficient. The convective velocity is given by Darcy's law, which does not depend on acoustic pressure. From the numerical results, the authors concluded that controlled drug release by heating with ultrasound allows a significant increase in drug penetration into the tumor.

In [44], experimental results of the effect of ultrasonic waves on solute transport in porous media are presented. The behavior of the solute concentration c, in an one-dimensional domain, is described by a convective-diffusion equation, where the convective velocity is given by $v(p) = v + v^*$, and the diffusion coefficient is $D(p) = \alpha_L v(p) + D_d$, where v denotes the steady state fluid velocity, v^* represents the enhanced velocity due to the acoustic pressure, D_d is the molecular diffusion coefficient, and α_L is the dispersivity.

The papers introduced before, namely, [24], [35] and [48], presenting a mathematical description of drug delivery enhanced by ultrasound, do not present any detail on the numerical methods used to compute the numerical results presented as well as on their convergence analysis. To the best of our knowledge, the mathematical analysis as well as the design of accurate and efficient numerical methods for the system (1.1)-(1.3) were not yet object of research. These facts are the main motivation for our work in what concerns the construction of numerical methods and the development of their mathematical foundations.

In this thesis, our aim is to propose a numerical method that can be used to accurately compute numerical approximations for the acoustic pressure, temperature and concentration described by (1.1)-(1.3), defined in a two-dimensional domain. To simplify we assume that the drug is initially dispersed in the domain and the previous system is complemented with Dirichlet boundary conditions for the three unknowns. While for the temperature and for the concentration, these type of conditions can be realistic in certain scenarios, the boundary conditions for the acoustic pressure should be more realistic and further studies need to be prosecuted.

The main obstacle in the design of numerical methods to approximate the solution of (1.1)-(1.3) is the nonlinear dependence of the drug convective velocity on the gradient of the acoustic pressure, and the nonlinear dependence of the drug diffusion coefficient on the temperature and on the acoustic pressure. The discretization of the wave equation (1.1) should lead to an accurate approximation for the gradient of the acoustic pressure that does not deteriorate the quality of the approximation for the concentration. The methods proposed in this work can be seen simultaneously as fully discrete in space piecewise linear finite element methods and finite difference methods. The theoretical support for the convergence of the proposed methods is provided in this thesis under lower smoothness assumptions on the solution of the initial boundary value problem for (1.1)-(1.3) than those used in the literature for similar problems. It is shown that the numerical approximation for the acoustic pressure is second order convergent with respect to a H^1- discrete norm while the approximations for the temperature and for the concentration are second order convergent but with respect to a L^2- discrete norm. In the scope of the finite difference methods, our results can be seen as a supraconvergence results because the method uses nonuniform rectangular grids where the correspondent truncation errors are only first order convergent with respect to the norm $\|\cdot\|_\infty$. As the method can be constructed considering piecewise linear finite element method, in the language of the finite element methods our results can be seen as superconvergence results. In fact, it is well known that piecewise linear finite element methods for elliptic equations lead to first order convergent approximations with respect to the usual H^1- norm.

Numerical results illustrating the theoretical support are also included, highlighting the sharpness of the smoothness assumption on the solutions of the multiphysics problem. It is reported in the literature the use of ultrasound to increase the drug transport and its absorption within the target tissue in different contexts, as for instance in cancer treatment. A simple version of the mathematical problem is studied in this work to illustrate the effectiveness of the use of ultrasound to enhance the drug transport.

The convergence analysis followed here is based on the approach introduced in [3] for one-dimensional problems and in [14] for two-dimensional. This approach is based on the use of Bramble-Hilbert Lemma ([5]), that allows the replacement of the spaces of continuous functions $C^4(\overline{\Omega})$ by the Sobolev space $H^3(\Omega)$. The second convergence order of our scheme is established assuming that $p(t), T(t), c(t) \in H^3(\Omega)$. We remark that in [2] numerical methods to approximate the solution of a differential system defined by an elliptic equation and an integro-differential equation were studied using the same approach. Bramble-Hilbert lemma is also the basis of the convergence analysis of the numerical methods introduced in [13] for a system of two parabolic equations.

1.1 Outline of the Thesis

In what follows, we describe summarily the organization of this thesis highlighting the main contributions in each chapter.

In Chapter 2, we consider the hyperbolic initial boundary value problem, defined by the telegraph equation (1.1) coupled with the initial condition (1.4) and homogeneous Dirichelet boundary conditions. We propose a numerical scheme obtained using the Method of Lines Approach: a spatial discretization that leads to a semi-discrete approximation (continuous in time) followed by a time integration. The spatial discretization is defined considering a piecewise linear finite element method combined with particular quadrature rules that lead to a fully discrete in space scheme. This fully discrete scheme can also be seen as a finite difference method defined in nonuniform rectangular meshes. The classical convergence analysis of the semi-discrete approximation using the finite difference language is based on the concept of truncation error. As we will see, the truncation error is only of first order with respect to the norm $\|\cdot\|_\infty$, provided $p(t) \in C^3(\overline{\Omega})$. However, using our approach we prove that the finite difference approximation for the solution of the hyperbolic IBVP defined by (1.1) is second order convergent with respect to a discrete H^1- norm, provided $p'(t),\ p(t) \in C^4(\overline{\Omega})$ (Theorem 2.2). This means that the corresponding discrete gradient is second order convergent with respect to a discrete L^2- norm. First of all, we remark that the obtained convergence order is unexpected. In fact, error estimates for the approximation of the correspondent elliptic equations have an important role in the traditional approach followed in the convergence analysis of this kind of methods. It is known that the piecewise linear finite element method for elliptic equations leads to a first order approximation for the gradient provided that the solution of the correspondent weak problem is in $H^2(\Omega)$. Following the approach introduced by Wheeler in [45] for parabolic problems, only first order of convergence is expected. The second question that we would like to address is the reduction of the smoothness assumptions imposed before. In fact, using the Bramble-Hilbert Lemma as main tool, we prove the second order of convergence for our numerical solution, provided $p'(t),\ p(t) \in H^3(\Omega)$ (Theorem 2.3 and Corollary 2.1). In what concerns the time integration, we present two numerical schemes. The first one only presents first order of convergence in time. However, rewriting our problem in an equivalent way and considering a Cranck-Nicolson approach we construct a fully discrete in space and time problem leading with second order convergence in time (Theorem 2.5 and Corollary 2.4). The main results of this chapter are included in [15].

In Chapter 3, a simplified version of the differential problem (1.1)-(1.3) is considered: the thermal effects induced by ultrasonic waves are discarded. Then we study the system of partial differential equations defined by the hyperbolic equation (1.1) and the following convection-diffusion-reaction equation, similar to (1.3),

$$\frac{\partial c}{\partial t} + \nabla \cdot (v(p, \nabla p)c) - \nabla \cdot (D(p)\nabla c) = f_1. \tag{1.14}$$

The main problem on the computation of numerical approximations for the solution of this hyperbolic-parabolic IBVP defined by (1.1) and (1.14) is the dependence of the convective term v in (1.14) on the solution of the hyperbolic equation and its gradient. Here, the results of the previous chapter have a crucial role, since to compute a second order approximation for the concentration we need to have second order approximation for the gradient of the solution of the hyperbolic problem. We recall that Corollary 2.1 establishes this result.

In this chapter, we propose a fully discrete piecewise linear finite element method for the concentration that allows the computation of a second order approximation for the solution c of (1.14) with respect to a L^2- norm. In Section 3.2 we present the fully discrete in space piecewise linear finite element method for (1.1), (1.14). Section 3.3 is the main section of this chapter devoted to the convergence analysis of the semi-discrete approximation. Theorem 3.1 and Corollary 3.1 are the main results of the chapter that establish the second order of convergence provided $p(t), c(t) \in H^3(\Omega)$. We remark that these results are not expected since the studied method is constructed using the piecewise linear finite element method that leads to a first order approximation with respect to H^1- norm. Again, as the traditional approach for the convergence analysis of this type of approximation for parabolic equations is based on error estimates for the solution of the piecewise linear finite element method applied to the corresponding elliptic equation, that establish first order of convergence with respect to the H^1- norm, we expect only first order convergence for the approximation of the concentration defined before. To illustrate the applicability of the differential system (1.1), (1.14) in the mathematical modeling of drug delivery enhanced by ultrasound, we consider a toy model where a wave equation is coupled with a simplified version of (1.14). Numerical results illustrating the convergence results established in this chapter are also included. The main results of this chapter are included in [16].

The study of the complete problem (1.1)-(1.9) is presented in Chapter 4. Here, we consider the thermal effects of the ultrasound propagation, and consequently, in the drug transport. Our main aim is to design a fully discrete in space piecewise linear finite element approximation for the differential system (1.1)-(1.9) that leads to a second order approximation for the drug concentration c with respect to a discrete L^2- norm. As we are considering the thermal effects and the diffusion coefficient D_c depends on the temperature T, an error estimate for temperature approximation defined using the fully discrete in space piecewise linear approximation is needed. The heat source term f_2 depends on the acoustic pressure p, and consequently the error estimate for the approximation for the temperature depends on the error estimates for the acoustic pressure. Such error estimates are established in Theorem 4.1 and Corollary 4.1 that show second order of convergence provided that $p(t), T(t) \in H^3(\Omega)$. Finally in Theorem 4.2 and Corollary 4.3, we conclude that the numerical approximation for the concentration remains with second convergence rate. The main results of this chapter can be found in [17].

This thesis ends with a last chapter summarizing conclusions and open problems that will be object of study in the near future.

Chapter 2

Acoustic Pressure Propagation

2.1 Introduction

In this chapter, we consider the hyperbolic acoustic pressure equation (1.1) coupled with (1.4), (1.7), with $\Omega = (0,1)^2$ and $p : \overline{\Omega} \times [0,T_f] \to \mathbb{R}$. In (1.1), the coefficient functions a, b and E are space dependent, such that $a \geq a_0 > 0$, $b \geq b_0 > 0$ in $\overline{\Omega}$, and E is a second order diagonal matrix with entries $e_i,\ i = 1,2$, such that $e_i \geq e_0 > 0$ in $\overline{\Omega}$, for $i = 1,2$. Note, that the assumption $b_0 > 0$ is considered for simplicity, since similar results can be achieved for $b_0 \in \mathbb{R}$. In what follows, if $w : \overline{\Omega} \times [0,T_f] \to \mathbb{R}$, then for $t \in [0,T_f]$, $w(t) : \overline{\Omega} \to \mathbb{R}$ is given by $w(t)(x,y) = w(x,y,t)$, $(x,y) \in \overline{\Omega}$.

Our main goal in this chapter is the construction of an accurate numerical scheme to compute a numerical approximation for the solution p of the IBVP (1.1), (1.4), (1.7). We start by presenting some notations, after in Section 2.3, we define our semi-discrete numerical scheme, being its convergence analysis developed in Section 2.4. Theorem 2.1 establishes first order estimates for the error for the semi-discretization taking into account the expression of the correspondent truncation error. A careful mathematical manipulation of the term involving the truncation error can be used to improve the quality of the error estimate at least when the acoustic pressure is a smooth function. In Sections 2.4.2 and 2.4.3 we achieve improved convergence results considering $p(t) \in C^4(\overline{\Omega})$ and $p(t) \in H^3(\Omega)$, respectively. Bramble Hilbert Lemma is the main tool in the convergence analysis of the last result when $p(t) \in H^3(\Omega)$. Fully discrete, in time and space, methods are studied in Section 2.5. Numerical results illustrating the theoretical results established in the previous section are presented in Section 2.6. Finally, we draw some conclusions in Section 2.7.

The existence and uniqueness of the solution of the IBVP based in the hyperbolic equation (1.1) is not analyzed in this work. We remark that such results can be established using the results presented in Chapter 7 of [11].

2.2 Some Notations

We start by introducing some notations and definitions. In the usual Sobolev space $H^n(\Omega)$ we consider the usual norm

$$\|w\|_{H^n(\Omega)} = \left(\sum_{|\alpha| \leq n} \|D^\alpha w\|^2 \right)^{1/2}, w \in H^n(\Omega),$$

where, for $\alpha = (\alpha_1, \alpha_2) \in \mathbb{N}_0 \times \mathbb{N}_0$, $D^\alpha w = \dfrac{\partial^{|\alpha|} w}{\partial x^{\alpha_1} \partial y^{\alpha_2}}$. For $n = 0$ we take $H^0(\Omega) = L^2(\Omega)$ where we consider the usual inner product $(\cdot,\cdot)$ and the correspondent induced norm $\|\cdot\|$. Let $((\cdot,\cdot))$ be the usual inner product in $[L^2(\Omega)]^2$ and $\|\cdot\|$ the correspondent norm. By $H_0^1(\Omega)$ we represent the usual Sobolev space where we take the usual norm $\|\cdot\|_1$.

Let X denote a vector space of functions equipped with the norm $\|\cdot\|_X$. By $C^m([0,T_f],X)$ we represent the space of functions $w : [0,T_f] \to X$ such that $w^{(j)} : [0,T_f] \to X$, $j = 0,\ldots,m$, are continuous and

$$\|w\|_{C^m(X)} = \|w\|_{C^m([0,T_f],X)} = \sum_{j=0}^{m} \max_{0\le t\le T_f} \left\|w^{(j)}(t)\right\|_X < +\infty.$$

By $H^m(0,T_f,X)$ we represent the space of functions $w : (0,T_f) \to X$ with weak derivatives $w^{(j)} : (0,T_f) \to X$, $j = 0,\ldots,m$, such that

$$\|w\|_{H^m(X)} = \|w\|_{H^m(0,T_f,X)} = \left(\sum_{j=0}^{m} \int_0^{T_f} \left\|w^{(j)}(t)\right\|_X^2 \, dt\right)^{1/2} < +\infty.$$

We also consider $L^\infty(0,T_f,X)$ the space of all measurable functions $w : (0,T_f) \to X$ with

$$\|w\|_{L^\infty(0,T_f,X)} = \operatorname{ess}\sup_{0\le t\le T_f} \|w(t)\|_X < +\infty.$$

2.3 Semi-Discrete Numerical Scheme

In this section, we present a fully discrete in space method that allows the computation of an approximation for the solution of the following variational problem: find $p(t) \in H_0^1(\Omega)$ such that $p^{(j)}(t) \in L^2(\Omega)$, $j = 1,2$, $t \in (0,T_f]$, and

$$(ap''(t),w) + (bp'(t),w) = -((E\nabla p(t),\nabla w)) + (f_3(t),w), t \in (0,T_f], \tag{2.1}$$

for $w \in H_0^1(\Omega)$, and

$$\begin{cases} (p'(0),w) = (p_{v,0},w), & \forall w \in L^2(\Omega), \\ (p(0),q) = (p_0,q), & \forall q \in L^2(\Omega). \end{cases} \tag{2.2}$$

In $\overline{\Omega}$ we introduce an arbitrary nonuniform rectangular mesh defined by $H = (h,k)$ with

(i) $h = (h_1,\ldots,h_N)$, $N \in \mathbb{N}$, a vector of positive entries such that $\sum_{i=1}^{N} h_i = 1$;

(ii) $k = (k_1,\ldots,k_M)$, $M \in \mathbb{N}$, a vector of positive entries such that $\sum_{j=1}^{M} k_j = 1$.

Let $x_i, i = 0,\ldots,N$, and $y_j, j = 0,\ldots,M$, be the nonuniform grids induced by h and k in $[0,1]$, respectively, with $h_i = x_i - x_{i-1}$ and $k_j = y_j - y_{j-1}$. In $\overline{\Omega}$ we define the rectangular grid

$$\overline{\Omega}_H = \left\{(x_i,y_j), i = 0,\ldots,N, j = 0,\ldots,M\right\},$$

depending on H. Also, we define $\Omega_H = \Omega \cap \overline{\Omega}_H$ and $\partial\Omega_H = \partial\Omega \cap \overline{\Omega}_H$.

Let $H_{\max} = \max\left\{h_i, k_j; i = 1,\dots,N; j = 1,\dots,M\right\}$ and let Λ be a sequence of vectors $H = (h,\ k)$ such that $H_{\max}$ goes to 0. Let W_H be the space of grid functions defined in $\overline{\Omega}_H$ and $W_{H,0} = \{w_H \in W_H : w_H = 0 \text{ on } \partial\Omega_H\}$. By $\mathscr{T}_H$ we denote a triangulation of $\overline{\Omega}$ using the set $\overline{\Omega}_H$ as vertices. The notation diamΔ represents the diameter of the triangle $\Delta \in \mathscr{T}_H$. For $w_H \in W_H$, $P_H w_H$ denotes the continuous piecewise linear interpolant of w_H with respect to $\mathscr{T}_H$.

In order to construct a fully discrete in space approximation we define now discrete inner products and the corresponding norms. In $W_{H,0}$ we introduce the inner product

$$(v_H, w_H)_H = \sum_{(x_i,y_j)\in\overline{\Omega}_H} |\Box_{i,j}| v_H(x_i,y_j) w_H(x_i,y_j),\ v_H, w_H \in W_{H,0},$$

where $\Box_{i,j} = (x_{i-1/2}, x_{i+1/2}) \times (y_{j-1/2}, y_{j+1/2}) \cap \Omega$, $|\Box_{i,j}|$ denotes the area of $\Box_{i,j}$, and $x_{i+1/2} = x_i + \dfrac{h_{i+1}}{2}$, $x_{i-1/2} = x_i - \dfrac{h_i}{2}$, $h_{i+1/2} = x_{i+1/2} - x_{i-1/2}$ being $y_{j\pm 1/2}$ and $k_{j+1/2}$ defined analogously. Let $\|\cdot\|_H$ be the corresponding norm.

For $v_H = (v_{1,H}, v_{2,H})$, $w_H = (w_{1,H}, w_{2,H})$, and $v_{\ell,H}, w_{\ell,H} \in W_H$, for $\ell = 1,2$, we use the notation

$$((v_H, w_H))_H = (v_{1,H}, w_{1,H})_{H,x} + (v_{2,H}, w_{2,H})_{H,y},$$

where

$$(v_{1,H}, w_{1,H})_{H,x} = \sum_{i=1}^{N} \sum_{j=1}^{M-1} h_i k_{j+1/2} v_{1,H}(x_i,y_j) w_{1,H}(x_i,y_j),$$

being $(v_{2,H}, w_{2,H})_{H,y}$ defined analogously.

Let D_{-x} and D_{-y} be the first order backward finite difference operators with respect to the variables x and y, respectively,

$$D_{-x} v_H(x_i,y_j) = \frac{v_H(x_i,y_j) - v_H(x_{i-1},y_j)}{h_i}$$

and D_{-y} is defined analogously. Let ∇_H be the discrete version of the gradient operator ∇ defined by $\nabla_H v_H = (D_{-x} v_H, D_{-y} v_H)$. We use the following notations

$$\begin{aligned}\|\nabla_H v_H\|_H &= \Big((D_{-x}v_H, D_{-x}v_H)_{H,x} + (D_{-y}v_H, D_{-y}v_H)_{H,y}\Big)^{1/2} \\ &= \Big(\|D_{-x}v_H\|_H^2 + \|D_{-y}v_H\|_H^2\Big)^{1/2}, v_H \in W_H.\end{aligned}$$

Moreover, a straightforward calculation shows that the following Poincaré-Friedrichs inequality holds

$$\|v_H\|_H^2 \le \frac{1}{2} \|\nabla_H v_H\|_H^2, \forall v_H \in W_{H,0}. \tag{2.3}$$

Note that $\|\cdot\|_H$ and $\|\nabla_H \cdot\|_H$ can be seen as discrete versions of L^2- norm, and H^1- seminorm, respectively. Then $\|\cdot\|_{1,H} = \Big(\|\cdot\|_H^2 + \|\nabla_H \cdot\|_H^2\Big)^{1/2}$ is a discrete version of H^1- norm.

We are now in position to define our numerical scheme. The piecewise linear finite element method for the wave IBVP (1.1), (1.4), (1.7) is defined as follows: find $p_H(t) \in W_{H,0}$ such that

$P_H p_H(t)$ satisfies

$$(aP_H p_H''(t), P_H w_H) + (bP_H p_H'(t), P_H w_H) = -((E\nabla P_H p_H(t), \nabla P_H w_H)) + (f_3(t), P_H w_H), \tag{2.4}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, and

$$\begin{cases} (P_H p_H'(0), P_H w_H) = (P_H R_H p_{v,0}, P_H w_H), & \forall w_H \in W_{H,0}, \\ (P_H p_H(0), P_H q_H) = (P_H R_H p_0, P_H q_H), & \forall q_H \in W_{H,0}, \end{cases} \tag{2.5}$$

where $R_H : C(\overline{\Omega}) \to W_H$ denotes the restriction operator and $C(\overline{\Omega})$ represents the space of continuous functions in $\overline{\Omega}$.

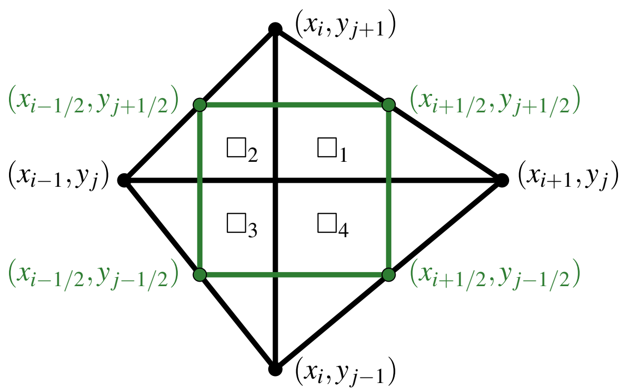


Fig. 2.1 Scheme of the partition used for the quadrature rules.

For $i = 0, \ldots, N$, $j = 0, \ldots, M$, we consider the following partition of $\square_{i,j}$, illustrated in the Figure 2.1: $\square_{i,j} = \cup_{l=1}^{4} (\square_l \cap \Omega)$, with

$$\begin{aligned} \square_1 &= (x_i, x_{i+1/2}) \times (y_j, y_{j+1/2}), \\ \square_2 &= (x_{i-1/2}, x_i) \times (y_j, y_{j+1/2}), \\ \square_3 &= (x_{i-1/2}, x_i) \times (y_{j-1/2}, y_j), \\ \square_4 &= (x_i, x_{i+1/2}) \times (y_{j-1/2}, y_j). \end{aligned}$$

In order to construct a fully discrete in space finite element problem, we consider the following approximation formulas:

$$\int_{\square_l} aP_H p_H''(t) P_H w_H dxdy \simeq |\square_l| a(x_i, y_j) p_H''(x_i, y_j, t) w_H(x_i, y_j), l = 1, 2, 3, 4. \tag{2.6}$$

Then, taking into account that our problem has homogeneous Dirichlet boundary conditions, we have

$$(aP_H p_H''(t), P_H w_H) = \int_\Omega aP_H p_H''(t) P_H w_H dxdy \simeq \left(a_H p_H''(t), w_H\right)_H,$$

where $a_H = R_H a$. Analogously we introduce the following approximation

$$(bP_H p_H'(t), P_H w_H) \simeq (b_H p_H'(t), w_H)_H,$$

where $b_H = R_H b$. If $f_{3,H}$ denotes the following grid function

$$f_{3,H}(t)(x_i, y_j) = \frac{1}{|\Box_{i,j}|} \int_{\Box_{i,j}} f_3(x, y, t)\, dxdy, \tag{2.7}$$

then, from the same quadrature rule, we obtain

$$(f_3(t), P_H w_H) \simeq (f_{3,H}(t), w_H)_H.$$

In the initial conditions (2.5) we consider the same approximation formulas. For the integral term associated with the second order spatial derivatives with respect to x, and $(x_i, y_j) \in \overline{\Omega}_H$, we have

$$\int_{\Box_l} e_1 \frac{\partial}{\partial x}(P_H p_H(t)) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq |\Box_l|\, e_1(x_{i+1/2}, y_j) D_{-x} p_H(x_{i+1}, y_j, t) D_{-x} w_H(x_{i+1}, y_j),\ l = 1, 4$$

and

$$\int_{\Box_l} e_1 \frac{\partial}{\partial x}(P_H p_H(t)) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq |\Box_l|\, e_1(x_{i-1/2}, y_j) D_{-x} p_H(x_i, y_j, t) D_{-x} w_H(x_i, y_j),\ l = 2, 3.$$

The last approximation quadrature rules allow us to introduce

$$((E\nabla P_H p_H(t), \nabla P_H w_H)) \simeq ((E_H \nabla_H p_H(t), \nabla_H w_H))_H,$$

where E_H denotes the 2×2 diagonal matrix with the following diagonal entries: $e_{1,H}(x_i, y_j) = e_1(x_{i-1/2}, y_j)$ and $e_{2,H}(x_i, y_j) = e_2(x_i, y_{j-1/2})$.

Then, considering the previous quadrature rules to approximate the integrals, we replace (2.4), (2.5) by the following fully discrete in space finite element problem: find $p_H(t) \in W_{H,0}$ such that

$$(a_H p_H''(t), w_H)_H + (b_H p_H'(t), w_H)_H = -((E_H \nabla_H p_H(t), \nabla_H w_H))_H + (f_{3,H}(t), w_H)_H, \tag{2.8}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, and

$$\begin{cases} (p_H'(0), w_H)_H = (R_H p_{v,0}, w_H)_H, & \forall w_H \in W_{H,0}, \\ (p_H(0), q_H)_H = (R_H p_0, q_H)_H, & \forall q_H \in W_{H,0}. \end{cases} \tag{2.9}$$

We observe that the fully discrete in space finite element problem (2.8), (2.9) can be rewritten as a finite difference method. In order to define such equivalent method, we introduce the finite difference operator $\nabla_H^* = (D_x^-, D_y^-)$ where

$$D_x^- v_H(x_i, y_j) = \frac{v_H(x_{i+1}, y_j) - v_H(x_i, y_j)}{h_{i+1/2}},$$

and D_y^- is defined analogously. Then, considering in (2.8) $w_H \in W_{H,0}$ equals to 1 in (x_i, y_j) and 0 in the remaining grid nodes, for each $(x_i, y_j) \in \Omega_H$, we obtain that (2.8), (2.9) can be seen as: find $p_H \in W_{H,0}$ such that

$$a_H p_H''(t) + b_H p_H'(t) = \nabla_H^* \cdot (E_H \nabla_H p_H(t)) + f_{3,H}(t) \text{ in } \Omega_H, t \in (0, T_f], \tag{2.10}$$

coupled with the boundary condition

$$p_H(t) = 0 \text{ on } \partial\Omega_H \times (0, T_f], \tag{2.11}$$

and the initial conditions

$$\begin{cases} p_H'(0) = R_H p_{v,0}, \\ p_H(0) = R_H p_0. \end{cases} \tag{2.12}$$

The existence of a smooth solution of the IBVP (2.10)-(2.12) can be easily established considering that such problem can be rewritten as the following differential system

$$a_H p_H''(t) + b_H p_H'(t) = A p_H(t) + f_{3,H}(t),\ t \in (0, T_f], \tag{2.13}$$

coupled with the initial conditions (2.12), where the entries of the matrix A depend on the coefficient functions e_i, $i = 1, 2$. For instance, if $f_{3,H}(t)$ is a continuous function, then (2.13), (2.12) has a unique solution $p_H(t) \in C^2((0, T_f]) \cap C^1([0, T_f])$ ([7]).

2.4 Convergence Analysis - Spatial Discretization

2.4.1 Classical Convergence Analysis

The classical convergence analysis of a semi-discrete finite difference method is based on the truncation error $T_{H,p}(t)$ associated with the spatial discretization, and upper bounds for the spatial discretization error are established depending on the norm of the $T_{H,p}(t)$.

Let $e_{H,p}(t) = R_H p(t) - p_H(t)$ be the spatial discretization error induced by the numerical scheme (2.10)-(2.12). Then

$$(a_H e_{H,p}''(t), w_H)_H + (b_H e_{H,p}'(t), w_H)_H = -((E_H \nabla_H e_{H,p}(t), \nabla_H w_H))_H + (T_{H,p}(t), w_H)_H, \tag{2.14}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, and

$$\begin{cases} e_{H,p}'(0) = 0 \\ e_{H,p}(0) = 0, \end{cases}$$

with

$$T_{H,p}(t) = R_H(\nabla \cdot (E \nabla p(t))) - \nabla_H^* \cdot (E_H \nabla_H R_H p(t)) + R_H f_3(t) - f_{3,H}(t).$$

Considering in (2.14) $w_H = e_{H,p}'(t)$, we obtain

$$(a_H e_{H,p}''(t), e_{H,p}'(t))_H + (b_H e_{H,p}'(t), e_{H,p}'(t))_H = -((E_H \nabla_H e_{H,p}(t), \nabla_H e_{H,p}'(t)))_H + (T_{H,p}(t), e_{H,p}'(t))_H,$$

which implies

$$\frac{1}{2}\frac{d}{dt}\|\sqrt{a_H}e'_{H,p}(t)\|_H^2 + b_0\|e'_{H,p}(t)\|_H^2 + \frac{1}{2}\frac{d}{dt}\|\sqrt{E_H}\nabla_H e_{H,p}(t)\|_H^2 \leq (T_{H,p}(t), e'_{H,p}(t))_H, \tag{2.15}$$

that leads to

$$\frac{d}{dt}\left(\frac{1}{2}\|\sqrt{a_H}e'_{H,p}(t)\|_H^2 + b_0\int_0^t \|e'_{H,p}(s)\|_H^2 ds + \frac{1}{2}\|\sqrt{E_H}\nabla_H e_{H,p}(t)\|_H^2\right) \leq \|T_{H,p}(t)\|_H\|e'_{H,p}(t)\|_H, \tag{2.16}$$

where $\sqrt{E}$ denotes the diagonal matrix with diagonal entries $\sqrt{e_i}, i=1,2$. To establish a representation of the spatial truncation error $T_{H,p}(t)$ we remark that if $f_3(t) \in C^2(\overline{\Omega})$, then

$$f_3(x_i,y_j,t) - f_{3,H}(x_i,y_j,t) = -\frac{h_{i+1}-h_i}{4}\frac{\partial f_3}{\partial x}(x_i,y_j,t) - \frac{k_{j+1}-k_j}{4}\frac{\partial f_3}{\partial y}(x_i,y_j,t) + \mathscr{O}(H_{max}^2), \tag{2.17}$$

for $i=1,\dots,N-1$, $j=1,\dots,M-1$ and $t\in(0,T_f]$. If $p(t)\in C^4(\overline{\Omega})$, $e_l\in C^3(\overline{\Omega})$, $l=1,2$, then, for $i=1,\dots,N-1$, $j=1,\dots,M-1$, $t\in(0,T_f]$, we have

$$\begin{aligned}
D_x^-(e_1(x_{i+1/2},y_j)D_{-x}R_H p(x_i,y_j,t)) - \frac{\partial}{\partial x}\left(e_1(x_i,y_j)\frac{\partial p}{\partial x}(x_i,y_j,t)\right) = \\
= \frac{h_{i+1}-h_i}{4}\frac{\partial^2 e_1}{\partial x^2}(x_i,y_j)\frac{\partial p}{\partial x}(x_i,y_j,t) + \frac{h_{i+1}-h_i}{2}\frac{\partial e_1}{\partial x}(x_i,y_j)\frac{\partial^2 p}{\partial x^2}(x_i,y_j,t) \\
+ \frac{h_{i+1}-h_i}{3}e_1(x_i,y_j)\frac{\partial^3 p}{\partial x^3}(x_i,y_j,t) + \mathscr{O}(H_{\max}^2).
\end{aligned} \tag{2.18}$$

Note that, we can obtain a similar expression for the term with respect to y.

Finally, from (2.17) and (2.18), for $i=1,\dots,N-1$, $j=1,\dots,M-1$, $t\in(0,T_f]$, we obtain

$$\begin{aligned}
T_{H,p}(x_i,y_j,t) = -(h_{i+1}-h_i)\Bigg(&\frac{1}{4}\frac{\partial^2 e_1}{\partial x^2}(x_i,y_j)\frac{\partial p}{\partial x}(x_i,y_j,t) + \frac{1}{2}\frac{\partial e_1}{\partial x}(x_i,y_j)\frac{\partial^2 p}{\partial x^2}(x_i,y_j,t) \\
&+ \frac{1}{3}e_1(x_i,y_j)\frac{\partial^3 p}{\partial x^3}(x_i,y_j,t) + \frac{1}{4}\frac{\partial f_3}{\partial x}(x_i,y_j,t)\Bigg) \\
-(k_{j+1}-k_j)\Bigg(&\frac{1}{4}\frac{\partial^2 e_2}{\partial y^2}(x_i,y_j)\frac{\partial p}{\partial y}(x_i,y_j,t) + \frac{1}{2}\frac{\partial e_2}{\partial y}(x_i,y_j)\frac{\partial^2 p}{\partial y^2}(x_i,y_j,t) \\
&+ \frac{1}{3}e_2(x_i,y_j)\frac{\partial^3 p}{\partial y^3}(x_i,y_j,t) + \frac{1}{4}\frac{\partial f_3}{\partial y}(x_i,y_j,t)\Bigg) + \mathscr{O}(H_{\max}^2)
\end{aligned}$$

provided that $p(t)\in C^4(\overline{\Omega})$, $e_l\in C^3(\overline{\Omega})$, $l=1,2$, $f_3(t)\in C^2(\overline{\Omega})$. The term $\mathscr{O}(H_{\max}^2)$ represents a term such that there exists a positive constant C_t, H, t, p and f_3 independent, satisfying

$$|\mathscr{O}(H_{\max}^2)| \leq C_t H_{\max}^2\left(\|e_1\|_{C^3(\overline{\Omega})}\|p(t)\|_{C^4(\overline{\Omega})} + \|e_2\|_{C^3(\overline{\Omega})}\|p(t)\|_{C^4(\overline{\Omega})} + \|f_3(t)\|_{C^2(\overline{\Omega})}\right),$$

where $\|\cdot\|_{C^m(\overline{\Omega})}$ denotes the usual norm in $C^m(\overline{\Omega})$, $m \in \mathbb{N}_0$. This means, there exists a positive constant C, H, t, p and f_3 independent, such that

$$\begin{aligned}|T_{H,p}(x_i,y_j,t)| \le C|h_{i+1}-h_i| \Big(\|e_1\|_{C^2(\overline{\Omega})}\|p(t)\|_{C^3(\overline{\Omega})} + \|f_3(t)\|_{C^1(\overline{\Omega})}\Big)\\ + C|k_{j+1}-k_j| \Big(\|e_2\|_{C^2(\overline{\Omega})}\|p(t)\|_{C^3(\overline{\Omega})} + \|f_3(t)\|_{C^1(\overline{\Omega})}\Big) + \big|\mathscr{O}(H_{\max}^2)\big|,\end{aligned}$$

for $i = 1,\ldots,N-1$, $j = 1,\ldots,M-1$, $t \in (0,T_f]$ and then

$$\|T_{H,p}(t)\|_H \le 2CH_{\max}\Big(\Big(\|e_1\|_{C^2(\overline{\Omega})} + \|e_2\|_{C^2(\overline{\Omega})}\Big)\|p(t)\|_{C^3(\overline{\Omega})} + \|f_3(t)\|_{C^1(\overline{\Omega})}\Big) + \big|\mathscr{O}(H_{\max}^2)\big|. \quad (2.19)$$

An inequality similar to (2.19) can be established for lower smoothness functions. In fact,

$$\|T_{H,p}(t)\|_H \le CH_{\max}\Big(\Big(\|e_1\|_{C^2(\overline{\Omega})} + \|e_2\|_{C^2(\overline{\Omega})}\Big)\|p(t)\|_{C^3(\overline{\Omega})} + \|f_3(t)\|_{C^1(\overline{\Omega})}\Big)$$

can be obtained, for some positive constant C, H, t, p and f_3 independent, provided that $p(t) \in C^3(\overline{\Omega})$, $e_l \in C^2(\overline{\Omega})$, $l = 1,2$, $f_3(t) \in C^1(\overline{\Omega})$.

Inequality (2.16) leads to

$$\begin{aligned}\frac{d}{dt}\Big(\frac{1}{2}\|\sqrt{a_H}e'_{H,p}(t)\|_H^2 + b_0\int_0^t \|e'_{H,p}(s)\|_H^2\,ds + \frac{1}{2}\|\sqrt{E_H}\nabla_H e_{H,p}(t)\|_H^2\Big)\\ \le CH_{\max}\Big(\Big(\|e_1\|_{C^2(\overline{\Omega})} + \|e_2\|_{C^2(\overline{\Omega})}\Big)\|p(t)\|_{C^3(\overline{\Omega})} + \|f_3(t)\|_{C^1(\overline{\Omega})}\Big)\big\|e'_{H,p}(t)\big\|_H.\end{aligned}$$

As $a \ge a_0,\ b \ge b_0,\ e_i \ge e_0,\ i = 1,2$, in $\overline{\Omega}$, from the last inequality we obtain, for $\varepsilon \neq 0$, the following inequality

$$\begin{aligned}\frac{1}{2}a_0\|e'_{H,p}(t)\|_H^2 + \big(b_0-\varepsilon^2\big)\int_0^t \|e'_{H,p}(s)\|_H^2\,ds + \frac{1}{2}\sqrt{e_0}\|\nabla_H e_{H,p}(t)\|_H^2\\ \le \frac{C}{4\varepsilon^2}H_{max}^2\int_0^t \Big(\Big(\|e_1\|_{C^2(\overline{\Omega})}^2 + \|e_2\|_{C^2(\overline{\Omega})}^2\Big)\|p(s)\|_{C^3(\overline{\Omega})}^2 + \|f_3(s)\|_{C^1(\overline{\Omega})}^2\Big)\,ds.\\ + \frac{1}{2}\|\sqrt{a_H}e'_{H,p}(0)\|_H^2 + \frac{1}{2}\|\sqrt{E_H}\nabla_H e_{H,p}(0)\|_H^2,\end{aligned}$$

where C is a positive constant, H, t, p, and f_3 independent. Fixing ε such that $b_0-\varepsilon^2 > 0$, and taking into account the initial conditions for $e_{H,p}(t)$ we easily obtain the following estimate

$$\begin{aligned}\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2\,ds + \|\nabla_H e_{H,p}(t)\|_H^2\\ \le CH_{\max}^2\int_0^t \Big(\Big(\|e_1\|_{C^2(\overline{\Omega})}^2 + \|e_2\|_{C^2(\overline{\Omega})}^2\Big)\|p(s)\|_{C^3(\overline{\Omega})}^2 + \|f_3(s)\|_{C^1(\overline{\Omega})}^2\Big)\,ds.\end{aligned}$$

for $t \in [0,T_f]$. Taking into account now the inequality (2.3) we conclude

$$\|e_{H,p}(t)\|_{1,H}^2 \le CH_{\max}^2\Big(\Big(\|e_1\|_{C^2(\overline{\Omega})}^2 + \|e_2\|_{C^2(\overline{\Omega})}^2\Big)\|p\|_{C(C^3)}^2 + \|f_3\|_{C(C^1)}^2\Big), \quad (2.20)$$

for $t \in [0,T_f]$, where C is a positive constant, H, t, p and f_3 independent. Inequality (2.20) establishes that the discrete H^1- norm of the error is at least first order convergent.

The last result can be summarized as follows:

Theorem 2.1. *If the solution p of the IBVP (1.1), (1.4), (1.7) is in $C([0,T_f],C^3(\overline{\Omega}))\cap C^2([0,T_f],C(\overline{\Omega}))$, $e_i \in C^2(\overline{\Omega})$, $i=1,2$, and $f_3 \in C([0,T_f],C^1(\overline{\Omega}))$, and the coefficient functions $a \geq a_0 > 0$, $b \geq b_0 > 0$, $e_i \geq e_0 > 0, i=1,2$, then there exists a positive constant C, independent of p, f_3, H, and t, such that for $H \in \Lambda$, the error $e_{H,p}(t) = R_H p(t) - p_H(t)$, where $p_H(t)$ is defined by (2.8), (2.9) (or, equivalently by (2.10)-(2.12)), satisfies the following*

$$\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2\, ds + \|\nabla_H e_{H,p}(t)\|_H^2 \\ \leq CH_{\max}^2 \left(\left(\|e_1\|^2_{C^2(\overline{\Omega})} + \|e_2\|^2_{C^2(\overline{\Omega})}\right)\|p\|^2_{C(C^3)} + \|f_3\|^2_{C(C^1)}\right),\ t \in [0,T_f].$$

From this first attempt based on the truncation error to obtain an estimate for $\|e_{H,p}(t)\|^2_{1,H}$, we conclude that our discretization has at least first order of convergence. However, if we are dealing with uniform grids, as $\|T_H(t)\|_\infty \leq C\max\{h^2,k^2\}$, we obtain in this case

$$\|e_{H,p}(t)\|^2_{1,H} \leq C\max\{h^4,k^4\}.$$

2.4.2 Supra-Superconvergence: Smooth Case

In this section our aim is to establish an improvement to Theorem 2.1. We will show that our method (2.8), (2.9) is in fact second order convergent. In this second attempt to get the desired convergence order we will pay a serious price - an increase on the smoothness imposed to the solution p ($p(t) \in C^4(\overline{\Omega})$).

Theorem 2.2. *If the solution p of the IBVP (1.1), (1.4), (1.7) is in $C^1([0,T_f],C^4(\overline{\Omega}))\cap C^2([0,T_f],C(\overline{\Omega}))$ and $f_3 \in C^1([0,T_f],C^2(\overline{\Omega}))$, $e_i \in C^3(\overline{\Omega})$, $i=1,2$, and the coefficient functions $a \geq a_0 > 0$, $b \geq b_0 > 0$, $e_i \geq e_0 > 0, i=1,2$, then there exist positive constants C_1 and C_2, independent of p, f_3, H, and t, such that, for $H \in \Lambda$, the error $e_{H,p}(t) = R_H p(t) - p_H(t)$, where $p_H(t)$ is defined by (2.8), (2.9), satisfies the following*

$$\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2\, ds + \|e_{H,p}(t)\|_H^2 + \|\nabla_H e_{H,p}(t)\|_H^2 \\ \leq C_1 H_{\max}^4 e^{C_2 t}\left(\left(\|e_1\|^2_{C^3(\overline{\Omega})} + \|e_2\|^2_{C^3(\overline{\Omega})}\right)\|p\|^2_{C^1(C^4)} + \|f_3\|^2_{C^1(C^2)}\right),\ t \in [0,T_f]. \tag{2.21}$$

Proof. As in the proof of Theorem 2.1, (2.15) holds. To get the desired upper bound we need to get the right form for the error term $(T_{H,p}(t), e'_{H,p}(t))_H$. We observe that

$$(T_{H,p}(t), e'_{H,p}(t))_H = \frac{d}{dt}(T_{H,p}(t), e_{H,p}(t))_H - (T'_{H,p}(t), e_{H,p}(t))_H, \tag{2.22}$$

where, for $i=1,\dots,N-1,\ j=1,\dots,M-1,\ t\in(0,T_f]$,

$$\begin{aligned}
T'_{H,p}(x_i,y_j,t) = &-(h_{i+1}-h_i)\Bigg(\frac{1}{4}\frac{\partial^2 e_1}{\partial x^2}(x_i,y_j)\frac{\partial^2 p}{\partial t\partial x}(x_i,y_j,t)+\frac{1}{2}\frac{\partial e_1}{\partial x}(x_i,y_j)\frac{\partial^3 p}{\partial t\partial x^2}(x_i,y_j,t)\\
&+\frac{1}{3}e_1(x_i,y_j)\frac{\partial^4 p}{\partial t\partial x^3}(x_i,y_j,t)+\frac{1}{4}\frac{\partial^2 f_3}{\partial t\partial x}(x_i,y_j,t)\Bigg)\\
&-(k_{j+1}-k_j)\Bigg(\frac{1}{4}\frac{\partial^2 e_2}{\partial y^2}(x_i,y_j)\frac{\partial^2 p}{\partial t\partial y}(x_i,y_j,t)+\frac{1}{2}\frac{\partial e_2}{\partial y}(x_i,y_j)\frac{\partial^3 p}{\partial t\partial y^2}(x_i,y_j,t)\\
&+\frac{1}{3}e_2(x_i,y_j)\frac{\partial^4 p}{\partial t\partial y^3}(x_i,y_j,t)+\frac{1}{4}\frac{\partial^2 f_3}{\partial t\partial y}(x_i,y_j,t)\Bigg)+\mathscr{O}(H^2_{\max}),
\end{aligned}$$

with $|\mathscr{O}(H^2_{max})|\le C_t H^2_{max}\Big(\|e_1\|_{C^3(\overline{\Omega})}\|p'(t)\|_{C^4(\overline{\Omega})}+\|e_2\|_{C^3(\overline{\Omega})}\|p'(t)\|_{C^4(\overline{\Omega})}+\|f'_3(t)\|_{C^2(\overline{\Omega})}\Big)$.

From (2.15) and (2.22), taking into account the initial conditions for $e_{H,p}(t)$, we get

$$\begin{aligned}
\|\sqrt{a_H}e'_{H,p}(t)\|^2_H+2b_0\int_0^t\|e'_{H,p}(s)\|^2_H ds+\|\sqrt{E_H}\nabla_H e_{H,p}(t)\|^2_H &\le 2(T_{H,p}(t),e_{H,p}(t))_H\\
&-2\int_0^t (T'_{H,p}(s),e_{H,p}(s))_H ds,\ t\in(0,T_f]. \qquad (2.23)
\end{aligned}$$

To obtain upper bounds for the terms $(T_{H,p}(t),e_{H,p}(t))_H$, $(T'_{H,p}(s),e_{H,p}(s))_H$ we consider the generic term

$$T_{G,x}(t)=\sum_{i=1}^{N-1}\sum_{j=1}^{M-1}h_{i+1/2}k_{j+1/2}(h_{i+1}-h_i)v_1(x_i,y_j,t)e_{H,p}(x_i,y_j,t).$$

We have successively

$$\begin{aligned}
T_{G,x}(t) &= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1}k_{j+1/2}h_i^2\Big(v_1(x_i,y_j,t)e_{H,p}(x_i,y_j,t)-v_1(x_{i-1},y_j,t)e_{H,p}(x_{i-1},y_j,t)\Big)\\
&= -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1}k_{j+1/2}h_i^2\int_{x_{i-1}}^{x_i}\frac{\partial v_1}{\partial x}(x,y_j,t)dx\, e_{H,p}(x_i,y_j,t)\\
&\quad -\frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1}k_{j+1/2}h_i^3 v_1(x_{i-1},y_j,t)D_{-x}e_{H,p}(x_i,y_j,t)\\
&:= T^{(1)}_{G,x}(t)+T^{(2)}_{G,x}(t).
\end{aligned}$$

For the term $T^{(1)}_{G,x}(t)$ it can be shown the following

$$
\begin{aligned}
\left|T^{(1)}_{G,x}(t)\right| &\leq \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2} h_i^{5/2}\left(\int_{x_{i-1}}^{x_i}\left(\frac{\partial v_1}{\partial x}(x,y_j,t)\,dx\right)^2\right)^{1/2} |e_{H,p}(x_i,y_j,t)| \\
&\leq \frac{1}{2}H^2_{\max}\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2} h_i\left\|\frac{\partial v_1}{\partial x}(t)\right\|_{C(\overline{\Omega})} |e_{H,p}(x_i,y_j,t)| \\
&\leq H^2_{\max}\|v_1(t)\|_{C^1(\overline{\Omega})}\left(\sum_{i=1}^{N-1}\sum_{j=1}^{M-1} k_{j+1/2}h_{i+1/2}\right)^{1/2}\left(\sum_{i=1}^{N-1}\sum_{j=1}^{M-1} k_{j+1/2}h_{i+1/2}(e_{H,p}(x_i,y_j,t))^2\right)^{1/2} \\
&\leq H^2_{\max}\|v_1(t)\|_{C^1(\overline{\Omega})}\|e_{H,p}(t)\|_H \\
&\leq \frac{1}{4\eta_1^2}H^4_{\max}\|v_1(t)\|^2_{C^1(\overline{\Omega})} + \eta_1^2\|e_{H,p}(t)\|^2_H,
\end{aligned}
$$

while for $T^{(2)}_{G,x}(t)$ we have

$$
\begin{aligned}
\left|T^{(2)}_{G,x}(t)\right| &\leq \frac{1}{2}\left(\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i^4 h_i (v_1(x_{i-1},y_j,t))^2\right)^{1/2}\left(\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i(D_{-x}e_{H,p}(x_i,y_j,t))^2\right)^{1/2} \\
&\leq \frac{1}{2}H^2_{\max}\left(\sum_{i=1}^{N}\sum_{j=1}^{M-1} k_{j+1/2}h_i(v_1(x_{i-1},y_j,t))^2\right)^{1/2}\|D_{-x}e_{H,p}(t)\|_H \\
&\leq \frac{1}{2}H^2_{\max}\,\|v_1(t)\|_{C^0(\overline{\Omega})}\,\|D_{-x}e_{H,p}(t)\|_H \\
&\leq \frac{1}{16\eta_2^2}H^4_{\max}\|v_1(t)\|^2_{C^0(\overline{\Omega})} + \eta_2^2\|D_{-x}e_{H,p}(t)\|^2_H,
\end{aligned}
$$

where η_i, $i = 1,2$, are non-zero constants. Consequently we obtain

$$
|T_{G,x}(t)| \leq \frac{1}{4\eta_1^2}H^4_{\max}\|v_1(t)\|^2_{C^1(\overline{\Omega})} + \eta_1^2\|e_{H,p}(t)\|^2_H + \frac{1}{16\eta_2^2}H^4_{\max}\|v_1(t)\|^2_{C^0(\overline{\Omega})} + \eta_2^2\|D_{-x}e_{H,p}(t)\|^2_H.
$$

Analogously, for the correspondent term in y direction

$$
T_{G,y}(t) = \sum_{i=1}^{N-1}\sum_{j=1}^{M-1} h_{i+1/2}k_{j+1/2}(k_{j+1}-k_j)v_2(x_i,y_j,t)e_{H,p}(x_i,y_j,t)
$$

it can be shown that

$$
|T_{G,y}(t)| \leq \frac{1}{4\eta_3^2}H^4_{\max}\|v_2(t)\|^2_{C^1(\overline{\Omega})} + \eta_3^2\|e_{H,p}(t)\|^2_H + \frac{1}{16\eta_4^2}H^4_{\max}\|v_2(t)\|^2_{C^0(\overline{\Omega})} + \eta_4^2\|D_{-y}e_{H,p}(t)\|^2_H,
$$

where η_i, $i = 3,4$, are non-zero constants.

Let $\eta_1 = \eta_3$ and $\eta_2 = \eta_4$, then we deduce

$$
\begin{aligned}
&|T_{G,x}(t)| + |T_{G,y}(t)| \\
&\quad\leq \Big(\frac{1}{4\eta_1^2} + \frac{1}{16\eta_2^2}\Big)H^4_{\max}\left(\|v_1(t)\|^2_{C^1(\overline{\Omega})} + \|v_2(t)\|^2_{C^1(\overline{\Omega})}\right) + 2\eta_1^2\|e_{H,p}(t)\|^2_H + \eta_2^2\|\nabla_H e_{H,p}(t)\|^2_H.
\end{aligned}
$$

Considering now the term $(T_{H,p}(t), e_{H,p}(t))_H$ and choosing the convenient terms $v_i(t), i = 1,2$, we conclude

$$\begin{aligned}
|(T_{H,p}(t), e_{H,p}(t))_H| \leq \Big(\frac{1}{4\xi_1^2} + \frac{1}{16\xi_2^2}\Big) H_{\max}^4 \Big(2(\|e_1\|_{C^3(\overline{\Omega})} + \|e_2\|_{C^3(\overline{\Omega})})\|p(t)\|_{C^4(\overline{\Omega})} \\
+ \frac{1}{2}\|f_3(t)\|_{C^2(\overline{\Omega})}\Big)^2 + 3\xi_1^2 \|e_{H,p}(t)\|_H^2 + \xi_2^2 \|\nabla_H e_{H,p}(t)\|_H^2 \\
+ \frac{1}{4\xi_1^2} C_t^2 H_{\max}^4 \Big(\Big(\|e_1\|_{C^3(\overline{\Omega})} + \|e_2\|_{C^3(\overline{\Omega})}\Big) \|p(t)\|_{C^4(\overline{\Omega})} + \|f_3(t)\|_{C^2(\overline{\Omega})}\Big)^2,
\end{aligned} \tag{2.24}$$

where $\xi_i, i = 1,2$, are non-zero constants. Analogously for $(T'_{H,p}(s), e_{H,p}(s))$ we get the upper bound

$$\begin{aligned}
|(T'_{H,p}(s), e_{H,p}(s))_H| \leq \Big(\frac{1}{4\xi_3^2} + \frac{1}{16\xi_4^2}\Big) H_{\max}^4 \Big(2(\|e_1\|_{C^3(\overline{\Omega})} + \|e_2\|_{C^3(\overline{\Omega})})\|p'(s)\|_{C^4(\overline{\Omega})} \\
+ \frac{1}{2}\|f'_3(s)\|_{C^2(\overline{\Omega})}\Big)^2 + 3\xi_3^2 \|e_{H,p}(s)\|_H^2 + \xi_4^2 \|\nabla_H e_{H,p}(s)\|_H^2 \\
+ \frac{1}{4\xi_3^2} C_t^2 H_{\max}^4 \Big(\Big(\|e_1\|_{C^3(\overline{\Omega})} + \|e_2\|_{C^3(\overline{\Omega})}\Big) \|p'(s)\|_{C^4(\overline{\Omega})} + \|f'_3(s)\|_{C^2(\overline{\Omega})}\Big)^2,
\end{aligned} \tag{2.25}$$

where ξ_i, $i = 3,4$, are non-zero constants.

Taking (2.24) and (2.25) into (2.23), and using the discrete Poincaré inequality (2.3), we obtain

$$\begin{aligned}
a_0\|e'_{H,p}(t)\|_H^2 + 2b_0 \int_0^t \|e'_{H,p}(s)\|_H^2 ds + \Big(e_0 - 6\xi_1^2\Big)\|e_{H,p}(t)\|_H^2 + \Big(\frac{e_0}{2} - 2\xi_2^2\Big)\|\nabla_H e_{H,p}(t)\|_H^2 \\
\leq \int_0^t 2\Big(\xi_4^2 \|\nabla_H e_{H,p}(s)\|_H^2 + 3\xi_3^2 \|e_{H,p}(s)\|_H^2\Big) ds + C H_{max}^4 \Big(R(t) + \int_0^t R(s) ds\Big), \, t \in [0, T_f],
\end{aligned}$$

where C depends on the previous constants $\xi_i, i = 1,2,3,4$, and C_t, and $R(\mu) = \|f_3(\mu)\|^2_{C^2(\overline{\Omega})} + \|f'_3(\mu)\|^2_{C^2(\overline{\Omega})} + \Big(\|e_1\|^2_{C^3(\overline{\Omega})} + \|e_2\|^2_{C^3(\overline{\Omega})}\Big)\Big(\|p(\mu)\|^2_{C^4(\overline{\Omega})} + \|p'(\mu)\|^2_{C^4(\overline{\Omega})}\Big)$. Fixing ξ_1 and ξ_2 such that $e_0 - 6\xi_1^2 > 0$, $\frac{e_0}{2} - 2\xi_2^2 > 0$, it follows that there exist positive constants C_i, $i = 1,2$, p, f_3, H and t independent, such that

$$\begin{aligned}
\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2 ds + \|e_{H,p}(t)\|_H^2 + \|\nabla_H e_{H,p}(t)\|_H^2 \\
\leq C_1 H_{\max}^4 \Big(R(t) + \int_0^t R(s) ds\Big) + C_2 \int_0^t \Big(\|\nabla_H e_{H,p}(s)\|_H^2 + \|e_{H,p}(s)\|_H^2\Big) ds.
\end{aligned} \tag{2.26}$$

Applying Gronwall's Lemma ([6]) to (2.26) we arrive at

$$\begin{aligned}
\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2 \, ds + \|e_{H,p}(t)\|_H^2 + \|\nabla_H e_{H,p}(t)\|_H^2 \\
\leq C_1 H_{\max}^4 e^{C_2 t} \Big(\Big(\|e_1\|^2_{C^3(\overline{\Omega})} + \|e_2\|^2_{C^3(\overline{\Omega})}\Big) \|p\|^2_{C^1(C^4)} + \|f_3\|^2_{C^1(C^2)}\Big), \, t \in [0, T_f],
\end{aligned}$$

which gives us the desired result. □

Such result enables us to conclude that $\|e_{H,p}(t)\|_{1,H} \leq CH_{\max}^2$ although $\|T_{H,p}(t)\|_\infty \leq CH_{\max}$. In the context of finite element approach, our result cannot be obtained following the approach introduced by Wheeler for parabolic equations in [45]. In fact, this approach is based on the split of the spatial discretization error into two terms introducing the numerical approximation for an elliptic problem associated with our hyperbolic equation

$$\begin{aligned} p(t) - P_H p_H(t) &= p(t) - P_H \tilde{p}_H(t) + P_H \tilde{p}_H(t) - P_H p_H(t) \\ &= \rho_H(t) + \theta_H(t), \end{aligned} \tag{2.27}$$

where, to simplify, taking $a = 1, b = 0, E = I_2$ (the identity matrix of order 2), $\tilde{p}_H(t)$ satisfies the following

$$((\nabla P_H \tilde{p}_H(t), \nabla P_H w_H)) = -\left(p''(t), P_H w_H\right) + (f_3(t), P_H w_H),$$

for $w_H \in W_{H,0}$ and $t \in (0, T_f]$, and $P_H p_H(t)$ is the solution of (2.4), (2.5). It is known that

$$\|\rho_H(t)\| \leq CH_{\max}^2, \quad \|\rho_H(t)\|_1 \leq CH_{\max},$$

provided that $p(t) \in H^2(\Omega) \cap H_0^1(\Omega)$ and assuming that the family of triangulations associated with our rectangular grids are quasi-uniform ([19]). It can be shown that $\theta_H(t)$ satisfies the following differential equation

$$\left(\theta_H''(t), P_H w_H\right) + ((\nabla \theta_H(t), \nabla P_H w_H)) = \left(\rho_H''(t), P_H w_H\right), t \in (0, T_f].$$

Then

$$\begin{aligned} &\left\|\theta_H'(t)\right\|^2 + \|\nabla \theta_H(t)\|^2 + \int_0^t e^{t-s} \|\nabla \theta_H(s)\|^2 ds \\ &\qquad \leq e^t \left(\left\|\theta_H'(0)\right\| + \|\nabla \theta_H(0)\|^2\right) + \int_0^t e^{t-s} \left\|\rho_H''(s)\right\|^2 ds, t \in [0, T_f]. \end{aligned}$$

If we assume that $p''(t) \in H^2(\Omega) \cap H_0^1(\Omega)$, and

$$\left\|\theta_H'(0)\right\| + \|\nabla \theta_H(0)\|^2 \leq CH_{\max}^4,$$

then

$$\|\nabla \theta_H(t)\|^2 \leq CH_{\max}^4.$$

However, from (2.27) we get

$$\|p(t) - P_H p_H(t)\|_1 \leq \|\rho_H(t)\|_1 + \|\theta_H(t)\|_1 \leq CH_{\max}.$$

If we look to our method as a fully discrete piecewise linear method, then we have shown that

$$\|e_{H,p}(t)\|_{1,H} \leq CH_{\max}^2,$$

which can be seen as a superconvergence result. It is clear that this upper bound was obtained under severe smoothness assumptions. In what follows we study the accuracy of $p_H(t)$ under weaker assumptions than those considered here.

In what concerns the geometry of the triangulations associated with the nonuniform rectangular grids, they do not need to be quasi-uniform. In fact, we can have triangles with interior angles whose amplitude is arbitrarily small ([19]).

2.4.3 Supra-Superconvergence: Non-Smooth Case

In this section, we establish an upper bound analogous to (2.21) but under weaker assumptions than those used in the proof of Theorem 2.2, namely $p \in C^1([0,T_f],C^4(\overline{\Omega})) \cap C^2([0,T_f],C(\overline{\Omega}))$ and $f_3 \in C^1([0,T_f],C^2(\overline{\Omega}))$. The main tool used in the proof of the next result is the Bramble-Hilbert Lemma ([5]). Let us assume that

$$p \in H^3(0,T_f,H^2(\Omega)) \cap H^1(0,T_f,H^3(\Omega) \cap H^1_0(\Omega)).$$

We remark that if $p \in H^m(0,T_f,H^r(\Omega))$ then $p \in C^{m-1}([0,T_f],H^r(\Omega))$, $m \in \mathbb{N}$, $r \in \mathbb{N}_0$ (see [1]).

Theorem 2.3. *If the solution p of the IBVP (1.1), (1.4), (1.7) belongs to* $H^1(0,T_f,H^3(\Omega) \cap H^1_0(\Omega)) \cap H^3(0,T_f,H^2(\Omega))$*, the coefficient functions* $a,b,e_i, i=1,2 \in W^{2,\infty}(\Omega)$*, and* $a \geq a_0 > 0$*,* $b \geq b_0 > 0$*,* $e_i \geq e_0 > 0, i=1,2$*, then there exist positive constants* $C_i, i=1,2$*, p, H, and t independent, such that, for* $H \in \Lambda$*, the spatial discretization error* $e_{H,p}(t) = R_H p(t) - p_H(t)$*, where* $p_H(t)$ *is defined by (2.8), (2.9), satisfies the following*

$$\begin{aligned}
&\|e'_{H,p}(t)\|^2_H + \int_0^t \|e'_{H,p}(s)\|^2_H ds + \|\nabla_H e_{H,p}(t)\|^2_H \\
&\quad \leq C_1 e^{C_2 t} \sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \Big(\|p\|^2_{H^1(H^3)} + \|p\|^2_{H^3(H^2)} \Big), t \in [0,T_f].
\end{aligned}$$

Proof. It is easy to show that the spatial discretization error $e_{H,p}(t)$ is solution of the discrete variational equation

$$\begin{aligned}
(a_H e''_{H,p}(t), w_H)_H + (b_H e'_{H,p}(t), w_H)_H = &-((E_H \nabla_H e_{H,p}(t), \nabla_H w_H))_H \\
&+ T_1(p(t), w_H) + T_2(p(t), w_H), t \in (0,T_f], \forall w_H \in W_{H,0},
\end{aligned} \tag{2.28}$$

where

$$T_1(p(t),w_H) = ((E_H \nabla_H (R_H p(t)), \nabla_H w_H))_H - (-(\nabla \cdot (E \nabla p(t)))_H, w_H)_H$$

and

$$T_2(p(t),w_H) = (R_H(ap''(t)+bp'(t)) - (ap''(t)+bp'(t))_H, w_H)_H.$$

In the definition of $T_1(p(t),w_H)$ and $T_2(p(t),w_H)$, $(g(t))_H$ for $g(t) = ap''(t)+bp'(t), g(t) = \nabla \cdot (E\nabla p(t))$, is given by (2.7) with $f_3(t)$ replaced by $g(t)$.

Lemma 5.1 of [14] allows us to conclude the following estimate

$$
\begin{aligned}
|T_1(p(t),w_H)| &\leq \left|(e_{1,H}D_{-x}(R_Hp(t)),D_{-x}w_H)_{H,x} - \left(-\left(\frac{\partial}{\partial x}\left(e_1\frac{\partial}{\partial x}p(t)\right)\right)_H, w_H\right)_H\right| \\
&\quad + \left|(e_{2,H}D_{-y}(R_Hp(t)),D_{-y}w_H)_{H,y} - \left(-\left(\frac{\partial}{\partial y}\left(e_2\frac{\partial}{\partial y}p(t)\right)\right)_H, w_H\right)_H\right| \\
&\leq C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|p(t)\|^2_{H^3(\Delta)}\Big)^{1/2}\|\nabla_Hw_H\|_H, \qquad (2.29)
\end{aligned}
$$

for $w_H \in W_{H,0}$, where C is a positive constant p, H and t independent.

Moreover, Lemma 5.7 of [14] leads to

$$
\begin{aligned}
|T_2(p(t),w_H)| &\leq \left|((ap''(t))_H - R_H(ap''(t)),w_H)_H\right| + \left|((bp'(t))_H - R_H(bp'(t)),w_H)_H\right| \\
&\leq C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\left(\|p'(t)\|^2_{H^2(\Delta)} + \|p''(t)\|^2_{H^2(\Delta)}\right)\Big)^{1/2}\|\nabla_Hw_H\|_H, \qquad (2.30)
\end{aligned}
$$

for $w_H \in W_{H,0}$, and where C denotes a positive constant p, H and t independent which is not necessarily the one that arises in (2.29).

If we take in (2.28) $w_H = e'_{H,p}(t)$ then we obtain

$$
\begin{aligned}
(a_He''_{H,p}(t),e'_{H,p}(t))_H + (b_He'_{H,p}(t),e'_{H,p}(t))_H &= -((E_H\nabla_He_{H,p}(t),\nabla_He'_{H,p}(t)))_H \\
&\quad + T_1(p(t),e'_{H,p}(t)) + T_2(p(t),e'_{H,p}(t)). \qquad (2.31)
\end{aligned}
$$

As we have

$$
T_i(p(t),e'_{H,p}(t)) = \frac{d}{dt}T_i(p(t),e_{H,p}(t)) - T_i(p'(t),e_{H,p}(t)),\, i = 1,2,
$$

from (2.31), we deduce

$$
\begin{aligned}
\frac{d}{dt}\|\sqrt{a_H}e'_{H,p}(t)\|^2_H + 2\|\sqrt{b_H}e'_{H,p}(t)\|^2_H + \frac{d}{dt}\|\sqrt{E_H}\nabla_He_{H,p}(t)\|^2_H &= 2\frac{d}{dt}T_1(p(t),e_{H,p}(t)) \\
&\quad + 2\frac{d}{dt}T_2(p(t),e_{H,p}(t)) - 2T_1(p'(t),e_{H,p}(t)) - 2T_2(p'(t),e_{H,p}(t)).
\end{aligned}
$$

That leads to

$$
\begin{aligned}
\frac{d}{dt}\Bigg(&\|\sqrt{a_H}e'_{H,p}(t)\|^2_H + 2\int_0^t\|\sqrt{b_H}e'_{H,p}(s)\|^2_H ds + \|\sqrt{E_H}\nabla_He_{H,p}(t)\|^2_H \\
&- 2T_1(p(t),e_{H,p}(t)) - 2T_2(p(t),e_{H,p}(t)) + 2\int_0^t T_1(p'(s),e_{H,p}(s)) + T_2(p'(s),e_{H,p}(s))ds\Bigg) = 0.
\end{aligned}
$$

From the last identity we easily obtain

$$
\begin{aligned}
&a_0\|e'_{H,p}(t)\|^2_H + 2b_0\int_0^t\|e'_{H,p}(s)\|^2_H ds + e_0\|\nabla_He_{H,p}(t)\|^2_H \\
&\quad\leq 2T_1(p(t),e_{H,p}(t)) + 2T_2(p(t),e_{H,p}(t)) - 2\int_0^t T_1(p'(s),e_{H,p}(s)) + T_2(p'(s),e_{H,p}(s))ds,
\end{aligned}
$$

because we are assuming that $e_{H,p}(0) = e'_{H,p}(0) = 0$. Taking into account the upper bounds (2.29) and (2.30) in the last inequality, we get

$$
\begin{aligned}
a_0\|e'_{H,p}(t)\|_H^2 + 2b_0\int_0^t \|e'_{H,p}(s)\|_H^2 ds + (e_0 - 4\xi_1^2)\|\nabla_H e_{H,p}(t)\|_H^2 \\
\leq \frac{C}{2\xi_1^2}\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(\|p(t)\|^2_{H^3(\Delta)} + \sum_{\ell=1}^{2}\|p^{(\ell)}(t)\|^2_{H^2(\Delta)}\Big) \\
+\frac{C}{2\xi_2^2}\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\int_0^t\Big(\|p'(s)\|^2_{H^3(\Delta)} + \sum_{\ell=2}^{3}\|p^{(\ell)}(s)\|^2_{H^2(\Delta)}\Big)ds \\
+4\xi_2^2\int_0^t \|\nabla_H e_{H,p}(s)\|_H^2 ds,
\end{aligned}
$$

where $\xi_i, i = 1,2$, are non-zero constants and C a positive constant, p, H and t independent. Fixing ξ_1 such that $e_0 - 4\xi_1^2 > 0$, we conclude the existence of two positive constants $C_i, i = 1,2$, such that

$$
\begin{aligned}
\|e'_{H,p}(t)\|_H^2 + \int_0^t \|e'_{H,p}(s)\|_H^2 ds + \|\nabla_H e_{H,p}(t)\|_H^2 \\
\leq C_1\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(\|p\|^2_{H^1(H^3)} + \|p\|^2_{H^3(H^2)}\Big) \\
+C_2\int_0^t \|\nabla_H e_{H,p}(s)\|_H^2 ds.
\end{aligned}
$$

Finally, applying Gronwall's Lemma, we obtain the desired result. □

We point out that Lemmas 5.1 and 5.7 of [14] were considered to obtain (2.29) and (2.30). We remark that the Bramble-Hilbert Lemma is the main tool used in the proofs of those lemmas.

Corollary 2.1. *Under the assumptions of Theorem 2.3, we conclude that there exists a positive constant C, H, and t independent, such that*

$$
\|e_{H,p}(t)\|^2_{1,H} \leq CH^4_{\max},\ t\in[0,T_f],\ H\in\Lambda. \tag{2.32}
$$

Proof. We remark that (2.32) follows immediately from Theorem 2.3 and (2.3). □

As Theorem 2.2, Theorem 2.3 and Corollary 2.1 can also be seen as supra-superconvergence results. These last results were established under weaker smoothness assumption on p than those considered in Theorem 2.2.

In what follows, we study the boundness of the sequences $(\|p_H(t)\|_\infty)_{H\in\Lambda}$ and $(\|\nabla_H p_H(t)\|_\infty)_{H\in\Lambda}$, where

$$
\|p_H(t)\|_\infty = \max_{(x,y)\in\overline{\Omega}_H}|p_H(x,y,t)|, \tag{2.33}
$$

$$
\|\nabla_H p_H(t)\|_\infty = \max_{i=1,\dots,N,j=1,\dots,M-1}\left|D_{-x}p_H(x_i,y_j,t)\right| + \max_{i=1,\dots,N-1,j=1,\dots,M}\left|D_{-y}p_H(x_i,y_j,t)\right|. \tag{2.34}
$$

As we will see later, these boundnesses have an important role in the error analysis for the numerical approximation for the concentration c (defined by (1.3) or (1.14)) that we will introduce in the next chapters. To guarantee this property for $p_H(t)$ and its gradient $\nabla_H p_H(t)$ we need to consider a condition on the spatial grids $\overline{\Omega}_H$ for $H \in \Lambda$. We assume that for $H \in \Lambda$, $H_{\max}$ small enough, there exists a positive constant C_m such that

$$\frac{H_{\max}}{H_{\min}} \leq C_m, \tag{2.35}$$

where $H_{\min} = \min\{h_i, k_j; i = 1, \ldots, N; j = 1, \ldots, M\}$.

To show that (2.33) and (2.34) are bounded we start by noting that

$$\|p_H(t)\|_\infty^2 \leq 2\frac{1}{H_{\min}^2}\|e_{H,p}(t)\|_H^2 + 2\|R_H p(t)\|_\infty^2.$$

Then, from Corollary 2.1, we get

$$\|p_H(t)\|_\infty^2 \leq C\frac{H_{\max}^4}{H_{\min}^2} + 2\|p(t)\|_\infty^2, H \in \Lambda,$$

and we derive the boundness of (2.33) by the fact that $p(t) \in C(\overline{\Omega})$ when $p(t) \in H^3(\Omega) \cap H_0^1(\Omega)$.

To prove the boundness of (2.34), we observe that we have successively

$$\begin{aligned}
\|\nabla_H p_H(t)\|_\infty^2 &\leq 2\frac{1}{H_{\min}^2}\|\nabla_H e_{H,p}(t)\|_H^2 + 2\|\nabla_H R_H p(t)\|_\infty^2 \\
&\leq C\frac{H_{\max}^4}{H_{\min}^2} + 2\|\nabla_H R_H p(t)\|_\infty^2 \\
&\leq C\frac{H_{\max}^4}{H_{\min}^2} + 2\|\nabla p(t)\|_\infty^2,
\end{aligned}$$

where C denotes a positive constant, p, H and t independent. The boundness of (2.34) follows from the fact that $p(t) \in C^1(\overline{\Omega})$ when $p(t) \in H^3(\Omega) \cap H_0^1(\Omega)$.

Corollary 2.2. *Under the assumptions of Theorem 2.3, if the sequence of step-sizes Λ satisfies (2.35) then, there exists a positive constant C, H and t independent, such that*

$$\|p_H(t)\|_\infty \leq C \quad \textit{and} \quad \|\nabla_H p_H(t)\|_\infty \leq C,\ t \in [0, T_f],$$

for $H \in \Lambda$ with $H_{\max}$ small enough.

2.5 Fully Discrete Approximation in Time and Space

In this section, we consider fully discrete approximations in time and space for our acoustic pressure problem (1.1), (1.4), (1.7), considering the discretization in space presented before. For that, we introduce in $[0, T_f]$ the uniforme time grid $\{t_n = n\Delta t, n = 0, \ldots, M_t\}$ with $t_{M_t} = T_f$ and where Δt is the time step.

We present two different methods with different convergence orders: order one in Section 2.5.1 and order two in Section 2.5.2.

2.5.1 First Order Scheme

Let $D_{2,t}$ be the second order centered finite difference operator in time and let D_{-t} be the backward finite difference operator in time. The fully discrete in time and space approximation for the solution of the IBVP (1.1), (1.4), (1.7) is defined by

$$(a_H D_{2,t} p_H^n, w_H)_H + (b_H D_{-t} p_H^{n+1}, w_H)_H = -((E_H \nabla_H p_H^{n+1}, \nabla_H w_H))_H \\ + (f_{3,H}(t_{n+1}), w_H)_H, \, n = 1, \ldots, M_t - 1, \quad (2.36)$$

for $w_H \in W_{H,0}$, with the initial conditions

$$\begin{cases} (D_{-t} p_H^1, w_H)_H = (R_H p_{v,0}, w_H)_H, & \forall w_H \in W_{H,0}, \\ (p_H^0, q_H)_H = (R_H p_0, q_H)_H, & \forall q_H \in W_{H,0}, \end{cases} \quad (2.37)$$

and the boundary condition

$$p_H^n = 0 \text{ on } \partial\Omega_H, \, n = 1, \ldots, M_t. \quad (2.38)$$

Equivalently, equation (2.36) can be written as

$$a_H D_{2,t} p_H^n + b_H D_{-t} p_H^{n+1} = \nabla_H^* \cdot (E_H \nabla_H p_H^{n+1}) + f_{3,H}(t_{n+1}) \text{ in } \Omega_H, \, n = 1, \ldots, M_t - 1, \quad (2.39)$$

and (2.37) replaced by

$$\begin{cases} D_{-t} p_H^1 = R_H p_{v,0}, \\ p_H^0 = R_H p_0. \end{cases} \quad (2.40)$$

The main theorem of this section is stated next.

Theorem 2.4. *If the solution p of the IBVP (1.1), (1.4), (1.7) is in $H^1(0, T_f, H^3(\Omega) \cap H_0^1(\Omega)) \cap H^3(0, T_f, H^2(\Omega)) \cap C^3([0, T_f], C(\overline{\Omega})) \cap C^2([0, T_f], C^1(\overline{\Omega})) \cap C^1([0, T_f], C^2(\Omega))$, a, b, e_i, $i = 1, 2 \in W^{2,\infty}(\Omega)$, and $a \geq a_0 > 0$, $b \geq b_0 > 0$, $e_i \geq e_0 > 0$, $i = 1, 2$, then, for $H \in \Lambda$, there exists a positive constant C, p, H and Δt independent, such that for the error $e_{H,p}^n = R_H p(t_n) - p_H^n$, where p_H^n is defined by (2.36), (2.37), (2.38), $n = 1, \ldots, M_t$, holds the following*

$$\|D_{-t} e_{H,p}^n\|_H^2 + \Delta t \sum_{j=1}^n \|D_{-t} e_{H,p}^j\|_H^2 + \|\nabla_H e_{H,p}^n\|_H^2 \\ \leq C\Big(\Delta t^2 \Big(\|p\|_{C^2(C)}^2 + \Delta t^2 \|p\|_{C^2(C^1)}^2 + \Delta t \, \|p\|_{C^3(C)}^2 + H_{\max}^2 \|p\|_{C^1(C^2)}^2\Big) \\ + \sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \Big(\|p\|_{C(H^3)}^2 + \|p\|_{C^2(H^2)}^2 + \|p\|_{H^1(H^3)}^2 + \|p\|_{H^3(H^2)}^2\Big)\Big). \quad (2.41)$$

Proof. It can be shown that the error $e_{H,p}^n$ satisfies the following equation

$$(a_H D_{2,t} e_{H,p}^n, D_{-t} e_{H,p}^{n+1})_H + (b_H D_{-t} e_{H,p}^{n+1}, D_{-t} e_{H,p}^{n+1})_H = -((E_H \nabla_H e_{H,p}^{n+1}, \nabla_H D_{-t} e_{H,p}^{n+1}))_H \\ + \sum_{\ell=1}^3 T_\ell(p(t_{n+1}), D_{-t} e_{H,p}^{n+1}), \quad (2.42)$$

where

$$T_1(p(t_{n+1}),w_H) = ((E_H\nabla_H(R_Hp(t_{n+1})),\nabla_H w_H))_H + ((\nabla\cdot(E\nabla p(t_{n+1})))_H,w_H)_H,$$

$$T_2(p(t_{n+1}),w_H) = (R_H(ap''(t_{n+1})+bp'(t_{n+1})) - ((ap''(t_{n+1})+bp'(t_{n+1}))_H),w_H)_H,$$

and

$$T_3(p(t_{n+1}),w_H) = (a_H(D_{2,t}R_Hp(t_n)-R_Hp''(t_{n+1}))+b_H(D_{-t}R_Hp(t_{n+1})-R_Hp'(t_{n+1})),w_H)_H,$$

for $w_H\in W_{H,0}$.

As we have successively

$$\begin{aligned}\left(e_{1,H}D_{-x}e^{n+1}_{H,p},D_{-x}D_{-t}e^{n+1}_{H,p}\right)_{H,x} &= \frac{1}{\Delta t}\left(\left\|\sqrt{e_{1,H}}D_{-x}e^{n+1}_{H,p}\right\|^2_H - \left(\sqrt{e_{1,H}}D_{-x}e^{n+1}_{H,p},\sqrt{e_{1,H}}D_{-x}e^{n}_{H,p}\right)_{H,x}\right)\\ &\geq \frac{1}{\Delta t}\left(\left\|\sqrt{e_{1,H}}D_{-x}e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{e_{1,H}}D_{-x}e^{n}_{H,p}\|_H\left\|\sqrt{e_{1,H}}D_{-x}e^{n+1}_{H,p}\right\|_H\right)\\ &\geq \frac{1}{2\Delta t}\left(\left\|\sqrt{e_{1,H}}D_{-x}e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{e_{1,H}}D_{-x}e^{n}_{H,p}\|^2_H\right),\end{aligned}$$

and a similar result holds for the term $\left(e_{2,H}D_{-y}e^{n+1}_{H,p},D_{-y}D_{-t}e^{n+1}_{H,p}\right)_{H,y}$, then we deduce

$$\left(\left(E_H\nabla_H e^{n+1}_{H,p},\nabla_H D_{-t}e^{n+1}_{H,p}\right)\right)_H \geq \frac{1}{2\Delta t}\left(\left\|\sqrt{E_H}\nabla_H e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{E_H}\nabla_H e^{n}_{H,p}\|^2_H\right). \tag{2.43}$$

We also have successively

$$\begin{aligned}(a_HD_{2,t}e^n_{H,p},D_{-t}e^{n+1}_{H,p})_H &= \frac{1}{\Delta t}\left(\left\|\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right\|^2_H - \left(\sqrt{a_H}D_{-t}e^{n}_{H,p},\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right)_H\right)\\ &\geq \frac{1}{\Delta t}\left(\left\|\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{a_H}D_{-t}e^{n}_{H,p}\|_H\left\|\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right\|_H\right)\\ &\geq \frac{1}{2\Delta t}\left(\left\|\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{a_H}D_{-t}e^{n}_{H,p}\|^2_H\right),\end{aligned} \tag{2.44}$$

and

$$T_\ell(p(t_{n+1}),D_{-t}e^{n+1}_{H,p}) = D_{-t}T_\ell(p(t_{n+1}),e^{n+1}_{H,p}) - T_\ell(D_{-t}p(t_{n+1}),e^n_{H,p}),\ \ell=1,2. \tag{2.45}$$

Taking in (2.42) the estimates (2.43), (2.44) and (2.45), we get

$$\begin{aligned}&\frac{1}{2\Delta t}\left(\left\|\sqrt{a_H}D_{-t}e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{a_H}D_{-t}e^{n}_{H,p}\|^2_H\right) + b_0\left\|D_{-t}e^{n+1}_{H,p}\right\|^2_H\\ &\leq -\frac{1}{2\Delta t}\left(\left\|\sqrt{E_H}\nabla_H e^{n+1}_{H,p}\right\|^2_H - \|\sqrt{E_H}\nabla_H e^{n}_{H,p}\|^2_H\right) + T_3(p(t_{n+1}),D_{-t}e^{n+1}_{H,p})\\ &\qquad + \sum_{\ell=1}^2 D_{-t}T_\ell(p(t_{n+1}),e^{n+1}_{H,p}) - \sum_{\ell=1}^2 T_\ell(D_{-t}p(t_{n+1}),e^n_{H,p}),\end{aligned}$$

which gives

$$\|\sqrt{a_H}D_{-t}e_{H,p}^{n+1}\|_H^2+2\Delta t b_0\|D_{-t}e_{H,p}^{n+1}\|_H^2-2\sum_{\ell=1}^2 T_\ell(p(t_{n+1}),e_{H,p}^{n+1})+\|\sqrt{E_H}\nabla_H e_{H,p}^{n+1}\|_H^2$$
$$\leq \|\sqrt{a_H}D_{-t}e_{H,p}^{n}\|_H^2+\|\sqrt{E_H}\nabla_H e_{H,p}^{n}\|_H^2-2\sum_{\ell=1}^2 T_\ell(p(t_n),e_{H,p}^{n})$$
$$-2\Delta t\sum_{\ell=1}^2 T_\ell(D_{-t}p(t_{n+1}),e_{H,p}^n)+2\Delta t T_3(p(t_{n+1}),D_{-t}e_{H,p}^{n+1}), \tag{2.46}$$

for $n=1,\dots,M_t-1$. Inequality (2.46) leads to

$$\|\sqrt{a_H}D_{-t}e_{H,p}^{n+1}\|_H^2+2\Delta t b_0\sum_{j=1}^{n+1}\|D_{-t}e_{H,p}^{j}\|_H^2-2\sum_{\ell=1}^2 T_\ell(p(t_{n+1}),e_{H,p}^{n+1})+\|\sqrt{E_H}\nabla_H e_{H,p}^{n+1}\|_H^2$$
$$\leq \|\sqrt{a_H}D_{-t}e_{H,p}^{1}\|_H^2+2\Delta t b_0\|D_{-t}e_{H,p}^{1}\|_H^2+\|\sqrt{E_H}\nabla_H e_{H,p}^{1}\|_H^2-2\sum_{\ell=1}^2 T_\ell(p(t_1),e_{H,p}^{1})$$
$$-2\Delta t\sum_{j=1}^{n}\Big(\sum_{\ell=1}^2 T_\ell(D_{-t}p(t_{j+1}),e_{H,p}^j)+T_3(p(t_{j+1}),D_{-t}e_{H,p}^{j+1})\Big), \tag{2.47}$$

for $n=1,\dots,M_t-1$.

The terms $T_\ell(p(t_{n+1}),e_{H,p}^{n+1})$, $\ell=1,2$ satisfy (2.29) and (2.30), respectively, with $w_H=e_{H,p}^{n+1}$, and for $T_\ell(D_{-t}p(t_{n+1}),e_{H,p}^n)$, $\ell=1,2$, we get

$$|T_1(D_{-t}p(t_{n+1}),e_{H,p}^n)|\leq C\frac{1}{\sqrt{\Delta t}}\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|p\|^2_{H^1(t_n,t_{n+1},H^3(\Delta))}\Big)^{1/2}\|\nabla_H e_{H,p}^n\|_H \tag{2.48}$$

and

$$|T_2(D_{-t}p(t_{n+1}),e_{H,p}^n)|\leq C\frac{1}{\sqrt{\Delta t}}\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|p\|^2_{H^3(t_n,t_{n+1},H^2(\Delta))}\Big)^{1/2}\|\nabla_H e_{H,p}^n\|_H. \tag{2.49}$$

Since, in Ω_H, we have

$$\big|D_{2,t}R_H p(t_n)-R_H p''(t_{n+1})\big|\leq C\Delta t\,\|p\|_{C^3(C)},$$

where C is a positive constant, p, H and Δt independent, then for $T_3(p(t_{n+1}),D_{-t}e_{H,p}^{n+1})$ we get

$$|T_3(p(t_{n+1}),D_{-t}e_{H,p}^{n+1})|\leq C\Delta t\|p\|_{C^3(C)}\|D_{-t}e_{H,p}^{n+1}\|_H. \tag{2.50}$$

Considering now in (2.47) the upper bounds (2.29), (2.30) for $|T_\ell(p(t_{n+1}),e_{H,p}^{n+1})|$, $\ell=1,2$, and (2.48), (2.49) for $|T_\ell(D_{-t}p(t_{n+1}),e_{H,p}^n)|$, $\ell=1,2$, and (2.50) for $|T_3(p(t_{n+1}),D_{-t}e_{H,p}^{n+1})|$, we establish

$$
\begin{aligned}
&a_0\|D_{-t}e_{H,p}^{n+1}\|_H^2 + 2\Delta t(b_0-\xi_3^2)\sum_{j=1}^{n+1}\|D_{-t}e_{H,p}^j\|_H^2 + \big(e_0-4\xi_1^2\big)\|\nabla_H e_{H,p}^{n+1}\|_H^2 \\
&\quad\leq \|\sqrt{a_H}D_{-t}e_{H,p}^1\|_H^2 + 2\Delta t b_0\|D_{-t}e_{H,p}^1\|_H^2 + \|\sqrt{E_H}\nabla_H e_{H,p}^1\|_H^2 - 2\sum_{\ell=1}^2 T_\ell(p(t_1),e_{H,p}^1) \\
&\qquad + \Delta t\sum_{j=1}^n 4\xi_2^2\|\nabla_H e_{H,p}^j\|_H^2 + T_{n+1}(p)
\end{aligned}
$$

for $n=1,\dots,M_t-1$, and

$$
\begin{aligned}
T_{n+1}(p) = C\Big(&\frac{1}{2\xi_1^2}\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(\|p(t_{n+1})\|_{H^3(\Delta)}^2 + \sum_{\ell=1}^2\|p^{(\ell)}(t_{n+1})\|_{H^2(\Delta)}^2\Big) \\
&+\sum_{j=1}^n\Big(\frac{1}{2\xi_2^2}\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(\|p\|_{H^1(t_j,t_{j+1},H^3(\Delta))}^2 + \|p\|_{H^3(t_j,t_{j+1},H^2(\Delta))}^2\Big) \\
&+\frac{1}{2\xi_3^2}\Delta t^3\|p\|_{C^3(C)}^2\Big)\Big)
\end{aligned}
\tag{2.51}
$$

with $\xi_i, i=1,2,3$, non-zero constants, and C, a p, H and Δt independent positive constant. Fixing ξ_1 and ξ_3 such that $e_0-4\xi_1^2>0$, $b_0-\xi_3^2>0$, we conclude that there exist positive constants C_1,C_2, p, H and Δt independent, such that

$$
\begin{aligned}
&\|D_{-t}e_{H,p}^{n+1}\|_H^2 + \Delta t\sum_{j=1}^{n+1}\|D_{-t}e_{H,p}^j\|_H^2 + \|\nabla_H e_{H,p}^{n+1}\|_H^2 \\
&\quad\leq C_1\left(\|D_{-t}e_{H,p}^1\|_H^2 + \|\nabla_H e_{H,p}^1\|_H^2 + \sum_{\ell=1}^2|T_\ell(p(t_1),e_{H,p}^1)| + T_{n+1}(p)\right) + C_2\Delta t\sum_{j=1}^n\|\nabla_H e_{H,p}^j\|_H^2.
\end{aligned}
$$

Applying the discrete Gronwall's Lemma (Lemma 2 of [23]) we obtain the next upper inequality

$$
\begin{aligned}
&\|D_{-t}e_{H,p}^{n+1}\|_H^2 + \Delta t\sum_{j=1}^{n+1}\|D_{-t}e_{H,p}^j\|_H^2 + \|\nabla_H e_{H,p}^{n+1}\|_H^2 \\
&\quad\leq C\Big(\|D_{-t}e_{H,p}^1\|_H^2 + \|\nabla_H e_{H,p}^1\|_H^2 + \sum_{\ell=1}^2|T_\ell(p(t_1),e_{H,p}^1)| + \max_{j=2,\dots,n+1}T_j(p)\Big)\Big(1+T_f e^{C_2 n\Delta t}\Big),
\end{aligned}
\tag{2.52}
$$

for $n=1,\dots,M_t-1$.

Finally, to obtain the final error estimate we need to compute upper bounds for $\|D_{-t}e_{H,p}^1\|_H^2$, $\|\nabla_H e_{H,p}^1\|_H^2$ and $|T_\ell(p(t_1),e_{H,p}^1)|$, $\ell=1,2$. From the first relation of (2.40) we easily get

$$
D_{-t}e_{H,p}^1 = D_{-t}R_H p(t_1) - R_H p'(t_0),
$$

that leads to

$$
\|D_{-t}e_{H,p}^1\|_H^2 \leq \frac{1}{4}\Delta t^2\|p\|_{C^2(C)}^2. \tag{2.53}
$$

To obtain an upper bound for $\|\nabla_H e^1_{H,p}\|^2_H$ we start by remarking that in what concerns $\nabla_H D_{-t} e^1_{H,p}$ we have

$$\nabla_H D_{-t} e^1_{H,p} = \nabla_H D_{-t} R_H p(t_1) - \nabla_H R_H p'(t_0),$$

and consequently, in Ω_H,

$$\left|\nabla_H D_{-t} e^1_{H,p} - \left(\nabla_H D_{-t} R_H p(t_1) - R_H \nabla p'(t_0)\right)\right| \leq C H_{\max} \|p\|_{C^1(C^2)}.$$

Moreover, in Ω_H, we also have

$$\left|\nabla_H D_{-t} R_H p(t_1) - R_H \nabla p'(t_0)\right| \leq C\left(H_{\max}\|p\|_{C^1(C^2)} + \Delta t \|p\|_{C^2(C^1)}\right).$$

Leading to

$$((\nabla_H D_{-t} e^1_{H,p}, \nabla_H e^1_{H,p}))_H = ((T_r(p(t_1)), \nabla_H e^1_{H,p}))_H,$$

with

$$|T_r(p(t_1))| \leq C\Big(\Delta t \|p\|_{C^2(C^1)} + H_{\max}\|p\|_{C^1(C^2)}\Big).$$

The previous estimates allow us to write

$$\begin{aligned}
\|\nabla_H e^1_{H,p}\|^2_H &= \Delta t((T_r(p(t_1)), \nabla_H e^1_{H,p}))_H + ((\nabla_H e^0_{H,p}, \nabla_H e^1_{H,p}))_H \\
&\leq \frac{1}{2}\|\nabla_H e^0_{H,p}\|^2_H + \frac{1}{2}\|\nabla_H e^1_{H,p}\|^2_H + \frac{\Delta t^2}{4\xi^2}\|T_r(p(t_1))\|^2_H + \xi^2 \|\nabla_H e^1_{H,p}\|^2_H,
\end{aligned}$$

where $\xi \neq 0$ is an arbitrary constant. Consequently,

$$\left(1 - 2\xi^2\right)\|\nabla_H e^1_{H,p}\|^2_H \leq \|\nabla_H e^0_{H,p}\|^2_H + \frac{\Delta t^2}{2\xi^2}\|T_r(p(t_1))\|^2_H,$$

and as $e^0_{H,p} = 0$, then, there exists a positive constant C, p, H and Δt independent, such that

$$\|\nabla_H e^1_{H,p}\|^2_H \leq C\Delta t^2\Big(\Delta t^2 \|p\|^2_{C^2(C^1)} + H^2_{\max}\|p\|^2_{C^1(C^2)}\Big). \tag{2.54}$$

Furthermore, from (2.29) and (2.30),

$$\left|T_1(p(t_1), e^1_{H,p})\right| \leq C \sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \|p(t_1)\|^2_{H^3(\Delta)} + \frac{1}{2}\left\|\nabla_H e^1_{H,p}\right\|^2_H, \tag{2.55}$$

and

$$\left|T_2(p(t_1), e^1_{H,p})\right| \leq C \sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \left(\left\|p'(t_1)\right\|^2_{H^2(\Delta)} + \left\|p''(t_1)\right\|^2_{H^2(\Delta)}\right) + \frac{1}{2}\left\|\nabla_H e^1_{H,p}\right\|^2_H. \tag{2.56}$$

Combining (2.51), (2.53), (2.54), (2.55) and (2.56) with (2.52) we conclude (2.41).

□

From (2.3), Theorem 2.4 allows us to conclude the following corollary that establishes that the numerical scheme (2.36), (2.37), (2.38) or (2.39), (2.40), (2.38) has first order of convergence in time, and second order of convergence in space.

Corollary 2.3. *Under the assumptions of Theorem 2.4 we conclude that there exists a positive constant C, H and Δt independent, such that*

$$\|D_{-t}e^n_{H,p}\|^2_H + \|e^n_{H,p}\|^2_{1,H} \leq C\big(\Delta t^2 + H^4_{\max}\big),$$

for $H \in \Lambda$ and $n = 1, \ldots, M_t$.

2.5.2 Second Order Scheme

The first order in time upper bound (2.41) arises due to the use of the backward operator to discretize the first order terms in time in the wave equation, as well as, in its initial velocity. To increase the order of the term defined by the stepsize in time in the mentioned upper bound, we need to invest in the time discretization of the two previous first order terms. We rewrite the IBVP (1.1), (1.4) and (1.7), in the equivalent form

$$\begin{cases} a\dfrac{\partial p}{\partial t} = w - bp \\ \dfrac{\partial w}{\partial t} = \nabla \cdot (E\nabla p) + f_3, \qquad \text{in } \Omega \times (0, T_f], \end{cases}$$

with the initial conditions

$$\begin{cases} w(x,y,0) = ap_{v,0}(x,y) + bp_0(x,y) \\ p(x,y,0) = p_0(x,y), \qquad\qquad (x,y) \in \Omega, \end{cases}$$

and the boundary conditions

$$\begin{cases} w(x,y,t) = 0 \\ p(x,y,t) = 0, \qquad\qquad (x,t) \in \partial\Omega \times (0, T_f]. \end{cases}$$

In this section, to simplify, we assume that a, b, $e_i, i = 1,2$ are positive constant functions.

To get a second order approximation for p and w we use a standard procedure used in first order time derivative problems: we consider the Crank-Nicolson approach. Let p^n_H and w^n_H be the corresponding approximations defined by the finite difference scheme

$$\begin{cases} aD_{-t}p^{n+1}_H = \dfrac{w^{n+1}_H + w^n_H}{2} - b\dfrac{p^{n+1}_H + p^n_H}{2} \\ D_{-t}w^{n+1}_H = \nabla^*_H \cdot \Big(E\nabla_H\Big(\dfrac{p^{n+1}_H + p^n_H}{2}\Big)\Big) + \dfrac{f_{3,H}(t_{n+1}) + f_{3,H}(t_n)}{2} \qquad \text{in } \Omega_H, \end{cases} \tag{2.57}$$

for $n = 0, \ldots, M_t - 1$,

$$\begin{cases} w^0_H = aR_H p_{v,0} + bR_H p_0 \\ p^0_H = R_H p_0, \qquad\qquad \text{in } \Omega_H, \end{cases} \tag{2.58}$$

and

$$\begin{cases} w_H^n = 0 \\ p_H^n = 0, \qquad \text{on } \partial\Omega_H \times \{1,\dots,M_t\}. \end{cases} \tag{2.59}$$

We observe that from (2.57) we easily get

$$\begin{cases} \left(aD_{-t}p_H^{n+1}, v_H\right)_H = \left(\dfrac{w_H^{n+1}+w_H^n}{2}, v_H\right)_H - \left(b\dfrac{p_H^{n+1}+p_H^n}{2}, v_H\right)_H \\ \left(D_{-t}w_H^{n+1}, v_H\right)_H = -\left(\left(E\nabla_H\Big(\dfrac{p_H^{n+1}+p_H^n}{2}\Big), \nabla_H v_H\right)\right)_H + \left(\dfrac{f_{3,H}(t_{n+1})+f_{3,H}(t_n)}{2}, v_H\right)_H, \end{cases}$$

for all $v_H \in W_{H,0}$. We remark that we also have,

$$\begin{aligned} \left(\left(aED_{-t}\nabla_H p_H^{n+1}, \nabla_H v_H\right)\right)_H = {} & \left(\left(E\nabla_H\Big(\frac{w_H^{n+1}+w_H^n}{2}\Big), \nabla_H v_H\right)\right)_H \\ & - \left(\left(bE\nabla_H\Big(\frac{p_H^{n+1}+p_H^n}{2}\Big), \nabla_H v_H\right)\right)_H, \end{aligned} \tag{2.60}$$

for all $v_H \in W_{H,0}$.

For the error $e_p^n = R_H p(t_n) - p_H^n$ and $e_w^n = R_H w(t_n) - w_H^n$ we obtain

$$(D_{-t}e_w^{n+1}, v_H)_H = -\left(\left(E\nabla_H\left(\frac{e_p^{n+1}+e_p^n}{2}\right), \nabla_H v_H\right)\right)_H + (T_{1,H}^n(p), v_H)_H, \tag{2.61}$$

for all $v_H \in W_{H,0}$, where

$$\begin{aligned} \left(T_{1,H}^n(p), v_H\right)_H = {} & -\left(\left(\frac{1}{2}\left(w'(t_{n+1})+w'(t_n)\right)\right)_H - D_{-t}R_H w(t_{n+1}), v_H\right)_H \\ & + \left(\left(\nabla\cdot\left(E\nabla\left(\frac{p(t_{n+1})+p(t_n)}{2}\right)\right)\right)_H, v_H\right)_H + \left(\left(E\nabla_H\left(\frac{R_H p(t_{n+1})+R_H p(t_n)}{2}\right), \nabla_H v_H\right)\right)_H. \end{aligned}$$

To get an estimate for $T_{1,H}^n(p)$ we observe that we have $\left|\left(T_{1,H}^n(p), v_H\right)_H\right| \leq |T_{1,1}^n| + |T_{1,2}^n|$, with

$$T_{1,1}^n = \left(\left(\frac{1}{2}\left(w'(t_{n+1})+w'(t_n)\right)\right)_H - D_{-t}R_H w(t_{n+1}), v_H\right)_H$$

and

$$T_{1,2}^n = \left(\left(E\nabla_H\left(\frac{R_H p(t_{n+1})+R_H p(t_n)}{2}\right), \nabla_H v_H\right)\right)_H + \left(\left(\nabla\cdot\left(E\nabla\left(\frac{p(t_{n+1})+p(t_n)}{2}\right)\right)\right)_H, v_H\right)_H.$$

Note that, for $T_{1,1}^n$, we have

$$\begin{aligned} T_{1,1}^n = {} & \left(\left(\frac{w'(t_{n+1})+w'(t_n)}{2}\right)_H - R_H\left(\frac{w'(t_{n+1})+w'(t_n)}{2}\right), v_H\right)_H \\ & + \left(R_H\left(\frac{w'(t_{n+1})+w'(t_n)}{2}\right) - D_{-t}R_H w(t_{n+1}), v_H\right)_H. \end{aligned}$$

An estimate for the first term of $T^n_{1,1}$ is obtained considering Lemma 5.7 of [14]. In fact, from this lemma, there exists a positive constant C, p, w, H and Δt independent, such that

$$\begin{aligned}
&\left| \left(\left(\frac{w'(t_{n+1})+w'(t_n)}{2} \right)_H - R_H\left(\frac{w'(t_{n+1})+w'(t_n)}{2} \right), v_H \right)_H \right| \\
&\leq C\left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \left(\frac{\|w'(t_{n+1})\|^2_{H^2(\Delta)} + \|w'(t_n)\|^2_{H^2(\Delta)}}{2} \right) \right)^{1/2} \|\nabla_H v_H\|_H \\
&\leq C\left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \|p\|^2_{C^2(H^2)} \right)^{1/2} \|\nabla_H v_H\|_H .
\end{aligned}$$

For the second term of $T^n_{1,1}$, we also guarantee the existence of a positive constant C, p, w, H and Δt independent, such that, in Ω_H,

$$\begin{aligned}
\left| R_H\left(\frac{w'(t_{n+1})+w'(t_n)}{2} \right) - D_{-t}R_H w(t_{n+1}) \right| &\leq C\Delta t^2 \|w\|_{C^3(C)} \\
&\leq C\Delta t^2 \|p\|_{C^4(C)} .
\end{aligned}$$

Therefore

$$\left| \left(R_H\left(\frac{w'(t_{n+1})+w'(t_n)}{2} \right) - D_{-t}R_H w(t_{n+1}), v_H \right)_H \right| \leq C\Delta t^2 \|p\|_{C^4(C)} \|v_H\|_H .$$

Finally,

$$|T^n_{1,1}| \leq C\left[\left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \|p\|^2_{C^2(H^2)} \right)^{1/2} \|\nabla_H v_H\|_H + \Delta t^2 \|p\|_{C^4(C)} \|v_H\|_H \right] . \tag{2.62}$$

An estimate for $T^n_{1,2}$ is easily obtained considering (2.29). In fact, there exists a positive constant C, p, H and Δt independent, such that

$$\left|T^n_{1,2}\right| \leq C\left[\left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \|p(t_{n+1})\|^2_{H^3(\Delta)} \right)^{1/2} + \left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \|p(t_n)\|^2_{H^3(\Delta)} \right)^{1/2} \right] \|\nabla_H v_H\|_H . \tag{2.63}$$

Then, from (2.62) and (2.63), there exists a positive constant C, p, w, H and Δt independent, such that

$$\begin{aligned}
\left| \left(T^n_{1,H}(p), v_H \right)_H \right| \leq C\Bigg[&\Delta t^2 \|p\|_{C^4(C)} \|v_H\|_H \\
&+ \left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \left(\|p\|^2_{C^2(H^2)} + \|p\|^2_{C(H^3)} \right) \right)^{1/2} \|\nabla_H v_H\|_H \Bigg] .
\end{aligned} \tag{2.64}$$

Taking $v_H = e_w^{n+1} + e_w^n$ in (2.61), we obtain

$$\|e_w^{n+1}\|_H^2 = \|e_w^n\|_H^2 - \Delta t\left(\left(E\nabla_H\left(\frac{e_p^{n+1}+e_p^n}{2}\right), \nabla_H(e_w^{n+1}+e_w^n)\right)\right)_H + \Delta t(T_{1,H}^n(p), e_w^{n+1}+e_w^n)_H. \tag{2.65}$$

From (2.60), it can be shown the next equality,

$$\begin{aligned}\left(\left(E\nabla_H\left(\frac{e_w^{n+1}+e_w^n}{2}\right), \nabla_H v_H\right)\right)_H &= ((aED_{-t}\nabla_H e_p^{n+1}, \nabla_H v_H))_H \\ &+\left(\left(bE\nabla_H\left(\frac{e_p^{n+1}+e_p^n}{2}\right), \nabla_H v_H\right)\right)_H \\ &+((T_{2,H}^n(p), \nabla_H v_H))_H,\end{aligned} \tag{2.66}$$

for $v_H \in W_{H,0}$, with

$$\begin{aligned}\big((T_{2,H}^n(p), \nabla_H v_H)\big)_H = &\left(\left(E\nabla_H\left(\frac{R_H w(t_{n+1}) + R_H w(t_n)}{2}\right), \nabla_H v_H\right)\right)_H \\ &-((aED_{-t}\nabla_H(R_H p(t_{n+1})), \nabla_H v_H))_H \\ &-\left(\left(bE\nabla_H\left(\frac{R_H p(t_{n+1}) + R_H p(t_n)}{2}\right), \nabla_H v_H\right)\right)_H.\end{aligned}$$

We observe that we have the following equivalent representations

$$((aED_{-t}\nabla_H e_p^{n+1}, \nabla_H(e_p^{n+1}+e_p^n)))_H = \frac{1}{\Delta t}\left\|\sqrt{aE}\nabla_H e_p^{n+1}\right\|_H^2 - \frac{1}{\Delta t}\left\|\sqrt{aE}\nabla_H e_p^n\right\|_H^2$$

and

$$\left(\left(bE\nabla_H\left(\frac{R_H p(t_{n+1}) + R_H p(t_n)}{2}\right), \nabla_H(e_p^{n+1}+e_p^n)\right)\right)_H = \frac{1}{2}\left\|\sqrt{bE}\nabla_H(e_p^{n+1}+e_p^n)\right\|_H^2.$$

Consequently, from (2.65), we have

$$\begin{aligned}\|e_w^{n+1}\|_H^2 + \|\sqrt{aE}\nabla_H e_p^{n+1}\|_H^2 = &\|e_w^n\|_H^2 + \|\sqrt{aE}\nabla_H e_p^n\|_H^2 - \frac{\Delta t}{2}\left\|\sqrt{bE}\nabla_H(e_p^{n+1}+e_p^n)\right\|_H^2 \\ &+ \Delta t(T_{1,H}^n(p), e_w^{n+1}+e_w^n)_H - \Delta t((T_{2,H}^n(p), \nabla_H(e_p^{n+1}+e_p^n)))_H.\end{aligned} \tag{2.67}$$

In order to find an upper bound to $((T_{2,H}^n(p), \nabla_H v_H))_H$, observe that

$$((T_{2,H}^n(p), \nabla_H v_H))_H = \left(\left(aE\nabla_H\left[\frac{R_H(p'(t_{n+1})) + R_H(p'(t_n))}{2} - D_{-t}R_H p(t_{n+1})\right], \nabla_H v_H\right)\right)_H$$

and, for $i = 1, \ldots, N$, $j = 1, \ldots, M-1$, $n = 0, \ldots, M_t - 1$,

$$
\begin{aligned}
&D_{-x}\Big(\frac{1}{2}\Big(\frac{\partial p}{\partial t}(x_i,y_j,t_{n+1})+\frac{\partial p}{\partial t}(x_i,y_j,t_n)\Big)-D_{-t}p(x_i,y_j,t_{n+1})\Big)\\
&\qquad=\frac{1}{h_i}\int_{x_{i-1}}^{x_i}\frac{1}{2}\Big(\frac{\partial^2 p}{\partial x\partial t}(s,y_j,t_{n+1})+\frac{\partial^2 p}{\partial x\partial t}(s,y_j,t_n)\Big)-D_{-t}\frac{\partial p}{\partial x}(s,y_j,t_{n+1})\,ds.
\end{aligned}
$$

With,

$$
\left|\frac{1}{2}\Big(\frac{\partial^2 p}{\partial x\partial t}(s,y_j,t_{n+1})+\frac{\partial^2 p}{\partial x\partial t}(s,y_j,t_n)\Big)-D_{-t}\frac{\partial p}{\partial x}(s,y_j,t_{n+1})\right|\leq C\Delta t^2\left\|\frac{\partial p}{\partial x}\right\|_{C^3(C)}\leq C\Delta t^2\|p\|_{C^3(C^1)}.
$$

Then

$$
\left|((T^n_{2,H}(p),\nabla_H v_H))_H\right|\leq C\Delta t^2\|p\|_{C^3(C^1)}\left\|\sqrt{aE}\nabla_H v_H\right\|_H, \tag{2.68}
$$

where C is a positive constant, p, w, H and Δt independent.

Using, in (2.67), (2.64) and (2.68), for $\varepsilon\neq 0$,

$$
\begin{aligned}
&(1-2\varepsilon^2\Delta t)\left(\|e_w^{n+1}\|_H^2+\left\|\sqrt{aE}\nabla_H e_p^{n+1}\right\|_H^2\right)\\
&\qquad\leq(1+2\varepsilon^2\Delta t)\left(\|e_w^n\|_H^2+\left\|\sqrt{aE}\nabla_H e_p^n\right\|_H^2\right)+\varepsilon^2\Delta t\left\|\nabla_H(e_w^{n+1}+e_w^n)\right\|_H^2\\
&\qquad\quad+\frac{C\Delta t}{4\varepsilon^2}\Big(\Delta t^4\left(\|p\|^2_{C^4(C)}+\|p\|^2_{C^3(C^1)}\right)+\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\left(\|p\|^2_{C^2(H^2)}+\|p\|^2_{C(H^3)}\right)\Big).
\end{aligned}\tag{2.69}
$$

In order to find an upper bound for $\|\nabla_H(e_w^{n+1}+e_w^n)\|_H$, (2.66) leads to

$$
\begin{aligned}
&\frac{1}{2}\min\{e_1,e_2\}\left\|\nabla_H(e_w^{n+1}+e_w^n)\right\|_H^2\\
&\leq\frac{\sqrt{\max\{e_1,e_2\}}(2a+b\Delta t)}{2\sqrt{2a}\Delta t}\left(\|\sqrt{aE}\nabla_H e_p^{n+1}\|_H+\|\sqrt{aE}\nabla_H e_p^n\|_H\right)\|\nabla_H(e_w^{n+1}+e_w^n)\|_H\\
&\quad+C\Delta t^2\|p\|_{C^3(C^1)}\|\nabla_H(e_w^{n+1}+e_w^n)\|_H,
\end{aligned}
$$

with C a positive constant, p, w, H and Δt independent. Therefore we have

$$
\begin{aligned}
\Delta t\left\|\nabla_H(e_w^{n+1}+e_w^n)\right\|_H^2\leq{}&\frac{2(2a+\Delta tb)^2\max\{e_1,e_2\}}{a\Delta t(\min\{e_1,e_2\})^2}\left(\left\|\sqrt{aE}\nabla_H e_p^{n+1}\right\|_H^2+\left\|\sqrt{aE}\nabla_H e_p^n\right\|_H^2\right)\\
&+2C\Delta t^5\|p\|^2_{C^3(C^1)}.
\end{aligned}
$$

Considering $r=\dfrac{(2a+\Delta tb)^2\max\{e_1,e_2\}}{a\Delta t(\min\{e_1,e_2\})^2}$, from (2.69), we achieve to

$$\begin{aligned}
\|e_w^{n+1}\|_H^2 + \left\|\sqrt{aE}\nabla_H e_p^{n+1}\right\|_H^2 \leq & \frac{1+2\varepsilon^2\Delta t+2\varepsilon^2 r}{1-2\varepsilon^2\Delta t-2\varepsilon^2 r}\left(\|e_w^n\|_H^2 + \left\|\sqrt{aE}\nabla_H e_p^n\right\|_H^2\right) + \\
& + \frac{C\Delta t}{4\varepsilon^2(1-2\varepsilon^2\Delta t-2\varepsilon^2 r)}\Big(\Delta t^4\Big((8\varepsilon^4+1)\|p\|^2_{C^3(C^1)} + \|p\|^2_{C^4(C)}\Big) \\
& + \sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\left(\|p\|^2_{C^2(H^2)} + \|p\|^2_{C(H^3)}\right)\Big) \\
\leq & \frac{CT_f}{4\varepsilon^2(1-2\varepsilon^2\Delta t-2\varepsilon^2 r)} e^{\frac{4\varepsilon^2 n(\Delta t+r)}{1-2\varepsilon^2\Delta t-2\varepsilon^2 r}}\Bigg(\Delta t^4\Big((8\varepsilon^4+1)\|p\|^2_{C^3(C^1)} \\
& + \|p\|^2_{C^4(C)}\Big) + \sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\left(\|p\|^2_{C^2(H^2)} + \|p\|^2_{C(H^3)}\right)\Bigg),
\end{aligned}$$

where $\varepsilon \neq 0$ such that $1-2\varepsilon^2\Delta t-2\varepsilon^2 r > 0$, and $e_w^0 = e_p^0 = 0$.
Finally, using (2.3), we conclude the following result.

Theorem 2.5. *If the solution of the IBVP (1.1), (1.4), (1.7) is in*

$$C^4([0,T_f],C(\overline{\Omega}))\cap C^3([0,T_f],C^1(\overline{\Omega}))\cap C^2([0,T_f],H^2(\Omega))\cap C([0,T_f],H^3(\Omega)\cap H_0^1(\Omega)),$$

and a, b, $e_i, i=1,2$ are positive constants, then, for $H\in\Lambda$, there exists a positive constant C, independent of p, w, H and Δt, such that for the errors $e_p^n = R_H p(t_n) - p_H^n$ and $e_w^n = R_H w(t_n) - w_H^n$, where p_H^n, w_H^n are defined by (2.57), (2.58), (2.59), $n = 0,\ldots,M_t-1$, holds the following

$$\begin{aligned}
&\|e_w^{n+1}\|_H^2 + \|\nabla_H e_p^{n+1}\|_H^2 + \|e_p^{n+1}\|_H^2 \\
&\qquad \leq C\Big(\Delta t^4\left(\|p\|^2_{C^3(C^1)} + \|p\|^2_{C^4(C)}\right) + \sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\left(\|p\|^2_{C^2(H^2)} + \|p\|^2_{C(H^3)}\right)\Big).
\end{aligned}$$

From Theorem 2.5, we finally conclude the second order of convergence of our fully discrete scheme (2.57), (2.58), (2.59). This result is presented in the following corollary.

Corollary 2.4. *Under the assumptions of Theorem 2.5, we conclude that there exists a positive constant C, H and Δt independent, such that*

$$\|e_w^n\|_H^2 + \|e_p^n\|_{1,H}^2 \leq C\Big(\Delta t^4 + H_{\max}^4\Big),$$

for $H\in\Lambda$ and $n = 1,\ldots,M_t$.

We remark that to obtain the last result an increase in the smoothness of the solution p was required. We were not able to prove the same result for lower smooth solutions.

2.6 Numerical Results

In this section we present some numerical experiments which illustrate the results of this chapter. In the Examples 2.1 and 2.2, we consider the fully discrete in time and space numerical scheme given by (2.39), (2.40), (2.38), with $T_f = 0.05$ and $\Delta t = 10^{-5}$. Moreover, we consider $a(x,y) = x^2$, $b(x,y) = 1+x+y$, $e_1(x,y) = 2+y^2$, $e_2(x,y) = 1+x$. We observe that the coefficient function a does not satisfy the condition $a(x,y) \geq a_0 > 0$, for $(x,y) \in \overline{\Omega}$. However, our numerical results are the expected, despite that.

Example 2.1. *To illustrate the result of Theorem 2.2, we consider the problem (1.1), (1.4), (1.7) with initial conditions and f_3, such that, its exact solution is given by*

$$p(x,y,t) = e^t(1-x)(1-cos(4\pi y))sin(xy).$$

Note that $p \in C^1([0,T_f], C^4(\overline{\Omega})) \cap C^2([0,T_f], C(\overline{\Omega}))$, and $f_3 \in C^1([0,T_f], C^2(\overline{\Omega}))$.

Example 2.2. *In this example, we intend to illustrate the sharpness of the smoothness conditions imposed in Theorem 2.3. We expect to lose the convergence order obtained in this result for lower smoothness solutions. We define f_3 and the initial conditions of the problem (1.1), (1.4), (1.7) such that*

$$p(x,y,t) = e^t sin(xy)(2x-2)(y-1)|2y-1|^{1+\alpha}, \alpha \in \mathbb{R},$$

is the exact solution of our IBVP (1.1), (1.4), (1.7). Note that, for $\alpha = 2.1$, p is under the conditions of Theorem 2.3 (but not under the conditions of Theorem 2.2). Otherwise, for $\alpha = 1.1$, we have $p(t) \in H^2(\Omega)$, but $p(t) \notin H^3(\Omega)$.

To obtain the numerical approximations for the IBVPs defined in Examples 2.1 and 2.2, we consider a sequence of grids H_k, $k = 1,\dots,6$, of increasing size. H_1 is a nonuniform mesh defined randomly with $N = 6$ and $M = 8$. H_k, $k = 2\dots,6$, are constructed inserting grid points at the midpoints of H_{k-1}. To obtain the numerical rate of convergence we define the error

$$E_{H,p} = \max_{n=1,\dots,M_t} \left\|D_{-t}e^n_{H,p}\right\|_H + \left\|\nabla_H e^n_{H,p}\right\|_H.$$

The time step Δt is fixed small enough satisfying $\Delta t \leq CH^2_{\max}$.

Example 2.1		Example 2.2 ($\alpha = 2.1$)		Example 2.2 ($\alpha = 1.1$)	
$H_{\max}$	$E_{H,p}$	$H_{\max}$	$E_{H,p}$	$H_{\max}$	$E_{H,p}$
3.404e-1	7.128e-1	2.007e-1	2.111e-2	1.763e-1	4.676e-2
1.702e-1	1.899e-1	1.003e-1	5.658e-3	8.814e-2	2.052e-2
8.510e-2	4.451e-2	5.017e-2	1.372e-3	4.407e-2	9.533e-3
4.255e-2	1.112e-2	2.508e-2	3.594e-4	2.204e-2	4.470e-3
2.128e-2	2.775e-3	1.254e-2	8.965e-5	1.102e-2	2.091e-3
1.064e-2	6.931e-4	6.271e-3	2.232e-5	5.509e-3	9.741e-4

Table 2.1 The errors $E_{H,p}$ on successively refined meshes: Example 2.1 and 2.2.

Using the data from Table 2.1, we plot in Figures 2.2 and 2.3 the $\log(E_{H,p})$ versus $\log(H_{\max})$ for the Examples 2.1 and 2.2, respectively. Assuming that the errors $E_{H,p}$ are proportional to $H^r_{\max}$, for some $r \in \mathbb{R}$, the slope of the best fitting least square line illustrates the convergence rate.

For Example 2.1 the obtained estimated value is 2.0094, which illustrates the theoretical second order of convergence obtained in the Theorem 2.2. The obtained data for the Example 2.2, with

$\alpha = 2.1$ verifies the second order convergence rate of the smooth case, as expected by Theorem 2.3. However, considering the second example with $\alpha = 1.1$ ($p(t) \in H^2(\Omega)$), the obtained numerical rate of convergence is approximately one. This fact suggests that the assumption $p(t) \in H^3(\Omega)$ in Theorem 2.3 is optimal in Sobolev spaces. As illustration, we present in Figure 2.4 the numerical solution and the square of the error $e_{H,p}^{M_t}$, at time T_f, for each of the considered examples. We remark that, using the results established in [14] and following the steps of Theorem 2.3, it can be proved that the rate of convergence is in fact one when $p(t) \in H^2(\Omega)$.

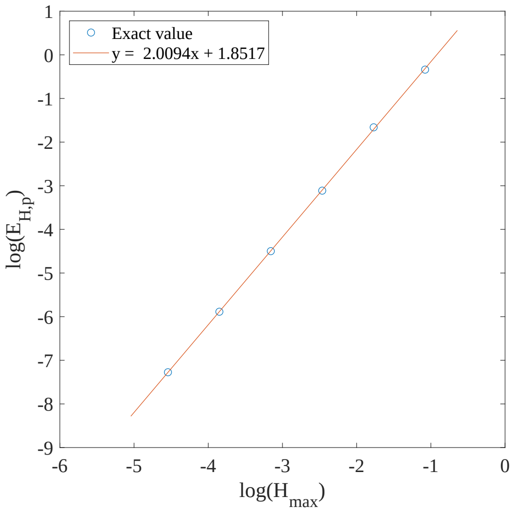
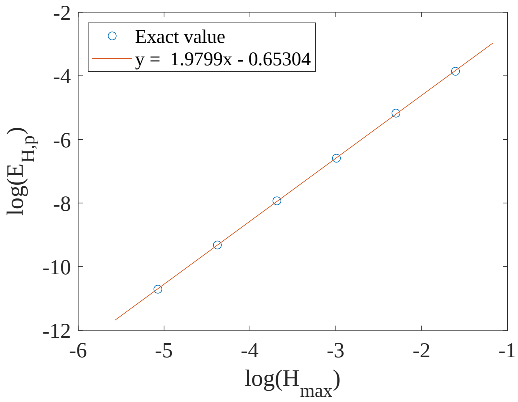


Fig. 2.2 Log-log plot of $E_{H,p}$ versus $H_{\max}$ for Example 2.1. In the solid line is shown the best fitting least square line.



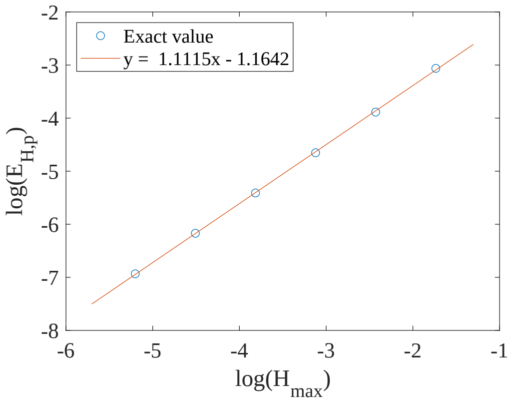


Fig. 2.3 From left to right: Log-log plot of $E_{H,p}$ versus $H_{\max}$ for Example 2.2 with $\alpha = 2.1$ and $\alpha = 1.1$. In the solid line is shown the best fitting least square line.

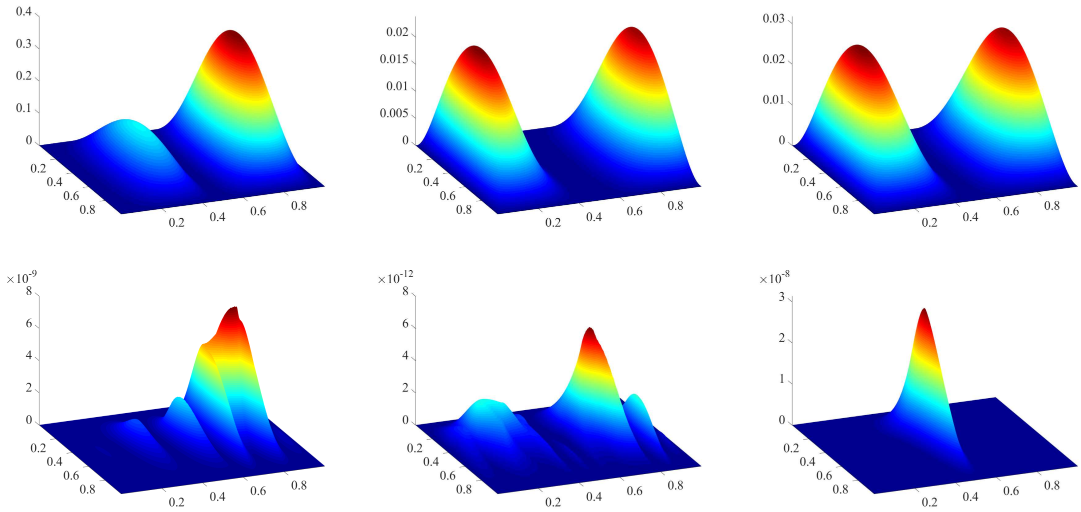


Fig. 2.4 From left to right: numerical solution $p_H^{M_t}$ (first row) and square of the error $e_{H,p}^{M_t}$ (second row) on the grid H_6; for Example 2.1 and Example 2.2 with $\alpha = 2.1$ and $\alpha = 1.1$.

Example 2.3. *In order to study the time convergence of the presented numerical schemes in the Sections 2.5.1 and 2.5.2, consider the IBVP (1.1), (1.4), (1.7) with coefficient functions* $a(x,y) = 5(1+x)$*,* $b(x,y) = xy$*,* $e_1(x,y) = 1+x$*, and* $e_2(x,y) = y$*, whose solution is given by*

$$p(x,y,t) = e^t(x-1)\sin(\pi x)(y-1)sin(\pi y),$$

with initial conditions and f_3 *defined properly.*

To examine the rate of convergence in time, we use Example 2.3. For that, we consider successively smaller time stepsizes using a fixed spatial grid with $H_{\max} = 3.913e-3$, and $T_f = 3$.

In Table 2.2 we present the numerical results considering the error term $E_{H,p}$ defined before to study the behavior of the first order scheme (2.39), (2.40), (2.38), and

$$E_{H,2} = \max_{n=1,\ldots,M_t} \|e_w^n\|_H + \left\|\nabla_H e_p^n\right\|_H + \left\|e_p^n\right\|_H$$

to study the behavior of the second order scheme (2.57), (2.58), (2.59).

In Figure 2.5 we plot the $\log(E_{H,p})$ and $\log(E_{H,2})$ versus $\log(\Delta t)$, for Example 2.3, considering the first and second order schemes, respectively. The best fitting least square lines are also presented. In this figure it is illustrated the convergence rate established in Corollary 2.3, as well as the convergence rate equal to 2 established in Corollary 2.4 for the scheme (2.57), (2.58), (2.59).

Note that, in this example, the coefficient functions are not constants, as we assume in the proof of Theorem 2.5. However this fact can be used to infer that this result remains true for non constant coefficient functions. We need to revisit the proof of this result in order to extend it for non constant coefficient functions. In the Figure 2.6 we present some illustrative images.

Example 2.3 (2nd order scheme)		Example 2.3 (1st order scheme)	
Δt	$E_{H,2}$	Δt	$E_{H,p}$
5.000e-1	3.950e-1	5.000e-1	24.89e-1
2.500e-1	9.949e-2	2.500e-1	13.78e-1
1.250e-1	2.486e-2	1.250e-1	7.285e-1
6.250e-2	6.151e-3	6.250e-2	3.754e-1
3.125e-2	1.478e-3	3.125e-2	1.907e-1

Table 2.2 The errors $E_{H,2}$ and $E_{H,p}$ for successively smaller time stepsizes: Example 2.3.

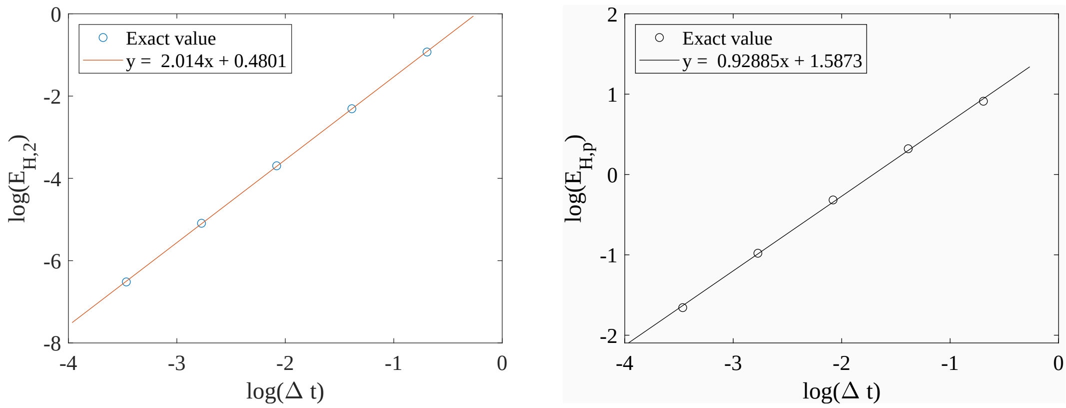


Fig. 2.5 From left to right: Log-log plots of $E_{H,p}$ and $E_{H,2}$ versus Δt for Example 2.3 with the first order and second order schemes, respectively. In the solid line is shown the best fitting least square line.

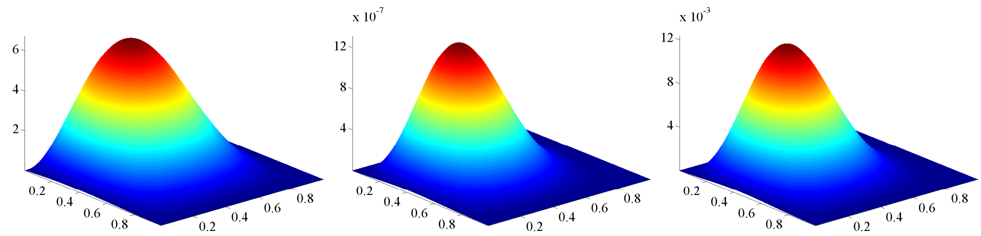


Fig. 2.6 From left to right: numerical solution $p_H^{M_t}$ obtained with the second order in time scheme and square of the error $e_p^{M_t}$ for the second order in time scheme and the first order in time scheme; results for Example 2.3 using $\Delta t = 0.0625$.

2.7 Conclusions

In this chapter, we consider a hyperbolic IBVP arising in the context of acoustic pressure propagation. Our main goal was to establish conditions that allow us to obtain second order approximations, in space and time, with respect to a discrete H^1- norm.

The main results in this chapter are Theorems 2.2 and 2.3. In these theorems convergence proprieties of the semi-discrete solution defined by the fully discrete in space piecewise linear finite element method (2.8), (2.9), which is equivalent to the finite difference method (2.10), (2.11), (2.12), were analyzed, considering smooth and non-smooth assumptions for the solution of the correspondent continuous IBVP. For each case, two complete different techniques of analysis were followed to derive second order approximations in respect to a discrete H^1- norm. Theorem 2.2 corresponds to the smooth case and Theorem 2.3 to the non-smooth case. The discretization in time was studied in Section 2.5. We present two fully discrete in space and time schemes, proving first order of convergence in time of the first scheme, and second order when we consider Crank-Nicolson approach.

Numerical experiments illustrating the obtained theoretical results were also included. In particular, Example 2.2 with $\alpha = 1.1$, illustrates that the convergence rate established in Theorem 2.3 is optimal in the sense that if $p(t) \in H^2(\Omega)$ then the rate of convergence is only one.

Chapter 3

Coupling: Acoustic Pressure Propagation and Drug Transport

3.1 Introduction

In this chapter, we consider the system defined by the telegraph equation (1.1) coupled with the convection-diffusion-reaction equation (1.14) in $\Omega \times (0, T_f]$. This system is complemented with homogeneous Dirichlet boundary conditions (1.7) and (1.9), and the initial conditions (1.4) and (1.6). As previously mentioned, the system of differential equations (1.1), (1.14) can be used to describe the drug transport enhanced by ultrasound when the heat effects are not explicitly considered. This means that this chapter is an intermediate stage between Chapter 2 and Chapter 4. In fact, in Chapter 2 only the telegraph equation is studied, while in Chapter 4 we analyze the differential system (1.1)-(1.3) where ultrasound, thermal effects and drug transport are taken into account.

As well as previously, we assume $\Omega = (0,1)^2$ and $p,\ c : \overline{\Omega} \times [0, T_f] \to \mathbb{R}$. The assumptions imposed over the telegraph model in the previous chapter, are also going to be considered here. In addition, in equation (1.14), $D(p)$ is a second order diagonal matrix with entries $d_i : \mathbb{R} \to \mathbb{R}$, $i = 1,2$, with a positive lower bound d_0 in $\mathbb{R}$. We assume that $v : \mathbb{R}^3 \to \mathbb{R}^2$ that arises in the convective velocity of (1.14) is such that its components $v_i : \mathbb{R}^2 \to \mathbb{R}$, $i = 1,2$, are given by $v(x,y,z) = (v_1(x,y), v_2(x,z)), x,y,z \in \mathbb{R}$.

In this chapter, we propose a fully discrete piecewise linear finite element method, that can be seen as a finite difference method, to approximate p and c, that leads to second order approximations with respect to a discrete H^1- norm and L^2- norm, respectively.

Section 3.2 is devoted to the design of the semi-discrete scheme, and the convergence analysis of the proposed method is given in Section 3.3. The results obtained in previous chapter have a crucial role in what follows. In the main results, Theorem 3.1 and Corollary 3.1, we establish the second order of convergence. In Section 3.4, we present some numerical experiments illustrating the last convergence results. In this section we also include an illustrative example in the scope of the drug transport enhanced by ultrasound, where the efficacy of the use of ultrasound is showed. Lastly, we present some conclusions for this chapter.

Before continuing, we present a small remark about the existence and uniqueness of solution of the IBVP (1.1), (1.14), (1.4), (1.6), (1.7) and (1.9). Following Chapter 7 of [11], the section about parabolic equations, it is possible to define weak solution of this problem and prove an existence and uniqueness result. However, we need to consider $p \in L^\infty(0,T_f,L^\infty(\Omega))$, $\nabla p \in L^\infty(0,T_f,[L^\infty(\Omega)]^2)$, since the convective term of (1.14) depends on p, ∇p, and the diffusion is p dependent. To obtain such regularity for the weak solution of the hyperbolic problem, we can adapt to our case the Theorems 2, 5 and 6 of Section 7.1.2 of [11]. It is clear that in this case, it is mandatory to increase the smoothness of f_3, p_0 and $p_{v,0}$.

3.2 Semi-Discrete Numerical Scheme

Our aim in this section is to construct a fully discrete in space finite element method for the presented coupled hyperbolic-parabolic problem (1.1), (1.14), (1.4), (1.6), (1.7) and (1.9).

We start by introducing the following variational problem: find $(p(t),c(t)) \in [H_0^1(\Omega)]^2$ such that

(i) $p^{(j)}(t) \in L^2(\Omega)$, $j=1,2$, $t \in (0,T_f]$, and (2.1) holds for $w \in H_0^1(\Omega)$, coupled with (2.2);

(ii) $c'(t) \in L^2(\Omega)$, $t \in (0,T_f]$, and

$$(c'(t),w) - ((v(p(t),\nabla p(t))c(t),\nabla w)) + ((D(p(t))\nabla c(t),\nabla w)) = (f_1(t),w),\ t \in (0,T_f],$$

for $w \in H_0^1(\Omega)$, and

$$(c(0),q) = (c_0,q), \quad \forall q \in L^2(\Omega).$$

For the acoustic pressure, it is considered the fully discrete FEM constructed in Section 2.3:

(i) find $p_H(t) \in W_{H,0}$ such that (2.8) holds for $t \in (0,T_f]$, $w_H \in W_{H,0}$, with initial conditions given by (2.9).

Note that, as referred in Section 2.3, this fully discrete FEM can be seen as the following finite difference problem: find $p_H(t) \in W_{H,0}$ such that (2.10), (2.11), (2.12) hold.

Now, we intend to construct a fully discrete in space finite element scheme for the convection-diffusion equation (1.14). With that goal, we start by introducing the following piecewise linear finite element approximation for the concentration: find $c_H(t) \in W_{H,0}$ such that

$$\begin{aligned}(P_H c_H'(t),P_H w_H) - ((P_H c_H(t) v(P_H p_H(t),\nabla P_H p_H(t)),\nabla P_H w_H)) \\ = -((D(P_H p_H(t))\nabla P_H c_H(t),\nabla P_H w_H)) + (f_1(t),P_H w_H),\end{aligned} \tag{3.1}$$

for $t \in (0,T_f]$, $w_H \in W_{H,0}$, and

$$(P_H c_H(0),P_H q_H) = (P_H R_H c_0, P_H q_H),\ \forall q_H \in W_{H,0}. \tag{3.2}$$

Following the approach introduced in Section 2.3, for $i=0,\dots,N$, $j=0,\dots,M$, consider $\square_{i,j} = \cup_{l=1}^4 (\square_l \cap \Omega)$ illustrated in Figure 2.1. In what follows, we intend to construct a fully discrete in space piecewise linear finite element approximation for the concentration. For that, we need to use adequate quadrature rules, which will be presented in what follows.

We consider

$$\left(P_H c_H'(t),P_H w_H\right) \simeq \left(c_H'(t),w_H\right)_H,$$

$$(f_1(t), P_H w_H) \simeq (f_{1,H}(t), w_H)_H\,,$$

and

$$(P_H c_H(0), P_H w_H) \simeq (R_H c_0, w_H)_H\,,$$

using the quadrature rule presented in (2.6), where $f_{1,H}$ is given by (2.7) with $f_3(t)$ replaced by $f_1(t)$.

Now, let D_H^* be the finite difference operator $D_H^* w_H = \big(D_h^* w_H, D_k^* w_H\big)$, $w_H \in W_H$, with

$$D_h^* w_H(x_i, y_j) = \frac{h_i D_{-x} w_H(x_{i+1}, y_j) + h_{i+1} D_{-x} w_H(x_i, y_j)}{h_i + h_{i+1}}, i = 1, \dots, N-1,$$

$$D_h^* w_H(x_N, y_j) = D_{-x} w_H(x_N, y_j),\; D_h^* w_H(x_0, y_j) = D_{-x} w_H(x_1, y_j),$$

for $j = 1, \dots, M-1$, being $D_k^* w_H$ defined analogously. M_H represents the average operator given by

$$M_H(w_1, w_2) = (M_h w_1, M_k w_2), \quad M_h(w_1(x_i, y_j)) = \frac{1}{2}(w_1(x_{i-1}, y_j) + w_1(x_i, y_j)),$$

being M_k defined analogously and $(w_1, w_2) \in [W_{H,0}]^2$.

For $(x_i, y_j) \in \overline{\Omega}_H$, we introduce the following quadrature rutes

$$\int_{\square_l} P_H c_H(t) v_1\left(P_H p_H(t), \frac{\partial}{\partial x}(P_H p_H(t))\right) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq$$
$$\simeq |\square_l|\, M_h(c_H(x_{i+1}, y_j, t) v_1(p_H(x_{i+1}, y_j, t), D_h^* p_H(x_{i+1}, y_j, t))) D_{-x} w_H(x_{i+1}, y_j),\; l = 1, 4,$$

and

$$\int_{\square_l} P_H c_H(t) v_1\left(P_H p_H(t), \frac{\partial}{\partial x}(P_H p_H(t))\right) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq$$
$$\simeq |\square_l|\, M_h(c_H(x_i, y_j, t) v_1(p_H(x_i, y_j, t), D_h^* p_H(x_i, y_j, t))) D_{-x} w_H(x_i, y_j),\; l = 2, 3,$$

with similar definitions for the term associated with the derivatives with respect to y. Then we obtain

$$((P_H c_H(t) v(P_H p_H(t), \nabla P_H p_H(t)), \nabla P_H w_H)) \simeq ((M_H(c_H(t) v_H(t)), \nabla_H w_H))_H\,,$$

with $v_H(t) = \big(v_1(p_H(t), D_h^* p_H(t)), v_2(p_H(t), D_k^* p_H(t))\big)$.

We also consider

$$((D(P_H p_H(t)) \nabla P_H c_H(t), \nabla P_H w_H)) \simeq ((D_H(t) \nabla_H c_H(t), \nabla_H w_H))_H\,,$$

where $D_H(t)$ is the 2×2 diagonal matrix with diagonal elements $d_{1,H}(t) = d_1(M_h p_H(t))$ and $d_{2,H}(t) = d_2(M_k p_H(t))$. To obtain this approximation, for $(x_i, y_j) \in \overline{\Omega}_H$, we set

$$\int_{\square_l} d_1(P_H p_H(t)) \frac{\partial}{\partial x}(P_H c_H(t)) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq$$
$$\simeq |\square_l|\, d_1(M_h p_H(x_{i+1}, y_j, t)) D_{-x} c_H(x_{i+1}, y_j, t) D_{-x} w_H(x_{i+1}, y_j),\; l = 1, 4,$$

and

$$\int_{\square_l} d_1(P_H p_H(t)) \frac{\partial}{\partial x}(P_H c_H(t)) \frac{\partial}{\partial x}(P_H w_H)\, dxdy \simeq$$
$$\simeq |\square_l|\, d_1(M_h p_H(x_i,y_j,t)) D_{-x} c_H(x_i,y_j,t) D_{-x} w_H(x_i,y_j),\ l = 2,3,$$

considering similar approximations for the term related to the y variable. Then, the initial value problem (3.1), (3.2) is replaced by the following fully discrete in space finite element problem: find $c_H(t) \in W_{H,0}$ such that

$$\begin{aligned}(c_H'(t), w_H)_H - ((M_H(c_H(t)v_H(t)), \nabla_H w_H))_H = -((D_H(t)\nabla_H c_H(t), \nabla_H w_H))_H \\ + (f_{1,H}(t), w_H)_H, \qquad (3.3)\end{aligned}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, and

$$(c_H(0), q_H)_H = (R_H c_0, q_H)_H,\ \forall q_H \in W_{H,0}. \qquad (3.4)$$

This finite element problem can be seen as a finite difference method, given by

$$c_H'(t) + \nabla_{c,H} \cdot (c_H(t)v_H(t)) = \nabla_H^* \cdot (D_H(t)\nabla_H c_H(t)) + f_{1,H}(t) \text{ in } \Omega_H,\ t \in (0, T_f], \qquad (3.5)$$

with the initial condition

$$c_H(0) = R_H c_0 \text{ in } \Omega_H, \qquad (3.6)$$

and the boundary condition

$$c_H(t) = 0 \text{ on } \partial\Omega_H. \qquad (3.7)$$

Here $\nabla_{c,H}$ denotes a finite difference operator defined by

$$\nabla_{c,H} \cdot (w_1, w_2) = D_{c,x} w_1 + D_{c,y} w_2, \text{ and } D_{c,x} w_1(x_i, y_j) = \frac{w_1(x_{i+1}, y_j) - w_1(x_{i-1}, y_j)}{h_i + h_{i+1}},$$

where $(w_1, w_2) \in [W_{H,0}]^2$, being $D_{c,y}$ defined analogously.

In what concerns the existence and uniqueness of the semi-discrete approximation $c_H(t)$, we remark that (3.5) can be written in the following equivalent form

$$c_H'(t) + B(t)c_H(t) = f_{1,H}(t),\ t \in (0, T_f], \qquad (3.8)$$

where the entries of the matrix $B(t)$ depend on $v_H(t)$ and $D_H(t)$, this means that it also depends on the solution $p_H(t)$ of (2.13), (2.12). As it is well known, establishing conditions to guarantee the continuity of $B(t)$ and $f_{1,H}(t)$ is enough to assure the existence and uniqueness of a solution $c_H(t) \in C^1((0, T_f]) \cap C([0, T_f])$ for the initial value problem (3.8), (3.6) ([7]).

3.3 Convergence Analysis

The fully discrete in space piecewise linear FEM proposed for the coupled IBVP (1.1), (1.14), (1.4), (1.6), (1.7), (1.9), is obtained coupling:

(i) (2.8), (2.9) to compute an approximation for the acoustic pressure;

(ii) (3.3), (3.4) to compute an approximation for the concentration.

As explained in Section 2.4, for the fully discrete in space approximation of p, it was expected

$$\|R_H p(t) - p_H(t)\|_H + \|\nabla_H (R_H p(t) - p_H(t))\|_H \leq CH_{\max}.$$

For the concentration, it is also well known that the continuous version of the IBVP (3.3), (3.4) leads

$$\|c(t) - P_H c_H(t)\| \leq CH^2_{\max}, \quad \|c(t) - P_H c_H(t)\|_1 \leq CH_{\max},$$

with $c(t) \in H^2(\Omega) \cap H^1_0(\Omega)$ ([19], [42], [45]). As the convective velocity for the concentration depends on ∇p, then the coupled piecewise linear FEM should lead to a first order approximation for the concentration with respect to the L^2- norm. Should be expected that this result also holds for the fully discrete coupled method proposed. However, we have that the fully discrete acoustic pressure approximation $p_H(t)$ is second order convergent with respect to the discrete version of the H^1- norm considered in this work (Corollary 2.1), which means that its discrete gradient is a second order approximation to $\nabla p(t)$ with respect to a discrete version of the L^2- norm. These facts allow us to prove that $c_H(t)$ is also a second order approximation for $c(t)$, with respect to the discrete version of the norm L^2 ($\|\cdot\|_H$), assuming $p(t), c(t) \in H^3(\Omega) \cap H^1_0(\Omega)$. The uniform boundness of the numerical approximation $p_H(t)$ for the acoustic pressure $p(t)$, and of its discrete gradient $\nabla_H p_H(t)$ established in Corollary 2.2 is a main tool in the proof of such result.

We observe that the coupled method (2.8), (2.9), (3.3), (3.4) is equivalent to the finite difference coupling

(i) (2.10), (2.11), (2.12) for the acoustic pressure $p_H(t)$,

(ii) (3.5), (3.6), (3.7) for the concentration $c_H(t)$.

Each finite difference IBVP is defined in a nonuniform rectangular grid Ω_H. If we assume that $p(t),\ c(t) \in C^3(\overline{\Omega})$, then it can be shown that the truncation errors of each subproblem is only first order, with respect to the norm $\|\cdot\|_\infty$ (for $p_H(t)$ this fact is proved in Section 2.4.1). Based on stability and consistency we can expect that the global semi-discrete error for $c_H(t)$ will be only of first order. Attending the equivalence between the two coupled problems described before: the fully discrete FEM IBVPs (2.8), (2.9) and (3.3), (3.4), and the finite difference IBVPs (2.10), (2.11), (2.12) and (3.5), (3.6), (3.7), we conclude that the finite difference approximation $p_H(t)$, $c_H(t)$ have exactly the convergence properties of the correspondent fully discrete piecewise linear FE approximations.

In what follows, it is obtained an estimate for the spatial discretization error $e_{H,c}(t) = R_H c(t) - c_H(t)$ induced by the spatial discretization introduced for the concentration. To obtain the desired upper bound, we do not follow the split introduced by Wheeler in [45] and largely followed in the finite element and finite differences communities, and considered before for $P_H p_H(t)$, solution of the FEM given by (2.4), (2.5), in Section 2.4.2. Our approach is based on the direct analysis of the error equation for $e_{H,c}(t)$.

We start by remarking that $e_{H,c}(t) \in W_{H,0}$ and it satisfies the following

$$\begin{aligned}(e'_{H,c}(t), w_H)_H = &-((D_H(t)\nabla_H e_{H,c}(t), \nabla_H w_H))_H \\ &+ (((D_H(t) - D^*_H(t))\nabla_H R_H c(t), \nabla_H w_H))_H \\ &+ ((M_H(v_H(t) e_{H,c}(t)), \nabla_H w_H))_H \\ &- ((M_H((v_H(t) - v^*_H(t)) R_H c(t)), \nabla_H w_H))_H \\ &+ \tau_D(w_H) + \tau_v(w_H) + \tau_c(w_H),\end{aligned} \tag{3.9}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, where $D^*_H(t)$ is defined as $D_H(t)$ with p_H replaced by $R_H p$, and $v^*_H(t)$ is defined as $v_H(t)$ with p_H replaced by $R_H p$. In (3.9), $\tau_D(w_H)$, $\tau_v(w_H)$ and $\tau_c(w_H)$ are defined by

$$\tau_D(w_H) = ((D^*_H(t)\nabla_H R_H c(t), \nabla_H w_H))_H + ((\nabla\cdot(D(p(t))\nabla c(t)))_H, w_H)_H, \tag{3.10}$$

$$\tau_v(w_H) = -((M_H(v^*_H(t) R_H c(t)), \nabla_H w_H))_H - ((\nabla\cdot(v(p(t), \nabla p(t)) c(t)))_H, w_H)_H, \tag{3.11}$$

and

$$\tau_c(w_H) = (R_H c'(t), w_H)_H - ((c'(t))_H, w_H)_H. \tag{3.12}$$

Note that $(\nabla\cdot(c(t)v(t)))_H$, $(\nabla\cdot(D(t)\nabla c(t)))_H$ and $(c'(t))_H$ are defined by (2.7) with $f_3(t)$ replaced by $\nabla\cdot(c(t)v(t))$, $\nabla\cdot(D(t)\nabla c(t))$ and $c'(t)$, respectively. To establish an estimate for $\|e_{H,c}(t)\|_H$ we study the functionals $\tau_v(w_H)$, $\tau_D(w_H)$ and $\tau_c(w_H)$ when $w_H \in W_{H,0}$.

Proposition 3.1. *Let us suppose that v_i, $i = 1,2$, are L_v- Lipschitz functions and $p(t) \in H^3(\Omega) \cap H^1_0(\Omega)$, $c(t) \in H^2(\Omega) \cap H^1_0(\Omega)$, $\dfrac{\partial^2 p}{\partial x \partial y}(t) = \dfrac{\partial^2 p}{\partial y \partial x}(t)$ in Ω and $v(t)c(t) \in [H^2(\Omega)]^2$. Then for the functional $\tau_v : W_{H,0} \to \mathbb{R}$, defined by (3.11), there exists a positive constant C, H, t, p and c independent, such that*

$$\begin{aligned}|\tau_v(w_H)| \le C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(&\|v(t)c(t)\|^2_{[H^2(\Delta)]^2} \\ &+ L_v^2\|c(t)\|^2_{C(\Delta)}\|p(t)\|^2_{H^3(\Delta)}\Big)\Big)^{1/2}\|\nabla_H w_H\|_H,\end{aligned} \tag{3.13}$$

for $w_H \in W_{H,0}$, $H \in \Lambda$.

Proof. We start by observing that $\tau_v(w_H)$ admits the representation

$$\tau_v(w_H) = \tau_v^{(1)}(w_H) + \tau_v^{(2)}(w_H),$$

where

$$\tau_v^{(1)}(w_H) = -((\nabla\cdot(v(t)c(t)))_H, w_H)_H - ((M_H(R_H(v(t)c(t))), \nabla_H w_H))_H$$

and

$$\tau_v^{(2)}(w_H) = ((M_H(R_H(v(t)c(t))),\nabla_H w_H))_H - ((M_H(v_H^*(t)R_Hc(t)),\nabla_H w_H))_H.$$

Using Lemma 5.5 of [14], we can state the following estimate for $\tau_v^{(1)}$

$$\begin{aligned}\left|\tau_v^{(1)}(w_H)\right| &\leq C\Bigg(\bigg(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|v_1(t)c(t)\|^2_{H^2(\Delta)}\bigg)^{1/2}\\ &\qquad+\bigg(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|v_2(t)c(t)\|^2_{H^2(\Delta)}\bigg)^{1/2}\Bigg)\|\nabla_H w_H\|_H\\ &\leq C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|v(t)c(t)\|^2_{[H^2(\Delta)]^2}\Big)^{1/2}\|\nabla_H w_H\|_H, \end{aligned} \tag{3.14}$$

where C denotes a positive constant, H, t, p and c independent.

To get an estimate for $\tau_v^{(2)}(w_H)$ we introduce the notation $g_1(x_i,y_j,t) = \frac{\partial p}{\partial x}(x_i,y_j,t) - D_h^* p(x_i,y_j,t)$. We have

$$\begin{aligned}|k_{j+1/2}g_1(x_i,y_j,t)| &= \int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(x_i,y_j,t)|dy\\ &\leq \int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(x_i,y,t)|dy + \int_{y_{j-1/2}}^{y_{j+1/2}}\int_y^{y_j}\left|\frac{\partial g_1}{\partial y}(x_i,s,t)\right|dsdy\\ &\leq \int_{y_{j-1/2}}^{y_{j+1/2}}\Big(k_{j+1/2}\left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right| + |g_1(x_i,y,t)|\Big)dy. \end{aligned} \tag{3.15}$$

Following [30], we consider

$$|g_1(x_i,y,t)| = \frac{1}{h_i+h_{i+1}}\left|w'(\mu_1) - \left(\mu_2(w(1)-w(\mu_1)) + \frac{1}{\mu_2}(w(\mu_1)-w(0))\right)\right| = \frac{1}{h_i+h_{i+1}}|\lambda(w)|,$$

for $w(\xi) = p(x_{i-1}+\xi(h_i+h_{i+1}),y,t)$, $\xi\in[0,1]$, $\mu_1 = \dfrac{h_i}{h_i+h_{i+1}}$, $\mu_2 = \dfrac{h_i}{h_{i+1}}$ and $\lambda : W^{3,1}(0,1)\to\mathbb{R}$ with

$$\lambda(g) = g'(\mu_1) - \left(\mu_2(g(1)-g(\mu_1)) + \frac{1}{\mu_2}(g(\mu_1)-g(0))\right),\ g\in W^{3,1}(0,1).$$

Since $\lambda(g) = 0$ for $g = 1,\xi,\xi^2$, and λ is bounded in $W^{3,1}(0,1)$, by Bramble-Hilbert Lemma, we get

$$|\lambda(g)| \leq C\int_0^1|g'''(\xi)|d\xi,\ g\in W^{3,1}(0,1),$$

which, under the smoothness assumption for p, allows us to conclude the estimate

$$\int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(x_i,y,t)|dy \leq C(h_i+h_{i+1})\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i-1}}^{x_{i+1}}\left|\frac{\partial^3 p}{\partial x^3}(x,y,t)\right|dxdy.$$

Analogously, by Bramble-Hilbert Lemma, we obtain

$$\int_{y_{j-1/2}}^{y_{j+1/2}} \left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right| dy \le C \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1}}^{x_{i+1}} \left|\frac{\partial^3 p}{\partial x^2 \partial y}(x,y,t)\right| dxdy,$$

for a positive constant C, H, t and p independent, leading to

$$\begin{aligned} |k_{j+1/2} g_1(x_i,y_j,t)| \le C\Big(k_{j+1/2} \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1}}^{x_{i+1}} \left|\frac{\partial^3 p}{\partial x^2 \partial y}(x,y,t)\right| dxdy \\ + (h_i+h_{i+1}) \int_{y_{j-1/2}}^{y_{j+1/2}} \int_{x_{i-1}}^{x_{i+1}} \left|\frac{\partial^3 p}{\partial x^3}(x,y,t)\right| dxdy\Big). \end{aligned} \tag{3.16}$$

For $g_2(x_i,y_j,t) = \frac{\partial p}{\partial y}(x_i,y_j,t) - D_k^* p(x_i,y_j,t)$ we can establish an estimate analogous to (3.16).

Finally, using the Lipschitz assumption for v, we have

$$\begin{aligned} |\tau_v^{(2)}(w_H)| \le L_v \Bigg[\|D_{-x} w_H\|_H \left(\sum_{i=1}^{N-1} \sum_{j=1}^{M-1} h_{i+1/2} k_{j+1/2} |g_1(x_i,y_j,t)|^2 |c(x_i,y_j,t)|^2 \right)^{1/2} \\ + \|D_{-y} w_H\|_H \left(\sum_{i=1}^{N-1} \sum_{j=1}^{M-1} k_{j+1/2} h_{i+1/2} |g_2(x_i,y_j,t)|^2 |c(x_i,y_j,t)|^2 \right)^{1/2} \Bigg], \end{aligned}$$

and from (3.16) we conclude

$$|\tau_v^{(2)}(w_H)| \le C L_v \Big(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \|c(t)\|^2_{C(\Delta)} \|p(t)\|^2_{H^3(\Delta)} \Big)^{1/2} \|\nabla_H w_H\|_H, \tag{3.17}$$

for a positive constant C, H, t, p and c independent. Considering (3.17) and (3.14) we get (3.13). □

Proposition 3.2. *If d_i, $i=1,2$, are L_D- Lipschitz functions, $p(t) \in H^2(\Omega)$, $c(t) \in H^3(\Omega)$, $d_i(p(t)) \in L^\infty(\Omega), i=1,2$, and $D(t)\nabla c(t) \in [H^2(\Omega)]^2$ then, for the functional $\tau_D : W_{H,0} \to \mathbb{R}$ defined by (3.10), there exists a positive constant C, H, t, p and c independent, such that*

$$\begin{aligned} |\tau_D(w_H)| \le C\Big(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \big(L_D^2 \|p(t)\|^2_{H^2(\Delta)} \|c(t)\|^2_{C^1(\Delta)} \\ + \|D(p(t))\|^2_{\infty, L^\infty(\Delta)} \|c(t)\|^2_{H^3(\Delta)} + \|D(p(t))\nabla c(t)\|^2_{[H^2(\Delta)]^2} \big) \Big)^{1/2} \|\nabla_H w_H\|_H, \end{aligned}$$

for $w_H \in W_{H,0}$, $H \in \Lambda$, where $\|D(p(t))\|_{\infty, L^\infty(\Delta)} = \max_{i=1,2} \|d_i(p(t))\|_{L^\infty(\Delta)}$.

Proof. We start observing that the functional (3.10) admits the representation

$$\tau_D(w_H) = \sum_{i=1}^{2} \tau_D^{(i)}(w_H), w_H \in W_{H,0}, \tag{3.18}$$

with

$$\tau_D^{(1)}(w_H) = (((D_H^*(t) - \tilde{D}_H(t)) \nabla_H R_H c(t), \nabla_H w_H))_H,$$

where the diagonal entries of $\tilde{D}_H(t)$ at (x_i,y_j) are given by $d_1(p(x_{i-1/2},y_j,t))$, $d_2(p(x_i,y_{j-1/2},t))$, and

$$\tau_D^{(2)}(w_H) = ((\tilde{D}_H(t)\nabla_H R_H c(t), \nabla_H w_H))_H + ((\nabla\cdot(D(p(t))\nabla c(t)))_H, w_H)_H.$$

We start by noting that $\tau_D^{(1)}(w_H)$ can be written in the following equivalent form

$$\begin{aligned}\tau_D^{(1)}(w_H) &= (d_1(M_h R_H p(t))D_{-x}R_H c(t), D_{-x}w_H)_{H,x} - (d_1(p(M_h(t)))D_{-x}R_H c(t), D_{-x}w_H)_{H,x}\\ &\quad + (d_2(M_k R_H p(t))D_{-y}R_H c(t), D_{-y}w_H)_{H,y} - (d_2(p(M_k(t)))D_{-y}R_H c(t), D_{-y}w_H)_{H,y}\\ &:= \tau_x(w_H) + \tau_y(w_H).\end{aligned}$$

First, we estimate $\tau_x(w_H)$. Let us introduce

$$g_1(x_i,y_j,t) = \frac{1}{2}\left(p(x_{i-1},y_j,t) + p(x_i,y_j,t)\right) - p(x_{i-1/2},y_j,t),$$

satisfying (as in (3.15))

$$k_{j+1/2}|g_1(x_i,y_j,t)| \le \int_{y_{j-1/2}}^{y_{j+1/2}} |g_1(x_i,y,t)|dy + k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}} \left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right| dy.$$

Note that g_1 can be written as follows

$$g_1(x_i,y,t) = \frac{w(0)+w(1)}{2} - w\left(\frac{1}{2}\right) = \lambda(w),$$

where $w(\xi) = p(x_{i-1}+h_i\xi,y,t)$, $\xi\in[0,1]$, and $\lambda : W^{2,1}(0,1)\to\mathbb{R}$ with

$$\lambda(g) = \frac{g(0)+g(1)}{2} - g\left(\frac{1}{2}\right),\ g\in W^{2,1}(0,1).$$

Then, an estimate for g_1 is obtained estimating $\lambda(w)$. The functional λ is bounded in $W^{2,1}(0,1)$ and vanishes for $g = 1,\xi$. By Bramble-Hilbert Lemma, there exists a positive constant C, such that

$$|\lambda(g)| \le C\int_0^1 |g''(\xi)|d\xi,\ g\in W^{2,1}(0,1).$$

Consequently,

$$|g_1(x_i,y,t)| = |\lambda(w)| \le Ch_i\int_{x_{i-1}}^{x_i}\left|\frac{\partial^2 p}{\partial x^2}(x,y,t)\right| dx.$$

Analogously, we get

$$\left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right| \le C\int_{x_{i-1}}^{x_i}\left|\frac{\partial^2 p}{\partial x\partial y}(x,y,t)\right| dxdy,$$

with C a positive constant. Then we obtain

$$\begin{aligned}|k_{j+1/2}g_1(x_i,y_j,t)| &\leq \int_{y_{j-1/2}}^{y_{j+1/2}} |g_1(x_i,y,t)|dy + k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}} \left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right| dy \\ &\leq C\Big(h_i \int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i-1}}^{x_{i+1}} \left|\frac{\partial^2 p}{\partial x^2}(x,y,t)\right| dxdy + k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}}\int_{x_{i-1}}^{x_i} \left|\frac{\partial^2 p}{\partial x \partial y}(x,y,t)\right| dxdy\Big).\end{aligned} \tag{3.19}$$

Since we are assuming that d_i, $i = 1,2$, are L_D-Lipschitz functions,

$$\begin{aligned}&k_{j+1/2}\left|d_1\left(M_h(R_H p(x_i,y_j,t))\right) - d_1\left(p(M_h(x_i,y_j,t))\right)\right| \\ &\qquad \leq L_D k_{j+1/2}|g_1(x_i,y_j,t)|,\end{aligned}$$

and taking into account the estimates (3.19), we establish

$$\begin{aligned}|\tau_x(w_H)| &\leq L_D \sum_{i=1}^{N}\sum_{j=1}^{M-1}\left(h_i\left(\int_{y_{j-1/2}}^{y_{j+1/2}}|g_1(x_i,y,t)|\,dy + k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}}\left|\frac{\partial g_1}{\partial y}(x_i,y,t)\right|dy\right)\right. \\ &\qquad \left. \times |D_{-x}c(x_i,y_j,t)||D_{-x}w_H(x_i,y_j)|\right) \\ &\leq CL_D\left(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|c(t)\|^2_{C^1(\Delta)}\|p(t)\|^2_{H^2(\Delta)}\right)^{1/2}\|D_{-x}w_H\|_H,\end{aligned}$$

for C a positive constant, H, t, p and c independent. Adapting the followed procedures, an estimate for $\tau_y(w_H)$ can be easily deduced, and we obtain

$$|\tau_D^{(1)}(w_H)| \leq CL_D\left(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|c(t)\|^2_{C^1(\Delta)}\|p(t)\|^2_{H^2(\Delta)}\right)^{1/2}\|\nabla_H w_H\|_H. \tag{3.20}$$

To estimate $\tau_D^{(2)}(w_H)$, directly from the proof of Lemma 5.1 of [14], we get

$$\begin{aligned}|\tau_D^{(2)}(w_H)| \leq C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(&\|D(p(t))\|^2_{\infty,L^\infty(\Delta)}\|c(t)\|^2_{H^3(\Delta)} \\ &+\|D(p(t))\nabla c(t)\|^2_{[H^2(\Delta)]^2}\Big)\Big)^{1/2}\|\nabla_H w_H\|_H,\end{aligned} \tag{3.21}$$

where C is a positive constant, H, t, p and c independent.

To conclude the proof, it is enough to consider (3.20) and (3.21) in (3.18). □

Proposition 3.3. *If $c'(t)\in H^2(\Omega)$ then, for the functional $\tau_c : W_{H,0}\to\mathbb{R}$ defined by (3.12), there exists a positive constant C, H, t, p and c independent, such that*

$$|\tau_c(w_H)| \leq C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|c'(t)\|^2_{H^2(\Delta)}\Big)^{1/2}\|\nabla_H w_H\|_H,$$

for $w_H\in W_{H,0}$, $H\in\Lambda$.

Proof. This result follows directly from Lemma 5.7 of [14]. □

With the previous three propositions we have the conditions to state the main result of this chapter, Theorem 3.1, where an upper bound for $\|e_{H,c}(t)\|_H$ is established. Here and in what follows, in what concerns the time regularity of p and/or T we implicitly assume the needed smoothness for the results.

Theorem 3.1. *Let us suppose the following:*

(i) the sequence of grids $\overline{\Omega}_H$, $H \in \Lambda$, satisfies (2.35) for $H_{\max}$ small enough;

(ii) $p(t) \in H^3(\Omega) \cap H_0^1(\Omega)$, where p is solution of the IBVP (1.1), (1.4), (1.7);

(iii) the solution c of the IBVP (1.14), (1.6), (1.9) belongs to $L^2(0,T_f,H^3(\Omega) \cap H_0^1(\Omega)) \cap H^1(0,T_f,H^2(\Omega))$ and $R_H c \in C^1((0,T_f],W_{H,0})$;

(iv) the solution c_H of the initial value problem (3.3), (3.4) belongs to $C^1((0,T_f],W_{H,0}) \cap C([0,T_f],W_{H,0})$;

(v) v_i satisfies $|v_i(z_1,z_2)| \leq C_v(|z_1|+|z_2|)$, $\forall z_1,z_2 \in \mathbb{R}$, $i=1,2$;

(vi) $d_i \geq d_0 > 0$ in $\mathbb{R}$, $i=1,2$;

(vii) the assumptions of Propositions 3.1 and 3.2 hold.

Then, there exist a positive constant C, H, t, p and c independent, such that for the spatial error $e_{H,c}(t) = R_H c(t) - c_H(t)$ the following holds

$$\begin{aligned}
&\|e_{H,c}(t)\|_H^2 + 2(d_0 - 6\varepsilon^2)\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\|\nabla_H e_{H,c}(s)\|_H^2 ds \leq e^{\int_0^t g_H(p_H(\mu))d\mu}\|e_{H,c}(0)\|_H^2\\
&\quad + \frac{1}{\varepsilon^2}L_D^2\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\|e_{H,p}(s)\|_H^2\|\nabla_H R_H c(s)\|_\infty^2 ds\\
&\quad + \frac{4}{\varepsilon^2}L_v^2\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\Big(\|e_{H,p}(s)\|_H^2 + 2C_m\|\nabla_H e_{H,p}(s)\|_H^2\Big)\|R_H c(s)\|_\infty^2 ds\\
&\quad + \int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\tau_{c,H}(s)ds,
\end{aligned} \tag{3.22}$$

for $t \in [0,T_f]$, $H \in \Lambda$ and $H_{\max}$ small enough. In (3.22), $\varepsilon \neq 0$ is an arbitrary constant,

$$\begin{aligned}
\tau_{c,H}(t) = \frac{C}{2\varepsilon^2}\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\Big(&\|D(t)\|_{\infty,L^\infty(\Delta)}^2\|c(t)\|_{H^3(\Delta)}^2 + \|D(t)\nabla c(t)\|_{[H^2(\Delta)]^2}^2 + \|v(t)c(t)\|_{[H^2(\Delta)]^2}^2\\
&+ \|c(t)\|_{C^1(\Delta)}^2\|p(t)\|_{H^3(\Delta)}^2 + \|c'(t)\|_{H^2(\Delta)}^2\Big),
\end{aligned} \tag{3.23}$$

and

$$g_H(p_H(t)) = \frac{2}{\varepsilon^2}C_v^2\big(\|p_H(t)\|_\infty^2 + \|\nabla_H p_H(t)\|_\infty^2\big).$$

Proof. Note that, since $d_i,\ i=1,2$, are L_D- Lipschitz functions, then

$$\begin{aligned}
&|(((D_H(t) - D_H^*(t))\nabla_H R_H c(t), \nabla_H w_H))_H|\\
&\qquad \leq \sqrt{2}L_D\|e_{H,p}(t)\|_H\|\nabla_H R_H c(t)\|_\infty\|\nabla_H w_H\|_H.
\end{aligned} \tag{3.24}$$

Also,

$$|D_h^* p_H(x_i, y_j, t)| \leq \|D_{-x} p_H(t)\|_\infty$$

and, of course, $|D_k^* p_H(x_i, y_j, t)| \leq \|D_{-y} p_H(t)\|_\infty$. Considering that v satisfies

$$|v_i(z_1, z_2)| \leq C_v(|z_1| + |z_2|), \forall z_1, z_2 \in \mathbb{R},\ i = 1, 2,$$

we have

$$|((M_H(v_H(t) e_{H,c}(t)), \nabla_H w_H))_H| \leq \sqrt{2} C_v ||e_{H,c}(t)||_H \left(\|p_H(t)\|_\infty + \|\nabla_H p_H(t)\|_\infty\right) \|\nabla_H w_H\|_H. \quad (3.25)$$

To estimate $|-((M_H((v_H(t) - v_H^*(t)) R_H c(t)), \nabla_H w_H))_H|$, we assume that the condition (2.35) holds for the sequence of grids $\overline{\Omega}_H$, $H \in \Lambda$. For $H \in \Lambda$, with $H_{\max}$ small enough, for $i = 1, \ldots, N-1$, $j = 1, \ldots, M-1$, we have

$$h_{i+1/2} \frac{h_i^2}{(h_{i+1} + h_i)^2} = \frac{h_i^2 h_{i+1}}{2 h_{i+1}(h_{i+1} + h_i)} \leq \frac{C_m}{2} h_{i+1} \text{ and } h_{i+1/2} \frac{h_{i+1}^2}{(h_{i+1} + h_i)^2} \leq \frac{C_m}{2} h_i.$$

Taking also into account that $v_i,\ i = 1, 2$, are L_v- Lipschitz functions, we obtain

$$\begin{aligned} &|-((M_H((v_H(t) - v_H^*(t)) R_H c(t)), \nabla_H w_H))_H| \\ &\qquad \leq 2 L_v \|R_H c(t)\|_\infty \left(\|e_{H,p}(t)\|_H + \sqrt{2Cm} \|\nabla_H e_{H,p}(t)\|_H\right) \|\nabla_H w_H\|_H, \end{aligned} \quad (3.26)$$

for $w_H \in W_{H,0}$, $H \in \Lambda$ with $H_{\max}$ small enough.

Taking in (3.9), $w_H = e_{H,c}(t)$, considering (3.24), (3.25), (3.26) we have

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} \|e_{H,c}(t)\|_H^2 + d_0 \|\nabla_H e_{H,c}(t)\|_H^2 \leq\ & \sqrt{2} L_D \|e_{H,p}(t)\|_H \|\nabla_H R_H c(t)\|_\infty \|\nabla_H e_{H,c}(t)\|_H \\ & + \sqrt{2} C_v \left(\|p_H(t)\|_\infty + \|\nabla_H p_H(t)\|_\infty\right) \|e_{H,c}(t)\|_H \|\nabla_H e_{H,c}(t)\|_H \\ & + 2 L_v \left(\|e_{H,p}(t)\|_H + \sqrt{2C_m} \|\nabla_H e_{H,p}(t)\|_H\right) \|R_H c(t)\|_\infty \|\nabla_H e_{H,c}(t)\|_H \\ & + |\tau_D(e_{H,c}(t))| + |\tau_v(e_{H,c}(t))| + |\tau_c(e_{H,c}(t))|. \end{aligned} \quad (3.27)$$

From (3.27), considering Propositions 3.1-3.3, we obtain

$$\begin{aligned} \frac{d}{dt} \|e_{H,c}(t)\|_H^2 + 2(d_0 - 6\varepsilon^2) \|\nabla_H e_{H,c}(t)\|_H^2 \leq\ & \frac{1}{\varepsilon^2} L_D^2 \|e_{H,p}(t)\|_H^2 \|\nabla_H R_H c(t)\|_\infty^2 \\ & + \frac{2}{\varepsilon^2} C_v^2 \left(\|p_H(t)\|_\infty^2 + \|\nabla_H p_H(t)\|_\infty^2\right) \|e_{H,c}(t)\|_H^2 \\ & + \frac{4}{\varepsilon^2} L_v^2 \left(\|e_{H,p}(t)\|_H^2 + 2C_m \|\nabla_H e_{H,p}(t)\|_H^2\right) \|R_H c(t)\|_\infty^2 + \tau_{c,H}(t), \end{aligned} \quad (3.28)$$

with $\tau_{c,H}(t)$ given by (3.23) and $\varepsilon \neq 0$ an arbitrary constant.

Multiplying everything by $e^{-\int_0^t g_H(p_H(s))ds}$, inequality (3.28) leads to

$$\frac{d}{dt}\Bigg(e^{-\int_0^t g_H(p_H(s))ds}\|e_{H,c}(t)\|_H^2+2(d_0-6\varepsilon^2)\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\|\nabla_H e_{H,c}(s)\|_H^2 ds$$
$$-\frac{1}{\varepsilon^2}L_D^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\|e_{H,p}(s)\|_H^2\|\nabla_H R_H c(s)\|_\infty^2 ds$$
$$-\frac{4}{\varepsilon^2}L_v^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\left(\|e_{H,p}(s)\|_H^2+2C_m\|\nabla_H e_{H,p}(s)\|_H^2\right)\|R_H c(s)\|_\infty^2 ds$$
$$-\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\tau_{c,H}(s)ds\Bigg)\leq 0,\ t\in(0,T_f],$$

that allows us to obtain

$$e^{-\int_0^t g_H(p_H(s))ds}\|e_{H,c}(t)\|_H^2+2(d_0-6\varepsilon^2)\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\|\nabla_H e_{H,c}(s)\|_H^2 ds$$
$$-\frac{1}{\varepsilon^2}L_D^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\|e_{H,p}(s)\|_H^2\|\nabla_H R_H c(s)\|_\infty^2 ds$$
$$-\frac{4}{\varepsilon^2}L_v^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\left(\|e_{H,p}(s)\|_H^2+2C_m\|\nabla_H e_{H,p}(s)\|_H^2\right)\|R_H c(s)\|_\infty^2 ds$$
$$-\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\tau_{c,H}(s)ds\leq\|e_{H,c}(0)\|_H^2,\ t\in[0,T_f].$$

Finally, from the last inequality we easily get (3.22). □

In Theorem 3.1, we fix $\varepsilon\neq 0$ such that $d_0-6\varepsilon^2>0$. Note that Corollary 2.2 gives us the uniform boundness of $g_H(p_H(t))$, for $H\in\Lambda$, for $H_{\max}$ small enough. Also, from Theorem 2.3, we have an upper bound for $\|e_{H,p}(t)\|_H$, $\|\nabla_H e_{H,p}(t)\|_H$. From these observations together with Theorem 3.1 we conclude the following result:

Corollary 3.1. *Under the assumptions of Theorems 2.3 and 3.1, there exists a positive constant C, H and t independent, such that*

$$\|e_{H,c}(t)\|_H^2+\int_0^t\|\nabla_H e_{H,c}(s)\|_H^2 ds\leq CH_{\max}^4,\ t\in[0,T_f],$$

for $H\in\Lambda$ and $H_{\max}$ small enough.

3.4 Numerical Results

3.4.1 An Implicit Scheme

In this section, we include some numerical experiments. We start presenting a time discretization method for the coupled wave-concentration problem (2.10), (2.11), (2.12), (3.5), (3.6), (3.7). Remarking that in this section we are focused on the spatial discretization, the wave equation (1.1) is solved by the implicit first-order method studied in the Section 2.5.1. For the concentration equation (1.14), note that all the coefficient functions are independent on the concentration, so our parabolic problem (dependent on the wave IBVP) can also be solved by a first-order implicit method. For the temporal domain $[0,T_f]$, we define the uniform time grid $\{t_n = n\Delta t, n = 0,\ldots,M_t\}$, with $t_{M_t} = T_f$, where Δt is the time step. Let us denote by p_H^n and c_H^n the numerical approximations for $p_H(t_n)$ and $c_H(t_n)$, respectively, defined by the following implicit method

$$a_H \frac{p_H^{n+1} - 2p_H^n + p_H^{n-1}}{\Delta t^2} + b_H \frac{p_H^{n+1} - p_H^n}{\Delta t} = \nabla_H^* \cdot (E_H \nabla_H p_H^{n+1}) + f_{3,H}^{n+1} \text{ in } \Omega_H, \tag{3.29}$$

for $n = 1,\ldots,M_t - 1$,

$$\frac{c_H^{n+1} - c_H^n}{\Delta t} + \nabla_{c,H} \cdot (c_H^{n+1} v_H^{n+1}) = \nabla_H^* \cdot (D_H^{n+1} \nabla_H c_H^{n+1}) + f_{1,H}^{n+1} \text{ in } \Omega_H, \tag{3.30}$$

for $n = 0,\ldots,M_t - 1$, and with the initial conditions

$$\frac{p_H^1 - p_H^0}{\Delta t} = R_H p_{v,0},\ p_H^0 = R_H p_0,\ c_H^0 = R_H c_0 \text{ in } \Omega_H, \tag{3.31}$$

and boundary conditions

$$c_H^n = 0,\ p_H^n = 0 \text{ on } \partial\Omega_H,\ n = 0,\ldots,M_t.$$

Note that the acoustic pressure approximation in (3.30), in v_H and D_H, is evaluated at time level t_{n+1}. This strategy allows us to solve the coupled problem in a sequential way. From time level t_n to time level t_{n+1} we first solve equation (3.29) (or we use (3.31) if $n = 0$) to obtain p_H^{n+1} and then we solve equation (3.30) to obtain c_H^{n+1}. Let us now define the errors

$$e_{H,p}^n = R_H p(t_n) - p_H^n \quad \text{and} \quad e_{H,c}^n = R_H c(t_n) - c_H^n.$$

In the next section we present a numerical experiment that intends to illustrate the theorical space convergence rate established in Theorems 2.3 and 3.1, and Corollaries 2.1 and 3.1. To finish this chapter, in the Section 3.4.3 we present a toy model for the drug transport enhanced by ultrasound obtained by simplifying the system of partial differential equations studied here. Numerical experiments illustrating the effects of the parameters of the model are also included.

3.4.2 Convergence Rate Tests

In what follows, we consider an example of the coupled problem (1.1), (1.4), (1.7), (1.14), (1.6), (1.9). We fix the following coefficient functions for the wave equation $a(x,y) = y^2$, $b(x,y) = x+y$, $e_1(x,y) = xy$, and $e_2(x,y) = x$, while for the parabolic equation we set $v(p,\nabla p) = (1+p+\frac{\partial p}{\partial x}, 2p+\frac{\partial p}{\partial y})$, $d_1(p) = 5+p$, and $d_2(p) = 10+p$. In addition, the initial conditions of the coupled problem and the functions f_3 and f_1 are defined such that the exact solution of the coupled system is given by

$$p(x,y,t) = e^t \sin(2\pi y)(1-\cos(2\pi x)),$$
$$c(x,y,t) = e^t \sin(\pi(2x-1))\sin(\pi(2y-1)).$$

Note that the smoothness conditions imposed in Theorem 3.1 hold, however the assumption that the coefficients functions a, b and e_i, $i=1,2$, have a positive lower bound in $\overline{\Omega}$ is not verified. Nevertheless, we observe numerically that the obtained convergence rate is two.

We take $T_f = 0.1$ and the time step $\Delta t =$1e-05. This time step is small enough so that the influence of the time discretization on the numerical error is negligible. To measure the numerical rate of convergence we define the error

$$E_{H,p} = \max_{n=1,\ldots,M_t} \|D_{-t}e^n_{H,p}\|_H + \|\nabla_H e^n_{H,p}\|_H,$$

which is associated with the discretization of the wave equation (1.1), and the error

$$E_{H,c} = \max_{n=1,\ldots,M_t} \|e^n_{H,c}\|_H + \|\nabla_H e^n_{H,c}\|_H,$$

which is associated with the discretization of the parabolic equation (1.14). For the simulation the domain Ω is first divided into $N\times M$ nonuniform intervals. Then, we subdivide each interval by considering the midpoint of each interval to obtain two intervals.

In Table 3.1 we present the errors $E_{H,p}$ and $E_{H,c}$ for several mesh sizes, from $N\times M = 12\times 14$ to $N\times M = 192\times 224$.

$H_{\max}$	$E_{H,p}$	$E_{H,c}$
9.921e-02	2.012e-01	1.255e-01
4.960e-02	5.061e-02	3.182e-02
2.480e-02	1.266e-02	7.983e-03
1.240e-02	3.166e-03	1.998e-03
6.201e-03	7.927e-04	4.996e-04

Table 3.1 The errors $E_{H,p}$ and $E_{H,c}$ on successively refined meshes for the coupled wave-parabolic problem.

Using the data from Table 3.1, we plot in Figure 3.1 the $\log(E_{H,p})$ and $\log(E_{H,c})$ versus $\log(H_{\max})$. Assuming that the errors $E_{H,p}$ and $E_{H,c}$ are proportional to $H^r_{\max}$, for some $r\in\mathbb{R}$, the convergence rate can be estimated by the slope of the best fitting least square line. The obtained estimated values are 1.9974 for $E_{H,p}$ and 1.9938 for $E_{H,c}$ that confirm the theoretical convergence rates. Plots illustrating the numerical solutions and the numerical errors are given in Figure 3.2.

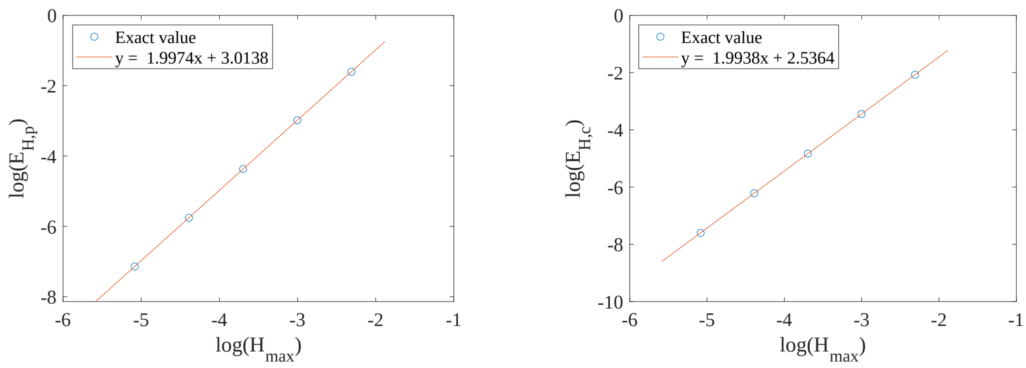


Fig. 3.1 From left to right: Log-log plots of $E_{H,p}$ and $E_{H,c}$ versus $H_{\max}$. The best fitting least square line is shown as a solid line.

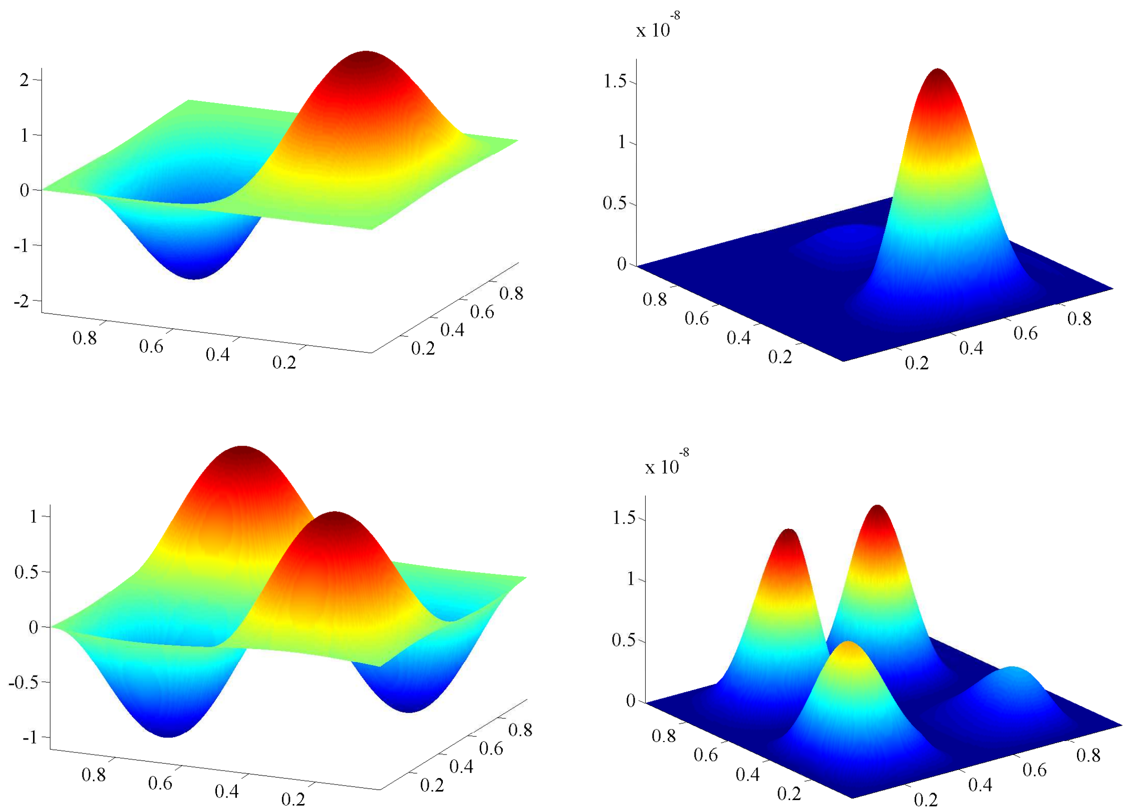


Fig. 3.2 From left to right: Numerical approximation and square error of p_H^n (first row) and c_H^n (second row) at the final simulation time $T_f = 0.1$ and at the finer mesh.

3.4.3 Application to Ultrasound Enhanced Drug Transport

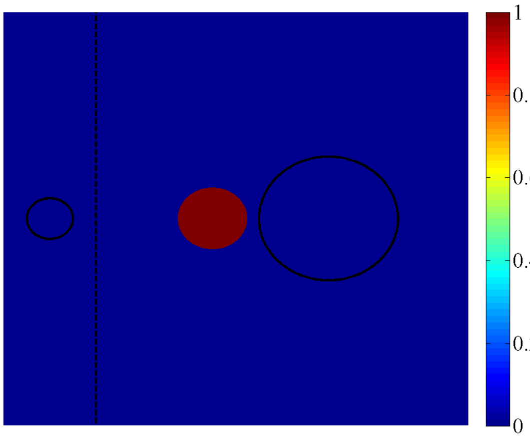
To finish this chapter we present some numerical results that intend to illustrate the use of the mathematical problem studied within this chapter in the mathematical modeling of the drug transport enhanced by ultrasound. To simplify we assume that we have a target tissue with constant density where we have an initial drug distribution. If we neglect the attenuation effects, then the acoustic pressure p is defined by the wave equation

$$\frac{\partial^2 p}{\partial t^2} = c_p^2 \Delta p, \tag{3.32}$$

considered here to model the ultrasound propagation. Our aim is to observe the drug distribution in time and space when the transport is enhanced by the acoustic pressure. The drug concentration c is defined by the convection-diffusion equation

$$\frac{\partial c}{\partial t} + \nabla \cdot (vc) = \nabla \cdot (D_m \nabla c), \tag{3.33}$$

where D_m is the diffusion coefficient, and v is the convective field generated by the ultrasound wave. Note that both D_m and v depend on the acoustic pressure p. This dependence will be specified later. The physical situation that we are interested in is described in Figure 3.3 (on the left), where we represent a tumor in a healthy tissue, the initial distribution of the drug and the localization of the ultrasound source. In the Figure 3.3 (on the right) we present the time profile of the intensity of the acoustic pressure source with expression $100e^{-(1.2t-3)^2} sin(10\pi t)$, with $t \in [0,5]$.



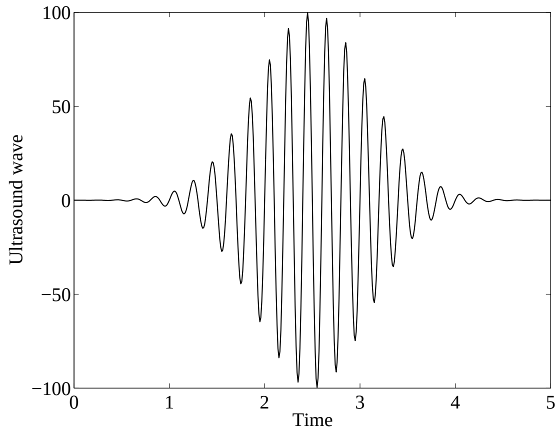


Fig. 3.3 On the left: Initial drug concentration and simulation scenario. The tumor tissue is represented by the black circle on the right and the ultrasound source is represented by the black circle on the left. On the right: time profile of the ultrasound source wave.

Note that the system (3.32), (3.33) can be seen a particular case of the coupled problem studied in this chapter. To finish its description, we explain how the convective velocity and the diffusion coefficient depend on the ultrasound wave. We consider that the convective velocity field is radial around the wave source origin (x_0, y_0) and has magnitude proportional to the acoustic pressure intensity, i.e,

$$v(x,y,t) = C_1 p(x,y,t)^2 \left(\frac{(x-x_0)}{\sqrt{(x-x_0)^2+(y-y_0)^2}}, \frac{(y-y_0)}{\sqrt{(x-x_0)^2+(y-y_0)^2}} \right), \quad \text{with } C_1 \geq 0.$$

Moreover, to model the effects of ultrasound waves on cell membrane permeabilization, we consider that the drug molecular diffusion in the tumor tissue, denoted by D_{m,T_u} (T_u represents the tumor domain), is a scalar that depends on the pressure wave intensity trough the following relation for

$(x,y) \in T_u$

$$D_{m,T_u}(x,y,t) = \begin{cases} D_{m,c} & \text{if } \max\limits_{(x,y)\in T_u} (p(x,y,t)^2) \leq C_2 \\ D_{m,p} & \text{if } \max\limits_{(x,y)\in T_u} (p(x,y,t)^2) > C_2 \end{cases}$$

with C_2 a positive constant ($D_{m,p} > D_{m,c}$). This means that the drug diffusion coefficient increases when the acoustic pressure intensity is greater than a certain threshold. The diffusion and acoustic parameters used in the following simulation were: $c_p = 2$, $D_m =$ 1e-03, $D_{m,p} =$ 1e-04, $D_{m,c} =$ 1e-06, $C_1 =$ 2e-04, and $C_2 = 20$. We remark that for simplicity units are omitted.

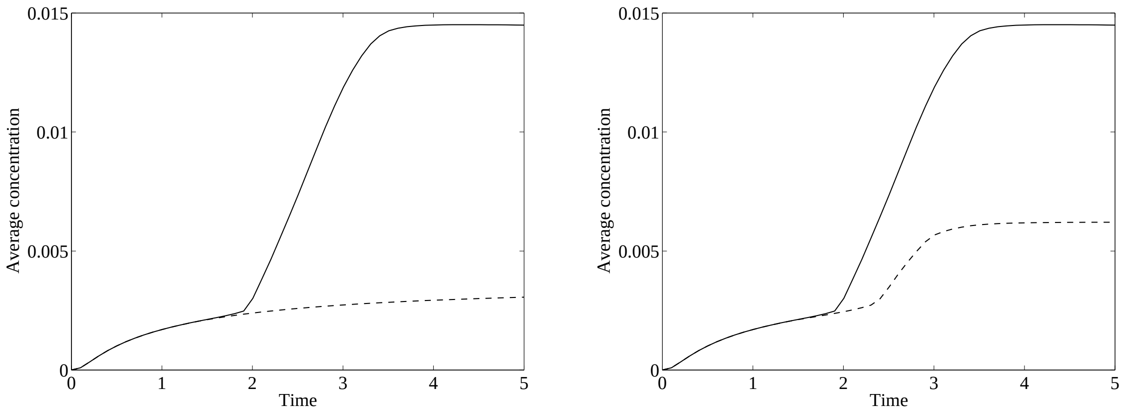


Fig. 3.4 Time evolution of the average concentration of drug in the tumor tissue. On the left: Passive diffusion (dash line) and ultrasound enhanced (solid line). On the right: Ultrasound enhanced with maximum wave amplitude equal 100 (solid line) and equal 50 (dash line).

In Figure 3.4, we present some results of our computational experiments. On the left we consider two simulation scenarios: drug transport under the influence of the ultrasound wave, and drug transport only by passive diffusion, i.e., without the application of the ultrasound wave. As can be observed when ultrasound is applied the average concentration of drug inside the tumor tissue at the final time is considerably higher than the one obtained only with passive diffusion. We can also observe that the higher flux of drug to the tumor tissue can be related with the ultrasound profile, once can be observed that between time equal 2 and time equal to 3.5 the flux of drug is larger, and it coincides with the higher intensity of the generated ultrasound wave (see Figure 3.3). The sensitivity analysis of the model to the ultrasound wave is shown in the right plot of Figure 3.4. In particular, we consider the same parameters as before but where the maximum wave amplitude is reduced from 100 to 50. As expected the final average concentration of drug in the tumor tissue is lower. The lower ultrasound amplitude also explains why the high flux of drug occurs during a shorter period of time. In Figure 3.5, we show snapshots of drug concentration in our domain at different values of time. We present the case of passive diffusion (right column) and passive diffusion plus ultrasound (left column), in order to observe the influence of the ultrasound wave. The effect of the convective transport on the concentration plume is clear on the images in the left column. We remark that in the tumor domain it is represented the average concentration, allowing a better visualization. Lastly, in Figure 3.6 the pressure wave and the velocity field are shown. We refer that a time step equal 1e-02 and a uniform mesh with $H_{\max} =$ 3.125e-03 were used. To minimize boundary effects the domain was enlarged.

We remark that this is a simple illustration, since the main aim of this chapter is the analysis of the convergence of the numerical coupled method.

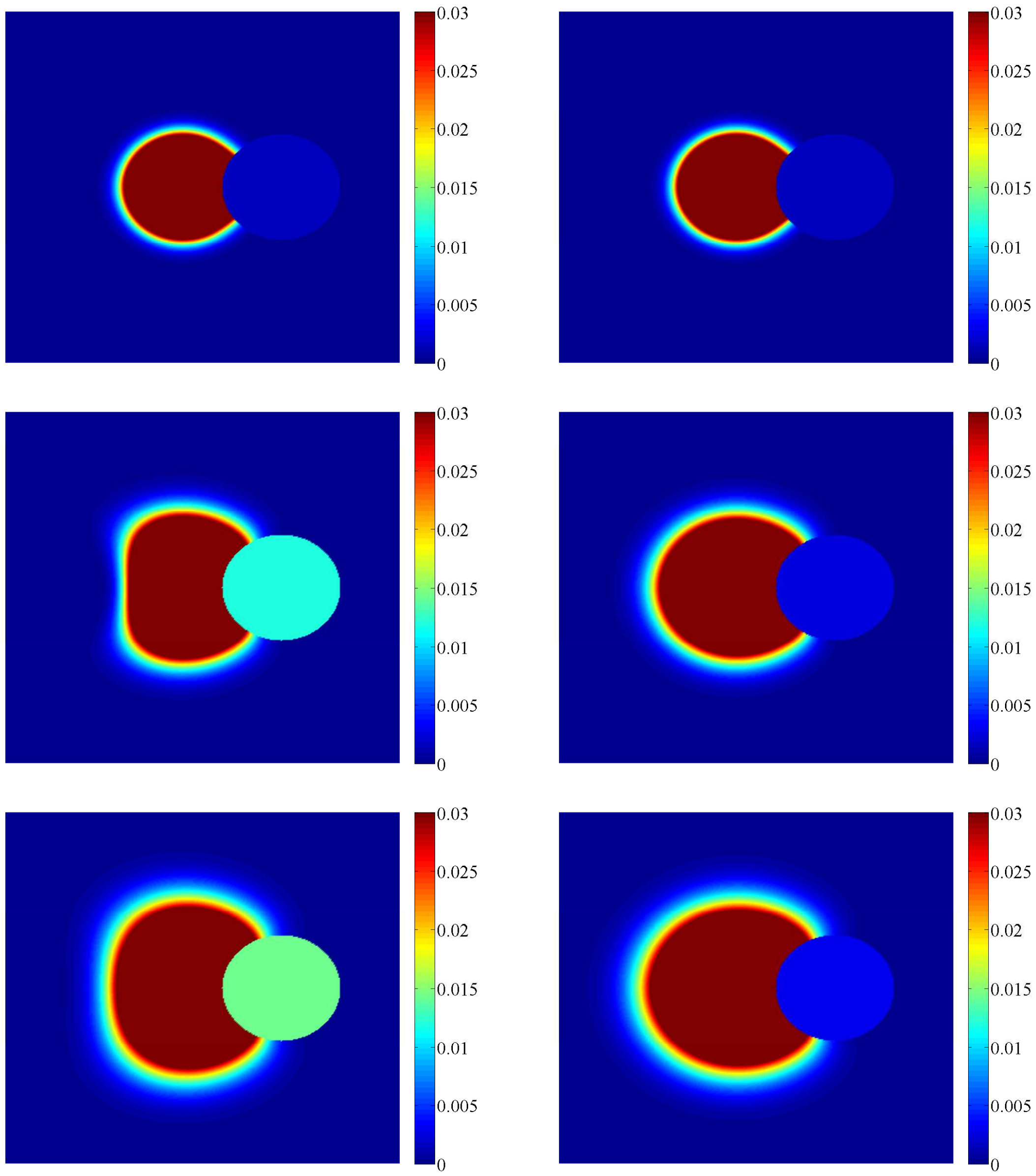


Fig. 3.5 From top to bottom: Drug concentration at time equal 1, 3, and final time 5. From left to right: Transport by diffusion and ultrasound, and transport by diffusion only.

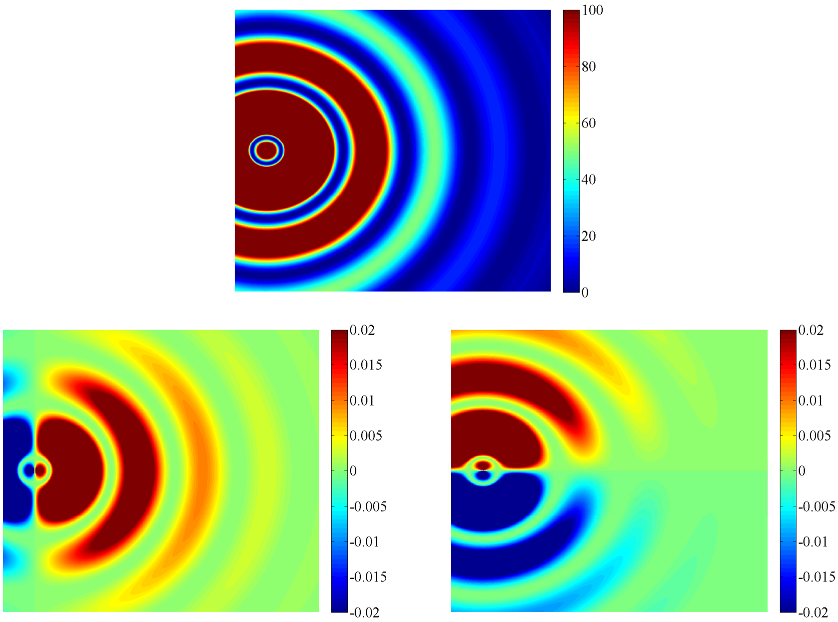


Fig. 3.6 Ultrasound intensity p^2 (first row) and velocity components x and y (second row) at time level equal 3.

3.5 Conclusions

In this chapter, we proposed a numerical method for a hyperbolic-parabolic IBVP that can be used, for example, to describe drug transport enhanced by ultrasound. This model is a simplification of our main problem. The devised numerical scheme is based on piecewise linear finite element spaces, and it can also be seen as a finite difference method defined on nonuniform rectangular partitions of the spatial domain.

The main results of this chapter are Theorem 3.1 and Corollary 3.1, where we proved that the considered numerical approximation of the solution of the parabolic IBVP (1.14), (1.6), (1.9) is second-order accurate with respect to a discrete L^2- norm. The proof of this theorem depends on Theorem 2.3 where we established that the numerical approximation for the acoustic pressure is second-order accurate with respect to a H^1- norm. These results were obtained assuming that $p(t),\ c(t) \in H^3(\Omega)$. It should be highlighted that our results were obtained imposing weaker smoothness conditions on the solution of the coupled IBVP (1.1), (1.14), (1.4), (1.6), (1.7), (1.9) than those usually considered in the convergence analysis of finite difference schemes. It should be pointed out that the uniform boundness of $p_H(t)$ and $\nabla_H p_H(t)$ established in Corollary 2.2 has an important role in the convergence study for the semi-discrete approximation for the solution of the diffusion equation. We remark that these quadratic orders of convergence are unexpected results, meaning that we are under super-supraconvergence results.

Numerical experiments illustrating the established theoretical results are included. An application illustrating the increase of drug concentration in the target tissue when ultrasound are applied is also presented.

Chapter 4

Coupling: Acoustic Pressure Propagation, Heat and Drug Transport

4.1 Introduction

In this chapter, we consider the system of partial differential equations (1.1)-(1.9) in $\Omega \times (0,T_f]$, with $\Omega = (0,1)^2$ and $p,T,c : \overline{\Omega} \times [0,T_f] \to \mathbb{R}$. As mentioned before, this system can be used to mathematically describe the drug transport enhanced by ultrasound when heat effects are taken into account. As the differential system (1.1), (1.14), (1.4), (1.6), (1.7), (1.9), where the heat effects were neglected, was studied in the Chapter 3, this chapter can be seen as a generalization of the last one.

Here, we have a coupling of a hyperbolic equation - a telegraph equation (1.1), with two parabolic equations - a nonlinear diffusion-reaction equation (1.2) and a convection-diffusion-reaction equation (1.3). In this system of partial differential equations, the reaction term of the diffusion-reaction equation (1.2) depends on the solution of the wave equation (1.1), the convective velocity of the second diffusion equation depends on the solution of the hyperbolic equation (1.1) and its gradient, and the diffusion coefficient depends on the temperature T and on the acoustic pressure p.

The considered assumptions over the telegraph IBVP (1.1), (1.4), (1.7), in Chapter 2, will again be considered. Furthermore, in equation (1.2), D_T is a 2×2 diagonal matrix with positive entries $d_{T,i} : \mathbb{R} \to \mathbb{R}$, $i = 1,2$, with a positive lower bound β_0 in $\mathbb{R}$, and k represents a constant. Finally, in equation (1.3), we consider $D_c(p,T)$ a second order diagonal matrix with entries $d_{c,i} : \mathbb{R}^2 \to \mathbb{R}$, $i = 1,2$, that have positive lower bound β_1 in $\mathbb{R}$. As introduced in Chapter 3, the convective velocity of (1.3) is $v : \mathbb{R}^3 \to \mathbb{R}^2$ such that $v(x,y,z) = (v_1(x,y), v_2(x,z)),\ x,y,z \in \mathbb{R}$, and $v_i : \mathbb{R}^2 \to \mathbb{R}$, $i = 1,2$.

Our main aim in this chapter is the central objective of this thesis, the construction of an efficient numerical method for the system (1.1)-(1.9). We propose a fully discrete in space piecewise linear finite element method, that can also be seen as a finite difference method, to approximate p, T, and c that leads to a second order approximation with respect to a discrete H^1- norm for p, as we have seen in Chapter 2, and a second order approximation with respect to a discrete L^2- norm for T and c. These convergence results can be seen as super-supraconvergence results. The main ideas for this chapter are the ones presented in the previous chapter, however here we have more dependences to study, we need to carefully study some terms.

This chapter is organized as follows. In Section 4.2, we present a fully discrete piecewise linear finite element semi-discrete approximation for the solution $(p(t),T(t),c(t))$ of the IBVP (1.1)-(1.9). Note that the approximation considered for the wave equation is the one presented in Chapter 2, and for the concentration equation, we use the idea presented in the previous chapter, considering the adequate modification related with the temperature. Section 4.3 is focused on the convergence analysis of the semi-discrete approximation for the solution of the coupled problem (1.1)-(1.9). In Section 4.3.1, the convergence result for the numerical approximation for the temperature defined by the diffusion-reaction equation (1.2) is presented. In this result, Corollary 2.1 has an important role because the reaction term of (1.2), depends on the solution of (1.1). The main results for the numerical approximation for the temperature are Theorem 4.1 and Corollary 4.1. Finally, in the Section 4.3.2 we prove our main result, Corollary 4.3, where the second order of convergence is established for the numerical approximation for the concentration defined by equation (1.3). This result is consequence of Theorems 2.3, 4.1 and 4.2. We also include some numerical results illustrating the main conclusions of this work in Section 4.4. We end the chapter with some conclusions.

Before starting the construction of the numerical scheme, we observe that the existence and uniqueness of solution of (1.1)-(1.9) can be studied. For that, it is necessary to prove the existence of solution of (1.2). Note that this parabolic equation is nonlinear, so the approach can not be the same mentioned in the previous chapter. Some results can be found in Chapter 6 of [25]. Note that we need to impose smoothness conditions on the data of our problem, namely on f_2, T_0, $d_{T,i},\ i=1,2$, and remark that the reaction term of (1.2) depends on the solution of the hyperbolic problem (1.1), (1.4), (1.7). As we saw before, increasing the smoothness of the data of the wave problem (1.1), (1.4), (1.7) we can improve the regularity of p, and finally prove the existence and uniqueness of T in a certain sense. Finally to prove the existence and uniqueness of solution of (1.1)-(1.9), we can follow [11], taking into account that in this case the diffusion term also depends on T.

4.2 Semi-Discrete Numerical Scheme

In this section, we intend to introduce a fully discrete piecewise linear finite element semi-discrete approximation for the solution $(p(t),T(t),c(t))$ of the IBVP (1.1)-(1.9). For that purpose, we start defining a weak solution of the last problem. We say $(p(t),T(t),c(t))\in[H_0^1(\Omega)]^3$ is a weak solution of the IBVP (1.1)-(1.9) if

(i) $p^{(j)}(t)\in L^2(\Omega)$, $i=1,2$, $t\in(0,T_f]$, and (2.1) holds for $w\in H_0^1(\Omega)$, coupled with (2.2);

(ii) $T'(t)\in L^2(\Omega)$, $t\in(0,T_f]$, and

$$(T'(t),w)=-((D_T(T(t))\nabla T(t),\nabla w))+k(T(t),w)+(f_2(p(t)),w),\ t\in(0,T_f], \tag{4.1}$$

for $w\in H_0^1(\Omega)$, and

$$(T(0),q)=(T_0,q),\quad \forall q\in L^2(\Omega); \tag{4.2}$$

(iii) $c'(t) \in L^2(\Omega)$, $t \in (0, T_f]$, and

$$(c'(t), w) - ((v(p(t), \nabla p(t))c(t), \nabla w)) + ((D_c(p(t), T(t))\nabla c(t), \nabla w)) = (f_1(t), w),\ t \in (0, T_f], \tag{4.3}$$

for $w \in H_0^1(\Omega)$, and

$$(c(0), q) = (c_0, q), \quad \forall q \in L^2(\Omega). \tag{4.4}$$

Now, from the previous variational problem, we construct a piecewise linear finite element approximation for the coupling IBVP (1.1)-(1.9).

For the acoustic pressure we consider the fully discrete in space FEM constructed in Section 2.3

(i) find $p_H(t) \in W_{H,0}$ such that (2.8) holds for $t \in (0, T_f]$, $w_H \in W_{H,0}$, with initial conditions given by (2.9).

Again, we remark that this fully discrete FEM can be seen as the following finite difference problem: find $p_H(t) \in W_{H,0}$ verifying (2.10), (2.11), (2.12).

For the temperature defined by (4.1), (4.2) we introduce the piecewise linear FEM: find $T_H(t) \in W_{H,0}$ such that

$$\begin{aligned}(P_H T_H'(t), P_H w_H) = -((D_T(P_H T_H(t))\nabla P_H T_H(t), \nabla P_H w_H)) + k(P_H T_H(t), P_H w_H) \\ + (f_2(P_H p_H(t)), P_H w_H),\end{aligned} \tag{4.5}$$

for $w_H \in W_{H,0}$, $t \in (0, T_f]$, and

$$(P_H T_H(0), P_H q_H) = (P_H R_H T_0, P_H q_H), \forall q_H \in W_{H,0}. \tag{4.6}$$

In order to consider a discrete in space finite element problem, we need to establish adequate quadrature rules for the integral terms in (4.5), (4.6). Following the idea presented in Sections 2.3 and 3.2, we consider:

(i) $(P_H T_H'(t), P_H w_H) \simeq (T_H'(t), w_H)_H$;

(ii) $(P_H T_H(t), P_H w_H) \simeq (T_H(t), w_H)_H$;

(iii) $(f_2(P_H p_H(t)), P_H w_H) \simeq (f_2(p_H(t)), w_H)_H$;

(iv) $(P_H T_H(0), P_H w_H) \simeq (T_H(0), w_H)_H$;

(v) $(P_H R_H T_0, P_H w_H) \simeq (R_H T_0, w_H)_H$;

(vi) $((D_T(P_H T_H(t))\nabla P_H T_H(t), \nabla P_H w_H)) \simeq ((D_{T,H}(t)\nabla_H T_H(t), \nabla_H w_H))_H$;

where $D_{T,H}(t)$ is a 2×2 diagonal matrix with entries $d_{T,1}(M_h T_H(t))$ and $d_{T,2}(M_k T_H(t))$. Then, the piecewise linear FEM (4.5), (4.6) is replaced by the following discrete in space FEM: find $T_H(t) \in W_{H,0}$ such that

$$\big(T_H'(t), w_H\big)_H = -((D_{T,H}(t)\nabla_H T_H(t), \nabla_H w_H))_H + k(T_H(t), w_H)_H + (f_2(p_H(t)), w_H)_H, \tag{4.7}$$

for $w_H \in W_{H,0}$, $t \in (0,T_f]$, and

$$(T_H(0), q_H)_H = (R_H T_0, q_H)_H, \forall q_H \in W_{H,0}. \tag{4.8}$$

The fully discrete in space finite element problem (4.7), (4.8) can also be rewritten as the following finite difference problem:

$$T_H'(t) = \nabla_H^* \cdot (D_{T,H}(t)\nabla_H T_H(t)) + kT_H(t) + f_2(p_H(t)) \text{ in } \Omega_H, t \in (0,T_f], \tag{4.9}$$

with the initial condition

$$T_H(0) = R_H T_0, \tag{4.10}$$

and the boundary condition

$$T_H(t) = 0 \text{ on } \partial\Omega_H. \tag{4.11}$$

Note that (4.9) can be written as a matrix ordinary differential equation of the form

$$T_H'(t) = C(T_H(t))T_H(t) + f_2(p_H(t)), \tag{4.12}$$

where $p_H(t)$ is the solution of (2.13), (2.12). Since this system of ODEs is nonlinear, in order to prove existence and uniqueness of the solution of (4.12), (4.10), we need to impose conditions on C. As $d_{T,i}(t), i = 1,2$, depend on $T_H(t)$, we can guarantee that $C(T_H(t))T_H(t)$ is a Lipschitz function imposing regularity on $d_{T,i}$. Moreover, as $p_H(t)$ is continuous, $f_2(p_H(t))$ is also continuous provided that f_2 is a continuous function. Under such conditions, we can establish the existence and uniqueness of the solution T_H of the initial value problem (4.12), (4.10) with $T_H \in C([0,T_f]) \cap C^1((0,T_f])$ ([7]).

To complete our fully discrete piecewise linear FEM for our coupled IBVP, we need to consider the initial value problem (4.3), (4.4). The semi-discrete approximation for this problem is defined following the approach used in Section 3.2 for the concentration equation (1.14). We consider the following piecewise linear FEM: find $c_H(t) \in W_{H,0}$ such that

$$\begin{aligned}(P_H c_H'(t), P_H w_H) - ((P_H c_H(t) v(P_H p_H(t), \nabla P_H p_H(t)), \nabla P_H w_H)) \\ = -((D_c(P_H p_H(t), P_H T_H(t))\nabla P_H c_H(t), \nabla P_H w_H)) + (f_1(t), P_H w_H),\end{aligned}$$

for $w_H \in W_{H,0}$, $t \in (0,T_f]$, and

$$(P_H c_H(0), P_H q_H) = (P_H R_H c_0, P_H q_H), \forall q_H \in W_{H,0}.$$

We take

$$((D_c(P_H p_H(t), P_H T_H(t))\nabla P_H c_H(t), \nabla P_H w_H)) \simeq ((D_{c,H}(t)\nabla_H c_H(t), \nabla_H w_H))_H,$$

with $D_{c,H}(t)$ a 2×2 diagonal matrix with diagonal elements $d_{c,1}(M_h p_H(t), M_h T_H(t))$ and $d_{c,2}(M_k p_H(t), M_k T_H(t))$, where $p_H(t)$ is defined by (2.8), (2.9), and $T_H(t)$ by (4.7), (4.8).

Then, the last finite element problem for the concentration is replaced by the following fully discrete in space FEM: find $c_H(t) \in W_{H,0}$ such that

$$(c'_H(t), w_H)_H - ((M_H(c_H(t)v_H(t)), \nabla_H w_H))_H = -((D_{c,H}(t)\nabla_H c_H(t), \nabla_H w_H))_H + (f_{1,H}(t), w_H)_H, \tag{4.13}$$

for $w_H \in W_{H,0}$, $t \in (0, T_f]$, and

$$(c_H(0), q_H)_H = (R_H c_0, q_H)_H, \forall q_H \in W_{H,0}. \tag{4.14}$$

In (4.13), $v_H(t)$ is given by $(v_1(p_H(t), D_h^* p_H(t)), v_2(p_H(t), D_k^* p_H(t)))$ where $p_H(t)$ is defined by (2.8), (2.9).

To complete this section, we remark that the introduced fully discrete FEM for the concentration (4.13), (4.14) can be seen as the following finite difference scheme

$$c'_H(t) + \nabla_{c,H} \cdot (c_H(t)v_H(t)) = \nabla_H^* \cdot (D_{c,H}(t)\nabla_H c_H(t)) + f_{1,H}(t) \text{ in } \Omega_H, t \in (0, T_f], \tag{4.15}$$

with

$$c_H(0) = R_H c_0 \text{ in } \Omega_H, \tag{4.16}$$

$$c_H(t) = 0 \text{ on } \partial\Omega_H. \tag{4.17}$$

Note that this FDM is, in fact, a system of ordinary differential equation, which can be written in the matrix form

$$c'_H(t) + M(t)c_H(t) = f_{1,H}(t),\ t \in (0, T_f]. \tag{4.18}$$

However, in this case, the entries of the matrix $M(t)$ depend on $D_{c,H}(t)$ and $v_H(t)$, $D_{c,H}(t)$ depends on T_H and p_H that are solutions of (4.12), (4.10) and (2.13), (2.12), respectively, and $v_H(t)$ depends only on $p_H(t)$ defined as before. Assuming smoothness conditions on $d_{c,i},\ i = 1,2$ and $v_i, i = 1,2$, we can guarantee the continuity of $M(t)$. Moreover, the continuity of $f_{1,H}(t)$ is a natural consequence of the continuity of f_1. Then we can establish a set of conditions on the diffusion tensor, on the convective velocity v and on f_1 that lead to the existence and uniqueness of the solution c_H of the initial value problem (4.18), (4.16) with $c_H \in C([0, T_f]) \cap C^1((0, T_f])$ ([7]).

4.3 Convergence Analysis

From last section, we have completed the construction of our fully discrete piecewise linear FEM for the coupled IBVP (1.1)-(1.9). Such method is obtained by the coupling of:

(i) (2.8), (2.9) to compute an approximation for the acoustic pressure;

(ii) (4.7), (4.8) to compute an approximation for the temperature;

(iii) (4.13), (4.14) to compute an approximation for the concentration.

Once again, we point out that the continuous versions of these fully discrete in space FEMs lead to a second order approximation, with respect to the L^2- norm, and to a first order approximation with respect to the H^1- norm, since such methods are based on piecewise linear elements ([19], [42], [45]). As the convective velocity for the concentration depends on ∇p, then the coupled continuous piecewise linear FEM should lead to a first order approximation for the concentration with respect to the L^2- norm. Moreover, it is expected that these results are maintained for the space discrete coupled method proposed. In Chapter 2, we have shown that the fully discrete in space acoustic pressure approximation $p_H(t)$ is second order convergent with respect to a discrete version of the H^1- norm. In this chapter, we prove that $T_H(t)$ is a second order approximation for the temperature and, following the approach used in Chapter 3, we prove a result that is analogous to Theorem 3.1.

The coupled method (2.8), (2.9), (4.7), (4.8), (4.13), (4.14) is equivalent to the finite difference coupling:

(i) (2.10), (2.11), (2.12) for the acoustic pressure $p_H(t)$;

(ii) (4.9), (4.10), (4.11) for the temperature $T_H(t)$;

(iii) (4.15), (4.16), (4.17) for the concentration $c_H(t)$.

These finite difference problems are defined in a nonuniform rectangular grid Ω_H. The truncation error associated with the spatial discretizations that lead to each subproblem is only of first order with respect to the maximum norm $\|\cdot\|_\infty$ (this analysis is presented for the hyperbolic equation in the Section 2.4.1), provided that $p(t),\ T(t),\ c(t) \in C^3(\overline{\Omega})$. Based on stability and consistency we are expecting that the semi-discrete errors for $p_H(t)$, $T_H(t)$ and $c_H(t)$ are only of first order. Since each of the FEM with quadrature is equivalent to the correspondent FDM, we conclude that the finite difference approximations $p_H(t)$, $T_H(t)$ and $c_H(t)$ have exactly the convergence properties of the correspondent fully discrete piecewise linear FE approximations. We believe that these convergence properties can be improved if we assume that $p(t), T(t), c(t) \in C^4(\overline{\Omega})$ using the approach presented in Section 2.4.2. In what follows, we obtain the same convergence results assuming lower smoothness assumptions.

4.3.1 Heat Transport

In this section, we intend to establish an estimate for the spatial discretization error $e_{H,T}(t) = R_H T(t) - T_H(t)$ induced by the spatial discretization for the temperature (4.7), (4.8). To obtain such estimate, our technique, based on the direct analysis of the error equation for $e_{H,T}(t)$, allows us to reduce the regularity assumptions on the solution $T(t)$. Note that this result should depend on $p_H(t)$.

We start establishing the following identity to $e_{H,T}(t)$

$$\begin{aligned}
(e'_{H,T}(t), w_H)_H = &-((D_{T,H}(t)\nabla_H e_{H,T}(t), \nabla_H w_H))_H \\
&+(((D_{T,H}(t) - D^*_{T,H}(t))\nabla_H R_H T(t), \nabla_H w_H))_H \\
&+(R_H f_2(p(t)) - f_2(p_H(t)), w_H)_H \\
&+(kR_H T(t) - kT_H(t), w_H)_H \\
&+\tau_{D_T}(w_H) + \tau_k(w_H) + \tau_{f_2}(w_H) + \tau_d(w_H),
\end{aligned} \tag{4.19}$$

where $t \in (0,T_f]$, $w_H \in W_{H,0}$, and $D^*_{T,H}(t)$ is defined as $D_{T,H}(t)$ with $T_H(t)$ replaced by $R_H T(t)$, and

$$\tau_{D_T}(w_H) = ((D^*_{T,H}(t)\nabla_H R_H T(t), \nabla_H w_H))_H + ((\nabla \cdot (D_T(T(t))\nabla T(t)))_H, w_H)_H, \tag{4.20}$$

$$\tau_k(w_H) = ((kT(t))_H, w_H)_H - (kR_H T(t), w_H)_H, \tag{4.21}$$

$$\tau_{f_2}(w_H) = ((f_2(p(t)))_H, w_H)_H - (f_2(R_H p(t)), w_H)_H, \tag{4.22}$$

$$\tau_d(w_H) = (R_H T'(t) - (T'(t))_H, w_H)_H, \tag{4.23}$$

with $(\nabla \cdot (D_T(T(t))\nabla T(t)))_H$, $(kT(t))_H$, $(f_2(p(t)))_H$ and $(T'(t))_H$ given by (2.7) with $f_3(t)$ replaced by $\nabla \cdot (D_T(T(t))\nabla T(t))$, $kT(t)$, $f_2(p(t))$ and $T'(t)$, respectively.

We start our convergence analysis establishing adequate estimates for the functionals $\tau_{D_T}(w_H)$, $\tau_k(w_H)$, $\tau_{f_2}(w_H)$ and $\tau_d(w_H)$, for $w_H \in W_{H,0}$. The estimates presented in Propositions 4.1, 4.2, 4.3 follows directly from Lemma 5.7 of [14], being the Bramble-Hilbert Lemma the main tool used.

Proposition 4.1. *If $T(t) \in H^2(\Omega)$, for the functional $\tau_k : W_{H,0} \to \mathbb{R}$ defined by (4.21) holds the following*

$$|\tau_k(w_H)| \le C \left(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \|T(t)\|^2_{H^2(\Delta)} \right)^{1/2} \|\nabla_H w_H\|_H ,$$

for $w_H \in W_{H,0}$, $H \in \Lambda$, where C denotes a positive constant, T, H and t independent.

Proposition 4.2. *If $T'(t) \in H^2(\Omega)$, for the functional $\tau_d : W_{H,0} \to \mathbb{R}$ defined by (4.23) holds the following*

$$|\tau_d(w_H)| \le C \left(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \left\|T'(t)\right\|^2_{H^2(\Delta)} \right)^{1/2} \|\nabla_H w_H\|_H ,$$

for $w_H \in W_{H,0}$, $H \in \Lambda$, where C denotes a positive constant, T, H and t independent.

Proposition 4.3. *If f_2 is such that $f_2(p(t)) \in H^2(\Omega)$ then, for the functional $\tau_{f_2} : W_{H,0} \to \mathbb{R}$ defined by (4.22), there exists a positive constant C, p, H and t independent, such that*

$$|\tau_{f_2}(w_H)| \le C \left(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \|f_2(p(t))\|^2_{H^2(\Delta)} \right)^{1/2} \|\nabla_H w_H\|_H,$$

for $w_H \in W_{H,0}$, $H \in \Lambda$.

Proposition 4.4. *If $d_{T,i}$, $i = 1,2$, are L_{D_T}- Lipschitz functions, $T(t) \in H^3(\Omega)$, $d_{T,i}(T(t)) \in L^\infty(\Omega), i = 1,2$, and $D_T(t)\nabla T(t) \in [H^2(\Omega)]^2$, then for the functional $\tau_{D_T} : W_{H,0} \to \mathbb{R}$ defined by (4.20) we have*

$$\begin{aligned} |\tau_{D_T}(w_H)| \le & C \Bigg(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \Big(L^2_{D_T} \|T(t)\|^2_{C^1(\Delta)} \|T(t)\|^2_{H^2(\Delta)} \\ & + \|D_T(T(t))\|^2_{\infty, L^\infty(\Delta)} \|T(t)\|^2_{H^3(\Delta)} \\ & + \|D_T(t)\nabla T(t)\|^2_{[H^2(\Delta)]^2} \Big) \Bigg)^{1/2} \|\nabla_H w_H\|_H , \end{aligned}$$

for $w_H \in W_{H,0}$, $H \in \Lambda$, where C denotes a positive constant, T, H and t independent.

Proof. We start by noting that τ_{D_T} can be written as

$$\begin{aligned}\tau_{D_T}(w_H) &= (d_{T,1}(M_h R_H T(t))D_{-x}R_H T(t), D_{-x}w_H)_{H,x} + \left(\left(\frac{\partial}{\partial x}\left(d_{T,1}(t)\frac{\partial T}{\partial x}(t)\right)\right)_H, w_H\right)_H \\ &\quad + (d_{T,2}(M_k R_H T(t))D_{-y}R_H T(t), D_{-y}w_H)_{H,y} + \left(\left(\frac{\partial}{\partial y}\left(d_{T,2}(t)\frac{\partial T}{\partial y}(t)\right)\right)_H, w_H\right)_H \\ &:= \tau_x(w_H) + \tau_y(w_H).\end{aligned}$$

We also split τ_x as $\tau_x(w_H) = \tau_1(w_H) + \tau_2(w_H)$ with

$$\begin{aligned}\tau_1(w_H) &= (d_{T,1}(M_h R_H T(t))D_{-x}R_H T(t), D_{-x}w_H)_{H,x} - (d_{T,1}(T(M_h(t)))D_{-x}R_H T(t), D_{-x}w_H)_{H,x}, \\ \tau_2(w_H) &= (d_{T,1}(T(M_h(t)))D_{-x}R_H T(t), D_{-x}w_H)_{H,x} + \left(\left(\frac{\partial}{\partial x}\left(d_{T,1}(t)\frac{\partial T}{\partial x}(t)\right)\right)_H, w_H\right)_H.\end{aligned}$$

Following the proof of Proposition 3.2, it is now simple to prove that there exists a positive constant C, T, H and t independent, such that

$$\begin{aligned}|\tau_1(w_H)| &\le L_{D_T}\sum_{i=1}^{N}\sum_{j=1}^{M-1}\Bigg(h_i\left(\int_{y_{j-1/2}}^{y_{j+1/2}}|\sigma(x_i,y,t)|\,dy + k_{j+1/2}\int_{y_{j-1/2}}^{y_{j+1/2}}\left|\frac{\partial\sigma}{\partial y}(x_i,y,t)\right|dy\right) \\ &\qquad \times |D_{-x}T(x_i,y_j,t)||D_{-x}w_H(x_i,y_j)|\Bigg) \\ &\le CL_{D_T}\left(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\|T(t)\|^2_{C^1(\Delta)}\|T(t)\|^2_{H^2(\Delta)}\right)^{1/2}\|D_{-x}w_H\|_H,\end{aligned}$$

where $\sigma(x_i,y,t) = \dfrac{T(x_{i-1},y,t)+T(x_i,y,t)}{2} - T(x_{i-1/2},y,t)$.

From the proof of Lemma 5.1 of [14], we easily obtain the following estimate for $\tau_2(w_H)$

$$|\tau_2(w_H)| \le C\Big(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(\|d_{T,1}(t)\|^2_{L^\infty(\Delta)}\|T(t)\|^2_{H^3(\Delta)} + \left\|d_{T,1}(t)\frac{\partial T}{\partial x}(t)\right\|^2_{H^2(\Delta)}\Big)\Big)^{1/2}\|\nabla_H w_H\|_H,$$

and therefore

$$\begin{aligned}|\tau_x(w_H)| \le C\Bigg(\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Bigg(&L^2_{D_T}\|T(t)\|^2_{C^1(\Delta)}\|T(t)\|^2_{H^2(\Delta)} + \|d_{T,1}(t)\|^2_{L^\infty(\Delta)}\|T(t)\|^2_{H^3(\Delta)} \\ &+ \left\|d_{T,1}(t)\frac{\partial T}{\partial x}(t)\right\|^2_{H^2(\Delta)}\Bigg)\Bigg)^{1/2}\|\nabla_H w_H\|_H.\end{aligned}$$

Proceeding analogously, we can obtain a similar result for $\tau_y(w_H)$, and finally get the inequality

$$|\tau_{D_T}(w_H)| \leq C\left(\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\Big(L_{D_T}^2\|T(t)\|_{C^1(\Delta)}^2\|T(t)\|_{H^2(\Delta)}^2 + \max_{i=1,2}\|d_{T,i}(t)\|_{L^\infty(\Delta)}^2\|T(t)\|_{H^3(\Delta)}^2 + \|D_T(t)\nabla T(t)\|_{[H^2(\Delta)]^2}^2\Big)\right)^{1/2}\|\nabla_H w_H\|_H,$$

where C denotes a positive constant, T, H and t independent. □

From the previous propositions, we can now derive the main result of this section, an upper bound for $\|e_{H,T}(t)\|_H$.

Theorem 4.1. *Assuming the following:*

(i) the solution T of the IBVP (1.2), (1.5), (1.8) satisfies $R_H T \in C^1((0,T_f],W_{H,0})$ and $T \in L^2(0,T_f,H^3(\Omega)\cap H_0^1(\Omega)) \cap H^1(0,T_f,H^2(\Omega))$;

(ii) the solution T_H of the initial value problem (4.7), (4.8) belongs to $C^1((0,T_f],W_{H,0})\cap C([0,T_f],W_{H,0})$;

(iii) f_2 is a L_{f_2}- Lipschitz function with $f_2(p(t))\in H^2(\Omega)$, where p is solution of the IBVP (1.1), (1.4), (1.7);

(iv) $d_{T,i}\geq \beta_0 > 0$, $i=1,2$, in $\mathbb{R}$;

(v) the assumptions of Proposition 4.4 hold.

Then, there exists a positive constant C, p, T, H and t independent, such that, for the spatial error $e_{H,T}(t) = R_H T(t) - T_H(t)$ holds the following

$$\begin{aligned}\|e_{H,T}(t)\|_H^2 &+ 2(\beta_0-5\varepsilon^2)\int_0^t e^{\int_s^t g_H(T(\mu))d\mu}\|\nabla_H e_{H,T}(s)\|_H^2 ds\\ &\leq e^{\int_0^t g_H(T(s))ds}\|e_{H,T}(0)\|_H^2 + L_{f_2}^2\int_0^t e^{\int_s^t g_H(T(\mu))d\mu}\|e_{H,p}(s)\|_H^2 ds\\ &+\int_0^t e^{\int_s^t g_H(T(\mu))d\mu}\tau_1(s)ds,\end{aligned}\tag{4.24}$$

for $t\in[0,T_f]$, $H\in\Lambda$, where

$$g_H(T(t)) = \frac{1}{\varepsilon^2}L_{D_T}^2\|\nabla_H R_H T(t)\|_\infty^2 + 1 + 2k,$$

$$\begin{aligned}\tau_1(t) = \frac{C}{2\varepsilon^2}\sum_{\Delta\in\mathcal{T}_H}(diam\Delta)^4\Big(&\big(L_{D_T}^2\|T(t)\|_{C^1(\Delta)}^2 + \|D_T(T(t))\|_{\infty,L^\infty(\Delta)}^2+1\big)\|T(t)\|_{H^3(\Delta)}^2\\ &+\|T'(t)\|_{H^2(\Delta)}^2 + \|D_T(t)\nabla T(t)\|_{[H^2(\Delta)]^2}^2 + \|f_2(p(t))\|_{H^2(\Delta)}^2\Big),\end{aligned}\tag{4.25}$$

and $\varepsilon\neq 0$ is an arbitrary constant.

Proof. Since $d_{T,i},\ i=1,2$, are L_{D_T}- Lipschitz functions, then

$$\begin{aligned}&|(((D_{T,H}(t)-D^*_{T,H}(t))\nabla_H R_H T(t),\nabla_H w_H))_H|\\&\quad\leq\sqrt{2}L_{D_T}\|e_{H,T}(t)\|_H\|\nabla_H R_H T(t)\|_\infty\|\nabla_H w_H\|_H.\end{aligned}\tag{4.26}$$

As f_2 is a L_{f_2}- Lipschitz function then

$$|(R_H f_2(p(t))-f_2(p_H(t)),w_H)_H|\leq L_{f_2}\|e_{H,p}(t)\|_H\|w_H\|_H.\tag{4.27}$$

Taking in (4.19) $w_H=e_{H,T}(t)$, considering (4.26) and (4.27), we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|e_{H,T}(t)\|_H^2+\beta_0\|\nabla_H e_{H,T}(t)\|_H^2&\leq\sqrt{2}L_{D_T}\|\nabla_H R_H T(t)\|_\infty\|e_{H,T}(t)\|_H\|\nabla_H e_{H,T}(t)\|_H\\&+L_{f_2}\|e_{H,p}(t)\|_H\|e_{H,T}(t)\|_H+k\|e_{H,T}(t)\|_H^2+|\tau_{D_T}(e_{H,T}(t))|+|\tau_k(e_{H,T}(t))|\\&+|\tau_{f_2}(e_{H,T}(t))|+|\tau_d(e_{H,T}(t))|.\end{aligned}$$

For the first term of the upper bound of the last inequality we easily get

$$\begin{aligned}&\sqrt{2}L_{D_T}\|\nabla_H R_H T(t)\|_\infty\|e_{H,T}(t)\|_H\|\nabla_H e_{H,T}(t)\|_H\\&\quad\leq\varepsilon^2\|\nabla_H e_{H,T}(t)\|_H^2+\frac{1}{2\varepsilon^2}L_{D_T}^2\|\nabla_H R_H T(t)\|_\infty^2\|e_{H,T}(t)\|_H^2,\end{aligned}$$

where $\varepsilon\neq 0$ is an arbitrary constant. Then taking into account Propositions 4.1 - 4.4, we get

$$\frac{d}{dt}\|e_{H,T}(t)\|_H^2+2(\beta_0-5\varepsilon^2)\|\nabla_H e_{H,T}(t)\|_H^2\leq L_{f_2}^2\|e_{H,p}(t)\|_H^2+g_H(T(t))\|e_{H,T}(t)\|_H^2+\tau_1(t),\tag{4.28}$$

where $\tau_1(t)$ is given by (4.25). Multiplying everything by $e^{-\int_0^t g_H(T(s))ds}$, inequality (4.28) leads to

$$\begin{aligned}&\frac{d}{dt}\Big(e^{-\int_0^t g_H(T(s))ds}\|e_{H,T}(t)\|_H^2+2(\beta_0-5\varepsilon^2)\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\|\nabla_H e_{H,T}(s)\|_H^2ds\\&\quad-L_{f_2}^2\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\|e_{H,p}(s)\|_H^2ds-\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\tau_1(s)ds\Big)\leq 0.\end{aligned}$$

Consequently,

$$\begin{aligned}&e^{-\int_0^t g_H(T(s))ds}\|e_{H,T}(t)\|_H^2+2(\beta_0-5\varepsilon^2)\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\|\nabla_H e_{H,T}(s)\|_H^2ds\\&-L_{f_2}^2\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\|e_{H,p}(s)\|_H^2ds-\int_0^t e^{-\int_0^s g_H(T(\mu))d\mu}\tau_1(s)ds\leq\|e_{H,T}(0)\|_H^2,\end{aligned}$$

that finally allows us to establish (4.24). □

Note that, since we are assuming $T(t)\in H^3(\Omega)$, then $T(t)\in C^1(\overline{\Omega})$, which gives us the uniform boundness of $g_H(T(t))$, for $H\in\Lambda$. Fixing, in Theorem 4.1, $\varepsilon\neq 0$ such that $\beta_0-5\varepsilon^2>0$, and taking into account the Corollary 2.1, we conclude the following result:

Corollary 4.1. *Under the assumptions of Theorems 2.3 and 4.1 we conclude that there exists a positive constant C, H and t independent, such that*

$$\|e_{H,T}(t)\|_H^2 + \int_0^t \|\nabla_H e_{H,T}(s)\|_H^2 ds \leq C H_{\max}^4,\ t \in [0,T_f],\ H \in \Lambda.$$

The Corollary 4.1 gives us the second order of convergence of our fully discrete in space FEM (2.8), (2.9), (4.7), (4.8) that defines an approximation for the solution of the system of partial differential equations (1.1), (1.4), (1.7), (1.2), (1.5), (1.8), with respect to the discrete norm $\|\cdot\|_H$. This is a supraconvergence result, since from the classical analysis for the correspondent FDM we only expect first order of convergence in relation to $\|\cdot\|_\infty$. In the language of FEM, this result can be seen as a superconvergence result.

In what follows, we present a result that gives us the boundness of the sequences $(\|T_H(t)\|_\infty)_{H\in\Lambda}$ and $\left(\int_0^t \|\nabla_H T_H(s)\|_\infty ds\right)_{H\in\Lambda}$, where

$$\|T_H(t)\|_\infty = \max_{(x,y)\in\overline{\Omega}_H} |T_H(x,y,t)|,$$
$$\|\nabla_H T_H(t)\|_\infty = \max_{i=1,\ldots,N,j=1,\ldots,M-1} \left|D_{-x}T_H(x_i,y_j,t)\right| + \max_{i=1,\ldots,N-1,j=1,\ldots,M} \left|D_{-y}T_H(x_i,y_j,t)\right|.$$

Corollary 4.2. *Under the conditions of Theorems 2.3 and 4.1, if the sequence of step-sizes Λ satisfies (2.35), we conclude that there exists a positive constant C, H and t independent, such that*

$$\|T_H(t)\|_\infty \leq C,\ \int_0^t \|\nabla_H T_H(s)\|_\infty ds \leq C,\ t \in [0,T_f],\ H \in \Lambda,$$

$H_{\max}$ *small enough.*

Proof. Taking into account Corollary 4.1, we have

$$\|T_H(t)\|_\infty^2 \leq 2\frac{1}{H_{\min}^2}\|e_{H,T}(t)\|_H^2 + 2\|R_H T(t)\|_\infty^2 \leq C\frac{H_{\max}^4}{H_{\min}^2} + 2\|T(t)\|_\infty^2,$$

for $H \in \Lambda$. The boundeness of $\|T(t)\|_\infty$ results from the fact that $T(t) \in C(\overline{\Omega})$ when $T(t) \in H^3(\Omega) \cap H_0^1(\Omega)$.

We also have,

$$\begin{aligned}\int_0^t \|\nabla_H T_H(s)\|_\infty^2 ds &\leq 2\frac{1}{H_{\min}^2}\int_0^t \|\nabla_H e_{H,T}(s)\|_H^2 ds + 2\int_0^t \|\nabla_H R_H T(s)\|_\infty^2 ds \\ &\leq C\frac{H_{\max}^4}{H_{\min}^2} + 2\int_0^{T_f} \|\nabla T(s)\|_\infty^2 ds,\end{aligned}$$

for C a positive constant. The result follows from the fact that $T(t) \in C^1(\overline{\Omega})$. □

4.3.2 Drug Transport

The aim of this subsection is to conclude the convergence analysis of the FE scheme: (2.8), (2.9) for the acoustic pressure, (4.7), (4.8) for the temperature, (4.13), (4.14) for the concentration, or equivalently, of the FD scheme (2.10), (2.11), (2.12) for the acoustic pressure $p_H(t)$, (4.9), (4.10), (4.11) for the temperature $T_H(t)$, (4.15), (4.16), (4.17) for the concentration $c_H(t)$. The main result of this section, Theorem 4.2, is in fact the central theorem of this thesis. In the proof of this result, Corollaries 2.1, 2.2 and 4.1 have a crucial role. Note that the approach in this section is similar to the one followed in Section 3.3.

Let $e_{H,c}(t) = R_H c(t) - c_H(t)$ be the spatial discretization error induced by the coupled scheme. From (4.13), we obtain

$$\begin{aligned}(e'_{H,c}(t), w_H)_H = &-((D_{c,H}(t)\nabla_H e_{H,c}(t), \nabla_H w_H))_H \\ &+ (((D_{c,H}(t) - D^*_{c,H}(t))\nabla_H R_H c(t), \nabla_H w_H))_H \\ &+ ((M_H(v_H(t)e_{H,c}(t)), \nabla_H w_H))_H \\ &- ((M_H((v_H(t) - v^*_H(t))R_H c(t)), \nabla_H w_H))_H \\ &+ \tau_{D_c}(w_H) + \tau_v(w_H) + \tau_c(w_H), \end{aligned} \tag{4.29}$$

for $t \in (0, T_f]$, $w_H \in W_{H,0}$, where $D^*_{c,H}(t)$ is defined as $D_{c,H}(t)$ with p_H and T_H replaced by $R_H p$ and $R_H T$, respectively, and $v^*_H(t)$ is defined as $v_H(t)$ with p_H replaced by $R_H p$. In (4.29), $\tau_{D_c}(w_H)$, $\tau_v(w_H)$ and $\tau_c(w_H)$ are defined by

$$\tau_{D_c}(w_H) = ((D^*_{c,H}(t)\nabla_H R_H c(t), \nabla_H w_H))_H + ((\nabla \cdot (D_c(p(t), T(t))\nabla c(t)))_H, w_H)_H, \tag{4.30}$$

$$\tau_v(w_H) = -((M_H(v^*_H(t)R_H c(t)), \nabla_H w_H))_H - ((\nabla \cdot (v(p(t), \nabla p(t))c(t)))_H, w_H)_H, \tag{4.31}$$

and

$$\tau_c(w_H) = (R_H c'(t), w_H)_H - ((c'(t))_H, w_H)_H. \tag{4.32}$$

We start establishing upper bounds for $\tau_{D_c}(w_H)$ and $\tau_c(w_H)$, for $w_H \in W_{H,0}$. Proposition 3.1 gives us an upper bound for $\tau_v(w_H)$, $w_H \in W_{H,0}$, define by (4.31).

Proposition 4.5. *If $d_{c,i},\ i = 1,2$, are L_{D_c}- Lipschitz functions, $p(t), T(t) \in H^2(\Omega)$, $c(t) \in H^3(\Omega)$, $d_{c,i}(p(t), T(t)) \in L^\infty(\Omega), i = 1,2$, and $D_c(t)\nabla c(t) \in [H^2(\Delta)]^2$ then, for the functional $\tau_{D_c} : W_{H,0} \to \mathbb{R}$ defined by (4.30), there exists a positive constant C, H, t, p, T and c independent, such that*

$$\begin{aligned}|\tau_{D_c}(w_H)| \le C\Big(\sum_{\Delta \in \mathscr{T}_H} (diam\Delta)^4 \big(L^2_{D_c}\big(\|T(t)\|^2_{H^2(\Delta)} + \|p(t)\|^2_{H^2(\Delta)}\big)\|c(t)\|^2_{C^1(\Delta)} \\ + \|D_c(p(t), T(t))\|^2_{\infty, L^\infty(\Delta)}\|c(t)\|^2_{H^3(\Delta)} \\ + \|D_c(p(t), T(t))\nabla c(t)\|^2_{[H^2(\Delta)]^2}\big)\Big)^{1/2} \|\nabla_H w_H\|_H\end{aligned}$$

for $w_H \in W_{H,0}$, $H \in \Lambda$.

Proof. This proof is similar to the proof of Proposition 3.2. Note that, the functional (4.30) admits the representation

$$\tau_{D_c}(w_H) = \sum_{i=1}^{2} \tau_i(w_H), w_H \in W_{H,0}, \tag{4.33}$$

with

$$\tau_1(w_H) = (((D^*_{c,H}(t) - \tilde{D}_{c,H}(t))\nabla_H R_H c(t), \nabla_H w_H))_H,$$

where the diagonal entries of $\tilde{D}_{c,H}(t)$ at (x_i, y_j) are given by $d_{c,1}(p(x_{i-1/2}, y_j, t), T(x_{i-1/2}, y_j, t))$ and $d_{c,2}(p(x_i, y_{j-1/2}, t), T(x_i, y_{j-1/2}, t))$, and

$$\tau_2(w_H) = ((\tilde{D}_{c,H}(t)\nabla_H R_H c(t), \nabla_H w_H))_H + ((\nabla\cdot(D_c(p(t), T(t))\nabla c(t)))_H, w_H)_H.$$

Following the steps of the proof of Proposition 3.2, it is now a simple task to prove that there exists a positive constant C, H, t, p, T and c independent, such that

$$|\tau_1(w_H)| \le C\Big(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 L^2_{D_c}\big(\|T(t)\|^2_{H^2(\Delta)} + \|p(t)\|^2_{H^2(\Delta)}\big)\|c(t)\|^2_{C^1(\Delta)}\Big)^{1/2}\|\nabla_H w_H\|_H. \quad (4.34)$$

Moreover, considering again the proof of Lemma 5.1 of [14], we get the following estimate for $\tau_2(w_H)$

$$\begin{aligned}|\tau_2(w_H)| \le C\Big(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \big(&\|D_c(p(t), T(t))\|^2_{\infty, L^\infty(\Delta)}\|c(t)\|^2_{H^3(\Delta)} \quad (4.35)\\ &+ \|D_c(p(t), T(t))\nabla c(t)\|^2_{[H^2(\Delta)]^2}\big)\Big)^{1/2}\|\nabla_H w_H\|_H,\end{aligned}$$

where C is a positive constant, H, t, p, T and c independent, and we finish the proof using (4.34) and (4.35) in (4.33).

□

The following proposition gives an estimate for $\tau_c(w_H)$.

Proposition 4.6. *If $c'(t) \in H^2(\Omega)$, for the functional $\tau_c : W_{H,0} \to \mathbb{R}$ defined by (4.32) we have*

$$|\tau_c(w_H)| \le C\left(\sum_{\Delta\in\mathscr{T}_H} (diam\Delta)^4 \|c'(t)\|^2_{H^2(\Delta)}\right)^{1/2}\|\nabla_H w_H\|_H,$$

for $w_H \in W_{H,0}$, $H \in \Lambda$, where C is a positive constant, H, t and c independent.

Proof. The inequality follows immediately from Lemma 5.7 of [14]. □

Finally, we are in condition to establish an estimate for the error $e_{H,c}(t)$. Note that, assuming that (2.35) holds, for $H \in \Lambda$, with $H_{\max}$ small enough, then we establish (3.26). Also, if v satisfies

$$|v_i(z_1, z_2)| \le C_v(|z_1| + |z_2|), \forall z_1, z_2 \in \mathbb{R},\ i = 1, 2,$$

we have (3.25). Moreover, considering $d_{c,i},\ i = 1, 2$, L_{D_c}- Lipschitz functions, we obtain the following upper bound,

$$\begin{aligned}&|(((D_{c,H}(t) - D^*_{c,H}(t))\nabla_H R_H c(t), \nabla_H w_H))_H| \\ &\quad \le 2L_{D_c}\big(\|e_{H,p}(t)\|_H + \|e_{H,T}(t)\|_H\big)\|\nabla_H R_H c(t)\|_\infty \|\nabla_H w_H\|_H. \quad (4.36)\end{aligned}$$

Now, it follows the main result of this work.

Theorem 4.2. *Let us assume that:*

(i) the sequence of grids $\overline{\Omega}_H, H \in \Lambda$, satisfies (2.35) for $H_{\max}$ small enough;

(ii) $p(t) \in H^3(\Omega) \cap H_0^1(\Omega)$, where p is solution of the IBVP (1.1), (1.4), (1.7);

(iii) $T(t) \in H^2(\Omega) \cap H_0^1(\Omega)$, where T is solution of the IBVP (1.2), (1.5), (1.8);

(iv) the solution c of the IBVP (1.3), (1.6), (1.9) satisfies $c \in L^2(0,T_f,H^3(\Omega) \cap H_0^1(\Omega)) \cap H^1(0,T_f,H^2(\Omega))$ and $R_H c \in C^1((0,T_f],W_{H,0})$;

(v) the solution c_H of the initial value problem (4.13), (4.14) belongs to $C^1((0,T_f],W_{H,0}) \cap C([0,T_f],W_{H,0})$;

(vi) v_i satisfies $|v_i(z_1,z_2)| \leq C_v(|z_1|+|z_2|)$, $\forall z_1 \in \mathbb{R}$, $\forall z_2 \in \mathbb{R}$, $i=1,2$;

(vii) $d_{c,i} \geq \beta_1 > 0$, $i=1,2$, in $\mathbb{R}^2$;

(viii) the assumptions of Propositions 3.1 and 4.5 hold.

Then, there exists a positive constant C, H, t, p, T and c independent, such that for the spatial error $e_{H,c}(t) = R_H c(t) - c_H(t)$ the following holds

$$
\begin{aligned}
&\|e_{H,c}(t)\|_H^2 + 2(\beta_1 - 6\varepsilon^2)\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\|\nabla_H e_{H,c}(s)\|_H^2 ds \leq e^{\int_0^t g_H(p_H(\mu))d\mu}\|e_{H,c}(0)\|_H^2\\
&+\frac{4}{\varepsilon^2}L_{D_c}^2\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\left(\|e_{H,p}(s)\|_H^2 + \|e_{H,T}(s)\|_H^2\right)\|\nabla_H R_H c(s)\|_\infty^2 ds\\
&+\frac{4}{\varepsilon^2}L_v^2\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\Big(\|e_{H,p}(s)\|_H^2 + 2C_m\|\nabla_H e_{H,p}(s)\|_H^2\Big)\|R_H c(s)\|_\infty^2 ds\\
&+\int_0^t e^{\int_s^t g_H(p_H(\mu))d\mu}\tau_c^*(s)ds, \qquad (4.37)
\end{aligned}
$$

for $t \in [0,T_f]$, $H \in \Lambda$ and $H_{\max}$ small enough. In (4.37),

$$g_H(p_H(t)) = \frac{2}{\varepsilon^2}C_v^2\left(\|p_H(t)\|_\infty^2 + \|\nabla_H p_H(t)\|_\infty^2\right),$$

$$
\begin{aligned}
\tau_c^*(t) = \frac{C}{2\varepsilon^2}\sum_{\Delta\in\mathscr{T}_H}(diam\Delta)^4\Big(&\|T(t)\|_{H^2(\Delta)}^2\|c(t)\|_{C^1(\Delta)}^2 + \|D_c(t)\|_{\infty,L^\infty(\Delta)}^2\|c(t)\|_{H^3(\Delta)}^2\\
&+\|D_c(t)\nabla c(t)\|_{[H^2(\Delta)]^2}^2 + \|v(t)c(t)\|_{[H^2(\Delta)]^2}^2\\
&+\|c(t)\|_{C^1(\Delta)}^2\|p(t)\|_{H^3(\Delta)}^2 + \|c'(t)\|_{H^2(\Delta)}^2\Big),
\end{aligned}
$$

where $\varepsilon \neq 0$ is an arbitrary constant.

Proof. From (4.29), with $w_H = e_{H,c}(t)$, taking into account (3.25), (3.26) and (4.36), using $d_{c,i} \geq \beta_1$ in $\mathbb{R}^2$, $i = 1,2$, we have

$$\begin{aligned}
\frac{1}{2}\frac{d}{dt}\|e_{H,c}(t)\|_H^2 + \beta_1\|\nabla_H e_{H,c}(t)\|_H^2 \leq\ & 2L_{D_c}(\|e_{H,p}(t)\|_H + \|e_{H,T}(t)\|_H)\|\nabla_H R_H c(t)\|_\infty \|\nabla_H e_{H,c}(t)\|_H \\
&+ \sqrt{2}C_v\big(\|p_H(t)\|_\infty + \|\nabla_H p_H(t)\|_\infty\big)\|e_{H,c}(t)\|_H\|\nabla_H e_{H,c}(t)\|_H \\
&+ 2L_v\Big(\|e_{H,p}(t)\|_H + \sqrt{2C_m}\|\nabla_H e_{H,p}(t)\|_H\Big)\|R_H c(t)\|_\infty\|\nabla_H e_{H,c}(t)\|_H \\
&+ |\tau_{D_c}(e_{H,c}(t))| + |\tau_v(e_{H,c}(t))| + |\tau_c(e_{H,c}(t))|.
\end{aligned}$$

Considering Propositions 3.1, 4.5 and 4.6, we get

$$\begin{aligned}
\frac{d}{dt}\|e_{H,c}(t)\|_H^2 + 2(\beta_1 - 6\varepsilon^2)\|\nabla_H e_{H,c}(t)\|_H^2 \leq\ & \frac{4}{\varepsilon^2}L_{D_c}^2\big(\|e_{H,p}(t)\|_H^2 + \|e_{H,T}(t)\|_H^2\big)\|\nabla_H R_H c(t)\|_\infty^2 \\
&+ \frac{2}{\varepsilon^2}C_v^2\big(\|p_H(t)\|_\infty^2 + \|\nabla_H p_H(t)\|_\infty^2\big)\|e_{H,c}(t)\|_H^2 \\
&+ \frac{4}{\varepsilon^2}L_v^2\Big(\|e_{H,p}(t)\|_H^2 + 2C_m\|\nabla_H e_{H,p}(t)\|_H^2\Big)\|R_H c(t)\|_\infty^2 + \tau_c^*(t),
\end{aligned}$$

with $\varepsilon \neq 0$. Finally, multiplying the last inequality by $e^{-\int_0^t g_H(p_H(s))ds}$, we obtain

$$\begin{aligned}
\frac{d}{dt}\Big(& e^{-\int_0^t g_H(p_H(s))ds}\|e_{H,c}(t)\|_H^2 + 2(\beta_1 - 6\varepsilon^2)\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\|\nabla_H e_{H,c}(s)\|_H^2 ds \\
&- \frac{4}{\varepsilon^2}L_{D_c}^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}(\|e_{H,p}(s)\|_H^2 + \|e_{H,T}(s)\|_H^2)\|\nabla_H R_H c(s)\|_\infty^2 ds \\
&- \frac{4}{\varepsilon^2}L_v^2\int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\big(\|e_{H,p}(s)\|_H^2 + 2C_m\|\nabla_H e_{H,p}(s)\|_H^2\big)\|R_H c(s)\|_\infty^2 ds \\
&- \int_0^t e^{-\int_0^s g_H(p_H(\mu))d\mu}\tau_c^*(s)ds\Big) \leq 0,
\end{aligned}$$

which gives us (4.37). □

Finally, we achieve the second order of convergence of our fully discrete in space FEM to approximate the solution of the coupled problem (1.1)-(1.9). In Theorem 4.2 we consider $\varepsilon \neq 0$, such that $\beta_1 - 6\varepsilon^2 > 0$. Corollary 2.2 guarantees the uniform boundness of $g_H(p_H(t))$, $H \in \Lambda$, for $H_{\max}$ small enough, and by Corollaries 2.1, 4.1, we conclude the following result:

Corollary 4.3. *Under the assumptions of Theorems 2.3, 4.1 and 4.2, there exists a positive constant C, H and t independent, such that*

$$\|e_{H,c}(t)\|_H^2 + \int_0^t \|\nabla_H e_{H,c}(s)\|_H^2 ds \leq CH_{\max}^4,\ t \in [0, T_f],$$

for $H \in \Lambda$ and $H_{\max}$ small enough.

4.4 Numerical Results

In this section we illustrate the theoretical convergence rates. For the spatial discretization we consider the FDMs introduce before:

(i) (2.10), (2.11), (2.12) for the acoustic pressure $p_H(t)$;

(ii) (4.9), (4.10), (4.11) for the temperature $T_H(t)$;

(iii) (4.15), (4.16), (4.17) for the concentration $c_H(t)$.

We start by defining the numerical strategy used for the time discretization of the previous FD methods. We define a uniform time mesh for $[0,T_f]$, given by $t_n = n\Delta t$, for $n = 0,\dots,M_t$, with $t_{M_t} = T_f$ and Δt the time step. By p_H^n, T_H^n, and c_H^n we denote the numerical approximations for $p_H(t_n)$, $T_H(t_n)$, and $c_H(t_n)$, respectively. We consider an implicit approach, except in the diffusion term of the equation for the temperature, where we consider an explicit term. To compute p_H^n, T_H^n, and c_H^n, we use the following numerical methods

$$a_H \frac{p_H^{n+1} - 2p_H^n + p_H^{n-1}}{\Delta t^2} + b_H \frac{p_H^{n+1} - p_H^n}{\Delta t} = \nabla_H^* \cdot (E_H \nabla_H p_H^{n+1}) + f_{3,H}^{n+1} \text{ in } \Omega_H,$$

for $n = 1,\dots,M_t - 1$,

$$\frac{T_H^{n+1} - T_H^n}{\Delta t} = \nabla_H^* \cdot \left(D_{T,H}^n \nabla_H T_H^{n+1}\right) + kT_H^{n+1} + f_2(p_H^{n+1}) + g_{2,H}^{n+1} \text{ in } \Omega_H,$$

for $n = 0,\dots,M_t - 1$,

$$\frac{c_H^{n+1} - c_H^n}{\Delta t} + \nabla_{c,H} \cdot (c_H^{n+1} v_H^{n+1}) = \nabla_H^* \cdot (D_{c,H}^{n+1} \nabla_H c_H^{n+1}) + f_{1,H}^{n+1} \text{ in } \Omega_H,$$

for $n = 0,\dots,M_t - 1$, complemented with the initial conditions

$$\frac{p_H^1 - p_H^0}{\Delta t} = R_H p_{v,0}, \quad p_H^0 = R_H p_0, \quad T_H^0 = R_H T_0, \quad \text{and} \quad c_H^0 = R_H c_0, \quad \text{in } \Omega_H,$$

and the boundary conditions

$$p_H^n = 0, \quad T_H^n = 0, \quad \text{and} \quad c_H^n = 0, \quad \text{on } \partial\Omega_H, n = 0,\dots,M_t.$$

We define the numerical errors associated with this fully discrete approximation by

$$e_{H,p}^n = R_H p(t_n) - p_H^n, \quad e_{H,T}^n = R_H T(t_n) - T_H^n, \quad \text{and} \quad e_{H,c}^n = R_H c(t_n) - c_H^n.$$

In the following, we introduce two examples that will be used to illustrate the theoretical results established in the previous section.

Example 4.1. *Regarding the coefficient functions of system* $(1.1)-(1.9)$ *we set*

$$a(x,y) = 1 + x, \quad b(x,y) = 2xy, \quad e_1(x,y) = x + y, \quad \textit{and} \quad e_2(x,y) = y$$

in the acoustic pressure equation (1.1),

$$d_{T,1}(T) = 1+2T, \quad d_{T,2}(T) = 1+T, \quad k=1, \quad \textit{and} \quad f_2(p) = p$$

in the temperature equation (1.2), and

$$v(p,\nabla p) = \left(p+\frac{\partial p}{\partial x}, p+\frac{\partial p}{\partial y}\right), \quad d_{c,1}(p,T) = 1+p+T, \quad \textit{and} \quad d_{c,2}(p,T) = 2+p^2+T^2$$

in the concentration equation (1.3). In order to obtain a problem with known solution, the initial conditions $(1.4)-(1.6)$ *and the functions* f_1*,* g_2*, and* f_3 *are defined such that the solution of the coupled system* $(1.1)-(1.9)$ *is given by*

$$p(x,y,t) = e^t xy(1-x)(1-\cos(2\pi y)), \quad T(x,y,t) = e^t x\sin(2\pi y)(x-1)(y-1)$$
$$\textit{and} \quad c(x,y,t) = e^t xy\sin(2\pi x-\pi)(1-y),$$

for $(x,y)\in[0,1]^2$*,* $t\in[0,T_f]$ *with* $T_f = 0.1$*.*

Note that in Example 4.1, b, e_1 and e_2 do not verify the assumption $b \geq b_0 > 0$, $e_i \geq e_0 > 0$, $i=1,2$, in $\overline{\Omega}$. However, the numerical results presented in what follows illustrate the convergence orders established in Corollaries 2.1, 4.1 and 4.3.

To estimate the rate of convergence we use the quantities

$$E_{H,p} = \max_{n=1,\ldots,M_t} \|D_{-t}e^n_{H,p}\|_H + \|\nabla_H e^n_{H,p}\|_H,$$
$$E_{H,T} = \max_{n=1,\ldots,M_t} \|e^n_{H,T}\|_H + \|\nabla_H e^n_{H,T}\|_H,$$
$$E_{H,c} = \max_{n=1,\ldots,M_t} \|e^n_{H,c}\|_H + \|\nabla_H e^n_{H,c}\|_H,$$

for acoustic pressure, temperature and concentration variables, respectively.

Just like in the previous chapters, for the numerical calculations, we consider an initial random mesh H_1 defined by a vector of size $N\times M$. The size of this mesh is successively increased (by two in each direction) by adding to the new mesh the midpoints of the current mesh. On each mesh H_j, $j\in\mathbb{N}$, we measure the errors $E_{H,p,j}$, $E_{H,T,j}$, and $E_{H,c,j}$.The time step is given by $\Delta t = H^2_{\min,j}$, which is small enough to ensure that the error of the time discretization is negligible.

N	M	$H_{\max}$	$E_{H,p}$	$E_{H,T}$	$E_{H,c}$
6	7	2.056e-01	4.083e-02	5.774e-02	6.299e-02
12	14	1.028e-01	1.384e-02	1.432e-02	1.635e-02
24	28	5.141e-02	3.641e-03	3.572e-03	4.121e-03
48	56	2.570e-02	8.999e-04	8.926e-04	1.032e-03
96	112	1.285e-02	2.253e-04	2.231e-04	2.582e-04
192	224	6.426e-03	5.664e-05	5.578e-05	6.455e-05

Table 4.1 The errors $E_{H,p}$, $E_{H,T}$ and $E_{H,c}$ on successively refined meshes for the coupled problem, for the Example 4.1.

In Table 4.1 the data and the obtained errors for each mesh are presented. Using the information of Table 4.1, we plot in Figure 4.1 the $\log(E_{H,p})$, $\log(E_{H,T})$ and $\log(E_{H,c})$ versus $\log(H_{\max})$. Assuming $E_{H,p}$, $E_{H,T}$ and $E_{H,c}$ are proportional to $H^r_{\max}$, for some $r \in \mathbb{R}$, the slope of the best fitting least square line estimates the convergence rate. The obtained estimated values are 1.9231 for $E_{H,p}$, 2.0026 for $E_{H,T}$ and 1.9887 for $E_{H,c}$. These values confirm the convergence rate equal to 2 proved in Corollaries 2.1, 4.1 and 4.3. Plots of the numerical solutions, considering the finest mesh with $T_f = 0.1$ are shown in Figure 4.2.

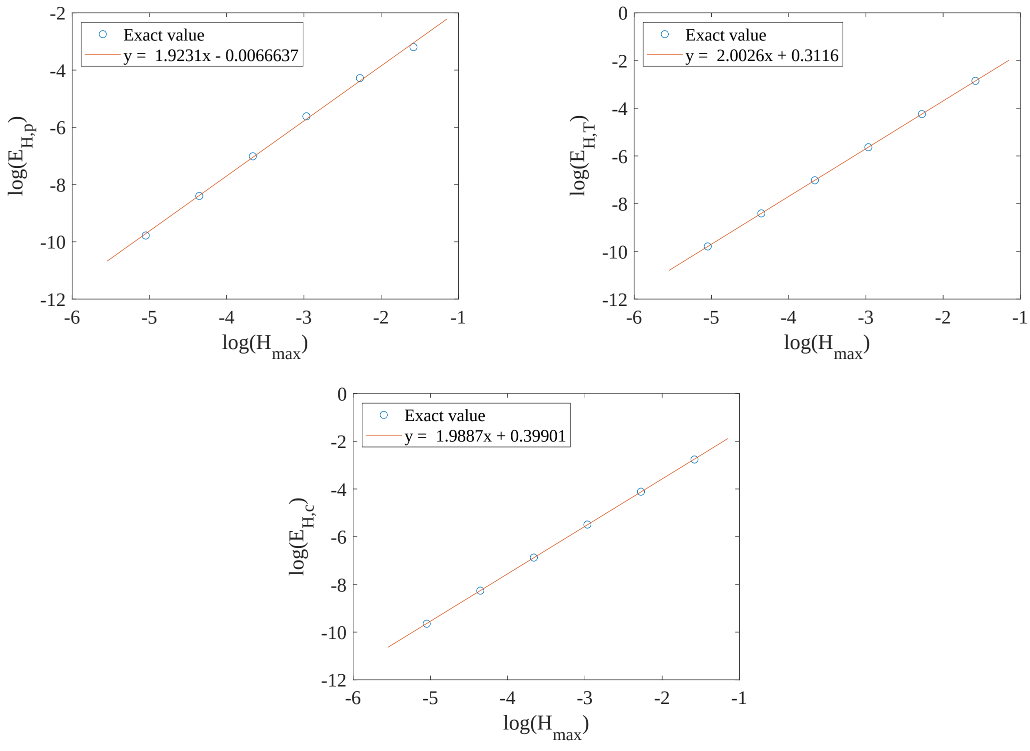


Fig. 4.1 Log-log plots of $E_{H,p}$, $E_{H,T}$ (first row - from left to right) and $E_{H,c}$ (second row) versus $H_{\max}$, for the Example 4.1. The best fitting least square line is shown as a solid line.

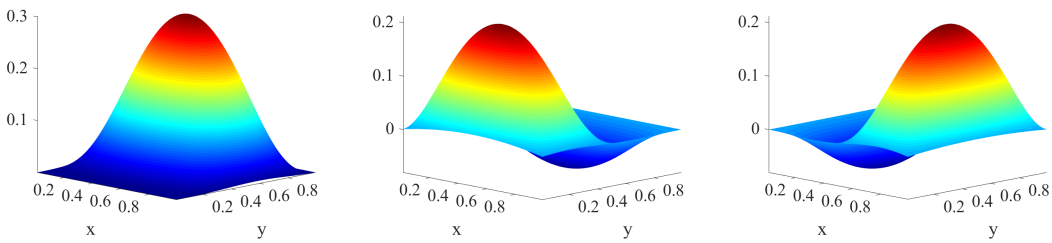


Fig. 4.2 From left to right: numerical approximations $p_H^{M_t}$, $T_H^{M_t}$ and $c_H^{M_t}$ with $N = 192$ and $M = 224$, for the Example 4.1.

Example 4.2. *In this second example, we test the sharpness of the smoothness condition imposed to $p(t)$, $T(t)$ and $c(t)$ on the convergence results: Theorems 2.3, 4.1 and 4.2. Namely, we set our* *problem (1.1)-(1.9) such that the solution of the concentration equation (1.3) is given by*

$$c(x,y,t) = 2e^t x^2 y(x-1)(y-1)|y-0.5|^{2.1}.$$

This solution function belongs only to $H^2(\Omega)$ and does not satisfy the conditions of Theorem 4.2, which requires solutions with higher regularity, at least $H^3(\Omega)$. Thus, a decrease in the convergence rate for the variable c may occur. All the other parameters are the same as the ones used in Example 4.1.

N	M	$H_{\max}$	$E_{H,p}$	$E_{H,T}$	$E_{H,c}$
6	8	2.046e-01	4.185e-02	5.830e-02	2.910e-03
12	16	1.023e-01	1.454e-02	1.434e-02	1.560e-03
24	32	5.116e-02	3.864e-03	3.570e-03	8.128e-04
48	64	2.558e-02	9.484e-04	8.916e-04	3.814e-04
96	128	1.279e-02	2.370e-04	2.229e-04	1.833e-04
192	256	6.395e-03	5.914e-05	5.571e-05	8.639e-05

Table 4.2 The errors $E_{H,p}$, $E_{H,T}$ and $E_{H,c}$ on successively refined meshes for the coupled problem, for the Example 4.2.

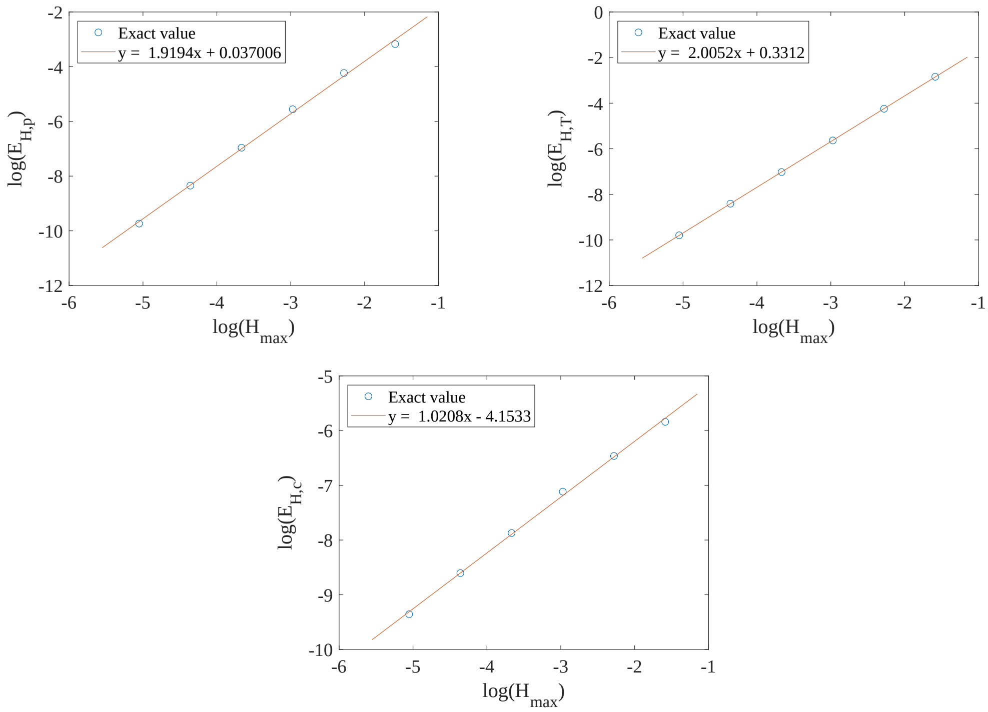


Fig. 4.3 Log-log plots of $E_{H,p}$, $E_{H,T}$ (first row - from left to right) and $E_{H,c}$ (second row) versus $H_{\max}$, for the Example 4.2. The best fitting least square line is shown as a solid line.

In Table 4.2, the results of $E_{H,p}$, $E_{H,T}$ and $E_{H,c}$ for each mesh, considering the Example 4.2, are given. In Figure 4.3, it is present the log-log plots of $E_{H,p}$, $E_{H,T}$ and $E_{H,c}$ versus $H_{\max}$, and the best fitting least square line for each case, where the slope illustrates the convergence rate. These results show that the convergence rate for the concentration variable c is only one, while for the other variables we still get second convergence rate. These results suggest that the regularity conditions imposed on the solutions of (1.1)-(1.9) are sharp, in the sense that if these restrictions do not hold, then a loss in convergence rate may appear. This behavior is in line with the findings of [14].

4.5 Conclusions

In this chapter we propose a numerical method for the coupling of the wave equation with two parabolic equations: the IBVP (1.1)-(1.9). The proposed semi-discrete method is defined by (2.8), (2.9), (4.7), (4.8), and (4.13), (4.14), and it can be seen as a piecewise linear finite element method with quadrature. This method can also be seen as the finite difference method (2.10), (2.11), (2.12), (4.9), (4.10), (4.11), and (4.15), (4.16), (4.17) defined on nonuniform rectangular mesh for the spatial domain.

The main results of this chapter give us the second order of convergence of the approximation for the temperature and concentration related to a discrete L^2- norm: Corollary 4.1, for the numerical approximation for the temperature which is obtained from Theorem 4.1 and Corollary 2.1; Corollary 4.3 which arises from Theorem 4.2 and Corollaries 2.1, 2.2 and 4.1, where the second order of convergence of $c_H(t)$ is stated. Corollary 4.3 is a supra-superconvergence result in the sense that it can be seen simultaneously in the finite difference and finite element contexts, and it was established assuming that $p(t)$, $T(t)$, $c(t) \in H^3(\Omega)$.

A set of numerical experiments were included to illustrate the main results of this chapter, Corollaries 4.1 and 4.3, as well as the sharpness of the imposed smoothness assumptions, $p(t), T(t), c(t) \in H^3(\Omega)$. If for instance $c(t) \in H^2(\Omega)$, then only first convergence rate is observed.

Chapter 5

Conclusions and Future Work

In drug delivery systems, the use of enhancers like ultrasound, light, electric and magnetic fields is becoming a common approach. Such enhancers can have three main roles: breaking biological barriers, increasing drug transport, and controlling drug release (avoiding side effects and maintaining a desired therapeutic level). To optimize the enhancer protocols, the study *in silico* of the drug transport through the target tissue, under the effect of the enhancer, is an important part of the puzzle. In this thesis, we consider a system of partial differential equations that can be used to mathematically describe the drug transport through a target tissue enhanced by ultrasound. The system takes into account all variables of interest: acoustic pressure, temperature, and concentration.

At the best of our knowledge, the differential problem has no explicit solution then, in order to study qualitatively and quantitatively the coupled IBVP, it is crucial to have a numerical method that allows an accurate computation of numerical approximations for the acoustic pressure, temperature, and drug concentration. This work intends to contribute to the solution of this problem - to introduce a numerical method and to develop the theoretical support that allows its safe use. Note that the main challenge is the dependence of the drug concentration equation on the gradient of the acoustic pressure, as well as on the temperature.

In Chapter 2, it is considered the wave problem (1.1), (1.4), (1.7). We construct the fully discrete in space piecewise linear finite element method (2.8), (2.9) to approximate the continuous solution, which can also be seen as the finite difference method in nonuniform meshes (2.10), (2.11), (2.12). We prove Theorem 2.3 and Corollary 2.1 that state the second order of convergence of the proposed semi-discrete method with respect to a discrete H^1- norm. This is a supra-superconvergence result because, as a FDM, the spatial discretization truncation error presents first order with respect to the norm $\|\cdot\|_\infty$. If we consider the piecewise linear FEM correspondent to our fully discrete in space FEM, it is known that it leads to a second order approximation with respect to the L^2- norm and first order approximation with respect to the usual H^1- norm. In this chapter, we also state the uniform boundness of the sequence of acoustic pressure approximations.

In Chapter 3, we consider the previously studied wave problem, coupled with the parabolic system (1.14), (1.6), (1.9). This is a simplified version of the system that we study in Chapter 4. We construct the fully discrete in space piecewise linear FEM (2.8), (2.9), (3.3), (3.4) to approximate the solution of this coupled system, which can also be seen as the finite difference method (2.10), (2.11), (2.12), (3.5), (3.6), (3.7). Since the convective term of (1.14) depends on ∇p, the results of Chapter 2 have a crucial role in the convergence analysis presented here. We prove that the approximation for the concentration has second order of convergence with respect to a discrete L^2- norm - Theorem 3.1 and Corollary 3.1.

Finally, in Chapter 4, we consider the complete coupled problem (1.1)-(1.9). We propose the semi-discrete method (2.8), (2.9), (4.7), (4.8), (4.13), (4.14) to compute an approximation for the solution of this problem. In Theorem 4.1 and Corollary 4.1, it is established that the proposed method leads to a second order approximation for the temperature with respect to a L^2- norm. Lastly, Theorem 4.2 and Corollary 4.3 present the main result of this work: the coupled method leads to a second order approximation for the concentration with respect to a discrete L^2- norm. Note that this result depends on the results for $p_H(t)$ and $T_H(t)$.

The convergence results were proved assuming that the solutions of the correspondent differential problems belong to $H^3(\Omega)$. The Bramble-Hilbert Lemma is the main tool used in the proofs of the convergence results that allows the reduction of the smoothness usually imposed in the convergence analysis of this kind of methods.

Finally, we would like to point out some questions related to the research developed in this work that will be studied in the near future. The drug transport through skin enhanced by ultrasound, and the correspondent validation, will be studied. Moreover, the acoustic pressure propagation was described in this work by a linear wave equation. However, to study the effects of the ultrasound, for example, in the skull, another approach should be followed. One idea is to model the particle displacement using the viscoelastic wave equation of solids (1.13), as in [34].

The accuracy of the semi-discrete approximations for the solutions of different problems were studied and error estimates were established. The convergence of the fully discrete in space and time approximations for the solutions of the coupled problems was not studied. We remark that results for the fully discrete approximations can be obtained considering the semi-discretization error and the error of the time integration of the semi-discrete approximation. However, estimates for the last error depend on the time derivatives of the semi-discrete approximations. To avoid such dependence, the accuracy of the fully discrete approximation should be studied considering the correspondent error equation. This task is particularly difficult for the fully discrete methods introduced here for the nonlinear coupled problems. This question will be addressed in the near future.

The convergence results for the semi-discrete approximation of different coupled problems were established analyzing carefully the error equation. However, the stability of such approximations is an important property that needs to be studied. As we were dealing with nonlinear problems, the stability analysis is not a simple task. In fact, it requires the uniform boundness of the semi-discrete solutions and it will be object of analysis.

In this work, we studied systems of partial differential equations that can be used to describe physical problems, coupling different phenomena occurring in the same spatial domain. However, in drug delivery enhanced by ultrasound, the drug can be transported by a nanocarrier that will be in contact with the target tissue. Then a set of phenomena that need to be considered take place in the nanocarrier. In this case, we have a set of phenomena that occur in different domains. Mathematically, these physical processes are described by systems of partial differential equations defined in different spatial domains. The construction of numerical methods for this kind of differential systems as well as their theoretical support needs to be studied.

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