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DRUG DELIVERY ASSISTED BY ULTRASOUND IN VISCOELASTIC MATERIALS

A MATHEMATICAL APPROACH

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Abstract

The main goal of this work is the analytical and numerical study of a differential system defined by an integro-differential equation of hyperbolic type and a convection-diffusion-reaction equation. This system arises in the mathematical modeling of drug delivery enhanced by ultrasound. In this case, the hyperbolic equation describes the target displacement generated by ultrasound and the second equation describes the drug transport. The parabolic equation depends on the displacement and eventually on its time derivative. The differential system is completed by initial conditions and homogeneous boundary conditions of Dirichlet type. We establish existence, uniqueness and stability results for the displacement and concentration in both the continuous and the semi-discrete cases. In the continuous case, the existence result for the displacement problem is established considering the method of separation of variables, the stability is proved considering the energy method that allows us to get an estimate for the potential and kinetic energies. The existence of concentration is obtained applying a known result. The stability is proved using again the energy method. In the stability analysis of the semi-discrete approximations for the displacement and concentration, we follow discrete versions of the arguments used in the continuous case. The convergence analysis of the semi-discrete approximations is also based in the discrete energy method and second convergence order is obtained. We observe that the spatial truncation error is only of first order with respect to the norm $\|\cdot\|_\infty$. The numerical results illustrating the theoretical results established are also included.

Resumo

O objectivo principal deste trabalho é o estudo analítico e numérico de um sistema diferencial definido por uma equação integro-diferencial do tipo hiperbólico e uma equação de convecção-difusão-reação. Este sistema surge na modelação matemática da administração de fármacos assistida por ultrassom. Neste caso, a equação hiperbólica descreve o deslocamento no meio gerado pelo ultrassom e a segunda equação descreve o transporte do fármaco. A equação parabólica depende do deslocamento e eventualmente da sua derivada temporal. O sistema diferencial é completado com condições iniciais e condições de fronteira homogéneas de Dirichlet. Estabelecemos resultados de existência, unicidade e estabilidade para o deslocamento e para a concentração tanto no caso contínuo como no caso semi-discreto. No caso contínuo, o resultado da existência para o problema do deslocamento é estabelecido considerando o método de separação de variáveis, a estabilidade é provada considerando o método da energia que nos permite encontrar uma estimativa para as energias potencial e cinética. A existência da concentração é obtida aplicando um resultado conhecido. A estabilidade é provada usando novamente o método da energia. Na análise da estabilidade da aproximação semi-discreta para o deslocamento, seguimos versões discretas dos argumentos usados no caso contínuo. A análise da convergência das aproximações semi-discretas é também baseada no método da energia discreto e é obtida segunda ordem de convergência. Observamos que o erro de truncatura espacial é apenas de primeira ordem em relação à norma $\|\cdot\|_\infty$. Os resultados numéricos ilustrando os resultados teóricos obtidos são também incluídos neste trabalho.

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Chapter 1

Introduction

The main goal of this work is to study the differential system defined by an integro-differential equation

$$\rho_0 u_{tt}(x,t) = E_0 u_{xx}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)u_{xx}(x,s)ds + f(x,t), x \in \Omega, t \in (0,T], \tag{1.1}$$

with $\Omega = (0,1)$, and the parabolic equation

$$c_t(x,t) + (c(x,t)v(u(x,t)))_x = Dc_{xx}(x,t) - \gamma c(x,t), x \in \Omega, t \in (0,T], \tag{1.2}$$

complemented with the initial conditions

$$u(x,0) = \phi(x), \frac{\partial u}{\partial t}(x,0) = \psi(x), x \in \Omega, \tag{1.3}$$

$$c(x,0) = c_0(x), x \in \Omega, \tag{1.4}$$

and the boundary conditions of Dirichlet type

$$u(0,t) = u(1,t) = 0, t \in (0,T], \tag{1.5}$$

$$c(0,t) = c(1,t) = 0, t \in (0,T], \tag{1.6}$$

In (1.1) $E(\mu)$ is a kernel function with specific properties that we will specify in what follows. The convective velocity v in (1.2) can be also dependent on u_x but in order to simplify the analysis we consider that v depends only on u.

The differential problem (1.1)-(1.6) can be used to describe mathematically the drug delivery enhanced by ultrasound, as for instance, in [5] and [8]. Ultrasound induces in the target tissue a complex set of phenomena that are characterized by the so called cavitation - expansion and contraction of endogenous or exogenous microbubbles that can be stable or unstable. In this last case, the collapse of the microbubbles can occur generating in the fluid environment several phenomena that can lead to the increase of the permeability of the media and also of the convective transport (see for instance [7]).

In the case of transdermal drug delivery, the ultrasound is used to disrupt the stratum corneum barrier. This layer is the outermost part of the epidermis, is flexible but relatively impermeable due to its brick structure made mostly from proteins and some lipids. The skin is a viscoelastic tissue whose mechanical properties are mainly determined by collagen fibers, elastic fibers, and proteoglycans (see for instance [1]). A viscoelastic material is a material with both elastic and viscous properties. Elasticity is a property of solid objects to deform under tension and then return to its original position. This deformation occurs instantly when the tension is applied and the return to the original position also occurs instantly after the tension is removed. Viscosity is a property of liquids to resist flow. A viscoelastic material has both properties and therefore has properties of both liquids and solids.

The ultrasound generates a pressure wave that propagates through the target tissue, for instance in the skin, that induces a displacement of the tissue. Such displacement can be described by the partial differential equation (1.1) where f denotes the source displacement (a force). Equation (1.2) can be used to describe the drug transport trough the target tissue induced by the tissue displacement and by diffusion. The convective term v can be considered depending on u, u_x or u_t. In what follows we assume that v depends on the displacement and its velocity.

As we mention before, equation (1.1) can be used to describe the displacement evolution of a target tissue under the action of an ultrasound. In fact, the ultrasound generates a pressure wave that induces a displacement in the target namely in viscoelastic materials.

The displacement u of a point $x \in \Omega$ at time t under the action of a force f in this point is described by

$$\rho_0 u_{tt}(x,t) = \sigma_x(x,t) + f(x,t), x \in (0,1), t \in (0,T], \tag{1.7}$$

where σ denotes the stress that is related with the strain ε by the convolution relation

$$\sigma(x,t) = \int_0^t E(t-s)\varepsilon_t(x,s)ds. \tag{1.8}$$

In (1.8), $E(s) = D'e^{-\frac{s}{\tau}}$, τ is a relaxation parameter that corresponds to the time needed to restore its initial state when deforms, and the strain ε is given by

$$\varepsilon(x,t) = u_x(x,t), x \in (0,1), t \in (0,T]. \tag{1.9}$$

From (1.8) and considering (1.9) we obtain successively

$$\begin{aligned} \sigma(x,t) &= \int_0^t E(t-s)\varepsilon_t(x,s)ds \\ &= \varepsilon(x,t)E(0) - \varepsilon(x,0)E(t) - \int_0^t E'(t-s)\varepsilon(x,s)ds \\ &= E_0 u_x(x,t) - \varepsilon(x,0)E(t) + \frac{1}{\tau}\int_0^t E(t-s)u_x(x,s)ds. \end{aligned}$$

Considering that we do not have any initial strain or it is constant, we derive

$$\sigma_x(x,t) = E_0 u_{xx}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)u_{xx}(x,s)ds. \tag{1.10}$$

Taking this expression in (1.7) we conclude (1.1).

Finally we observe that the stress-strain relation (1.8), usually called Maxwell model, can be established considering the differential formulation

$$\sigma + a\sigma_t = C_1 \varepsilon_t, \tag{1.11}$$

where a and C_1 are convenient constants that depend on the properties of the material under consideration.

The generalization of (1.8) is the so called Maxwell-Weichert model

$$\sigma(x,t) = \int_0^t \left(E_0 + \sum_{i=1}^{n} E_i e^{-\frac{t-s}{\tau_i}}\right)\varepsilon_t(x,s)ds,$$

where E_i and τ_i are fixed in function of the characteristics of the material was considered in [9] with $n = 2$ to describe the viscoelastic properties of collagen - a main ingredient in the human skin.

We note that other models can be considered like the Voigt model

$$\sigma = C_0\varepsilon + C_1 \varepsilon_t, \tag{1.12}$$

or Zener model

$$\sigma + a\sigma_t = C_0\varepsilon + C_1 \varepsilon_t, \tag{1.13}$$

(see [10]).

We observe that in [2], [3] and [4], the authors considered (1.1) replaced by the telegraph equation for the pressure intensity

$$u_{tt} + \alpha u_t = \beta u_{xx}, x \in (0,1), t \in (0,T].$$

In this case the authors do not consider the viscoelastic nature of the target tissue. It should be noted that other equations have been considered in the same context to describe the propagation of the pressure waves.

The main goal of this work is to propose a numerical method for the IBVP (1.1)-(1.6) using the so called Method of Lines Approach (MOL) that converts the IBVP (1.1)-(1.6) in a ordinary differential problem. Here we use finite differences approximations defined in nonuniform grids.

The main problem here is to define the right discretization of (1.1) that guarantees that the numerical approximation for (1.2) is sufficiently accurate. In fact, the convective term in the last equation depends u and u_t and consequently, the numerical approximation for the concentration can be deteriorated.

As we intend to work with spatial nonuniform grids, the second order centered finite difference operator for the second order spatial derivative leads to a truncation error of first order with respect to the norm $\|.\|_\infty$. Consequently, we expect that the approximations for the displacement and for the concentration are also of first order accuracy. We will show that such approximations are in fact second order convergent with respect to convenient norms. In the establishment of these results, is crucial the adaptation to our system of equations of the approach followed in [4]. The stability of the semi-discrete solutions is analysed as well error estimates are established.

This thesis is composed by five chapters. In the second chapter, *Mathematical Analysis*, we provide for the displacement and concentration results on the existence, uniqueness and stability. The third chapter, *Numerical Analysis*, is devoted to the study of semi-discrete approximations for the displacement and concentration. Here, we establish results on the existence, uniqueness and stability for such approximations. This chapter ends with the error analysis of the semi-discretization errors where we prove second order accuracy for both approximations - displacement and concentration. In the fourth chapter, *Numerical Simulation*, numerical experiments illustrating the theoretical results are included. The thesis ends with the last chapter, *Conclusions*.

Chapter 2

Mathematical Analysis

2.1 Introduction

In this chapter we present some existence, stability and uniqueness results for the differential problem (1.1), (1.3), (1.5) when $f = 0$. We remark that when $f \neq 0$ the same approach for the existence result can be followed with the convenient adaptations. The existence, stability and uniqueness of the displacement solution are established in Section 2.2. Section 2.3 is focused in the mathematical analysis of the concentrations, namely, we study existence and stability results.

2.2 Existence, stability and uniqueness of the displacement solution

This section aims to establish some existence, stability and uniqueness results for the solution of the IBVP (1.1), (1.3), (1.5) when $f = 0$.

2.2.1 An existence result for the displacement

In what follows we consider that $E(s) = D'e^{-\frac{s}{\tau}}$, where $D' > 0$ and $\tau > 0$ represents the relaxation coefficient that measures the time needed for the medium to restore its initial configuration when deforms subject to a force. To prove that there is at least one solution of the IBVP (1.1), (1.3), (1.5), we use the method of separation of variables.

Let us suppose that $u(x,t) = N(t)M(x)$. From (1.1) we obtain

$$\rho_0 N''(t)M(x) = E_0 N(t)M''(x) + M''(x)\frac{1}{\tau}\int_0^t E(t-s)N(s)ds$$

that, for $N(t)M(x) \neq 0$, leads to

$$\frac{\rho_0 N''(t)}{E_0 N(t) + \frac{1}{\tau}\int_0^t E(t-s)N(s)ds} = \frac{M''(x)}{M(x)}, x \in (0,1).$$

Consequently,

$$\rho_0 N''(t) = \lambda \left(E_0 N(t) + \frac{1}{\tau}\int_0^t E(t-s)N(s)ds \right), t > 0, \tag{2.1}$$

and

$$M''(x) = \lambda M(x), x \in (0,1).$$

From the boundary conditions (1.5) we get $M(0) = M(1) = 0$. Then conclude for M the following boundary value problem

$$\begin{cases} M''(x) = \lambda M(x), x \in (0,1) \\ M(0) = M(1) = 0. \end{cases} \tag{2.2}$$

It is well known that (2.2) has the null solution for $\lambda \geq 0$ and then we take $\lambda = -\beta^2$ with $\beta > 0$. Consequently, we establish

$$\beta = n\pi, n \in \mathbb{N}, M_n(x) = \sin(n\pi x), n \in \mathbb{N}. \tag{2.3}$$

To compute the solution of the ordinary differential equation (2.1), we observe that

$$\rho_0 N^{(3)}(t) = -(n\pi)^2 \left(E_0 N'(t) + E_0 N(t) + \frac{1}{\tau} \int_0^t E'(t-s) N(s) ds \right).$$

Taking into account that $E'(s) = -\frac{1}{\tau} E(s)$, we deduce

$$\rho_0 N^{(3)}(t) = -\beta^2 \left(E_0 N'(t) + E_0 N(t) - \frac{1}{\tau^2} \int_0^t E(t-s) N(s) ds \right).$$

As from (2.1) we have also

$$\int_0^t E(t-s) N(s) ds = -\frac{\tau \rho_0 N''(t) + \tau \beta^2 E_0 N(t)}{\beta^2},$$

we conclude for $N(t)$ the third order ordinary differential equation

$$\rho_0 N^{(3)}(t) + \frac{1}{\tau} \rho_0 N^{(2)}(t) + \beta^2 E_0 N'(t) + \beta^2 E_0 \left(\frac{1}{\tau} + 1 \right) N(t) = 0, t > 0. \tag{2.4}$$

Equation (2.4) is a third order differential equation with constant coefficients, its solution admits the representation

$$N_n(t) = \sum_{\ell=1}^{3} A_{\ell,n} e^{r_{n,\ell} t}, n \in \mathbb{N}, \tag{2.5}$$

where $r_\ell, \ell = 1,2,3$, are the roots of the third order polynomial equation

$$\rho_0 r^3 + \frac{1}{\tau} \rho_0 r^2 + \beta^2 E_0 r + \beta^2 E_0 \left(\frac{1}{\tau} + 1 \right) = 0. \tag{2.6}$$

We observe that the roots $r_\ell, \ell = 1,2,3$, are real or one is real and the other two are imaginary. Let us suppose that r_1 is the real solution and r_2, r_3 are complex solutions. For $n \in \mathbb{N}$, we assume, without loss of generality, that, for $n \leq p_0$, these roots are real and for $n > p_0$ only one root (r_1) is real and

$r_{2,n} = Re(r_{n,2}) + iIm(r_{2,n})$. Consequently,

$$N_n(t) = \sum_{\ell=1}^{3} A_{\ell,n} e^{r_{n,\ell} t}, \text{ for } n \leq p_0,$$

and

$$N_n(t) = \tilde{A}_{1,n} e^{r_{1,\ell} t} + e^{Re(r_{2,n})t} \Big(\tilde{A}_{2,n} \cos(Im(r_{2,n})t) + \tilde{A}_{3,n} \sin(Im(r_{2,n})t) \Big), \text{ for } n > p_0.$$

We are now in position to predict the expression of u. In fact, we have formally

$$\begin{aligned} u(x,t) = & \sum_{n=1}^{p_0} \left(\sum_{\ell=1}^{3} A_{\ell,n} e^{r_{\ell,n} t} \right) \sin(n\pi x) \\ & + \sum_{n=p_0+1}^{\infty} \Big(\tilde{A}_{1,n} e^{r_{1,n} t} + e^{Re(r_{2,n})t} \left(\tilde{A}_{2,n} \cos(Im(r_{2,n})t) + \tilde{A}_{3,n} \sin(Im(r_{2,n})t) \right) \Big) \sin(n\pi x) \\ & , x \in [0,1], t \in [0,T]. \end{aligned} \quad (2.7)$$

To finalize the definition of u, we need to specify conditions for the constants $A_{\ell,n}, \ell = 1,2,3$. From the initial condition (1.3) we should have

$$\begin{aligned} \phi(x) = & \sum_{n=1}^{p_0} \left(\sum_{\ell=1}^{3} A_{\ell,n} \right) \sin(n\pi x) \\ & + \sum_{n=p_0+1}^{\infty} \left(\tilde{A}_{1,n} + \tilde{A}_{2,n} \right) \sin(n\pi x), x \in [0,1], t \in [0,T]. \end{aligned}$$

Consequently, $\sum_{\ell=1}^{3} A_{\ell,n}$, for $n \leq p_0$, and $\tilde{A}_{1,n}, \tilde{A}_{2,n}$, for $n > p_0$, should be given in function of the Fourier coefficients of ϕ as a Fourier series of sines, that is

$$\begin{aligned} & \sum_{\ell=1}^{3} A_{\ell,n} = 2 \int_0^1 \phi(x) \sin(n\pi x)\, dx, n \in \mathbb{N}, n \leq p_0 \\ & \tilde{A}_{1,n} + \tilde{A}_{2,n} = 2 \int_0^1 \phi(x) \sin(n\pi x)\, dx, n \in \mathbb{N}, n > p_0. \end{aligned} \quad (2.8)$$

From the velocity condition of (1.3), we should have

$$\begin{aligned} \psi(x) = & \sum_{n=1}^{p_0} \left(\sum_{\ell=1}^{3} r_{\ell,n} A_{\ell,n} \right) \sin(n\pi x) \\ & + \sum_{n=p_0+1}^{\infty} \left(r_{1,n} \tilde{A}_{1,n} + Re(r_{2,n}) \tilde{A}_{2,n} + Im(r_{2,n}) \tilde{A}_{3,n} \right) \sin(n\pi x), x \in [0,1], t \in [0,T]. \end{aligned}$$

Then we obtain the following equations

$$\begin{aligned} & \sum_{\ell=1}^{3} r_{\ell,n} A_{\ell,n} = 2 \int_0^1 \psi(x) \sin(n\pi x)\, dx, n \in \mathbb{N}, n \leq p_0, \\ & r_{1,\ell} \tilde{A}_{1,n} + Re(r_{2,n}) \tilde{A}_{2,n} + Im(r_{2,n}) \tilde{A}_{3,n} = 2 \int_0^1 \psi(x) \sin(n\pi x)\, dx, n \in \mathbb{N}, n > p_0. \end{aligned} \quad (2.9)$$

The last conditions for the coefficients $A_{\ell,n}, \ell=1,2,3$, for $p \leq p_0$, and $\tilde{A}_{\ell,n}, \ell=1,2,3$, for $n > p_0$, are established considering that the differential equation (1.1) holds at $t=0$. From this assumption we have

$$\rho_0 u_{tt}(x,0) = E_0 u_{xx}(x,0).$$

Assuming that ϕ is smooth enough, namely, there exists ϕ'', we get

$$\rho_0 u_{tt}(x,0) = E_0 \phi''(x).$$

Combining this condition with (2.7), we deduce the last conditions

$$\begin{aligned} &\sum_{\ell=1}^{3} r_{\ell,n}^2 A_{\ell,n} = \frac{2E_0}{\rho_0}\int_0^1 \phi''(x)\sin(n\pi x)\,dx, n \in \mathbb{N}, n \leq p_0, \\ &r_{1,\ell}^2 \tilde{A}_{1,n} + (Re(r_{2,\ell}))^2 \tilde{A}_{2,n} + 2Re(r_{2,n}) Im(r_{2,n}) \tilde{A}_{3,n} \\ &\qquad -\tilde{A}_{2,n}(Im(r_{2,n}))^2 = 2\int_0^1 \psi(x)\sin(n\pi x)\,dx, n \in \mathbb{N}, n > p_0. \end{aligned} \tag{2.10}$$

The algebraic system (2.8)- (2.10) defines the coefficients $A_{n,\ell}, \ell=1,2,3$, for $n \leq p_0$, and $\tilde{A}_{\ell,n}, \ell = 1,2,3$, for $n > p_0$.

Finally, we state the existence result:

Theorem 2.2.1. *Let $A_{\ell,n}, \ell=1,2,3$, for $n \leq p_0$, and $\tilde{A}_{\ell,n}, \ell=1,2,3$, for $n > p_0$, be defined by the algebraic system (2.8)- (2.10). Then (2.7) defines a solution $u \in C^2([0,1]\times[0,T])$ of the IBVP (1.1), (1.3), (1.5) provided that ϕ and ψ are smooth enough.*

We remark that in the near future we intend to specify the minimum smoothness conditions for these two functions that allow us to prove that u is in fact solution of the IBVP (1.1), (1.3), (1.5).

2.2.2 Stability

The main goal of this section is the establishment of stability inequalities for the solution of the IBVP (1.1), (1.3), (1.5). As we are interested in the stability, then it is enough to take $f=0$.

Let $(.,.)_{L^2}$ be the usual inner product in $L^2(0,1)$ defined by

$$(f,g)_{L^2} = \int_0^1 f(x)g(x)dx,\ f,g \in L^2(0,1),$$

and let $\|.\|_{L^2}$ be the correspondent norm.

If $v:[0,1]\times[0,T] \to \mathbb{R}$, then, for $t \in [0,T]$, $v(t)$ denotes the following function $v(t):[0,1]\to\mathbb{R}$ such that $v(t)(x) = v(x,t), x \in [0,1]$.

By $C^m([0,T], C^p([0,1]))$ we denote the space of functions $v:[0,1]\times[0,T]\to\mathbb{R}$ such that, for $t \in [0,T]$, and $j=0,\ldots,m$, $v^{(j)}(t):[0,1]\to\mathbb{R}$ have continuous spatial derivatives of order less or equal than p in $[0,1]$.

Theorem 2.2.2. *Let* $u \in C^2([0,T],C([0,1])) \cap C^1([0,T],C^1([0,1])) \cap C([0,T],C^2([0,1]))$ *be solution of the IBVP (1.1), (1.3), (1.5). If* $\tau E_0 > 2$ *and* β *is a positive constant such that* $\beta < \tau E_0 < 2\beta$ *and*

$$m = \min\left\{\rho_0, \frac{(\tau E_0 - 2)(\tau E_0 - \beta)}{\tau^2 E_0}, \frac{2\beta - \tau E_0}{\tau^2 E_0 \beta}\right\},$$

then

$$\begin{aligned}\int_0^t \left(\|u_t(s)\|_{L^2}^2 + \|u_x(s)\|_{L^2}^2 + \left\|\int_0^s E(s-\mu)u_x(\mu)d\mu + \beta u_x(s)\right\|_{L^2}^2 ds\right)\\ \leq \frac{1}{E_0}\left(\rho_0\|\psi\|_{L^2}^2 + \left(E_0 - \frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2\right)\left(e^{\frac{E_0}{m\tau}t} - 1\right),\end{aligned} \tag{2.11}$$

for $t \in [0,T]$.

Proof. From (1.1) we easily get

$$\rho_0(u_{tt}(t),u_t(t))_{L^2} = E_0(u_{xx}(t),u_t(t))_{L^2} + \frac{1}{\tau}\left(\int_0^t E(t-s)u_{xx}(s)ds, u_t(t)\right)_{L^2}. \tag{2.12}$$

We have

$$\frac{1}{2}\frac{d}{dt}\|u_t(t)\|_{L^2}^2 = (u_{tt}(t),u_t(t))_{L^2}. \tag{2.13}$$

As

$$(u_{xx}(t),u_t(t))_{L^2} = u_x(1,t)u_t(1,t) - u_x(0,t)u_t(0,t) - (u_x(t),u_{xt}(t))_{L^2},$$

and $u_t(0,t) = u_t(1,t) = 0$, we have also

$$(u_{xx}(t),u_t(t))_{L^2} = -(u_x(t),u_{xt}(t))_{L^2}.$$

Furthermore,

$$\frac{d}{dt}\|u_x(t)\|_{L^2}^2 = 2(u_x(t),u_{xt}(t)),$$

leads to

$$\frac{1}{2}\frac{d}{dt}\|u_x(t)\|_{L^2}^2 = -(u_{xx}(t),u_t(t))_{L^2}. \tag{2.14}$$

We need now to deduce a representation of the term $\left(\int_0^t E(t-s)u_{xx}(s)ds, u_t(t)\right)_{L^2}$. Using again that $u_t(0,t) = u_t(1,t) = 0$, we get

$$\left(\int_0^t E(t-s)u_{xx}(s)ds, u_t(t)\right)_{L^2} = -\left(\int_0^t E(t-s)u_x(s)ds, u_{xt}(t)\right)_{L^2}.$$

We start by noting that we have

$$\begin{aligned}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2 &= 2\left(E_0-\frac{\beta}{\tau}\right)\left(\int_0^t E(t-s)u_x(s)ds, u_x(t)\right)_{L^2}\\ &-2\frac{1}{\tau}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2\\ &+\beta^2\frac{d}{dt}\|u_x(t)\|_{L^2}^2+2E_0\beta\|u_x(t)\|_{L^2}^2\\ &+2\beta\left(\int_0^t E(t-s)u_x(s)ds, u_{xt}(t)\right)_{L^2}.\end{aligned}$$

The last equality allow us to obtain

$$\begin{aligned}\left(\int_0^t E(t-s)u_x(s)ds, u_{xt}(t)\right)_{L^2} &= \frac{1}{2\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2\\ &+\frac{1}{\beta}\left(\frac{\beta}{\tau}-E_0\right)\left(\int_0^t E(t-s)u_x(s)ds, u_x(t)\right)_{L^2}\\ &+\frac{1}{\beta\tau}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2\\ &-\frac{\beta}{2}\frac{d}{dt}\|u_x(t)\|_{L^2}^2-E_0\|u_x(t)\|_{L^2}^2.\end{aligned} \tag{2.15}$$

Now we need to establish a representation for $\left(\int_0^t E(t-s)u_x(s)ds, u_x(t)\right)_{L^2}$. As we have

$$\begin{aligned}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2 &= 2E_0\left(\int_0^t E(t-s)u_x(s)ds, u_x(t)\right)_{L^2}\\ &-2\frac{1}{\tau}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2,\end{aligned}$$

we deduce

$$\begin{aligned}\left(\int_0^t E(t-s)u_x(s)ds, u_x(t)\right)_{L^2} &= \frac{1}{2E_0}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2\\ &+\frac{1}{E_0\tau}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2.\end{aligned} \tag{2.16}$$

Taking (2.16) into (2.15), we establish the following representation

$$\begin{aligned}\left(\int_0^t E(t-s)u_x(s)ds, u_{xt}(t)\right)_{L^2} &= \frac{1}{2\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2\\ &+\left(\frac{\beta}{\tau}-E_0\right)\frac{1}{2E_0\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2\\ &+\frac{1}{E_0\tau^2}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2\\ &-\frac{\beta}{2}\frac{d}{dt}\|u_x(t)\|_{L^2}^2-E_0\|u_x(t)\|_{L^2}^2.\end{aligned} \tag{2.17}$$

Inserting (2.13), (2.14) and (2.17) in (2.12), we conclude the following differential inequality

$$\frac{d}{dt}\left(\rho_0\|u_t(t)\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|u_x(t)\|_{L^2}^2+\frac{1}{\tau\beta}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2\right.$$
$$\left.+\frac{\beta-E_0\tau}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2-\frac{E_0}{\tau}\int_0^t\|u_x(s)\|_{L^2}^2ds\right)\le 0, t>0. \tag{2.18}$$

Taking into account the smoothness of u, from (2.18) we derive

$$\rho_0\|u_t(t)\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|u_x(t)\|_{L^2}^2$$
$$+\frac{1}{\tau\beta}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2+\frac{\beta-E_0\tau}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2$$
$$\le\rho_0\|\psi\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2+\frac{E_0}{\tau}\int_0^t\|u_x(s)\|_{L^2}^2ds\le 0, t\in[0,T]. \tag{2.19}$$

We note that $E_0-\frac{\beta}{\tau}$ and $\frac{\beta-E_0\tau}{\tau^2E_0\beta}$ have symmetric signs so we can manipulate in the following way

$$\frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds\right\|_{L^2}^2=\frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)-\beta u_x(t)\right\|_{L^2}^2$$
$$\le 2\frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2-2\beta\frac{E_0\tau-\beta}{\tau^2E_0\beta}\|u_x(t)\|_{L^2}^2 \tag{2.20}$$

getting us to

$$\rho_0\|u_t(t)\|_{L^2}^2+\frac{(\tau E_0-2)(\tau E_0-\beta)}{\tau^2E_0}\|u_x(t)\|_{L^2}^2+\frac{2\beta-\tau E_0}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)u_x(s)ds+\beta u_x(t)\right\|_{L^2}^2$$
$$\le\rho_0\|\psi\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2+\frac{E_0}{\tau}\int_0^t\|u_x(s)\|_{L^2}^2ds\le 0, t\in[0,T]. \tag{2.21}$$

Let $Z(t)$ be defined by

$$Z(t)=\int_0^t\left(\|u_t(s)\|_{L^2}^2+\|u_x(s)\|_{L^2}^2+\left\|\int_0^s E(s-\mu)u_x(\mu)d\mu+\beta u_x(s)\right\|_{L^2}^2\right.$$
$$\left.+\left\|\int_0^s E(s-\mu)u_x(\mu)d\mu\right\|_{L^2}^2\right)ds.$$

Then, from (2.21), we get

$$Z'(t)-\frac{E_0}{m\tau}Z(t)\le\frac{1}{m}\left(\rho_0\|\psi\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2\right), t\ge 0,$$

and consequently

$$Z(t)\le\frac{1}{E_0}\left(\rho_0\|\psi\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2\right)\left(e^{\frac{E_0}{m\tau}t}-1\right), t\in[0,T],$$

that leads to (2.11).

□

Corollary 1. *Under the assumptions of Theorem 2.2.2, we have*

$$\|u_t(t)\|_{L^2}^2 + \|u_x(t)\|_{L^2}^2 \leq \frac{1}{m}\left(\rho_0\|\psi\|_{L^2}^2 + \left(E_0 - \frac{\beta}{\tau}\right)\|\phi'\|_{L^2}^2\right)e^{\frac{E_0}{m\tau}t}, \tag{2.22}$$

Corollary 2. *Under the assumptions of Theorem 2.2.2, the IBVP (1.1), (1.3), (1.5) has at most one solution.*

Proof. Let us suppose that (1.1), (1.3), (1.5) has two solutions u and w and let $\omega = u - w$. We have

$$\|\omega_t(t)\|_{L^2} = 0, \|\omega_x(t)\|_{L^2} = 0, t \in [0,T].$$

From $\|\omega_t(t)\|_{L^2} = 0$, using the continuity of $\omega_t(x,t)$, we get $\omega(t) = g(x)$. Using now the fact that we have also $\omega_x(x,t) = 0$, we obtain $\omega(x,t) = const$. Then we conclude the proof taking into account that $\omega(x,0) = 0$. □

2.3 Coupling the displacement with the concentration

Taking into account the results established for the displacement u defined by IBVP (1.1), (1.3), (1.5), the main objective of this section is to establish the existence and the uniqueness of the concentration defined by the IBVP (1.2), (1.4) and (1.6).

2.3.1 An existence result

We observe that the differential equation (1.2) can be rewritten in the following equivalent form

$$c_t(x,t) - Lc(x,t) + (\gamma + (v(u(x,t)))_x)c(x,t) = 0, x \in \Omega, t \in (0,T],$$

where

$$Lc(x,t) = Dc_{xx}(x,t) - v(u(x,t))c_x(x,t).$$

The existence of the solution of the IBVP (1.2), (1.4) and (1.6) is given by Theorem 1.1 of [6].

We recall that a function $g \in C((0,1)\times(0,T])$ is said to be Hölder continuous with coefficient $\alpha \in (0,1)$ if

$$\sup_{x,y\in(0,1),t,t'\in(0,T]} \frac{|g(x,t) - g(y,t')|}{((t-t')^2 + (x-y)^2)^{\frac{\alpha}{2}}} < +\infty.$$

For $p,q \in \mathbb{N}_0$, by $C^{p,q}((0,1)\times(0,T])$ we represent the space of functions whose p time derivatives in x and q times derivatives in t are continuous in $(0,1)\times(0,T]$.

Theorem 2.3.1. *If $v'(u)u_x$ and $v(u)$ are Hölder continuous in $(0,1)\times(0,T]$ and $c_0(0) = c_0(1) = 0$, then the IBVP (1.2), (1.4) and (1.6) has a unique solution in $C([0,1]\times[0,T]) \cap C^{2,1}((0,1)\times(0,T])$.*

2.3.2 Stability for the concentration

In this section we will establish energy estimates for the solution of the IBVP (1.2), (1.4) and (1.6).

Theorem 2.3.2. *Let* $c \in C([0,1]\times[0,T]) \cap C^{2,1}((0,1)\times(0,T))$ *be the solution of the IBVP (1.2), (1.4) and (1.6). If*

$$|v(y)| \leq L_\infty |y|, y \in \mathbb{R}, \tag{2.23}$$

then

$$\|c(t)\|_{L^2}^2 + 2(D-\varepsilon^2)\int_0^t e^{\int_s^t g(u(\mu))d\mu}\|c_x(s)\|_{L^2}^2 ds \leq e^{\int_0^t g(u(s))ds}\|c_0\|_{L^2}^2, \tag{2.24}$$

for $t \in [0,T]$, *where*

$$g(u(t)) = \frac{1}{2\varepsilon^2}L_\infty^2\|u(t)\|_\infty^2 - 2\gamma \tag{2.25}$$

Proof. From (1.2), taking into account the homogeneous boundary conditions, we easily obtain

$$(c_t(t),c(t))_{L^2} + D\|c_x(t)\|_{L^2}^2 = (v(u(t))c(t),c_x(t))_{L^2} - \gamma\|c(t)\|_{L^2}^2. \tag{2.26}$$

Considering that $|v(y)| \leq L_\infty|y|, y \in \mathbb{R}$, we get successively

$$\begin{aligned}(v(u(t))c(t),c_x(t))_{L^2} &\leq L_\infty\|u(t)\|_\infty\|c(t)\|_{L^2}\|c_x(t)\|_{L^2}\\ &\leq \frac{1}{4\varepsilon^2}L_\infty^2\|u(t)\|_\infty^2\|c(t)\|_{L^2}^2 + \varepsilon^2\|c_x(t)\|_{L^2}^2,\end{aligned}$$

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

Then, from (2.26), and using the fact

$$(c_t(t),c(t))_{L^2} = \frac{1}{2}\frac{d}{dt}\|c(t)\|_{L^2}^2,$$

we have

$$\frac{d}{dt}\|c(t)\|_{L^2}^2 + 2(D-\varepsilon^2)\|c_x(t)\|_{L^2}^2 \leq \left(\frac{1}{2\varepsilon^2}L_\infty^2\|u(t)\|_\infty^2 - 2\gamma\right)\|c(t)\|_{L^2}^2,$$

for $t>0$, that can be rewritten in the following equivalent form

$$\frac{d}{dt}\left(\|c(t)\|_{L^2}^2 e^{-\int_0^t g(u(s))ds} + 2(D-\varepsilon^2)\int_0^t e^{-\int_0^s g(u(\mu))d\mu}\|c_x(s)\|_{L^2}^2 ds\right) \leq 0, \tag{2.27}$$

for $t>0$. In (2.27), $g(u)$ is defined by (2.25).

Inequality (2.27) finally leads to (2.24). □

Under the assumptions of Theorem 2.3.2 we have the stability inequality (2.24) that depends on $g(u)$ given by (2.25). Considering that

$$\|u(t)\|_\infty \leq \|u_x(t)\|_{L^2},$$

we have

$$g(u(s)) \leq \frac{m}{E_0}\left(\|\psi\|_{L^2}^2 + \left(E_0 - \frac{2\beta}{\tau}\right)\|\phi'\|_{L^2}^2\right)\left(e^{\frac{E_0}{m}s} - 1\right).$$

In the next result we establish the stability of the IBVP (1.2), (1.4) and (1.6) comparing two solutions: c and $\tilde{c}$ depending on u and $\tilde{u}$ that are defined by the IBVP (1.1), (1.3), (1.5) with initial conditions ϕ, ψ and $\tilde{\phi}, \tilde{\psi}$, respectively, and two initial concentrations c_0 and $\tilde{c}_0$, respectively.

Theorem 2.3.3. *Let $c, \tilde{c} \in C([0,1]\times[0,T]) \cap C^{2,1}((0,1)\times(0,T])$ be solutions of the IBVP (1.2), (1.4) and (1.6) with initial conditions c_0 and $\tilde{c}_0$ and depending on u and $\tilde{u}$ that are defined by the IBVP (1.1), (1.3), (1.5) with initial conditions ϕ, ψ and $\tilde{\phi}, \tilde{\psi}$, respectively. Let ω_c and ω_u be defined by $\omega_c = c - \tilde{c}$ and $\omega_u = u - \tilde{u}$. If v is bounded by $\|v\|_\infty$ and is a Lipschitz function*

$$|v(y) - v(\tilde{y})| \leq L_v|y - \tilde{y}|, y, \tilde{y} \in \mathbb{R}, \tag{2.28}$$

then

$$\begin{aligned}\|\omega_c(t)\|_{L^2}^2 + 2(D - 2\varepsilon^2)\int_0^t e^{g(v)(t-s)}\|\omega_{cx}(s)\|_{L^2}^2 ds \\ \leq e^{g(v)t}\|\omega_c(0)\|_{L^2}^2 + \frac{1}{2\varepsilon^2}L_v^2\int_0^t e^{g(v)(t-s)}\|\omega_u(s)\|_{L^2}^2\|c(s)\|_\infty^2 ds,\end{aligned} \tag{2.29}$$

for $t \in [0,T]$, where

$$g(v) = \frac{1}{2\varepsilon^2}\|v\|_\infty^2 - 2\gamma \tag{2.30}$$

Proof. Considering (1.2) for c and $\tilde{c}$, for ω_c we obtain the following

$$(\omega_{ct}(t), \omega_c(t))_{L^2} + D\|\omega_{cx}(t)\|_{L^2}^2 = (v(u(t))c(t) - v(\tilde{u}(t))\tilde{c}(t), \omega_{cx}(t))_{L^2} - \gamma\|\omega_c(t)\|_{L^2}^2. \tag{2.31}$$

Considering that v is a Lipschitz function, we deduce

$$\begin{aligned}(v(u(t))c(t) - v(\tilde{u}(t))\tilde{c}(t), \omega cx(t))_{L^2} &= ((v(u(t)) - v(\tilde{u}(t)))c(t), \omega_{cx}(t))_{L^2} \\ &\quad + (v(\tilde{u}(t)))\omega_c(t), \omega_{cx}(t))_{L^2} \\ &\leq L_v\|\omega_u(t)\|_{L^2}\|c(t)\|_\infty\|\omega_{cx}(t)\|_{L^2} \\ &\quad + \|v\|_\infty\|\omega_c(t)\|_{L^2}\|\omega_{cx}(t)\|_{L^2} \\ &\leq \frac{1}{4\varepsilon^2}L_v^2\|\omega_u(t)\|_{L^2}^2\|c(t)\|_\infty^2 + 2\varepsilon^2\|\omega_{cx}(t)\|_{L^2}^2 \\ &\quad + \frac{1}{4\varepsilon^2}\|v\|_\infty^2\|\omega_c(t)\|_{L^2}^2,\end{aligned}$$

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

As

$$(\omega_{ct}(t), \omega_c(t))_{L^2} = \frac{1}{2}\frac{d}{dt}\|\omega_c(t)\|_{L^2}^2,$$

we get

$$\begin{aligned}\frac{d}{dt}\|\omega_c(t)\|_{L^2}^2 + 2(D - 2\varepsilon^2)\|\omega_{cx}(t)\|_{L^2}^2 \leq & \left(\frac{1}{2\varepsilon^2}\|v\|_\infty^2 - 2\gamma\right)\|\omega_c(t)\|_{L^2}^2 \\ & + \frac{1}{2\varepsilon^2}L_v^2\|\omega_u(t)\|_{L^2}^2\|c(t)\|_\infty^2,\end{aligned}$$

for $t > 0$.

The last inequality is equivalent to the following one

$$\begin{aligned}&\frac{d}{dt}\Big(\|\omega_c(t)\|_{L^2}^2 e^{-g(v)t}+2(D-2\varepsilon^2)\int_0^t e^{-g(v)s}\|\omega_{cx}(s)\|_{L^2}^2 ds\\&-\frac{1}{2\varepsilon^2}L_v^2\int_0^t e^{-g(v)s}\|\omega_u(s)\|_{L^2}^2\|c(s)\|_\infty^2 ds\Big)\le 0,\end{aligned} \tag{2.32}$$

for $t>0$. In (2.32), $g(v)$ is defined by (2.30).

The inequality (2.29) is easily concluded from (2.32). □

We consider now the Corollary 1 for the stability of the displacement. Under the conditions of the Theorem 2.2.2, we have

$$\|\omega_{ut}(t)\|_{L^2}^2+\|\omega_{ux}(t)\|_{L^2}^2\le\frac{1}{m}\left(\rho_0\|\psi-\tilde{\psi}\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'-\tilde{\phi}'\|_{L^2}^2\right)\left(e^{\frac{E_0}{m\tau}t}-1\right). \tag{2.33}$$

Considering now the Poincaré inequality we also have

$$\|\omega_u(t)\|_{L^2}^2\le\frac{1}{m}\left(\rho_0\|\psi-\tilde{\psi}\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'-\tilde{\phi}'\|_{L^2}^2\right)\left(e^{\frac{E_0}{m\tau}t}-1\right),$$

Corollary 3. *Under the assumptions of Theorems 2.2.2 and 2.3.3, we have*

$$\begin{aligned}&\|\omega_c(t)\|_{L^2}^2+2(D-2\varepsilon^2)\int_0^t e^{g(v)(t-s)}\|\omega_{cx}(s)\|_{L^2}^2 ds\\&\quad\le\frac{1}{2\varepsilon^2}L_v^2\frac{1}{m}\left(\rho_0\|\psi-\tilde{\psi}\|_{L^2}^2+\left(E_0-\frac{\beta}{\tau}\right)\|\phi'-\tilde{\phi}'\|_{L^2}^2\right)\int_0^t e^{g(v)(t-s)}\left(e^{\frac{E_0}{m\tau}s}-1\right)\|c(s)\|_\infty^2 ds\\&\qquad+e^{g(v)t}\|\omega_c(0)\|_{L^2}^2,\end{aligned} \tag{2.34}$$

for $t\in[0,T]$, where $\varepsilon\neq 0$ is an arbitrary constant and $g(v)$ is defined by (2.30).

Corollary 3 allow us to conclude the stability of the coupled problem: displacement defined by the IBVP (1.1), (1.3), (1.5) with concentration defined by the IBVP (1.2), (1.4) and (1.6).

Chapter 3

Numerical Analysis

3.1 Introduction

In this chapter we introduce a ordinary differential system that defines approximations for the displacement and concentration defined by IBVP (1.1)-(1.6). This ordinary differential problem is introduced following the MOL approach- the spatial derivatives presented in the displacement and concentration equations are discretized considering centered finite difference operators defined in nonuniform grids.

In the first part of this chapter : Sections 3.2 and 3.3, we introduce the differential problems for semi-discrete approximations for the displacement and concentration, respectively, and we establish existence, uniqueness and stability results.

The last part, Section 3.4, is focused in the convergence analysis of such semi-discrete approximations. It should be pointed out that the truncation error is first order convergent with respect to the norm $\|\cdot\|_\infty$. However, we show that both approximations are second order accuracy with respect to convenient norms.

3.2 A semi-discrete approximation for the displacement

Let λ be a sequence of vectors $h = (h_1, \ldots, h_N)$ with positive entries, such that

$$h_{max} = \max_{i=1,\ldots,N} h_i \to 0,$$

and

$$\sum_{i=1}^{N} h_i = 1.$$

Considering $h \in \Lambda$ we introduce in $\overline{\Omega} = [0,1]$ the following grid

$$\overline{\Omega}_h = \{x_i, i = 0, \ldots, N : x_0 = 0, x_i = x_{i-1} + h_i, i = 1, \ldots, N\}.$$

We also consider the set of grid points $\Omega_h = \overline{\Omega}_h - \{x_0, x_N\}$.

By W_h we denote the space of grid functions defined in $\overline{\Omega}_h$. Let $W_{h,0}$ be the vector subspace of W_h of the grid functions that are null at the boundary points x_0 and x_N.

In $W_{h,0}$ we introduce the inner product

$$(u_h, w_h)_h = \sum_{i=1}^{N-1} \frac{h_i + h_{i+1}}{2} u_h(x_i) v_h(x_i), u_h, w_h \in W_{h,0},$$

and the corresponding norm is denoted by $\|.\|_h$.

We use the notation

$$(u_h, w_h)_+ = \sum_{i=1}^{N} h_i u_h(x_i) w_h(x_i), u_h, w_h \in W_h,$$

and

$$\|u_h\|_+ = \Big(\sum_{i=1}^{N} h_i u_h(x_i)^2\Big)^{1/2}, u_h, W_h.$$

To discretize the spacial derivatives in (1.1) we introduce the finite difference operator

$$D_2 u_h(x_i) = \frac{h_i u_h(x_{i+1}) - (h_i + h_{i+1}) u_h(x_i) + h_{i+1} u_h(x_{i-1})}{h_i h_{i+1} h_{i+1/2}}, i = 1, \ldots, N-1,$$

where $h_{i+1/2} = \dfrac{h_i + h_{i+1}}{2}$. We observe that if D_{-x} denotes the the backward operator, we have

$$D_2 u_h(x_i) = \frac{D_{-x} u_h(x_{i+1}) - D_{-x} u_h(x_i)}{h_{i+1/2}}, i = 1, \ldots, N-1.$$

Holds the following proposition:

Proposition 1. *For $u_h, w_h \in W_{h,0}$, we have*

$$(D_2 u_h, w_h)_h = -(D_{-x} u_h, D_{-x} w_h)_+. \tag{3.1}$$

Proof. As $w_h(x_0) = w_h(x_N) = 0$ we have successively

$$\begin{aligned}(D_2 u_h, w_h)_h &= \sum_{i=1}^{N-1} D_{-x} u_h(x_{i+1}) w_h(x_i) - \sum_{i=1}^{N-1} D_{-x} u_h(x_i) w_h(x_i) \\ &= \sum_{i=1}^{N} D_{-x} u_h(x_i) w_h(x_{i-1}) - \sum_{i=1}^{N} D_{-x} u_h(x_i) w_h(x_i) \\ &= -\sum_{i=1}^{N} h_i D_{-x} u_h(x_i) D_{-x} w_h(x_i) \\ &= -(D_{-x} u_h, D_{-x} w_h)_+.\end{aligned}$$

□

3.2.1 Existence and uniqueness

We introduce the semi-discrete approximation for the solution of the IBVP (1.1), (1.3), (1.5). Let $u_h(t) \in W_{h,0}, t \in [0,T]$, be defined by the following ordinary differential system

$$\rho_0 u_h''(t)(x_i,t) = E_0 D_2 u_h(x_i,t) + \frac{1}{\tau}\int_0^t E(t-s) D_2 u_h(x_i,s)ds + f(x_i,t), i = 1,\ldots,N-1, t \in (0,T], \tag{3.2}$$

complemented with the initial conditions

$$u_h(x_i,0) = \phi(x_i),\, u_h'(x_i,0) = \psi(x_i), i = 1,\ldots,N-1, \tag{3.3}$$

and the boundary conditions of Dirichlet type

$$u_h(x_0,t) = u_h(x_N,t) = 0, t \in (0,T]. \tag{3.4}$$

To prove that there exists a unique solution $u_h(t) \in W_{h,0}$, we consider $\rho_0 = 1$ to simplify and we remark that the system (3.2), (3.3), (3.4) can be written in the following equivalent form

$$u_h''(t) = E_0 A_h u_h(t) + \frac{1}{\tau}\int_0^t E(t-s) A_h u_h(s)ds + F_h(t), t \in (0,T], \tag{3.5}$$

with the initial conditions

$$u_h(0) = \phi_h, u_h'(0) = \psi_h. \tag{3.6}$$

In this representation $u_h(t)$ is identified with the vector with entries $u_h(x_i,t), i = 1,\ldots,N-1$, and A_h is the tridiagonal matrix induced by the operator D_2 and ϕ_h and ψ_h are identified with the vectors with entries $\phi(x_i)$ and $\psi(x_i)$, $i = 1,\ldots,N-1$, respectively. Finally, $F_h(t)$ represents the vector with entries $f(x_i,t), i = 1,\ldots,N-1$.

Let $Z_h(t)$ and $Q_h(t)$ be defined by

$$Z_h(t) = u_h'(t), \qquad Q_h(t) = \frac{1}{\tau}\int_0^t E(t-s) u_h(s)ds.$$

As we have

$$\begin{aligned} Q_h'(t) &= E(0)u_h(t) - \frac{1}{\tau^2}\int_0^t E(t-s)u_h(s)ds \\ &= \frac{E_0}{\tau}u_h(t) - \frac{1}{\tau}Q_h(t), \end{aligned}$$

and

$$\begin{aligned} Z_h'(t) &= u_h''(t) \\ &= E_0 A_h u_h(t) + A_h\Big(\frac{1}{\tau}\int_0^t E(t-s)u_h(s)ds\Big) + F_h(t) \\ &= E_0 A_h u_h(t) + A_h Q_h(t) + F_h(t), \end{aligned}$$

for the vector with entries $u_h(t), Z_h(t)$ and $Q_h(t)$ we establish the following initial value problem:

$$\begin{bmatrix} u_h'(t) \\ Z_h'(t) \\ Q_h'(t) \end{bmatrix} = \begin{bmatrix} 0 & I & 0 \\ E_0 A_h & 0 & A_h \\ \frac{E_0}{\tau} I & 0 & -\frac{1}{\tau} I \end{bmatrix} \begin{bmatrix} u_h(t) \\ Z_h(t) \\ Q_h(t) \end{bmatrix} + \begin{bmatrix} 0 \\ F_h(t) \\ 0 \end{bmatrix}, t > 0, \tag{3.7}$$

with the initial condition

$$\begin{bmatrix} u_h(0) \\ Z_h(0) \\ Q_h(0) \end{bmatrix} = \begin{bmatrix} \phi_h \\ \psi_h \\ 0 \end{bmatrix}. \tag{3.8}$$

Finally we conclude that there exists a unique solution of the IVP (3.7), (3.8) that admits the representation

$$\mathscr{U}_h(t) = e^{\mathscr{A}_h t}\mathscr{U}_h(0) + \int_0^t e^{\mathscr{A}_h(t-s)}\mathscr{F}_h(s)ds, t \geq 0,$$

where

$$\mathscr{U}_h(t) = \begin{bmatrix} u_h(t) \\ Z_h(t) \\ Q_h(t) \end{bmatrix}, \mathscr{A}_h = \begin{bmatrix} 0 & I & 0 \\ E_0 A_h & 0 & A_h \\ \frac{E_0}{\tau} I & 0 & -\frac{1}{\tau} I \end{bmatrix}, \mathscr{F}_h(t) = \begin{bmatrix} 0 \\ F_h(t) \\ 0 \end{bmatrix}.$$

3.2.2 Stability

Theorem 3.2.1. *Let $u \in W_{h,0}$ be solution of the IBVP (3.2), (3.3), (3.4). If $\tau E_0 > 2$ and β is a positive constant such that $\beta < \tau E_0 < 2\beta$ and m is given by*

$$m = \min\left\{\rho_0, \frac{(\tau E_0 - 2)(\tau E_0 - \beta)}{\tau}, \frac{2\beta - E_0\tau}{\beta E_0 \tau^2}\right\},$$

then

$$\begin{aligned} &\rho_0\|u_h'(t)\|_h^2 + \frac{(\tau E_0 - 2)(\tau E_0 - \beta)}{\tau}\|D_{-x}u_h(t)\|_+^2 + \frac{2\beta - E_0\tau}{\beta E_0\tau^2}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 \\ &\leq e^{\frac{\tau E_0^2}{(\tau E_0 - 2)(\tau E_0 - \beta)}t}\left(\rho_0\|\psi_h\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right)\|\phi_h'\|_+^2\right), \end{aligned} \tag{3.9}$$

for $t \in [0,T]$, and

$$\begin{aligned} &\int_0^t \left(\|u_h'(s)\|_h^2 + \|D_{-x}u_h(s)\|_+^2 + \left\|\int_0^s E(s-\mu)D_{-x}u_h(\mu)d\mu + \beta D_{-x}u_h(s)\right\|_+^2\right) ds \\ &\quad \leq \frac{1}{E_0}\left(\rho_0\|\psi_h\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right)\|\phi_h'\|_+^2\right)\left(e^{\frac{E_0}{m\tau}t} - 1\right), \end{aligned} \tag{3.10}$$

for $t \in [0,T]$.

Proof. From (3.2) we easily get

$$\rho_0(u_h'(t), u_h''(t))_h = E_0(D_2u_h(t), u_h'(t))_h + \frac{1}{\tau}\left(\int_0^t E(t-s)D_2u_h(s)ds, u_h'(t)\right)_h. \tag{3.11}$$

We have

$$\frac{1}{2}\frac{d}{dt}\|u_h'(t)\|_h^2 = (u_h''(t), u_h'(t))_h, \tag{3.12}$$

and

$$\begin{aligned} (D_2u_h(t), u_h'(t))_h &= -(D_{-x}u_h(t), D_{-x}u_h'(t))_+ \\ &= -\frac{1}{2}\frac{d}{dt}\|D_{-x}u_h(t)\|_+^2. \end{aligned} \tag{3.13}$$

We need now to deduce a representation of the term $\left(\int_0^t E(t-s)D_2u_h(s)ds, u_t(t)\right)_h$. Using again (3.1), we get

$$\left(\int_0^t E(t-s)D_2u_h(s)ds, u_h'(t)\right)_h = -\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h'(t)\right)_+.$$

As we have

$$\begin{aligned}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 &= -2\left(\frac{\beta}{\tau}-E_0\right)\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h(t)\right)_+ \\ &\quad -2\frac{1}{\tau}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 \\ &\quad +\beta^2\frac{d}{dt}\|D_{-x}u_h(t)\|_+^2 + 2E_0\beta\|D_{-x}u_h(t)\|_+^2 \\ &\quad +2\beta\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h'(t)\right)_+,\end{aligned}$$

we obtain

$$\begin{aligned}\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h'(t)\right)_+ &= \frac{1}{2\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 \\ &\quad +\frac{1}{\beta}\left(\frac{\beta}{\tau}-E_0\right)\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h(t)\right)_+ \\ &\quad +\frac{1}{\beta\tau}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 \\ &\quad -\frac{\beta}{2}\frac{d}{dt}\|D_{-x}u_h(t)\|_+^2 - E_0\|D_{-x}u_h(t)\|_+^2.\end{aligned} \tag{3.14}$$

Now we need to establish a representation for $\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h(t)\right)_+$. As we have

$$\begin{aligned}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 &= 2E_0\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h(t)\right)_+ \\ &\quad -2\frac{1}{\tau}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2,\end{aligned}$$

we deduce

$$\begin{aligned}\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h(t)\right)_+ &= \frac{1}{2E_0}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 \\ &\quad +\frac{1}{E_0\tau}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2.\end{aligned} \tag{3.15}$$

Taking (3.15) into (3.14), we establish the following representation

$$\left(\int_0^t E(t-s)D_{-x}u_h(s)ds, D_{-x}u_h'(t)\right)_+ = \frac{1}{2\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + D_{-x}u_h(t)\right\|_+^2 + \left(\frac{\beta}{\tau}-E_0\right)\frac{1}{2E_0\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 + \frac{1}{E_0\tau^2}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 - \frac{\beta}{2}\frac{d}{dt}\|D_{-x}u_h(t)\|_+^2 - E_0\|D_{-x}u_h(t)\|_+^2. \tag{3.16}$$

Inserting (3.12), (3.13) and (3.16) in (3.11) we conclude the following differential inequality

$$\frac{d}{dt}\left(\rho_0\|u_h'(t)\|_h^2 + \left(E_0-\frac{\beta}{\tau}\right)\|D_{-x}u_h(t)\|_+^2 + \frac{1}{\tau\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 + \frac{\beta-E_0\tau}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 - \frac{E_0}{\tau}\int_0^t\|D_{-x}u_h(s)\|_+^2ds\right) \le 0, t>0.$$

that leads to

$$\rho_0\|u_h'(t)\|_h^2 + \left(E_0-\frac{\beta}{\tau}\right)\|D_{-x}u_h(t)\|_+^2 + \frac{1}{\tau\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 + \frac{\beta-E_0\tau}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 \le \rho_0\|\psi_h\|_h^2 + \left(E_0-\frac{\beta}{\tau}\right)\|\phi_h'\|_+^2 + \frac{E_0}{\tau}\int_0^t\|D_{-x}u_h(s)\|_+^2ds, t\in[0,T]. \tag{3.17}$$

We note that $E_0-\frac{\beta}{\tau}$ and $\frac{\beta-E_0\tau}{\tau^2E_0\beta}$ have symmetric signs so we can manipulate in the following way

$$\frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds\right\|_+^2 = \frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t) - \beta D_{-x}u_h(t)\right\|_+^2 \le 2\frac{E_0\tau-\beta}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 - 2\beta\frac{E_0\tau-\beta}{\tau^2E_0\beta}\|D_{-x}u_h(t)\|_+^2 \tag{3.18}$$

getting us to

$$\rho_0\|u_h'(t)\|_h^2 + \frac{(\tau E_0-2)(\tau E_0-\beta)}{\tau^2E_0}\|D_{-x}u_h(t)\|_+^2 + \frac{2\beta-\tau E_0}{\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}u_h(s)ds + \beta D_{-x}u_h(t)\right\|_+^2 \le \rho_0\|\psi_h\|_h^2 + \left(E_0-\frac{\beta}{\tau}\right)\|\phi_h'\|_+^2 + \frac{E_0}{\tau}\int_0^t\|D_{-x}u_h(s)\|_+^2ds \le 0, t\in[0,T]. \tag{3.19}$$

Let $Z(t)$ be given by

$$Z(t) = \rho_0 \|u_h'(t)\|_h^2 + \frac{(\tau E_0 - 2)(\tau E_0 - \beta)}{\tau^2 E_0} \|D_{-x} u_h(t)\|_+^2 + \frac{2\beta - \tau E_0}{\tau^2 E_0 \beta} \left\| \int_0^t E(t-s) D_{-x} u_h(s) ds + \beta D_{-x} u_h(t) \right\|_+^2 .$$

Then (3.19) leads to

$$Z(t) \leq \rho_0 \|\psi_h\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right) \|\phi_h'\|_+^2 + \frac{\tau E_0^2}{(\tau E_0 - 2)(\tau E_0 - \beta)} \int_0^t Z(s) ds, t \in [0,T].$$

Gronwall Lemma allow us to obtain

$$Z(t) \leq e^{\frac{\tau E_0^2}{(\tau E_0 - 2)(\tau E_0 - \beta)} t} \left(\rho_0 \|\psi_h\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right) \|\phi_h'\|_+^2 \right), t \in [0,T],$$

which is equivalent to (3.9).

Let now $Z(t)$ be defined by

$$Z(t) = \int_0^t \left(\|u_h'(s)\|_h^2 + \|D_{-x} u_h(s)\|_+^2 + \left\| \int_0^s E(s-\mu) D_{-x} u_h(\mu) d\mu + \beta D_{-x} u_h(s) \right\|_+^2 \right) ds$$

Then (3.19) can be rewritten in the following equivalent form

$$Z'(t) - \frac{E_0}{m\tau} Z(t) \leq \frac{1}{m} \left(\rho_0 \|\psi\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right) \|\phi'\|_+^2 \right), t \geq 0,$$

and, consequently,

$$Z(t) \leq \frac{1}{E_0} \left(\rho_0 \|\psi\|_h^2 + \left(E_0 - \frac{\beta}{\tau}\right) \|\phi'\|_+^2 \right) \left(e^{\frac{E_0}{m\tau} t} - 1 \right), t \in [0,T],$$

which is equivalent to (3.10).

□

3.3 A semi-discrete approximation for the concentration

To define the semi-discrete approximation for the solution of the IBVP (1.2), (1.4), (1.6) we introduce the first order centered finite difference operator

$$D_c w_h(x_i) = \frac{w_h(x_{i+1}) - w_h(x_{i-1})}{h_i + h_{i+1}}, i = 1, \ldots, N-1,$$

and the average operator

$$M_h w_h(x_i) = \frac{1}{2}(w_h(x_{i-1}) + w_h(x_i)), i = 1, \ldots, N,$$

where $w_h \in W_h$.

Holds the following proposition:

Proposition 2. *If* $w_h \in W_{h,0}$ *then*

$$(D_c w_h, q_h)_h = -(M_h w_h, D_{-x} q_h)_+, \; w_h, q_h \in W_{h,0}. \tag{3.20}$$

Proof. As $w_h, q_h \in W_{h,0}$, we have successively

$$\begin{aligned}
(D_c w_h, q_h)_h &= \frac{1}{2}\sum_{i=1}^{N-1} w_h(x_{i+1}) q_h(x_i) - \frac{1}{2}\sum_{i=1}^{N-1} w_h(x_{i-1}) q_h(x_i) \\
&= \frac{1}{2}\sum_{i=1}^{N-1} w_h(x_i) q_h(x_{i-1}) - \frac{1}{2}\sum_{i=1}^{N-1} w_h(x_i) q_h(x_{i+1}) \\
&= \frac{1}{2}\sum_{i=1}^{N-1} w_h(x_i)(q_h(x_{i-1}) - q_h(x_{i+1})) \\
&= -\frac{1}{2}\sum_{i=1}^{N-1} h_i w_h(x_i) D_{-x} q_h(x_i) \\
&\quad -\frac{1}{2}\sum_{i=1}^{N-1} h_{i+1} w_h(x_i) D_{-x} q_h(x_{i+1}) \\
&= -\frac{1}{2}\sum_{i=1}^{N} h_i w_h(x_i) D_{-x} q_h(x_i) \\
&\quad -\frac{1}{2}\sum_{i=1}^{N} h_i w_h(x_{i-1}) D_{-x} q_h(x_i) \\
&= -\sum_{i=1}^{N} h_i M_h w_h(x_i) D_{-x} q_h(x_i) \\
&== -(M_h w_h, D_{-x} q_h)_+.
\end{aligned}$$

□

The semi-discrete approximation $c_h(t) \in W_{h,0}$ for the concentration defined by IBVP (1.2), (1.4), (1.6) is defined now by the following ordinary differential system

$$c_h'(x_i,t) + D_c(c_h(x_i,t) v(M_h(u_h(x_i,t), M_h u_h'(x_i,t)))) = D D_2 c_h(x_i,t) - \gamma c_h(x_i,t), \tag{3.21}$$

for $i = 1, \ldots, N-1$, and $t \in (0,T]$, complemented with the initial

$$c_h(x_i,0) = c_0(x_i), i = 1, \ldots, N-1, \tag{3.22}$$

and the boundary conditions of Dirichlet type

$$c_h(x_0,t) = c_h(x_N,t) = 0, t \in (0,T]. \tag{3.23}$$

In (3.21), the semi-discrete approximation for the displacement $u_h(t) \in W_{h,0}$ is defined by (3.2), (3.3), (3.4).

3.3.1 Existence and uniqueness

The ordinary differential system (3.21), (3.22) and (3.23) can be rewritten in the following equivalent form

$$c_h'(t) = \Big(DA_h - \gamma I - A_{c,h}\mathscr{V}(u_h(t))\Big)c_h(t), t > 0, \tag{3.24}$$

with

$$c_h(0) = c_{0,h}, \tag{3.25}$$

where $c_h(t)$ is identified with the vector with entries $c_h(x_i,t), i = 1,\dots,N-1$, as before A_h is the matrix associated with the finite difference operator D_2 and $A_{c,h}$ is the matrix associated with the finite difference operator D_c. In (3.24), $\mathscr{V}(u_h(t))$ is the diagonal matrix with entries $v(M_h u_h(x_i,t), M_h u_h'(x_i,t)), i = 1,\dots,N-1$, and, in (3.25), $c_{0,h}$ is identified with the vector with entries $c_0(x_i), i = 1,\dots,N-1$.

The unique solution of the IVP (3.24), (3.25) is now given by

$$c_h(t) = e^{\int_0^t \mathscr{A}(u_h(s))ds} c_{h,0}, \, t \geq 0,$$

with

$$\mathscr{A}(u_h(t)) = DA_h - \gamma I - A_{c,h}\mathscr{V}(u_h(t)),$$

which is a continuous matrix function provided that $u_h(t)$ and $u_h'(t)$ are continuous.

3.3.2 Stability

In this section we will establish energy estimates for the solution of the IBVP (3.21), (3.22) and (3.23).

Theorem 3.3.1. *Let $c_h \in W_{h,0}$ be the solution of the IBVP (3.21), (3.22) and (3.23). If*

$$|v(y)| \leq L_\infty |y|, y \in \mathbb{R}, \tag{3.26}$$

then

$$\|c_h(t)\|_h^2 + 2(D-\varepsilon^2)\int_0^t e^{\int_s^t g(u_h(\mu))d\mu}\|D_{-x}c_h(s)\|_+^2 ds \leq e^{\int_0^t g(u_h(s))ds}\|c_0\|_{L^2}^2, \tag{3.27}$$

for $t \in [0,T]$, where

$$g(u(t)) = \frac{1}{2\varepsilon^2}L_\infty^2\|u_h(t)\|_\infty^2 - 2\gamma \tag{3.28}$$

Proof. From (3.21) taking into account the homogeneous boundary conditions, we easily obtain

$$\frac{1}{2}\frac{d}{dt}\|c_h\|_h^2 - (M_h(c_h v(M_h u_h)), D_{-x}c_h)_+ = -D\|D_{-x}c_h\|_+^2 - \lambda\|c_h\|_h^2. \tag{3.29}$$

Considering that $|v(y)| \leq L_\infty |y|, y \in \mathbb{R}$, we get successively

$$\begin{aligned}(M_h(c_h(t)v(M_h u_h(t))), D_{-x}c_h(t))_+ &\leq L_\infty \|M_h u_h(t)\|_\infty \|M_h c_h(t)\|_+ \|D_{-x}c_h(t)\|_+ \\ &\leq \frac{1}{4\varepsilon^2}L_\infty^2\|M_h u_h(t)\|_\infty^2\|M_h c_h(t)\|_+^2 + \varepsilon^2\|D_{-x}c_h(t)\|_+^2,\end{aligned}$$

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

Then we have

$$\frac{d}{dt}\|c_h(t)\|_h^2 + 2(D-\varepsilon^2)\|D_{-x}c_h(t)\|_+^2 \leq \left(\frac{1}{2\varepsilon^2}L_\infty^2\|M_h u_h(t)\|_\infty^2 - 2\gamma\right)\|M_h c_h(t)\|_+^2,$$

that leads to

$$\frac{d}{dt}\|c_h(t)\|_h^2 + 2(D-\varepsilon^2)\|D_{-x}c_h(t)\|_+^2 \leq \left(\frac{1}{2\varepsilon^2}L_\infty^2\|u_h(t)\|_\infty^2 - 2\gamma\right)\|c_h(t)\|_h^2,$$

for $t > 0$. The last inequality can be rewritten in the following equivalent form

$$\frac{d}{dt}\left(\|c_h(t)\|_h^2 e^{-\int_0^t g(u(s))ds} + 2(D-\varepsilon^2)\int_0^t e^{-\int_0^s g(u(\mu))d\mu}\|D_{-x}c_h(s)\|_+^2 ds\right) \leq 0, \tag{3.30}$$

for $t > 0$, where $g(u)$ is defined by (3.28).

Inequality (3.30) finally leads to (3.27). □

Corollary 4. *Under the assumptions of Theorem 3.3.1, we have*

$$\|c_h(t)\|_h^2 + 2(D-\varepsilon^2)\int_0^t e^{-\gamma(t-s)}\|D_{-x}c_h(s)\|_+^2 ds \leq e^{\int_0^t g(u_h(s))ds}\|c_0\|_{L^2}^2, \tag{3.31}$$

for $t \in [0,T]$.

3.4 Error analysis

3.4.1 Displacement

Let $e_{h,u}(x_i,t)$ be the global spatial discretization error for the displacement given by $e_{h,u}(x_i,t) = u(x_i,t) - u_h(x_i,t), i = 0,\ldots,N$, where u is solution of the IBVP (1.1), (1.3), (1.5) and u_h is solution of the ordinary differential problem (3.2), (3.3) and (3.4).

The spatial error $e_{h,u}$ is defined by the second-order integro-differential equation

$$\rho_0 e''_{h,u}(x_i,t) = E_0 D_2 e_{h,u}(x_i,t) + \frac{1}{\tau}\int_0^t E(t-s)D_2 e_{h,u}(x_i,s)ds + T_h(x_i,t), i = 1,\ldots,N-1, t \in (0,T], \tag{3.32}$$

and the boundary conditions

$$e_{h,u}(x_0,t) = e_{h,u}(x_N,t) = 0, \tag{3.33}$$

and the initial condition

$$e_{h,u}(x_i,0) = e'_{h,u}(x_i,0) = 0, i = 1,\ldots,N-1. \tag{3.34}$$

In (3.32), $T_h(t)$ denotes the spatial truncation error induced by the spatial discretization defined by the finite difference operator D_2. This error admits the representation

$$T_h(x_i,t) = -\frac{1}{3}(h_{i+1}-h_i)S_1(x_i,t) - \frac{1}{12(h_i+h_{i+1})}\left(h_{i+1}^3 S_2(\xi_1(x_1,t),t) + h_i^3 S_2(\eta_1(x_1,t),t)\right),$$

where $\xi_1, \eta_1 \in [x_{i-1}, x_{i+1}]$,

$$S_1(x,t) = E_0 \frac{\partial^3 u}{\partial x^3}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)\frac{\partial^3 u}{\partial x^3}(x,s)ds$$

and

$$S_2(x,t) = E_0 \frac{\partial^4 u}{\partial x^4}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)\frac{\partial^4 u}{\partial x^4}(x,s)ds.$$

We observe that (3.32) is easily obtained taking into account that

$$e''_{h,u}(x_i,t) = \frac{\partial^2 u}{\partial t^2}(x_i,t) - u''_h(x_i,t),$$

$$\rho_0 e''_{h,u}(x_i,t) = E_0\left(\frac{\partial^2 u}{\partial x^2}(x_i,t) - D_2 u_h(x_i,t)\right) + \frac{1}{\tau}\int_0^t E(t-s)\left(\frac{\partial^2 u}{\partial x^2}(x_i,t) - D_2 u_h(x_i,t)\right)ds$$

and

$$D_2 u(x_i,t) = \frac{\partial^2 u}{\partial x^2}(x_i,t) + \frac{1}{3}(h_{i+1}-h_i)\frac{\partial^3 u}{\partial x^3}(x_i,t) + \frac{1}{12(h_{i+1}+h_i)}\left(h_{i+1}^3\frac{\partial^4 u}{\partial x^4}(\xi,t) + h_i^3\frac{\partial^4 u}{\partial x^4}(\eta,t)\right).$$

We note that $T_h(x_i,t) = Lu(x_i,t) - L_h u(x_i,t)$, where L is the spatial differential operator for the displacement equation and L_h is the corresponding finite difference operator. From that we take

$$\begin{aligned} T'_h(x_i,t) &= L\frac{\partial u}{\partial t}(x_i,t) - L_h\frac{\partial u}{\partial t}(x_i,t) \\ &= \frac{1}{3}(h_{i+1}-h_i)S_1(x_i,t) - \frac{1}{12(h_i+h_{i+1})}\left(h_{i+1}^3 S_2(\xi_2(x_1,t),t) + h_i^3 S_2(\eta_2(x_1,t),t)\right), \end{aligned}$$

where $\xi_2, \eta_2 \in [x_{i-1}, x_{i+1}]$,

$$S_3(x,t) = E_0\frac{\partial^4 u}{\partial x^3 \partial t}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)\frac{\partial^4 u}{\partial x^3 \partial t}(x,s)ds$$

and

$$S_4(x,t) = E_0\frac{\partial^5 u}{\partial x^4 \partial t}(x,t) + \frac{1}{\tau}\int_0^t E(t-s)\frac{\partial^5 u}{\partial x^4 \partial t}(x,s)ds.$$

In what follows we use the following notation: $L^2(0,T,V)$ denotes the space of functions $q : [0,T] \to V$ such that

$$\|q\|^2_{L^2(0,T,V)} = \int_0^T \|q(s)\|_V^2 ds < \infty,$$

where V is a normed vector space with the norm $\|.\|_V$.

In the next proposition we establish upper bounds for the terms involved in the truncation error and their derivatives. Although very technical, these estimates, will have an important role in the construction of the bounds for the error $e_{h,u}(t)$.

Proposition 3. *The following inequalities hold:*

$$\|S_1(t)\|_\infty^2 \leq 2E_0 \left\| \frac{\partial^3 u}{\partial x^3}(t) \right\|_\infty^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \left\| \frac{\partial^3 u}{\partial x^3} \right\|_{L^2(0,T,C([0,1]))}^2,$$

$$\|S_2(t)\|_\infty^2 \leq 2E_0 \left\| \frac{\partial^4 u}{\partial x^4}(t) \right\|_\infty^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \left\| \frac{\partial^4 u}{\partial x^4} \right\|_{L^2(0,T,C([0,1]))}^2,$$

$$\|S_3(t)\|_\infty^2 \leq 2E_0 \left\| \frac{\partial^4 u}{\partial x^3 \partial t}(t) \right\|_\infty^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \left\| \frac{\partial^4 u}{\partial x^3 \partial t} \right\|_{L^2(0,T,C([0,1]))}^2,$$

$$\|S_4(t)\|_\infty^2 \leq 2E_0 \left\| \frac{\partial^5 u}{\partial x^4 \partial t}(t) \right\|_\infty^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \left\| \frac{\partial^5 u}{\partial x^4 \partial t} \right\|_{L^2(0,T,C([0,1]))}^2,$$

$$\left\| \frac{\partial S_3}{\partial x}(t) \right\|_{L^2(0,1)}^2 \leq 2E_0 \left\| \frac{\partial^5 u}{\partial t \partial x^4}(t) \right\|_{L^2(0,1)}^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \|u\|_{L^2(0,T,H^5(0,1))}^2$$

and

$$\left\| \frac{\partial S_1}{\partial x}(t) \right\|_{L^2(0,1)}^2 \leq 2E_0 \left\| \frac{\partial^4 u}{\partial x^4}(t) \right\|_{L^2(0,1)}^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \|u\|_{L^2(0,T,H^4(0,1))}^2.$$

Proof. For $S_1(t)$ we have successively

$$\begin{aligned}
\|S_1(t)\|_\infty^2 &= \left\| E_0 \frac{\partial^3 u}{\partial x^3}(t) + \frac{1}{\tau} \int_0^t E(t-s) \frac{\partial^3 u}{\partial x^3}(s) ds \right\|_\infty^2 \\
&\leq 2E_0 \left\| \frac{\partial^3 u}{\partial x^3}(t) \right\|^2 + 2\frac{1}{\tau} \left\| \int_0^t E(t-s) \frac{\partial^3 u}{\partial x^3}(s) ds \right\|_\infty^2 \\
&\leq 2E_0 \left\| \frac{\partial^3 u}{\partial x^3} \right\|_\infty^2 + 2\frac{1}{\tau} \int_0^t |E(t-s)|^2 ds \int_0^t \left| \frac{\partial^3 u}{\partial x^3}(s) \right|_\infty^2 ds \\
&\leq 2E_0 \left\| \frac{\partial^3 u}{\partial x^3}(t) \right\|_\infty^2 + 2\frac{1}{\tau} \|E\|_{L^2(0,T)}^2 \left\| \frac{\partial^3 u}{\partial x^3} \right\|_{L^2(0,T,C([0,1]))}^2.
\end{aligned}$$

The construction of the estimate for $S_2(t)$, $S_3(t)$ and $S_4(t)$ follow the steps used in the establishment of the upper bound for $S_1(t)$.

For $\dfrac{\partial S_3}{\partial x}(t)$ we obtain successively

$$\begin{aligned}\left\|\frac{\partial S_3}{\partial x}(t)\right\|^2_{L^2(0,1)} &= \int_0^1 \left(E_0 \frac{\partial^5 u}{\partial x^4 \partial t}(x,t) + \frac{1}{\tau}\frac{\partial}{\partial x}\int_0^t E(t-s)\frac{\partial^4 u}{\partial x^3 \partial t}(x,s)ds\right)^2 dx \\ &\leq 2E_0 \int_0^1 \left(\frac{\partial^5 u}{\partial x^4 \partial t}(x,t)\right)^2 dx + 2\frac{1}{\tau}\int_0^1 \left(\int_0^t E(t-s)\frac{\partial^5 u}{\partial x^4 \partial t}(x,s)ds\right)^2 dx \\ &\leq 2E_0 \left\|\frac{\partial^5 u}{\partial t \partial x^4}(t)\right\|^2_{L^2(0,1)} + 2\frac{1}{\tau}\int_0^1 \int_0^t |E(t-s)|^2 ds \int_0^t \left|\frac{\partial^5 u}{\partial x^4 \partial t}(x,s)\right|^2 dsdx \\ &\leq 2E_0 \left\|\frac{\partial^5 u}{\partial t \partial x^4}(t)\right\|^2_{L^2(0,1)} + 2\frac{1}{\tau}\|E\|^2_{L^2(0,T)}\|u\|^2_{L^2(0,T,H^5(0,1))}.\end{aligned}$$

The construction of the estimate for $\dfrac{\partial S_1}{\partial x}(t)$ is analogous to the last one.

□

In the establishment of the error estimate for $e_{h,u}(t)$ we need the following Discrete Poincaré inequality.

Theorem 3.4.1. *If $v \in W_{h,0}$ then*

$$\|v_h\|_h^2 \leq \|D_{-x}v_h\|_+^2.$$

Proof. We start by observing that we have the following representation for $v_h(x_i)$ that we represent by v_i

$$v_h(x_i) = \sum_{j=0}^{i} v_j - \sum_{j=0}^{i-1} v_j.$$

Then

$$\begin{aligned} v_h(x_i) = & \sum_{j=1}^{i} v_j - \sum_{j=1}^{i} v_{j-1} \\ &= \sum_{j=1}^{i} h_j \frac{v_j - v_{j-1}}{h_j} \\ &= \sum_{j=1}^{i} h_j D_{-x} v_j. \end{aligned}$$

The last representation leads to

$$v_i^2 \leq \sum_{j=1}^{i} h_j (D_{-x}v_j)^2.$$

Consequently, to conclude the proof, we remark that

$$\sum_{i=1}^{N-1} h_{i+\frac{1}{2}} v_i^2 \leq \sum_{i=1}^{N-1} h_{i+\frac{1}{2}} \sum_{j=1}^{i} h_j (D_{-x}v_j)^2.$$

□

The main convergence result is now established.

Theorem 3.4.2. *If $\beta, \lambda, \omega, \mu$ are positive constants such that $\beta < \tau E_0 < 2\beta$ and*

$$\frac{(\tau E_0-2)(\tau E_0-\beta)}{2\tau^2E_0} > \lambda^2+2\omega^2+\mu^2$$

and

$$m=\min\left\{\frac{1}{2}\rho_0, \frac{(\tau E_0-2)(\tau E_0-\beta)}{2\tau^2E_0}-\lambda^2-2\omega^2-\mu^2, \frac{2\beta-\tau E_0}{\tau^2E_0\beta}\right\}, \tag{3.35}$$

then

$$\begin{aligned}\int_0^t \left\|\frac{de_{h,u}}{dt}(s)\right\|_h^2+\|D_{-x}e_{h,u}(s)\|_+^2+\left\|\int_0^s E(s-\mu)D_{-x}e_{h,u}(\mu)d\mu+\beta D_{-x}e_{h,u}(s)\right\|_+^2 \\ +\left\|\int_0^s E(s-\mu)D_{-x}e_{h,u}(\mu)d\mu\right\|_+^2 ds\frac{h_{max}^4e^{\frac{c}{m}t}}{m}\int_0^t\left(\int_0^s\Theta_1(\eta)d\eta+\Theta_2\right)e^{-\frac{c}{m}s}ds,\end{aligned} \tag{3.36}$$

for $t\in[0,T]$, *and*

$$\begin{aligned}\left\|\frac{de_{h,u}}{dt}(t)\right\|_h^2+\|D_{-x}e_{h,u}(t)\|_+^2+\left\|\int_0^s E(s-\mu)D_{-x}e_{h,u}(\mu)d\mu+\beta D_{-x}e_{h,u}(t)\right\|_+^2 \\ +\left\|\int_0^s E(s-\mu)D_{-x}e_{h,u}(\mu)d\mu\right\|_+^2 ds\le\frac{h_{max}^4e^{\frac{c}{m}t}}{m}\int_0^T(\Theta_1(s)+\Theta_2(s))ds\end{aligned} \tag{3.37}$$

where

$$\begin{aligned}\Theta_1(t)=&\frac{1}{2\sigma^2}\frac{1}{6^2}h_{max}^4\left(E_0\left\|\frac{\partial^4u}{\partial x^3\partial t}(t)\right\|_\infty^2+\frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^4u}{\partial x^3\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right) \\ &+\frac{1}{2\varepsilon^2}\frac{1}{6^2}h_{max}^4\left(E_0\left\|\frac{\partial^5u}{\partial t\partial x^4}(t)\right\|_{L^2(0,1)}^2+\frac{1}{\tau}\|E\|_{L^2(0,T)}^2\|u\|_{L^2(0,T,H^5(0,1))}^2\right) \\ &+\frac{1}{2\delta^2}\frac{1}{4^2}h_{max}^4\left(E_0\left\|\frac{\partial^5u}{\partial x^4\partial t}(t)\right\|_\infty^2+\frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^5u}{\partial x^4\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right),\end{aligned} \tag{3.38}$$

$$\begin{aligned}\Theta_2(t)\ =&\frac{1}{2\lambda^2}\frac{1}{6^2}\left(E_0\left\|\frac{\partial^3u}{\partial x^3}(t)\right\|_\infty^2+\frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^3u}{\partial x^3}\right\|_{L^2(0,T,C([0,1]))}^2\right) \\ &+\frac{1}{2\omega^2}\frac{1}{6^2}\left(E_0\left\|\frac{\partial^4u}{\partial x^4}(t)\right\|_\infty^2+\frac{1}{\tau}\|E\|_{L^2(0,T)}^2\|u\|_{L^2(0,T,H^4(0,1))}^2\right) \\ &+\frac{1}{2\phi^2}\frac{1}{4^2}\left(E_0\left\|\frac{\partial^4u}{\partial x^4}(t)\right\|_{L^2(0,1)}^2+\frac{1}{\tau}\|E\|_{L^2(0,T,C([0,1]))}^2\left\|\frac{\partial^4u}{\partial x^4}\right\|_{L^2(0,T,C([0,1]))}^2\right)\end{aligned} \tag{3.39}$$

and

$$c=\frac{E_0}{\tau}+\sigma^2+\delta^2+2\varepsilon^2.$$

Proof. We start by remarking that we have

$$\begin{aligned}\rho_0\left(e''_{h,u}(t),e'_{h,u}(t)\right)_h\ =&E_0\left(D_2e_{h,u}(t),e'_{h,u}(t)\right)_h+\frac{1}{\tau}\left(\int_0^tE(t-s)D_2e_{h,u}(s)ds,e'_{h,u}(t)\right)_h \\ &+\left(T_h(t),e'_{h,u}(t)\right)_h.\end{aligned} \tag{3.40}$$

As before, we get

$$\rho_0\left(e''_{h,u}(t),e'_{h,u}(t)\right)_h=\frac{1}{2}\rho_0\frac{d}{dt}\left\|e'_{h,u}(t)\right\|_h^2$$

$$E_0\left(D_2e_{h,u}(t),e'_{h,u}(t)\right)_h=-\frac{1}{2}E_0\frac{d}{dt}\left\|D_{-x}e_{h,u}(t)\right\|_+^2$$

and

$$\begin{aligned}\frac{1}{\tau}\left(\int_0^t E(t-s)D_2e_{h,u}(s)ds,\frac{de_{h,u}}{dt}(t)\right)_h = & -\frac{1}{2\tau\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds+\beta D_{-x}e_{h,u}(t)\right\|_+^2\\ & -\left(\frac{\beta}{\tau}-E_0\right)\frac{1}{2\tau E_0\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds\right\|_+^2\\ & -\frac{1}{E_0\tau^3}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds\right\|_+^2\\ & +\frac{\beta}{2\tau}\frac{d}{dt}\left\|D_{-x}e_{h,u}(t)\right\|_+^2+\frac{E_0}{\tau}\left\|D_{-x}e_{h,u}(t)\right\|_+^2.\end{aligned}$$

The new term $\left(T_h(t),e'_{h,u}(t)\right)_h$ can be written in the following equivalent form

$$\left(T_h(t),e'_{h,u}(t)\right)_h=\frac{d}{dt}\left(T_h(t),e_{h,u}(t)\right)_h-\left(T'_h(t),e_{h,u}(t)\right)_h.$$

In what follows we estimate $\left(T_h'(t), e_{h,u}(t)\right)_h$. Taking into account the upper bound obtained in Proposition 3, we have successively

$$
\begin{aligned}
-\left(T_h'(t), e_{h,u}(t)\right)_h &= \frac{1}{6}\sum_{i=1}^{n}\left(h_{i+1}^2 - h_i^2\right) S_3(x_i,t) e_{h,u}(x_i,t) \\
&\quad + \frac{1}{12}\sum_{i=1}^{n}\frac{1}{h_{i+1}+h_i}\left(h_{i+1}^3 S_4(x_i,t) + h_i^3 S_4 x_i,t)\right)\frac{h_{i+1}+h_i}{2} e_{h,u}(x_i,t) \\
&\le \frac{1}{6}\sum_{i=1}^{n} h_i^2 |S_3(x_i,t)||D_{-x}e_{h,u}(x_i,t)|h_i + \frac{1}{6}\sum_{i=1}^{n} h_i^2\left(|S_3(x_{i-1},t)| + |S_3(x_i,t)|\right)|e_{h,u}(x_i,t)| \\
&\quad + \frac{1}{12}\sum_{i=1}^{n}\frac{h_{i+1}^3 + h_i^3}{h_{i+1}+h_i}\|S_4(t)\|_\infty \frac{h_{i+1}+h_i}{2}|e_{h,u}(x_i,t)| \\
&\le \frac{1}{6} h_{max}^2\|S_3(t)\|_\infty \|D_{-x}e_{h,u}(t)\|_+ + \frac{1}{6}\sum_{i=1}^{n} h_i^2\left(\int_{x_{i-1}}^{x_i}\left(\frac{\partial S_3}{\partial x}(\zeta,t)\right)^2 d\zeta\right)^{\frac{1}{2}}\sqrt{h_i}|e_{h,u}(x_i,t)| \\
&\quad + \frac{1}{4} h_{max}^2\|S_4(t)\|_\infty \|e_{h,u}(t)\|_h \\
&\le \frac{1}{4\sigma^2}\frac{1}{6^2} h_{max}^4\|S_3(t)\|_\infty^2 + \sigma^2\|D_{-x}e_{h,u}(t)\|_+^2 + \frac{1}{4\varepsilon^2}\frac{1}{6^2} h_{max}^4\left\|\frac{\partial S_3}{\partial x}(t)\right\|_{L^2(0,1)}^2 + 2\varepsilon^2\|e_{h,u}(t)\|_h^2 \\
&\quad + \frac{1}{4\delta^2}\frac{1}{4^2} h_{max}^4\|S_4(t)\|_\infty^2 + \delta^2\|e_{h,u}(t)\|_h^2 \\
&\le \frac{1}{2\sigma^2}\frac{1}{6^2} h_{max}^4\left(E_0\left\|\frac{\partial^4 u}{\partial x^3\partial t}(t)\right\|_\infty^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^4 u}{\partial x^3\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right) + \sigma^2\|D_{-x}e_{h,u}(t)\|_+^2 \\
&\quad + \frac{1}{2\varepsilon^2}\frac{1}{6^2} h_{max}^4\left(E_0\left\|\frac{\partial^5 u}{\partial t\partial x^4}(t)\right\|_{L^2(0,1)}^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\|u\|_{L^2(0,T,H^5(0,1))}^2\right) + 2\varepsilon^2\|e_{h,u}(t)\|_h^2 \\
&\quad + \frac{1}{2\delta^2}\frac{1}{4^2} h_{max}^4\left(E_0\left\|\frac{\partial^5 u}{\partial x^4\partial t}(t)\right\|_\infty^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^5 u}{\partial x^4\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right) + \delta^2\|e_{h,u}\|_h^2.
\end{aligned}
$$

Finally, we get

$$
\begin{aligned}
&\frac{1}{2}\rho_0\frac{d}{dt}\left\|e_{h,u}'(t)\right\|_h^2 + \frac{1}{2}\left(E_0 - \frac{\beta}{\tau}\right)\frac{d}{dt}\|D_{-x}e_{h,u}(t)\|_+^2 + \frac{1}{2\tau\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds + \beta D_{-x}e_{h,u}(t)\right\|_+^2 \\
&\quad + \left(\frac{\beta}{\tau} - E_0\right)\frac{1}{2\tau E_0\beta}\frac{d}{dt}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds\right\|_+^2 - \frac{d}{dt}\left(T_h(t), e_{h,u}(t)\right)_h \\
&\le \frac{1}{2\sigma^2}\frac{1}{6^2} h_{max}^4\left(E_0\left\|\frac{\partial^4 u}{\partial x^3\partial t}(t)\right\|_\infty^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^4 u}{\partial x^3\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right) + \sigma^2\|D_{-x}e_{h,u}(t)\|_+^2 \\
&\quad + \frac{1}{2\varepsilon^2}\frac{1}{6^2} h_{max}^4\left(E_0\left\|\frac{\partial^5 u}{\partial t\partial x^4}(t)\right\|_{L^2(0,1)}^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\|u\|_{L^2(0,T,H^5(0,1))}^2\right) + 2\varepsilon^2\|e_{h,u}(t)\|_h^2 \\
&\quad + \frac{1}{2\delta^2}\frac{1}{4^2} h_{max}^4\left(E_0\left\|\frac{\partial^5 u}{\partial x^4\partial t}(t)\right\|_\infty^2 + \frac{1}{\tau}\|E\|_{L^2(0,T)}^2\left\|\frac{\partial^5 u}{\partial x^4\partial t}\right\|_{L^2(0,T,C([0,1]))}^2\right) + \delta^2\|e_{h,u}\|_h^2 \\
&\quad + \left(\frac{E_0}{\tau} + \sigma^2\right)\|D_{-x}e_{h,u}(t)\|_+^2 + (\delta^2 + 2\varepsilon^2)\|e_{h,u}(t)\|_h^2,
\end{aligned}
$$

where $\varepsilon, \delta, \sigma \neq 0$ are arbitrary constants.

The last differential inequality leads to

$$\frac{1}{2}\rho_0\left\|\frac{de_{h,u}}{dt}(t)\right\|_h^2+\frac{(\tau E_0-2)(\tau E_0-\beta)}{2\tau^2E_0}\|D_{-x}e_{h,u}(t)\|_+^2+\frac{2\beta-\tau E_0}{2\tau^2E_0\beta}\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds+\beta D_{-x}e_{h,u}(t)\right\|_+^2$$
$$\leq h_{max}^4\int_0^t\Theta_1(s)ds+\left(\frac{E_0}{\tau}+\sigma^2+\delta^2+2\varepsilon^2\right)\int_0^t\|D_{-x}e_{h,u}(s)\|_+^2ds+(T_h(t),e_h(t))_h$$

where $\Theta_1(t)$ is defined by (3.38).

It can be shown that for $(T_h(t),e_{h,u}(t))_h$ we have

$$(T_h(t),e_{h,u}(t))_h \quad \leq h_{max}^4\int_0^t\Theta_2(s)ds+\lambda^2\|D_{-x}e_{h,u}\|_+^2+2\omega^2\|e_{h,u}\|_h^2+\mu^2\|e_{h,u}\|_h^2,$$

where $\lambda,\omega,\mu\neq 0$ are arbitrary constants, and $\Theta_2(t)$ is defined by (3.39).

If m is given by (3.35), then we deduce

$$m\left(\left\|\frac{de_{h,u}}{dt}(t)\right\|_h^2+\|D_{-x}e_{h,u}(t)\|_+^2+\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds+\beta D_{-x}e_{h,u}(t)\right\|_+^2\right)$$
$$\leq h_{max}^4\int_0^t(\Theta_1(s)+\Theta_2(s))ds+\left(\frac{E_0}{\tau}+\sigma^2+\delta^2+2\varepsilon^2\right)\int_0^t\|D_{-x}e_{h,u}(s)\|_+^2\,ds.$$

Introducing

$$Y(t)=\left\|\frac{de_{h,u}}{dt}(t)\right\|_h^2+\|D_{-x}e_{h,u}(t)\|_+^2+\left\|\int_0^t E(t-s)D_{-x}e_{h,u}(s)ds+\beta D_{-x}e_{h,u}(t)\right\|_+^2,$$

the last inequality admits the representation

$$mY(t)\leq h_{max}^4\int_0^T(\Theta_1(s)+\Theta_2(s))ds+c\int_0^t Y(s)ds,$$

where $c=\frac{E_0}{\tau}+\sigma^2+\delta^2+2\varepsilon^2$.

Gronwall Lemma allow us to obtain

$$\int_0^t Y(s)ds\leq\frac{h_{max}^4}{m}\int_0^T(\Theta_1(s)+\Theta_2(s))ds \tag{3.41}$$

and to

$$Y(t)\leq\frac{h_{max}^4}{m}e^{\frac{c}{m}t}\int_0^T(\Theta_1(s)+\Theta_2(s))ds. \tag{3.42}$$

The inequalities (3.41), (3.42) lead to (3.36) and (3.37), respectively. □

3.4.2 Concentration

Let c be the solution of the IBVP (1.2), (1.4), (1.6) and let $c_h(t)$ be its semi-discrete approximation defined by the differential problem (3.21), (3.22) and (3.23) where, to simplify, we assume that v depends only on the displacement. The spatial discretization error for the semi-discrete approximation $c_h(t)$ is defined by $e_{h,c}(x_i,t)=c(x_i,t)-c_h(x_i,t), i=0,\dots,N$. This error is solution of the following differential problem

$$\frac{\partial e_{h,c}}{\partial t}(x_i,t)+D_c\left(v(u)e_{h,c}+(v(u)-v(u_h)c_h)\right)=DD_2e_{h,c}(x_i,t)-\gamma e_{h,c}(x_i,t)+T_h(x_i,t) \tag{3.43}$$

for $i=1,\dots,N-1$, and $t\in(0,T]$, complemented with the initial condition

$$e_{h,c}(x_i,0)=0, i=1,\dots,N-1, \tag{3.44}$$

and the boundary conditions

$$e_{h,c}(x_0,t)=e_{h,c}(x_N,t)=0, t\in(0,T]. \tag{3.45}$$

In (3.43), u and u_h are defined by the IBVP (1.1), (1.3), (1.5) and by the ordinary differential problem (3.2), (3.3), (3.4), respectively, and $T_h(t)$ denotes the truncation error induced by the spatial discretization considered in (3.21). This error admits the representation

$$\begin{aligned} T_h(x_i,t) &= -\frac{1}{3}(h_{i+1}-h_i)\frac{\partial^3 c}{\partial x^3}(x_i,t)-\frac{1}{12(h_i+h_{i+1})}\left(h_{i+1}^3\frac{\partial^4 c}{\partial x^4}(\xi_1,t)+h_i^3\frac{\partial^4 c}{\partial x^4}(\eta_1,t)\right)\\ &+\frac{1}{2}(h_{i+1}-h_i)\frac{\partial^2 (v(u)c)}{\partial x^2}(x_i,t)+\frac{1}{6(h_i+h_{i+1})}\left(h_{i+1}^3\frac{\partial^3 (v(u)c)}{\partial x^3}(\xi_2,t)+h_i^3\frac{\partial^3 (v(u)c)}{\partial x^3}(\eta_2,t)\right), \end{aligned}$$

where $\xi_1,\xi_2,\eta_1,\eta_2\in[x_{i-1},x_{i+1}]$, $i=1,\dots,N-1$. To get this representation we observe that

$$D_2c(x_i,t)=\frac{\partial^2 c}{\partial x^2}(x_i,t)+\frac{1}{3}(h_{i+1}-h_i)\frac{\partial^3 c}{\partial x^3}(x_i,t)+\frac{1}{12(h_{i+1}+h_i)}\left(h_{i+1}^3\frac{\partial^4 c}{\partial x^4}(\xi_1,t)+h_i^3\frac{\partial^4 c}{\partial x^4}(\eta_1,t)\right)$$

and

$$\begin{aligned} D_c(v(u)c)(x_i,t) &= \frac{\partial (v(u)c)}{\partial x}(x_i,t)+\frac{1}{2}(h_{i+1}-h_i)\frac{\partial^2 (v(u)c)}{\partial x^2}(x_i,t)\\ &+\frac{1}{6(h_{i+1}+h_i)}\left(h_{i+1}^3\frac{\partial^3 (v(u)c)}{\partial x^3}(\xi_2,t)+h_i^3\frac{\partial^3 (v(u)c)}{\partial x^3}(\eta_2,t)\right). \end{aligned}$$

The next proposition establishes an auxiliary result that will be used in the main convergence result for the concentration.

Proposition 4.

$$(M_he_{h,c},D_{-x}e_{h,c})_+ \quad \leq \frac{1}{2\varepsilon^2}\|e_{h,c}\|_h^2+\varepsilon^2\|D_{-x}e_{h,c}\|_+^2,$$

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

Proof. We have successively

$$\begin{aligned} (M_he_{h,c},D_{-x}e_{h,c})_+ &= \sum_i h_i\frac{e_{i-1,c}+e_{i,c}}{2}D_{-x}e_{i,c}\\ &\leq \frac{1}{4\varepsilon^2}\sum_i h_i\frac{2e_{i-1,c}^2+2e_{i,c}^2}{4}+\varepsilon^2\|D_{-x}e_{h,c}\|_+^2\\ &= \frac{1}{4\varepsilon^2}\left(\sum_i h_i\frac{e_{i-1,c}^2}{2}+\sum_i h_i\frac{e_{i,c}^2}{2}\right)+\varepsilon^2\|D_{-x}e_{h,c}\|_+^2\\ &= \frac{1}{2\varepsilon^2}\|e_{h,c}\|_h^2+\varepsilon^2\|D_{-x}e_{h,c}\|_+^2. \end{aligned}$$

□

Theorem 3.4.3. *Let c be the solution of the IBVP (1.2), (1.4), (1.6) and let $c_h(t)$ be its semi-discrete approximation defined by the differential problem (3.21), (3.22) and (3.23). If v is a Lipschitz function with Lipschits constant L_v, then the spatial discretization error for the concentration $e_{h,c}(x_i,t) = c(x_i,t) - c_h(x_i,t), i = 0,\dots,N$, satisfies the following*

$$\begin{aligned}\|e_{h,c}\|_h^2 + 2C_1\int_0^t e^{2\int_s^t C_2(\mu)d\mu}\,\|D_{-x}e_{h,c}\|_+^2\,ds \quad &\leq \frac{1}{\varepsilon_2^2}\int_0^t L_v^2\|c_h(s)\|_\infty^2 e^{2\int_s^t C_2(\mu)d\mu}\,\|e_{h,u}\|_h^2 ds \\ &+2h_{max}^4\int_0^t e^{2\int_s^t C_2(\mu)d\mu}\Theta(s)ds,\end{aligned} \tag{3.46}$$

for $t \in [0,T]$, where $\varepsilon_i \neq 0, i = 1,\dots,8$, are such that

$$C_1 = D - \varepsilon_1^2 - \varepsilon_2^2 - \varepsilon_3^2 - \varepsilon_6^2 > 0$$

$$C_2 = \frac{1}{2\varepsilon_1^2}L_\infty\|u\|_\infty + 2\varepsilon_4^2 + \varepsilon_5^2 + 2\varepsilon_7^2 + \varepsilon_8^2 - \gamma > 0,$$

u is the displacement defined by IBVP (1.1), (1.3), (1.5), and $\Theta(t)$ is defined by

$$\begin{aligned}\Theta(t) \quad &= \frac{1}{4\varepsilon_3^2}\frac{1}{6^2}\,\|c(t)\|_{C^3([0,1])}^2 + \frac{1}{4\varepsilon_4^2}\frac{1}{6^2}\,\|c(t)\|_{H^4(0,1)}^2 + \frac{1}{4\varepsilon_5^2}\frac{1}{4^2}\,\|c(t)\|_{C^4([0,1])}^2 \\ &+\frac{1}{4\varepsilon_6^2}\frac{1}{4^2}L_\infty\|u(t)\|_\infty\,\|c(t)\|_{C^2([0,1])}^2 + \frac{1}{4\varepsilon_7^2}\frac{1}{4^2}L_\infty\|u(t)\|_\infty\,\|c(t)\|_{H^3(0,1)}^2 + \frac{1}{4\varepsilon_8^2}\frac{1}{2^2}L_\infty\|u(t)\|_\infty\,\|c(t)\|_{C^3([0,1])}^2.\end{aligned} \tag{3.47}$$

Proof. From (3.43), we easily get

$$\begin{aligned}&\left(e'_{h,c}(t), e_{h,c}(t)\right)_h + \left(D_c(v(u(t))c(t)) - D_c\left(v(u_h(t))c_h(t)\right), e_{h,c}(t)\right)_h \\ = \quad & D\left(D_2e_{h,c}(t), e_{h,c}(t)\right)_h - \gamma(e_{h,c}(t), e_{h,c}(t))_h + (T_h(t), e_{h,c}(t))_h\end{aligned}$$

that leads to

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\,\|e_{h,c}(t)\|_h^2 + D\,\|D_{-x}e_{h,c}(t)\|_+^2 + \gamma\|e_{h,c}(t)\|_h^2 \\ = \quad & \left(M_h\left(v(u(t))e_{h,c}(t) + (v(u(t)) - v(u_h(t)))c_h(t)\right), D_{-x}e_{h,c}(t)\right)_+ + (T_h(t), e_{h,c}(t))_h.\end{aligned}$$

Considering now the Lipchitz property for v we obtain

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\,\|e_{h,c}(t)\|_h^2 + D\,\|D_{-x}e_{h,c}(t)\|_+^2 + \gamma\|e_{h,c}(t)\|_h^2 \quad &\leq L_\infty\|u(t)\|_\infty\left(M_he_{h,c}(t), D_{-x}e_{h,c}(t)\right)_+ \\ &+L_v\|c_(t)h\|_\infty(M_h|u-u_h|, |D_{-x}e_{h,c}(t)|)_+ \\ &+(T_h, e_{h,c})_h\end{aligned}$$

and, from Proposition 4, we deduce

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|e_{h,c}(t)\|_h^2+D\|D_{-x}e_{h,c}(t)\|_+^2+\gamma\|e_{h,c}(t)\|_h^2 \leq& \frac{1}{2\varepsilon_1^2}L_\infty^2\|u(t)\|_\infty^2\|e_{h,c}(t)\|_h^2+\varepsilon_1^2\|D_{-x}e_{h,c}(t)\|_+^2\\ &+\frac{1}{2\varepsilon_2^2}L_v^2\|c_h(t)\|_\infty^2\|e_{h,u}(t)\|_h^2+\varepsilon_2^2\|D_{-x}e_{h,c}(t)\|_+^2\\ &+(T_h(t),e_{h,c}(t))_h.\end{aligned} \tag{3.48}$$

It can be shown that for $(T_h(t),e_{h,c}(t))_h$ we have

$$\begin{aligned}(T_h(t),e_{h,c}(t))_h \leq& \frac{1}{4\varepsilon_3^2}\frac{1}{6^2}h_{max}^4\|c(t)\|_{C^3([0,1])}^2+\varepsilon_3^2\|D_{-x}e_{h,c}(t)\|_+^2+\frac{1}{4\varepsilon_4^2}\frac{1}{6^2}h_{max}^4\|c(t)\|_{H^4(0,1)}^2+2\varepsilon_4^2\|e_{h,c}(t)\|_h^2\\ &+\frac{1}{4\varepsilon_5^2}\frac{1}{4^2}h_{max}^4\|c(t)\|_{C^4([0,1])}^2+\varepsilon_5^2\|e_{h,c}(t)\|_h^2\\ &+\frac{1}{4\varepsilon_6^2}\frac{1}{4^2}h_{max}^4L_\infty\|u(t)\|_\infty\|c(t)\|_{C^2([0,1])}^2+\varepsilon_6^2\|D_{-x}e_{h,c}(t)\|_+^2\\ &+\frac{1}{4\varepsilon_7^2}\frac{1}{4^2}h_{max}^4L_\infty\|u(t)\|_\infty\|c(t)\|_{H^3(0,1)}^2+2\varepsilon_7^2\|e_{h,c}(t)\|_h^2\\ &+\frac{1}{4\varepsilon_8^2}\frac{1}{2^2}h_{max}^4L_\infty\|u(t)\|_\infty\|c(t)\|_{C^3([0,1])}^2+\varepsilon_8^2\|e_{h,c}(t)\|_h^2\end{aligned}. \tag{3.49}$$

Considering now the two inequalities (3.48) and (3.49) we conclude that

$$\frac{1}{2}\frac{d}{dt}\|e_{h,c}\|_h^2+C_1\|D_{-x}e_{h,c}\|_+^2\leq C_2\|e_{h,c}\|_h^2+\frac{1}{2\varepsilon_2^2}L_v^2\|c_h\|_\infty^2\|e_{h,u}\|_h^2+h_{max}^4\Theta(t) \tag{3.50}$$

where $\Theta(t)$ is given by (3.47).

Finally, the inequality (3.50) leads to (3.46). □

The last result establishes the second order accuracy for the concentration and it is a corollary the main results established in this work.

Corollary 5. *Under the assumption of Theorems 3.2.1, 3.4.2, 3.3.1 and 3.4.3, there exists a positive constant C, h and t independent, such that*

$$\|e_{h,c}(t)\|_h^2+\int_0^t\|D_{-x}e_{h,c}(s)\|_+^2\,ds\leq Ch_{max}^4, \tag{3.51}$$

for $t\in[0,T], h\in\Lambda$.

Chapter 4

Numerical Simulation

4.1 Introduction

This chapter aims to illustrate the theoretical results established in this work, namely, the convergence results Theorem 3.4.2 and Corollary 5. We would like to show numerically that the errors for the displacement and for the concentration are second order convergent.

We remark that the semi-discrete approximation for the displacement is defined by the second order integro-differential problem (3.2), (3.3), (3.4). To compute numerically its solution, we need to consider a numerical method for second order ordinary differential equations and the integral term needs also to be discretized.

In what concerns the numerical solution of the semi-discrete problem (3.21), (3.22) and (3.23) for the concentration we consider an implicit-explicit approach.

4.2 Displacement

In order to test the theoretical convergence of the solution, we implement the fully discrete finite difference method in *python*. As studied before we use a non-uniform mesh in space, and uniform mesh in $[0,T]$. We introduce the following finite difference operators and the following operators

$$D_{2,t}w_h(x_i,t_j) = \frac{w_h(x_i,t_{j-1}) - 2w_h(x_i,t_j) + w_h(x_i,t_{j+1})}{\Delta t^2}$$

and

$$D_{-t}w_h(x_i,t_j) = \frac{w_h(x_i,t_j) - w_h(x_i,t_{j-1})}{\Delta t}.$$

As we consider an implicit approximation on the integral term $\int_0^t E(t-s)D_{2,x}u_h(x_i,s)ds$, where the x in the operator D_2 indicates that this operator acts in space, we split it in two

$$\begin{aligned}\int_0^{t_{n+1}} E(t_{n+1}-s)D_{2,x}u_h(x_i,s)ds &= \int_0^{t_n} E(t_{n+1}-s)D_{2,x}u_h(x_i,s)ds + \int_{t_n}^{t_{n+1}} E(t_{n+1}-s)D_{2,x}u_h(x_i,s)ds \\ &= e^{-\frac{\Delta t}{\tau}} \int_0^{t_n} E(t_n-s)D_{2,x}u_h(x_i,s)ds + \int_{t_n}^{t_{n+1}} E(t_{n+1}-s)D_{2,x}u_h(x_i,s)ds \\ &= \tau e^{-\frac{\Delta t}{\tau}} \left(D_{2,t}u_h(x_i,t_{n-1}) - DD_{2,x}u_h(x_i,t_n) - f(x_i,t_{n-1})\right) \\ &+ \int_{t_n}^{t_{n+1}} E(t_{n+1}-s)D_{2,x}u_h(x_i,s)ds,\end{aligned}$$

and we approximate the remaining integral with the trapezoidal rule

$$\int_a^b g(x)dx \approx \frac{b-a}{2}\left(g(a)+g(b)\right).$$

Now we construct the implicit finite difference scheme for the displacement considering $U^n = [U_1^n \ U_2^n \ \dots \ U_{N-1}^n]^T$ with $U_i^n \simeq u_h(x_i,t_n)$, $\phi = [\phi(x_1) \ \phi(x_2) \ \dots \ \phi(x_{N-1})]^T$, $\psi = [\psi(x_1) \ \psi(x_2) \ \dots \ \psi(x_{N-1})]^T$ and $F^n = [F_1^n \ F_2^n \ \dots \ F_{N-1}^n]^T$ with $F_i^n = f(x_i,t_n)$.

$$\begin{cases} U^0 &= \phi \\ U^1 &= \phi + \Delta t \psi \\ \left(I - D\Delta t^2\left(1+\frac{\Delta t}{3\tau}\right)A_x\right)U^2 &= 2\left(I + \frac{2D\Delta t^3}{3\tau}A_x\right)U^1 - \left(I - \frac{D\Delta t^3}{3\tau}e^{-\frac{2\Delta t}{\tau}}A_x\right)U^0 + \Delta t^2 F^2 \\ \left(I - D\Delta t^2\left(1+\frac{\Delta t}{2\tau}\right)A_x\right)U^{n+1} &= \left(\left(2+e^{-\frac{\Delta t}{\tau}}\right)I + D\Delta t^2 e^{-\frac{\Delta t}{\tau}}\left(\frac{\Delta t}{2\tau}-1\right)A_x\right)U^n \\ &\quad -\left(1+e^{-\frac{\Delta t}{\tau}}\right)U^{n-1} + e^{-\frac{\Delta t}{\tau}}U^{n-2} + \Delta t^2\left(F^{n+1} - e^{-\frac{\Delta t}{\tau}}F^n\right) \end{cases} \tag{4.1}$$

In (4.1), I is the identity matrix and A_x denotes the matrix induced by the finite difference operator $D_{2,x}$

$$A_x = \begin{bmatrix} -\frac{2}{h_1h_2} & \frac{2}{h_1(h_1+h_2)} & 0 & \\ \frac{2}{h_2(h_2+h_3)} & -\frac{2}{h_2h_3} & \frac{2}{h_2(h_2+h_3)} & \cdots \\ 0 & \frac{2}{h_3(h_3+h_4)} & -\frac{2}{h_3h_4} & \\ & \vdots & & \ddots \end{bmatrix}.$$

We take the following constants

$$\begin{cases} D &= 10^{-2} \\ \tau &= 1.1 \\ T &= 1. \end{cases}$$

Now we iterate $N_l = 10\cdot 2^l$, $i = 0,1,2,3$ and set $\Delta t_l = \left(h_{max}^{(l)}\right)^2$ for each mesh. Then we calculate the order of convergence

$$p_l = \frac{log\left(\frac{e_{l-1}}{e_l}\right)}{log\left(\frac{h_{max}^{(l-1)}}{h_{max}^{(l)}}\right)}$$

where

$$e_l = \|e_{h,u}^{(l)}(T)\|_h + \|D_{-x}e_{h,u}^{(l)}(T)\|_+.$$

Let $u(x,t) = e^{-t}sin(\pi x)$, $x \in [0,1]$, $t \in [0,T]$, be the solution of the IBVP (1.1), (1.3), (1.5 with

$$f(x,t) = e^{-t}sin(\pi x)\left(1 + D\pi^2\left(1 + \frac{e^{\frac{\tau-1}{\tau}t} - 1}{\tau - 1}\right)\right)$$

and initial conditions

$$\begin{aligned} u(x,0) &= \phi(x) &= sin(\pi x) \\ u_x(x,0) &= \psi(x) &= -sin(\pi x). \end{aligned}$$

The convergence rates obtained are included in the following table. The results are in agreement with the error estimate in Theorem 3.4.2.

N	$h_{max}^{(l)}$	e_l	p_l
20	0.0904	0.0171	-
40	0.0475	0.0047	1.992
80	0.0244	0.0013	1.972
160	0.0114	0.0003	1.994

4.3 Concentration

To obtain a numerical approximation for the semi-discrete approximation for the concentration defined by (3.21), (3.22) and (3.23) we use an implicit finite difference scheme.

Let $C^n = [C_1^n \ \ C_2^n \ \ \dots \ \ C_{N-1}^n]^T$ with $C_i^n \simeq c_h(x_i,t_n)$, $c_0 = [c_0(x_1) \ \ c_0(x_2) \ \ \dots \ \ c_0(x_{N-1})]^T$ and $F^n = [F_1^n \ \ F_2^n \ \ \dots \ \ F_{N-1}^n]^T$ with $F_i^n = f(x_i,t_n)$. Then our implicit scheme is defined by

$$\left\{ \begin{aligned} C^0 &= c_0 \\ \left((1+\Delta t\gamma)I - \Delta t D A_x + \Delta t B_x^{(n)}\right) C^n &= C^{n-1} + F^n \end{aligned} \right. \tag{4.2}$$

where $B_x^{(n)}$ denotes the matrix induced by the operator D_c

$$B_x^{(n)} = \begin{bmatrix} 0 & \frac{v(U_2^n)}{h_1+h_2} & 0 & \\ \frac{v(U_1^n)}{h_2+h_3} & 0 & \frac{v(U_3^n)}{h_2+h_3} & \cdots \\ 0 & \frac{v(U_2^n)}{h_3+h_4} & 0 & \\ & \vdots & & \ddots \end{bmatrix}.$$

Let $c(x,t) = e^{-t} sin(\pi x)$, $x \in [0,1]$, $t \in [0,T]$, be the solution of the IBVP (1.2), (1.4), (1.6) with the initial condition

$$c_0(x) = sin(\pi x),$$

$$f(x,t) = e^{-t} sin(\pi x)\left(2\pi e^{-t} cos(\pi x) + D\pi^2 + \gamma - 1\right),$$

$v(u) = u$ and

$$\begin{cases} D & = 0.1 \\ \gamma & = 1 \\ T & = 1. \end{cases}$$

In our numerical experiments we take

$$e_l = \|e_{h,c}^{(l)}(T)\|_h + \|D_{-x} e_{h,c}^{(l)}(T)\|_+$$

and the obtained convergence rates are included in the following table. The results are in agreement with the error estimate in Corollary 5.

N	$h_{max}^{(l)}$	e_l	p_l
20	0.0904	0.0266	-
40	0.0475	0.0073	2.012
80	0.0244	0.0019	1.984
160	0.0114	0.0004	2.115

Chapter 5

Conclusions

In this thesis we studied a coupled initial boundary value problem that describes the time and space evolution of the displacement of a viscoelastic material and the drug transport enhanced by this displacement. It is assumed that the material displacement is induced by pressure waves that propagate through the material and the pressure waves are generated by ultrasound. This system can be used to model drug transport through the skin enhanced by ultrasound. As the skin is a viscoelastic material, the Maxwell model was used to deduce a wave equation with an integral term for the displacement. For the drug concentration, a convection-diffusion equation is considered with a velocity v depending on the displacement. We believe that similar results can be obtained by considering v as a function of u, $\frac{\partial u}{\partial t}$ and ∇u.

We establish existence, uniqueness and stability results for displacement and concentration and, using the Method of Lines approach, semi-discrete approximations were introduced presenting discrete properties that can be seen as discrete versions of the continuous ones. Error bounds for the semi-discrete approximations were established allowing us to confirm the unexpected second order convergence in non uniform meshes.

References

[1] Crichton, M., Donose, B., Chen, X., Raphael, A., Huang, H., and Kendall, M. (2011). The viscoelastic, hyperelastic and scale dependent behaviour of freshly excised individual skin layers. *Biomaterials, 32(20):4670-81*.

[2] Ferreira, J. A., Jordão, D., and Pinto, L. (2017). Second order approximations for kinetic and potential energies in maxwell's wave equations. *Applied Numerical Mathematics, 120: 125-140*.

[3] Ferreira, J. A., Jordão, D., and Pinto, L. (2018). Approximating coupled hyperbolic-parabolic systems arising in enhanced drug delivery. *Computers & Mathematics with Applications 761(1):81-97*.

[4] Jordão, D. (2020). *Coupling hyperbolic and parabolic IBVP: applications to drug delivery*. PhD thesis, Universidade de Coimbra.

[5] Lavon, I. and Kost, J. (2004). Ultrasound and transdermal drug delivery. *Drug discovery today, 9(19):827*.

[6] Pao, C. (1992). *Nonlinear Parabolic and Elliptic Equations*. Fems Symposium. Springer US.

[7] Pitt, W., Husseini, G., and Staples, B. (2004). Ultrasonic drug delivery - a general review. *Expert Opinion Drug Delivery, 1(1): 37-56*.

[8] Seah, B. and Teo, B. (2018). Ultrasound and transdermal drug delivery. *International Journal of Nanomedicine, 152(3): 330-348*.

[9] Shen, Z., Kahn, H., Ballarini, R., and Eppell, S. (2011). Viscoelastic properties of isolated collagen fibrils. *Biophysical Journal, 100(12):3008-15*.

[10] T.Brown, Du, S., Eruslu, H., and Sayas, F.-J. (2018). Analysis of models for viscoelastic wave propagation. *Applied Mathematics and Nonlinear Analysis, 3(1):55-96*.