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NUMERICAL ANALYSIS OF A POROUS-ELASTIC MODEL FOR CONVECTION ENHANCED DRUG DELIVERY

J.A. FERREIRA, L. PINTO AND R.F. SANTOS

ABSTRACT: Convection enhanced drug delivery (CED) is a technique used to make therapeutic agents reach, through a catheter, sites of difficult access. The name of this technique comes from the convective flow originated by a pressure gradient induced at the tip of the catheter. This flow enhances passive diffusion and allows a more efficient spread of the agents by the target site. CED is particularly useful in the treatment of diseases that affect the central nervous system, where the blood-brain barrier prevents the diffusion of most therapeutic agents from the cerebral blood vessels to the brain interstitial space.

In this work we deal with the numerical analysis of a coupled system of partial differential equations that can be used to simulate CED in an elastic medium like brain tissue. The model variables are the fluid velocity, pressure, tissue deformation, and agents concentration. We prove the stability of the coupled problem and from the numerical point of view we propose a fully discrete piecewise linear finite element method (FEM). The convergence analysis shows that the method has second order convergence for the pressure, displacement, and concentration. Numerical experiments illustrating the theoretical convergence rates and the behavior of the system are also given.

KEYWORDS: Convection enhanced drug delivery, finite difference method, finite element method, convergence analysis.

1. Introduction

The brain-blood barrier is an obstacle to most of the therapeutic agents used in the treatment of diseases of the central nervous system like brain tumors, epilepsy, and Alzheimer. Therefore, to bypass this barrier, new approaches that directly inject the agents into the brain tissue with the aid of catheters are being investigated. Avoiding the systemic circulation these approaches minimize unwanted side effects and the agents degradation. One of such approaches is CED, a technique that employs a pressure gradient to distribute drugs within the target site. CED has shown to be more efficient than passive diffusion techniques that rely only on local concentration gradients to distribute drugs [3, 12]. Despite promising results a fully understanding of

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the agents distribution trough the brain tissue is still lacking. This is a crucial step before CED can be successfully applied in medical treatment. The main factors that influence the agents distribution are: catheter technology and implantation methods, infused agents characteristics and protocols, and the dynamics of fluid flow trough the brain tissue [2]. Mathematical modeling is a valuable tool that is commonly used to shed light on these issues [17, 11, 16].

One of the first mathematical models for CED simulation was proposed in [13]. This model was based on Darcy equation for pressure and fluid velocity and on a parabolic advection-diffusion equation for the agents concentration. A number of strong simplifications like tissue homogeneity allowed the authors to obtained an analytical solution. Since then CED modeling and simulation has become the subject of intense research, and several new models have been proposed in the literature. One of the main improvements were the so-called elastic models [16, 4, 15]. In this type of models the brain tissue is viewed as an elastic porous medium. This is a more realistic assumption than the rigidity assumption assumed in earlier studies like [13]. For instance, in [16] the tissue is considered to behave as an isotropic linear elastic material that deforms by action of fluid movement. Thus, the model variables are the pressure, the tissue displacement, and the agents concentration. Tissue heterogeneities and dispersion anisotropy are also taken into account. Moreover, the influence of displacement in the porosity and permeability is also considered. In particular, empirical formulas that relate porosity and permeability with the displacement divergence are employed. Based on realistic numerical simulations the authors concluded that elastic models are more reliable than rigid ones to describe CED in the brain. The numerical discretization was performed using a finite volume scheme. Similar conclusions highlighting the importance of elastic models were given in [4]. Here, it is pointed out that such type of models allows the development of safe and efficient protocols in the sense that the optimal therapeutic range is delivered with the minimal tissue deformation.

In this paper our focus is the numerical analysis of a piecewise linear FEM method for a coupled partial differential system. The concerned system is defined on a one-dimensional domain and can be used, for instance, to model CED in brain tissue. In that context the model accounts for fluid velocity, pressure, agents concentration, and tissue deformation. That is, it belongs to the elastic-type models and allows for medium heterogeneities, namely, variable permeability and elasticity. Next, we briefly deduce the system of equations that define the CED model.

Let us assume that the injected therapeutic agent is fully miscible in the interstitial fluid. Neglecting chemical reactions, and assuming constant porosity, the transport equation for the agent is given by

$$\frac{\partial c}{\partial t} + \nabla \cdot (vc) = \nabla \cdot (D\nabla c) + f \text{ in } \Omega \times (0, T], \tag{1}$$

where c denotes the concentration of the agent, D represents the diffusion coefficient, and f accounts for source and sink terms. Still in (1), we denote by v the transport velocity. This velocity v is the sum of two velocities, v_ℓ and v_s, which represent the velocity of the fluid mixture and the velocity of the deformable medium Ω, respectively. Assuming infinitesimal deformation, and denoting by u the displacement of each point of Ω, we can write that

$$v_s = \frac{\partial u}{\partial t}.$$

On the other hand, based on the assumption that brain tissue can be seen as porous media, we consider that the fluid velocity v_ℓ is given by Darcy's law

$$v_\ell = -\frac{1}{\mu} K \nabla p, \tag{2}$$

where p denotes the pressure, K denotes the permeability of the medium, and μ denotes the viscosity of the interstitial fluid. Thus, the transport velocity, $v = v_\ell + v_s$, is written as follows

$$v = -\frac{1}{\mu} K \nabla p + \frac{\partial u}{\partial t}. \tag{3}$$

Let us assume that the porosity is constant and that the fluid phase and the solid phase are incompressible, i.e,

$$\nabla \cdot v = \nabla \cdot (v_\ell + v_s) = s \text{ in } \Omega \times (0, T], \tag{4}$$

where s defines source and sink terms of the fluid flow. From (3) and (4) we deduce the following equation for the pressure

$$-\nabla \cdot (\frac{K}{\mu} \nabla p) + \nabla \cdot \frac{\partial u}{\partial t} = s \text{ in } \Omega \times (0, T]. \tag{5}$$

Now we address the modeling of the displacement field u. The total force F that acts in the porous medium is given by

$$F = \sigma - p,$$

where σ denotes the stress in the solid matrix and p the fluid pressure. We recall that the deformation ϵ depends on the displacement that in the one-dimensional case takes the form

$$\epsilon = \nabla \cdot u.$$

Moreover, if we assume that the stress and the strain are given by Hooke's law

$$\sigma = E_0 \epsilon,$$

where E_0 denotes Young's modulus, we get the following wave equation for the displacement

$$\frac{\partial^2 u}{\partial t^2} = \nabla \cdot (E_0 \nabla u) - \nabla p + r \ \text{ in } \Omega \times (0, T]. \tag{6}$$

Here, the term r collects exterior body forces, and it is null when the forces in the solid and in the fluid phases are in equilibrium.

The coupled problem (1), (5) and (6), is complemented with suitable initial and boundary conditions. For the concentration we assume that

$$\begin{cases} c(x,0) = c_0(x),\ x \in \Omega, \\ c(x,t) = 0,\ x \in \partial\Omega,\ t \in (0,T], \end{cases} \tag{7}$$

for the pressure we consider Dirichlet boundary conditions

$$p(x,t) = p_0(x,t),\ x \in \partial\Omega, t \in (0,T], \tag{8}$$

and finally for the displacement u we assume the following

$$\begin{cases} \dfrac{\partial u}{\partial t}(x,0) = \psi(x),\ x \in \Omega, \\ u(x,0) = \phi(x),\ x \in \Omega, \\ u(x,t) = 0,\ \ x \in \partial\Omega, t \in (0,T]. \end{cases} \tag{9}$$

The system of equations (1), (5), and (6), complemented with (7), (8), and (9), is a simplified but meaningful model for CED simulation in a porous-elastic medium.

Although the extensive literature on the numerical simulation of CED models, a detailed theoretically analysis of the schemes is usually not presented. As already mentioned our main concerned is the design and analysis of a piecewise linear FEM method for the initial boundary value problem (IBVP) (1), (5) (6), (7), (8) and (9). The goal is to obtain a numerical method that presents second order convergence, with respect to a discrete L^2-norm, for the concentration c. From the numerical point of view the main issue to overcome is the fact that the transport velocity v in (1) depends, through (3), on the gradient of the pressure p and also on the displacement u. Being governed by equation (6), u also depends on the gradient of the pressure p. Therefore, we must get at least second order convergence approximations for p in a discrete H^1-norm and for u in a discrete L^2-norm.

For this work, we build on the methods proposed in [8, 7, 10, 9, 14, 5, 6]. Namely, in [14, 5, 6] second order convergence, in a discrete H^1-norm, for the solution of an elliptic equation similar to (5) (u independent) are established for a piecewise linear FEM. In [7], a piecewise linear FEM was applied to a wave-type equation similar to (6) (p independent), and again second order convergence, in a discrete H^1-norm, was obtained for the solution. Coupled problems were considered in [8, 10, 9]. In, [10, 9] a parabolic equation of type (1) was coupled with an elliptic equation. This system models, for instance, transport of a fully miscible flow where the velocity is governed by Darcy's law. Second order convergence for the concentration, in a discrete L^2-norm, was again deduced for a piecewise linear FEM. Finally, in [8], a wave-type equation was coupled with a parabolic-type equation. This system can be used, e.g., to describe drug delivery enhanced by ultrasound. A piecewise linear FEM was proposed and it was proved that the numerical approximation for the solution of the parabolic problem is second order convergence in a discrete L^2-norm. Let us note that in those works non-standard analysis techniques allow the authors to reduce the smoothness assumptions on the solutions of the correspondent continuous problems. Also, the fact that piecewise linear FEM present second order convergence in a discrete H^1-norm is unexpected. Such phenomenon is usually referred in the literature as supercloness. Since these FEM can be seen as finite differences methods this is also known as supraconvergence. Important is also that these results stand for non-uniform spatial meshes. Despite this background, we point out that the analysis of the IBVP (1), (5) (6), (7), (8) and (9), presents much new difficulties.

We organize the paper as follows. In Section 2 we prove some energy estimates that show the stability of the IBVP (1), (5) (6), (7), (8) and (9). The existence of solution is not object of analysis is this work. However, from the energy estimates of Section 2, we easily get uniqueness of the solution. In Section 3, we introduce a discrete version of the previous continuous problem that can be obtained following two different approaches: a finite element approach or a finite difference approach. For such discrete problem we give discrete energy estimates that are discrete version of the continuous ones. The convergence analysis of the discrete model is given in Section 4. We show that the discrete pressure, displacement, and concentration converge to the correspondent continuous quantities, being the convergence rates equal to two in suitable discrete norms. Since the discrete model is based on piecewise linear finite element approximations, the obtained convergence rates exhibit the so-called supercloseness property. Some numerical experiments illustrating the behavior of the mathematical model as well as the obtained theoretical results are included in Section 5. Finally, in Section 6, we present some conclusions.

2. Model Stability: energy estimates

In what follows we prove stability, by energy estimates, for the weak solution of our differential problem. To do that, we assume homogeneous boundary conditions for the pressure. We adopt standard notations for Sobolev spaces, namely, $H^m(\Omega)$, $H_0^m(\Omega)$, $m \in \mathbb{N}_0$, as well as for the corresponding inner products and norms. Let V be a norm space equipped with the norm $\|.\|_V$. By $C^m(0,T,V)$, $m \in \mathbb{N}_0$, we represent the space of continuous functions, $v^{(j)}(t) : [0,T] \to V$, $j = 0,\ldots,m$, and such that, $\max_{j=0,\ldots,m} \|v^{(j)}(t)\|_V^2 < +\infty$. By $H^m(0,T,V)$, $m \in \mathbb{N}_0$, we represent the space of functions, $v(t) : (0,T) \to V$, with weak derivatives $v^{(j)}(t) : (0,T) \to V$, $j = 1,\ldots,m$, and such that, $\sum_{j=0}^m \int_0^T \|v^{(j)}(t)\|_V^2 dt < +\infty$.

The variational formulation of our problem is: find $p \in L^2(0,T,H_0^1(\Omega))$, $u \in H^2(0,T,H_0^1(\Omega))$, and $c \in L^2(0,T,H_0^1(\Omega))$, such that,

$$(A\nabla p(t), \nabla w) - (u'(t), \nabla w) = (s(t), w) \text{ a.e. in } (0,T), w \in H_0^1(\Omega), \quad (10)$$

where $A = \dfrac{K}{\mu}$,

$$\begin{cases} (u''(t), q) + (E_0 \nabla u(t), \nabla q) = -(\nabla p(t), q) + (r(t), q), \\ u'(0) = \psi \\ u(0) = \phi \end{cases} \quad (11)$$

a.e. in $(0,T)$, $q \in H_0^1(\Omega)$ and

$$\begin{cases} (c'(t), z) - (vc(t), \nabla z) + (D\nabla c(t), \nabla z) = (f(t), z), \\ c(0) = c_0 \end{cases} \quad (12)$$

a.e. in $(0,T)$, $z \in H_0^1(\Omega)$.

We start by analyzing the pressure equation. Taking in (10) $w = p(t)$, and assuming that $A \geq A_{min} > 0$, we get

$$A_{min}\|\nabla p(t)\|^2_{L^2} \leq \frac{1}{4\epsilon_1^2}\|u'(t)\|^2_{L^2} + \epsilon_1^2\|\nabla p(t)\|^2_{L^2} + \frac{1}{4\epsilon_2^2}\|s(t)\|^2_{L^2} + \epsilon_2^2\|p(t)\|^2_{L^2}, \quad (13)$$

where $\epsilon_i \neq 0, i = 1, 2$. Since $\|p(t)\|_{L^2} \leq C\|\nabla p(t)\|_{L^2}$, with C a positive constant, from (13) we obtain

$$(A_{min} - \epsilon_1^2 - \epsilon_2^2 C)\|\nabla p(t)\|^2_{L^2} \leq \frac{1}{4\epsilon_1^2}\|u'(t)\|^2_{L^2} + \frac{1}{4\epsilon_2^2}\|s(t)\|^2_{L^2}. \quad (14)$$

Fixing $\epsilon_i, i = 1, 2$, satisfying

$$A_{min} - \epsilon_1^2 - \epsilon_2^2 C > 0,$$

we conclude that there exists a positive constant C_p such that

$$\|\nabla p(t)\|^2_{L^2} \leq C_p(\|u'(t)\|^2_{L^2} + \|s(t)\|^2_{L^2}). \quad (15)$$

Now we analyze the displacement equation. Taking in (11) $q = u'(t)$, we deduce

$$\frac{1}{2}\frac{d}{dt}\|u'(t)\|^2_{L^2} + \frac{1}{2}\frac{d}{dt}\|\sqrt{E_0}\nabla u(t)\|^2_{L^2} \leq \frac{1}{4\epsilon_3^2}\|\nabla p(t)\|^2_{L^2} + (\epsilon_3^2 + \epsilon_4^2)\|u'(t)\|^2_{L^2} + \frac{1}{4\epsilon_4^2}\|r(t)\|^2_{L^2}. \quad (16)$$

where $\epsilon_i \neq 0, i = 3, 4$. Assuming that $u \in C^2(0, T, L^2(\Omega)) \cap C^1(0, T, H^1_0(\Omega))$, inequality (16) leads to

$$\|u'(t)\|^2_{L^2} + \|\sqrt{E_0}\nabla u(t)\|^2_{L^2} \leq \frac{1}{2\epsilon_3^2}\int_0^t \|\nabla p(\zeta)\|^2_{L^2} d\zeta + 2(\epsilon_3^2 + \epsilon_4^2)\int_0^t \|u'(\zeta)\|^2_{L^2} d\zeta + \frac{1}{2\epsilon_4^2}\int_0^t \|r(\zeta)\|^2_{L^2} d\zeta + \|\psi\|^2_{L^2} + \|\sqrt{E_0}\nabla\phi\|^2_{L^2}, \quad (17)$$

provided that $\psi \in L^2(\Omega)$ and $\phi \in H^1(\Omega)$. Using the estimate (15) in (17), we get

$$\|u'(t)\|^2_{L^2} + \|\sqrt{E_0}\nabla u(t)\|^2_{L^2} \leq \Big(2(\epsilon_3^2 + \epsilon_4^2) + \frac{1}{2\epsilon_3^2}C_p\Big)\int_0^t \|u'(\zeta)\|^2_{L^2} d\zeta + \int_0^t \Big(\frac{1}{2\epsilon_4^2}\|r(\zeta)\|^2_{L^2} + \frac{1}{2\epsilon_3^2}C_p\|s(\zeta)\|^2_{L^2}\Big)d\zeta + \|\psi\|^2_{L^2} + \|\sqrt{E_0}\nabla\phi\|^2_{L^2}. \quad (18)$$

Applying Gronwall's lemma we conclude that there exist positive constants $C_{u,1}$ and $C_{u,2}$, such that,

$$\|u'(t)\|_{L^2}^2 + \|\nabla u(t)\|_{L^2}^2 \leq C_{u,1} e^{C_{u,2} t}\Big(\int_0^t \Big(\|r(\zeta)\|_{L^2}^2 + \|s(\zeta)\|_{L^2}^2 \Big) d\zeta + \|\psi\|_{L^2}^2 + \|\nabla \phi\|_{L^2}^2 \Big), \tag{19}$$

provided that $E_{max} \geq E_0 \geq E_{min} > 0$.

Now, taking into account (19), we rewrite the pressure estimate (15). We obtain,

$$\|\nabla p(t)\|_{L^2}^2 \leq C_p \Big(C_{u,1} e^{C_{u,2} t}\Big(\int_0^t \Big(\|r(\zeta)\|_{L^2}^2 + \|s(\zeta)\|_{L^2}^2 \Big) d\zeta + \|\psi\|_{L^2}^2 + \|\nabla \phi\|_{L^2}^2 \Big) + \|s(t)\|_{L^2}^2 \Big). \tag{20}$$

At last we consider the concentration equation. Taking in (12) $z = c(t)$, we find

$$\frac{1}{2}\frac{d}{dt}\|c(t)\|_{L^2}^2 + D_{min}\|\nabla c(t)\|_{L^2}^2 \leq \|c(t)\|_\infty (A_{max}\|\nabla p(t)\|_{L^2} + \|u'(t)\|_{L^2})\|\nabla c(t)\|_{L^2} + \frac{1}{4\epsilon_5^2}\|f(t)\|_{L^2}^2 + \epsilon_5^2 \|c(t)\|_{L^2}^2. \tag{21}$$

for $\epsilon_5 \neq 0$ and provided that $D \geq D_{min} > 0$ and $A_{max} \geq A \geq A_{min} > 0$. Using the fact that $\|c(t)\|_\infty \leq C_c \|\nabla c(t)\|_{L^2}$, for some positive constant C_c, from (21), we get

$$\frac{d}{dt}\|c(t)\|_{L^2}^2 + 2(D_{min} - G(r,s,\phi,\psi))\|\nabla c(t)\|_{L^2}^2 \leq \frac{1}{2\epsilon_5^2}\|f(t)\|_{L^2}^2 + 2\epsilon_5^2\|c(t)\|_{L^2}^2. \tag{22}$$

where

$$G(r,s,\phi,\psi) = C_c A_{max}\sqrt{C_p}\|s(t)\|_{L^2} + C_c\sqrt{C_{u,1}} e^{\frac{1}{2}C_{u,2}t}\Big(1 + A_{max}\sqrt{C_p}\Big) \times \Big(\int_0^t \big(\|r(\zeta)\|_{L^2}^2 + \|s(\zeta)\|_{L^2}^2 \big) d\zeta + \|\psi\|_{L^2}^2 + \|\nabla\phi\|_{L^2}^2 \Big) 1/2.$$

Assuming that $c \in C^1(0,T,L^2(\Omega)) \cap C(0,T,H_0^1(\Omega))$, we have from (22), that

$$\|c(t)\|_{L^2}^2 + 2\int_0^t \Big(D_{min} - G(r,s,\phi,\psi)\Big)\|\nabla c(\zeta)\|_{L^2}^2 d\zeta \leq \|c_0\|_{L^2}^2 + \frac{1}{2\epsilon_5^2}\int_0^t \|f(\zeta)\|_{L^2}^2 d\zeta + 2\epsilon_5^2 \int_0^t \|c(\zeta)\|_{L^2}^2 d\zeta,$$

and Gronwall's lemma leads to

$$\|c(t)\|_{L^2}^2 + 2\int_0^t \Big(D_{min} - G(r,s,\phi,\psi)\Big)\|\nabla c(\zeta)\|_{L^2}^2 d\zeta \leq e^{2\epsilon_5^2 t}\Big(\|c_0\|_{L^2}^2 + \frac{1}{2\epsilon_5^2}\int_0^t \|f(\zeta)\|_{L^2}^2 d\zeta\Big). \tag{23}$$

From estimate (23) we get a stability result provided that the data of our IBVP satisfies the inequality

$$D_{min} - G(r,s,\phi,\psi) \geq 0. \tag{24}$$

Moreover, if the coupled system is isolated in the sense that we do not have source or sink terms, then condition (24) reduces to

$$D_{min} - C_c\sqrt{C_{u,1}}e^{\frac{1}{2}C_{u,2}t}(1 + A_{max}\sqrt{C_p})(\|\psi\|_{L^2}^2 + \|\nabla\phi\|_{L^2}^2)^{1/2} \geq 0.$$

Our stability result is presented next and it follows directly from the previous estimates assuming no source or sink terms.

Proposition 1. *Let $(p,u,c), (\tilde{p},\tilde{u},\tilde{c})$ in $L^\infty(0,T,H_0^1(\Omega)) \times (C^2(0,T,L^2(\Omega)) \cap C^1(0,T,H_0^1(\Omega))) \times (C^1(0,T,L^2(\Omega)) \cap C(0,T,H_0^1(\Omega)))$ be solutions of the variational problem (10), (11), and (12), with the initial conditions ϕ, ψ, c_0 and $\tilde{\phi}$, $\tilde{\psi}$, $\tilde{c}_0$, respectively, where ϕ, c_0, $\tilde{\psi}$, $\tilde{c}_0 \in L^2(\Omega)$ and ϕ, $\tilde{\phi} \in H_0^1(\Omega)$. Then there exist positive constants C_p, $C_{u,1}$, $C_{u,2}$ and $C_{c,1}$, $C_{c,2}$ such that, for $t \in [0,T]$, we have*

$$\|\nabla(p(t) - \tilde{p}(t))\|_{L^2}^2 \leq C_p C_{u,1} e^{C_{u,2}t}\Big(\|\psi - \tilde{\psi}\|_{L^2}^2 + \|\nabla(\phi - \tilde{\phi})\|_{L^2}^2\Big), \tag{25}$$

$$\|u'(t) - \tilde{u}'(t)\|_{L^2}^2 + \|\nabla(u(t) - \tilde{u}(t))\|_{L^2}^2 \leq C_{u,1}e^{C_{u,2}t}\Big(\|\psi - \tilde{\psi}\|_{L^2}^2 + \|\nabla(\phi - \tilde{\phi})\|_{L^2}^2\Big), \tag{26}$$

and

$$\|c(t)-\tilde{c}(t)\|_{L^2}^2+2\int_0^t\Big(D_{min}-G(0,0,\phi-\tilde{\phi},\psi-\tilde{\psi})\Big)\|\nabla(c(\zeta)-\tilde{c}(\zeta)\|_{L^2}^2 d\zeta \leq e^{C_{c,2}t}\Big(\|c_0-\tilde{c}_0\|_{L^2}^2\Big), \quad (27)$$

where

$$G(0,0,d,g)=C_{c,1}\sqrt{C_{u,1}}e^{\frac{1}{2}C_{u,2}t}\Big(1+A_{max}\sqrt{C_p}\Big)\Big(\|g\|_{L^2}^2+\|\nabla d\|_{L^2}^2\Big)^{1/2}\geq 0$$

for $t\in[0,T]$, $g\in L^2(\Omega)$ *and* $d\in H_0^1(\Omega)$. ■

Corollary 1. *Under the assumptions of Proposition 1, if*

$$D_{min}-G(0,0,\phi-\tilde{\phi},\psi-\tilde{\psi})\geq 0,$$

then we conclude the stability of the variational problem (10), (11) and (12). ■

3. Numerical scheme: stability and convergence analysis

In this section we present a piecewise linear FEM for our problem. An equivalent finite difference method (FDM) is also given. Stability and convergence results are also provided.

3.1. A piecewise linear FEM. Let $h=(h_1,\dots,h_N)$ be the vector of positive entries, in a sequence Λ, such that $\sum_{i=1}^N h_i = |\Omega|$, with $|\Omega|$ the length of Ω, and let $h_{max}=\max_{i=1,\dots,N} h_i$ and $H_{min}=\min_{i=1,\dots,N} h_i$. We assume that the sequence Λ is such that $h\in\Lambda, h_{max}\to 0$. Let $\{x_i\}$ be the non-uniform grid induced by h in $\overline{\Omega}$ with $h_i=x_i-x_{i-1}$, $i=1,\dots,N$. By $\overline{\Omega}_h$ we represent the grid defined in $\overline{\Omega}$ that depends on h. By Ω_h we denote the interior set of nodes, $\Omega_h=\Omega\cap\overline{\Omega}_h$, and by $\partial\Omega_H$ we denote the boundary set of nodes, $\partial\Omega_h=\partial\Omega\cap\overline{\Omega}_h$.

By W_h we represent the space of grid functions defined in $\overline{\Omega}_h$ and by $W_{h,0}$ we represent the subspace of W_h of grid functions null on $\partial\Omega_h$. By $P_h v_h$ we denote the continuous piecewise linear interpolant of v_h with respect to the partition $\overline{\Omega}_h$. In $W_{h,0}$ we introduce the inner product

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

where $h_{i+1/2} = \frac{1}{2}(h_i + h_{i+1})$. Let $\|.\|_h$ be the corresponding norm. We set $x_{i+1/2} = x_i + \frac{1}{2}h_{i+1}$, $x_{i-1/2} = x_i - \frac{1}{2}h_i$, and we define

$$(z_h, w_h)_{h,+} = \sum_{i=1}^{N} h_i z_h(x_i) w_h(x_i) \quad \text{and} \quad \|z_h\|_{h,+} = \sqrt{(z_h, z_h)_{h,+}}$$

for $z_h, w_h \in W_h$. Let ∇_h be the first order backward finite difference operator. We note that holds the following Poincaré-Friedrichs inequality

$$\|w_H\|_h \le |\Omega| \|\nabla_h w_H\|_{h,+}, \ \forall w_H \in W_{H,0}. \tag{28}$$

By $W^{1,2}_{h,0}$ we denote the space of grid functions null on the boundary points and equipped with the norm

$$\|w_h\|_{1,h} = \Big(\|w_h\|_h^2 + \|\nabla_h w_h\|_{h,+}^2\Big)^{1/2}.$$

The piecewise linear finite element approximation of the coupled problem (10), (11), and (12) is given by: find $P_h p_h(t)$, $P_h u_H(t)$, $P_h c_H(t) \in H_0^1(\Omega)$, such that,

$$(A\nabla P_h p_h(t), \nabla P_h w_h) - (P_h u_h'(t), \nabla P_h w_h) = (s(t), P_h w_h), \ w_h \in W_{h,0}, \tag{29}$$

$$\begin{cases} (P_h u_h''(t), P_h q_h) + (E_0 \nabla P_h u_h(t), \nabla P_h q_h) = -(\nabla P_h p_h(t), P_h q_h) + (r(t), P_h q_h), \\ P_h u_h'(0) = P_h R_h \psi, \\ P_h u_h(0) = P_h R_h \phi, \end{cases} \tag{30}$$

for $q_h \in W_{h,0}$ and

$$\begin{cases} (P_h c_h'(t), P_h z_h) - (P_h v_h(t) P_h c_h(t), \nabla P_h z_h) + (D\nabla P_h c_h(t), \nabla P_h z_h) = (f(t), P_h z_h), \\ P_h c_h(0) = P_h R_h c_0, \end{cases} \tag{31}$$

for $z_h \in W_{h,0}$ and where $P_h v_h(x,t) = -A(x)\nabla P_h p_h(x,t) + P_h u_h'(x,t), x \in \Omega_h$. In (30) and (31), R_h denotes the restriction operator $R_h : C(\overline{\Omega}) \to W_h$, $R_h g(x) = g(x)$, $x \in \overline{\Omega}_h$.

Let us define the following functions in W_h

$$\begin{aligned} s_h(x_i) &= \tfrac{1}{h_{i+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} s(x)dx, \ i = 1, \dots, N-1, \\ s_h(x_0) &= \tfrac{1}{h_1/2} \int_{x_0}^{x_{1/2}} s(x)dx, \\ s_h(x_N) &= \tfrac{1}{h_N/2} \int_{x_{N-1/2}}^{x_N} s(x)dx, \end{aligned} \tag{32}$$

being $r_h(t)$ and $f_h(t)$ defined analogously. We also define the finite difference operator D_h^* by

$$D_h^* w_h(x_i) = \frac{h_{i+1}}{h_i + h_{i+1}} \nabla_h w_h(x_i) + \frac{h_i}{h_i + h_{i+1}} \nabla_h w_h(x_{i+1}),\ i = 1, \dots, N-1.$$

The coupled problem (29), (30), and (31) is then replaced by the following fully discrete piecewise linear FEM: find $p_h(t)$, $u_H(t)$, $c_H(t) \in W_{h,0}$, such that,

$$(A_h \nabla_h p_h(t), \nabla_h w_h)_{h,+} - (M_h(u_h'(t)), \nabla_h w_h)_{h,+} = (s_h(t), w_h)_h,\ w_h \in W_{h,0}, \tag{33}$$

where $A_h(x_i) = A(x_{i-1/2}), i = 1, \dots, N$, and M_h denotes the average operator

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

$$\begin{cases} (u_h''(t), q_h)_h + (E_{0,h} \nabla_h u_h(t), \nabla_h q_h)_{h,+} = -(D_h^* p_h(t), q_h)_h + (r_h(t), q_h)_h, \\ u_h'(0) = R_h \psi, \\ u_h(0) = R_h \phi, \end{cases} \tag{34}$$

for $q_h \in W_{h,0}$ and where $E_{0,h}(x_i) = E_0(x_{i-1/2}), i = 1, \dots, N$, and

$$\begin{cases} (c_h'(t), z_h)_h - (M_h(v_h(t) c_h(t)), \nabla_h z_h)_{h,+} + (D_h \nabla_h c_h(t), \nabla_h z_h)_{h,+} = (f_h(t), z_h)_h, \\ c_h(0) = R_h c_0, \end{cases} \tag{35}$$

for $z_h \in W_{h,0}$, where $D_h(x_i) = D(x_{i-1/2}), i = 1, \dots, N$, and $v_h(t)$ is defined by

$$v_h(x_i, t) = A(x_i) D_h^* p_h(x_i) + u_h'(x_i, t),\ i = 1, \dots, N-1, \tag{36}$$

$$v_h(x_0, t) = A(x_0) \nabla_h p_h(x_1, t), \tag{37}$$

$$v_h(x_N, t) = A(x_N) \nabla_h p_h(x_N, t). \tag{38}$$

Note that the definition of v_h at x_0 and x_N has no role in what follows because in (35) they arise multiplied by $c_h(x_0, t)$ and $c_h(x_N, t)$, respectively, which are both null.

3.2. An equivalent FDM. In what follows we present a finite difference method that is equivalent to the fully discrete piecewise linear FEM (33), (34), and (35). First, we introduce the first order centered operator

$$\nabla_{h,c} w_h(x_i) = \frac{w_h(x_{i+1}) - w_h(x_{i-1})}{h_i + h_{i+1}},\ i = 1, \dots, N-1,\ w_h \in W_h,$$

and the finite difference operator ∇_h^* given by,

$$\nabla_h^*(R_h B \nabla_h w_h)(x_i) = \frac{B(x_{i+1/2})\nabla_h w_h(x_{i+1}) - B(x_{i-1/2})\nabla_h w_h(x_i)}{h_{i+1/2}},$$

$i = 1, \dots, N-1$, for $w_h \in W_h$.

Then the FDM equivalent to the fully discrete pieceise linear FEM (33), (34), (35) is defined by the following systems

$$\begin{cases} -\nabla_h^*(A_h \nabla_h p_h(t)) + \nabla_{h,c} u_h'(t) = s_h(t) \text{ in } \Omega_h \times (0,T] \\ p_h(t) = 0 \text{ on } \partial\Omega, \end{cases} \tag{39}$$

$$\begin{cases} u_h''(t) = \nabla_h^*(E_{0,h} \nabla_h u_h(t)) - D_h^* p_h(t) + r_h(t) \text{ in } \Omega_h \times (0,T] \\ u_h(t) = 0 \text{ on } \partial\Omega_h \times (0,T] \\ u_h'(0) = R_h \psi \text{ in } \Omega_h, \\ u_h(0) = R_h \phi \text{ in } \Omega_h, \end{cases} \tag{40}$$

and

$$\begin{cases} c_h'(t) + \nabla_{h,c}(v_h(t) c_h(t)) = \nabla_h^*(D_h \nabla_h c_h(t)) + f_h(t) \text{ in } \Omega_h \times (0,T] \\ c_h(t) = 0 \text{ on } \partial\Omega_h \times (0,T], \\ c_h(0) = R_h c_0 \text{ in } \Omega_h, \end{cases} \tag{41}$$

where $v_h(t)$ is defined by (36).

The equivalence between (33), (34), (35) and (39), (40) and (41) is easily shown nothing that (33), (34), and (35) can be rewritten in the form

$$(-\nabla_h^*(A_h \nabla_h p_h(t)), w_h)_h + (\nabla_{h,c}(u_h'(t)), w_h)_h = (s_h(t), w_h),\ w_h \in W_{h,0},$$

using here summation by parts,

$$(u_h''(t), q_h)_h = (\nabla_h^*(E_{0,h} \nabla_h u_h(t)), q_h)_h - (D_h^* p_h(t), q_h)_h + (r_h(t), q_h)_h,\ q_h \in W_{h,0},$$

and

$$(c_h'(t), z_h)_h + (\nabla_{h,c}(v_h(t) c_h(t)), z_h)_h = (\nabla_h^*(D_h \nabla_h c_h(t)), z_h)_h + (f_h(t), z_h)_h,\ z_h \in W_{h,0},$$

respectively.

3.3. Stability analysis. In the following, we prove the stability of the piecewise linear FEM (33), (34), and (35). Naturally, this also proves the stability of the FDM (39), (40), and (41).

Proposition 2. *Let us suppose that the initial conditions for the displacement u_h are defined by ϕ_h and ψ_h and the initial condition for the concentration c_h is defined by $c_{0,h}$. Let $r, s, f \in C(0,T,C^0(\overline{\Omega}))$.*

The sequence Λ that defines the spatial grids in $\overline{\Omega}_h$ satisfies

$$\frac{h_{max}}{h_{min}} \le C_g, \tag{42}$$

for some positive constant C_g.

Then $u_h \in C^2(0,T,W_{h,0}), p_h \in C^0(0,T,W_{h,0}), c_h \in C^1(0,T,W_{h,0})$ and there exist positive constants $C_{u,1}$ and $C_{u,2}$ and C_p such that

$$\|u_h'(t)\|_h^2 + \|\nabla_h u_h(t)\|_{h,+}^2 \le C_{u,1} e^{C_{u,2}t}\Big(\int_0^t \Big(\|r_h(\zeta)\|_h^2 + \|s_h(\zeta)\|_h^2\Big) d\zeta + \|\psi_h\|_h^2 + \|\nabla_h \phi_h\|_{h,+}^2\Big), \tag{43}$$

$$\|\nabla_h p_h(t)\|_{h,+}^2 \le C_p\Big(C_{u,1} e^{C_{u,2}t}\Big(\int_0^t \Big(\|r_h(\zeta)\|_h^2 + \|s_h(\zeta)\|_h^2\Big) d\zeta + \|\psi_h\|_h^2 + \|\nabla_h \phi_h\|_{h,+}^2\Big) + \|s_h(t)\|_h^2\Big). \tag{44}$$

and, for $\epsilon \neq 0$,

$$\|c_h(t)\|_h^2 + \int_0^t \|\nabla_h c_h(\zeta)\|_{h,+}^2 d\zeta \le C_c e^{2\epsilon^2 t}\Big(\|c_{0,h}\|_h^2 + \frac{1}{2\epsilon^2}\int_0^t \|f_h(\zeta)\|_h^2 d\zeta\Big), \tag{45}$$

provide that

$$D_{min} - G_h(r_h, s_h, \phi_h, \psi_h) > 0. \tag{46}$$

where

$$G_h(r_h, s_h, \phi_h, \psi_h) = |\Omega|^{1/2} A_{max}\sqrt{C_p}\|s_h(t)\|_h + |\Omega|^{1/2}\sqrt{C_{u,1}} e^{\frac{1}{2}C_{u,2}t}\Big(1 + A_{max}\sqrt{C_p}\Big)\Big(\int_0^t \big(\|r_h(\zeta)\|_h^2 + \|s_h(\zeta)\|_h^2\big) d\zeta + \|\psi_h\|_{L^2}^2 + \|\nabla_h \phi_h\|_{h,+}^2\Big)^{1/2}.$$

Proof: We start with the pressure equation. Choosing $w_h = p_h(t)$ in (33), using the discrete Poincaré-Friedrichs inequality (28), and adapting the steps followed in the continuous case, it can be shown that there exist a positive constant C_p, such that,

$$\|\nabla_h p_h(t)\|^2_{h,+} \leq C_p\|u'_h(t)\|^2_h + \|s_h(t)\|^2_h. \tag{47}$$

Now we analyze the displacement equation. We start by remarking that u_h can be rewritten as a solution of a second order differential equation depending on s_h and r_h. If s and r are smooth, then $u_h \in C^2(0,T,W_{h,0})$ and consequently $u_h \in C^1(0,T,W^{1,2}_{h,0})$ and $p_h \in C^0(0,T,W_{h,0})$. We note also that

$$\begin{aligned}|(D^*_h p_h(t), q_h| &\leq \|D^*_h p_h(t)\|_h\|q_h\|_h \\ &\leq \sqrt{2C_g}\|\nabla_h p_h(t)\|_{h,+}\|q_h\|_h,\end{aligned}$$

Taking $q_h = u_h(t)$ in (34) and adapting the procedure used to obtain (19), we get that exist positive constants $C_{u,1}$, and $C_{u,2}$, such that (43) holds. Using (43), we can rewrite the pressure related inequality (47) as (44).

Now we focus on the concentration. First from straightforward calculations, we find

$$\begin{aligned}|(M_h(v_h(t)c_h(t)), \nabla_h c_h)_{h,+}| \leq \|c_h(t)\|_\infty(A_{max}&\|\nabla_h p_h(t)\|_{h,+} \\ &+ \|u'_h(t)\|_h)\|\nabla_h c_h(t)\|_{h,+}.\end{aligned} \tag{48}$$

Using the fact that $\|c_h(t)\|_\infty \leq |\Omega|^{1/2}\|\nabla_h c_h(t)\|_{h,+}$, taking $z_h = c_h(t)$ in (35), and adapting the procedure used to obtain (23), we get (45).

■

We conclude the uniform boundedness of $p_h(t), u_h(t)$ and $c_h(t)$ in Λ and $[0,T]$. We observe that (46) provides a compatibility condition between the diffusion coefficient and the data defined by ϕ_h, ψ_h, r and s.

In the following we derive estimates that will allow us to obtain a stability result considering perturbations of the solution (p_h, u_h, c_h) of the coupled system (33), (34), and (35).

Proposition 3. *Let us suppose that the sequence Λ that defines the spatial grids in $\overline{\Omega}_h$ satisfies (42) and, for $h \in \Lambda$, $(p_h, u_h, c_h) \in L^\infty(0,T,W_{h,0}) \times C^2(0,T,W_{h,0}) \times C^1(0,T,W_{h,0})$ with initial conditions defined by ϕ_h and ψ_h for the displacement and $c_{0,h}$ for the concentration. Let $(\tilde{p}_h, \tilde{u}_h, \tilde{c}_h) \in L^\infty(0,T,W_{h,0}) \times C^2(0,T,W_{h,0}) \times C^1(0,T,W_{h,0})$ be the solution of (33), (34), and (35) with the initial conditions defined by $\tilde{\psi}_h$, $\tilde{\phi}_h$, $\tilde{c}_{0,h}$, that we suppose to be such that $\|\tilde{\psi}_h\|_h$, $\|\nabla_h\tilde{\phi}_h\|_{h,+}$, $\|\tilde{c}_0\|_h, h \in \Lambda$, are bounded sequences. Then there* *exist positive constants C_p, $C_{u,1}, C_{u,2}$ and $C_{c,1}, C_{c,2}$ such that, for $\omega_{p,h}(t) = p_h(t) - \tilde{p}_h(t)$, $\omega_{u,h}(t) = u_h(t) - \tilde{u}_h(t)$ and $\omega_{c,h}(t) = c_h(t) - \tilde{c}_h(t)$, we have*

$$\|\nabla_h \omega_{p,h}(t)\|_{h,+}^2 \leq C_p C_{u,1} e^{C_{u,2}t}\Big(\|\psi_h - \tilde{\psi}_h\|_h^2 + \|\nabla_h(\phi_h - \tilde{\phi}_h)\|_{h,+}^2\Big), \tag{49}$$

$$\begin{aligned}\|\omega_{u,h}(t)'\|_h^2 + \|\nabla_h \omega_{u,h}(t)\|_{h,+}^2 \leq C_{u,1} e^{C_{u,2}t}\Big(&\|\psi_h - \tilde{\psi}_h\|_h^2 \\ &+ \|\nabla_h(\phi_h - \tilde{\phi}_h)\|_{h,+}^2\Big).\end{aligned} \tag{50}$$

$$\begin{aligned}\|\omega_{c,h}(t)\|_h^2 + \int_0^t \|\nabla_h \omega_{c,h}(s)\|_{h,+}^2 ds \leq C_{c,2}\|c_{0,h} - \tilde{c}_{0,h}\|_h^2 \\ + \frac{1}{\epsilon^2} C_{c,1}^2 C_{u,1} e^{C_{u,2}t} T\Big(\|\psi_h - \tilde{\psi}_h\|_h^2 + \|\nabla_h(\phi_h - \tilde{\phi}_h)\|_{h,+}^2\Big),\end{aligned} \tag{51}$$

for $t \in [0,T]$. In (51), ϵ is such that

$$D_{min} - \epsilon^2 - G(\psi_h, \phi_h) > 0, \tag{52}$$

and

$$G(\psi_h, \phi_h) = C_{c,1}\sqrt{C_{u,1}} e^{\frac{1}{2}C_{u,2}t}\Big(1 + A_{max}\sqrt{C_p}\Big)\Big(\|\psi_h\|_h^2 + \|\nabla_h \phi_h\|_{h,+}^2\Big)^{1/2}. \tag{53}$$

Proof: Following the steps that led to (44) and (43), we get that there exist positive constants C_p and $C_{u,1}, C_{u,2}$ such that, for $t \in [0,T]$ it holds (49), (50). The question now is to estimate the quantity

$$\|\omega_{c,h}(t)\|_h^2 + \int_0^t \|\nabla_h \omega_{c,h}(s)\|_{h,+} ds.$$

For that, we need an upper bound for

$$(M_h(v_h(t)c_h(t) - \tilde{v}_h \tilde{c}_h(t)), \nabla_h \omega_{c,h}(t))_{h,+}.$$

Since $v_h(t)$ and $\tilde{v}_h(t)$ are defined by (36) with $p_h(t), u_h'(t)$ and $\tilde{p}_h(t), \tilde{u}_h'(t)$, respectively, we can use (42), to conclude that there exists a positive constant

$C_{c,1}$, such that,

$$
\begin{aligned}
&|(M_h(v_h(t)c_h(t) - \tilde{v}_h\tilde{c}_h(t)), \nabla_h\omega_{c,h}(t))_{h,+}| \\
&\leq C_{c,1}\Big(\Big(A_{max}\|\nabla_h p_h(t)\|_{h,+} + \|u_h'(t)\|_h\Big)\|\omega_{c,h}(t)\|_\infty\|\nabla_h\omega_{c,h}(t)\|_{h,+} \\
&\quad + \|\tilde{c}_h(t)\|_\infty\Big(A_{max}\|\nabla_h\omega_{p,h}(t)\|_{h,+} + \|\omega_{u,h}'(t)\|_h\Big)\|\nabla_h\omega_{c,h}(t)\|_{h,+}\Big) \\
&\leq C_{c,1}\Big(\|\nabla_h p_h(t)\|_{h,+} + \|u_h'(t)\|_h\Big)\|\nabla_h\omega_{c,h}(t)\|^2_{h,+} \\
&\quad + \frac{1}{4\epsilon^2}C_c^2\|\tilde{c}_h(t)\|^2_\infty\Big(\|\nabla_h\omega_{p,h}(t)\|^2_{h,+} + \|\omega_{u,h}'(t)\|^2_h\Big) + \epsilon^2\|\nabla_h\omega_{c,h}(t)\|^2_{h,+} \\
&\leq C_{c,1}\sqrt{C_{u,1}}e^{\frac{1}{2}C_{u,2}t}\Big(1 + A_{max}\sqrt{C_p}\Big)\Big(\|\psi_h\|^2_h + \|\nabla_h\phi_h\|^2_{h,+}\Big)^{1/2}\|\nabla_h\omega_{c,h}(t)\|^2_{h,+} \\
&\quad + \frac{1}{4\epsilon^2}C_{c,1}^2C_{u,1}e^{C_{u,2}t}\Big(1 + A_{max}C_p\Big)\Big(\|\psi_h - \tilde{\psi}_h\|^2_h + \\
&\quad \|\nabla_h(\phi_h - \tilde{\phi}_h)\|^2_{h,+}\Big)\|\nabla_h\tilde{c}_h(t)\|^2_{h,+} + \epsilon^2\|\nabla_h\omega_{c,h}(t)\|^2_{h,+}.
\end{aligned}
$$

Then, we obtain

$$
\begin{aligned}
&\frac{1}{2}\|\omega_{c,h}(t)\|^2_h + (D_{min} - \epsilon^2 - G(\psi_h, \phi_h))\|\nabla_h\omega_{c,h}(t)\|^2_{h,+} \\
&\qquad\qquad \leq F(\phi_h, \tilde{\phi}_h, \psi_h, \tilde{\psi}_h)\|\nabla_h\tilde{c}_h(t)\|^2_{h,+}, \quad (54)
\end{aligned}
$$

where $G(\psi_h\psi_h)$ is defined by (53) and

$$
\begin{aligned}
F(\psi_h, \tilde{\psi}_h, \psi_h, \tilde{\psi}_h) = \frac{1}{4\epsilon_2^2}C_{c,1}^2C_{u,1}e^{C_{u,2}t}\Big(1 + A_{max}C_p\Big) \\
\times\Big(\|\psi_h - \tilde{\psi}_h\|^2_h + \|\nabla_h(\phi_h - \tilde{\phi}_h)\|^2_{h,+}\Big).
\end{aligned}
$$

Inequality (54) leads to

$$
\begin{aligned}
&\|\omega_{c,h}(t)\|^2_h + \int_0^t (D_{min} - \epsilon_2^2 - G(\psi_h, \phi_h))\|\nabla_h\omega_{c,h}(s)\|^2_{h,+}ds \\
&\qquad \leq \|c_{0,h} - \tilde{c}_{0,h}\|^2_h + \int_0^t F(\psi_h, \tilde{\psi}_h, \psi_h, \tilde{\psi}_h)\|\nabla_h\tilde{c}_h(s)\|^2_{h,+}ds,\ t \in [0, T]. \quad (55)
\end{aligned}
$$

Then for ϵ such that (52) holds and attending that $\int_0^t \|\nabla_h\tilde{c}_h(s)\|^2_{h,+}ds$ is uniformly bounded for $h \in \Lambda$ and $t \in [0, T]$ because $\|\tilde{c}_{0,h}\|_h, \|\tilde{\psi}_h\|_h, \|\nabla_h\tilde{\phi}_h\|_{h,+}$ $h \in \Lambda$, are bounded sequences, from (55) we conclude (51).

■

3.4. Convergence analysis. The main question in the construction of numerical methods for the coupled IBVP (1), (5) (6), (7), (8) and (9) is the possible loss of accuracy when we consider the numerical approximations for the pressure and displacement defined by equations (33) and (34), in the computation of the numerical approximation for the concentration defined by (35). In this section we show that $p_h(t)$ and $u_h(t)$ defined by (33) and (34), respectively, satisfy

$$\begin{aligned}\|\nabla_h(R_hp(t)-p_h(t))\|_+^2 &\leq Ch_{max}^4, \\ \|\nabla_h(R_hu(t)-u_h(t))\|_+^2 &\leq Ch_{max}^4,\end{aligned} \tag{56}$$

and

$$\|\nabla_h(R_hc(t)-c_h(t))\|_+^2 \leq Ch_{max}^4.$$

The results presented in [14] and the approach followed in [1] have an important role in the construction of the previous error estimates.

Let $E_p(t)=R_hp(t)-p_h(t)$, $E_u(t)=R_hu(t)-u_h(t)$, and $E_c(t)=R_hc(t)-c_h(t)$.

Proposition 4. *Let us suppose that the sequence Λ that defines the spatial grids in $\overline{\Omega}_h$ satisfies (42). If the solution of $p(t)$ and $u(t)$ of (1), (5) with Dirichlet boundary conditions are such that $p(t)\in H^3(\Omega)\cap H_0^1(\Omega), u'(t)\in H^2(\Omega)\cap H_0^1(\Omega)$, then there is a positive constant C_p independent of p, h and t such that*

$$\|\nabla_hE_p(t)\|_{h,+}^2 \leq C_p\Big(h_{max}^4\sum_{i=1}^N\Big(\|p(t)\|_{H^3(I_i)}^2+\|u'(t)\|_{H^2(I_i)}^2\Big)+\|E_u'(t)\|_h^2\Big), \tag{57}$$

where $I_i=(x_{i-1},x_i), i=1,\dots,N$.

Proof: It can be shown that

$$\begin{aligned}(A_h\nabla_hE_p(t),\nabla_hE_p(t))_{h,+}&-(M_h(E_u'(t)),\nabla_hE_p(t))_{h,+}\\ &=(\lambda_1(u'(t)),\nabla_hE_p(t))_{h,+}+(\lambda_2(p(t)),\nabla_hE_p(t))_{h,+},\end{aligned} \tag{58}$$

where

$$\lambda_1(u'(t))(x_i)=u'(x_{i-1/2},t)-M_h(u'(x_i,t)), i=1,\dots,N,$$

and

$$\lambda_2(p(t))(x_i)=A(x_i)(\nabla_hp(x_i,t)-\nabla p(x_{i-1/2},t), i=1,\dots,N.$$

Following [14], Bramble Hilbert Lemma leads to

$$
\begin{aligned}
|(\lambda_1(u'(t)), \nabla_h E_p(t))_{h,+}| &\leq C_1 h_{max}^2 \Big(\sum_{i=1}^{N} \|p(t)\|^2_{H^3(I_i)} \Big)^{1/2} \|\nabla_h E_p(t)\|_{h,+} \\
&\leq \frac{1}{4\epsilon_1^2} C_1 h_{max}^4 \sum_{i=1}^{N} \|p(t)\|^2_{H^3(I_i)} + \epsilon_1^2 \|\nabla_h E_p(t)\|^2_{h,+},
\end{aligned}
$$

and

$$
\begin{aligned}
|(\lambda_2(u'(t)), \nabla_h E_p(t))_{h,+}| &\leq C_2 h_{max}^2 \Big(\sum_{i=1}^{N} \|u'(t)\|^2_{H^2(I_i)} \Big)^{1/2} \|\nabla_h E_p(t)\|_{h,+} \\
&\leq \frac{1}{4\epsilon_2^2} C_1 h_{max}^4 \sum_{i=1}^{N} \|u'(t)\|^2_{H^2(I_i)} + \epsilon_1^2 \|\nabla_h E_p(t)\|^2_{h,+},
\end{aligned}
$$

where $\epsilon_i \neq 0, i = 1, 2$. Consequently we conclude the existence of a positive constant C_p satisfying (57).

■

Proposition 5. *Let us suppose that* $p \in H^1(0, T, H^3(\Omega) \cap H_0^1(\Omega))$, $u \in H^3(0, T, H^2(\Omega) \cap H_0^1(\Omega)) \cap H^2(0, T, H^2(\Omega) \cap H_0^1(\Omega))$, *and* $u_h \in C^2(0, T, W_{h,0})$. *If the sequence* Λ *that defines the spatial grids in* $\overline{\Omega}_h$ *satisfies assumption (42), then there exists a positive constant* C_u *that is independent of* u, p, h *and* t, *such that*

$$
\begin{aligned}
\|E_u'(t)\|_h^2 + \|\nabla_h E_u(t)\|^2_{h,+} \leq C_u h_{max}^4 \Big(&\|u\|^2_{H^3(0,T,H^2(\Omega))} \\
&+ \|u\|^2_{H^1(0,T,H^3(\Omega))} + \|p\|^2_{H^1(0,T,H^3(\Omega))} \Big),
\end{aligned}
\tag{59}
$$

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

Proof: Here we follow the approach used in [7]. For $E_u(t)$ we get successively

$$
\begin{aligned}
(E_u''(t), E_u'(t))_h &= ((u''(t))_h, E_u'(t))_h - (u_h''(t), E_u'(t))_h \\
&\qquad + (R_h u''(t) - (u''(t))_h, E_u'(t))_h \\
&= ((\nabla(E_0 \nabla u(t)))_h, E_u'(t))_h - ((\nabla p(t))_h, E_u'(t))_h \\
&\qquad + (E_{0,h} \nabla_h u_h(t), \nabla_h E_u'(t))_{h,+} + (D_h^* p_h(t), E_u'(t))_h \\
&\qquad + (R_h u''(t) - (u''(t))_h, E_u'(t))_h \\
&= -(E_{0,h} \nabla_h E_u(t), \nabla_h E_u'(t))_{h,+} - (D_h^* E_p(t), E_u'(t))_h \\
&\qquad + (R_h u''(t) - (u''(t))_h, E_u'(t))_h \\
&\qquad + (E_{0,h}(\nabla_h u(t) - \nabla \hat{u}(t)), \nabla_h E_u'(t))_h \\
&\qquad + (\nabla p(t) - (\nabla p(t))_h, E_u'(t))_h \\
&\qquad + (D_h^* p(t) - \nabla p(t), E_u'(t))_h,
\end{aligned}
$$

where, $(v)_h$ is defined as (32) for $v = u''(t), \nabla p(t)$ and $\hat{u}(x_i, t) = u(x_{i-1/2}, t)$. Then we conclude for $E_u(t)$ the following IVP

$$
\begin{cases}
(E_u''(t), E_u'(t))_h + (E_{0,h} \nabla_h E_u(t), \nabla_h E_u'(t))_{h,+} = -(D_h E_p(t), E_u'(t))_h + \displaystyle\sum_{j=1}^{4} T_j, \\
E_h'(0) = 0, \\
E_u(0) = 0,
\end{cases}
\tag{60}
$$

for $t \in (0, T]$, with

$$T_1 = (R_h u''(t) - (u''(t))_h, E_u'(t))_h,$$

$$T_2 = (E_{0,h}(\nabla_h u(t) - \nabla \hat{u}(t)), \nabla_h E_u'(t))_h,$$

$$T_3 = (\nabla p(t) - (\nabla p(t))_h, E_u'(t))_h$$

and

$$T_4 = (D_h p(t) - \nabla p(t), E_u'(t))_h.$$

(1) An estimate for T_1.
T_1 admits the representation

$$T_1 = \frac{d}{dt}(R_h u''(t) - (u''(t))_h, E_u(t))_h - (R_h u^{(3)}(t) - (u^{(3)}(t))_h,$$

where, from for the last term we have

$$|(R_h u^{(3)}(t) - (u^{(3)}(t))_h| \leq Ch_{max}^2 \Big(\sum_{i=1}^{N} \|u^{(3)}(t)\|_{H^2(I_i)}^2 \Big)^{1/2} \|\nabla_h E_u(t)\|_{h,+}. \quad (61)$$

(2) An estimate for T_2.
Analogously to T_1, for T_2 we have

$$T_2 = \frac{d}{dt}(E_{0,h}(\nabla_h u(t) - \nabla \hat{u}(t)), \nabla_h E_u(t))_h - (E_{0,h}(\nabla_h u'(t) - \nabla \hat{u}'(t)), \nabla_h E_u(t))_h,$$

and

$$\begin{aligned} &|(E_{0,h}(\nabla_h u'(t) - \nabla \hat{u}'(t)), \nabla_h E_u(t))_h| \\ &\qquad \leq Ch_{max}^2 \Big(\sum_{i=1}^{N} \|u'(t)\|_{H^3(I_i)}^2 \Big)^{1/2} \|\nabla_h E_u(t)\|_{h,+}. \end{aligned} \quad (62)$$

(3) An estimate for T_3.
It is easy to show that

$$T_3 = \frac{d}{dt}(\nabla p(t) - (\nabla p(t))_h, E_u(t))_h - (\nabla p'(t) - (\nabla p'(t))_h, E_u(t))_h,$$

where

$$|(\nabla p'(t) - (\nabla p'(t))_h, E_u(t))_h| \leq Ch_{max}^2 \Big(\sum_{i=1}^{N} \|p'(t)\|_{H^3(I_i)}^2 \Big)^{1/2} \|\nabla_h E_u(t)\|_{h,+}. \quad (63)$$

(4) An estimate for T_4.
For T_4 we have

$$T_4 = \frac{d}{dt}(D_h^* p(t) - \nabla p(t), E_u(t))_h - (D_h^* p'(t) - \nabla p'(t), E_u(t))_h,$$

where

$$|(D_h^* p'(t) - \nabla p'(t), E_u(t))_h| \leq Ch_{max}^2 \Big(\sum_{i=1}^{N} \|p'(t)\|_{H^3(I_i)}^2 \Big)^{1/2} \|\nabla_h E_u(t)\|_{h,+}. \quad (64)$$

Taking the obtained estimates into (60) we get

$$\begin{aligned}
&\frac{d}{dt}\|E_u'(t)\|_h^2+\frac{d}{dt}\|\sqrt{E_{0,h}}\nabla_h E_u(t)\|_{h,+}^2 \leq 2C_g\|\nabla_h E_p(t)\|_{h,+}^2+\|E_u'(t)\|_h^2\\
&\quad +2\frac{d}{dt}(R_h u''(t)-(u''(t))_h, E_u(t))_h+2\frac{d}{dt}(E_{0,h}(\nabla_h u(t)-\nabla\hat{u}(t)),\nabla_h E_u(t))_h\\
&\quad +2\frac{d}{dt}(\nabla p(t)-(\nabla p(t))_h, E_u(t))_h+2\frac{d}{dt}(D_h^* p(t)-\nabla p(t), E_u(t))_h\\
&\quad +2\epsilon_1^2\|\nabla_h E_u(t)\|_{h,+}^2+\tau(t), \qquad (65)
\end{aligned}$$

where $\epsilon_1 \neq 0$ and

$$|\tau(t)| \leq Ch_{max}^4\sum_{i=1}^N\Big(\|u^{(3)}(t)\|_{H^2(I_i)}^2+\|u'(t)\|_{H^3(I_i)}^2+\|p'(t)\|_{H^3(I_i)}^2\Big).$$

Taking into account that $E_h'(0)=0$ and $E_u(0)=0$, the inequality (65) leads to

$$\begin{aligned}
&\|E_u'(t)\|_h^2+\|\sqrt{E_{0,h}}\nabla_h E_u(t)\|_{h,+}^2 \leq \int_0^t\Big(2C_g\|\nabla_h E_p(s)\|_{h,+}^2 ds+\|E_u'(s)\|_h^2\Big)ds\\
&\quad +2\epsilon_1^2\int_0^t\|\nabla_h E_u(s)\|_{h,+}^2 ds+\int_0^t\tau(s)ds+2(R_h u''(t)-(u''(t))_h, E_u(t))_h\\
&\quad +2(E_{0,h}(\nabla_h u(t)-\nabla\hat{u}(t)),\nabla_h E_u(t))_h+2(\nabla p(t)-(\nabla p(t))_h, E_u(t))_h\\
&\quad +2(D_h^* p(t)-\nabla p(t), E_u(t))_h. \qquad (66)
\end{aligned}$$

Again, proceeding as in [14], we establish for the last four terms of the right hand side of (66) the following estimate

$$\begin{aligned}
&|2(R_h u''(t)-(u''(t))_h, E_u(t))_h+2(E_{0,h}(\nabla_h u(t)-\nabla\hat{u}(t)),\nabla_h E_u(t))_h\\
&\quad +2(\nabla p(t)-(\nabla p(t))_h, E_u(t))_h+2(D_h^* p(t)-\nabla p(t), E_u(t))_h|\\
&\qquad \leq Ch_{max}^4\sum_{i=1}^N\Big(\|u''(t)\|_{H^2(I_i)}^2+\|u(t)\|_{H^3(I_i)}^2+\|p(t)\|_{H^3(I_i)}^2\Big)\\
&\qquad\qquad +\epsilon_2^2\|\nabla_h E_u(t)\|_{h,+}^2, \qquad (67)
\end{aligned}$$

where $\epsilon_2 \neq 0$. Inserting (57) and (67) in (65) we easily establish that there exists a positive constant C_1 such that

$$\begin{aligned}\|E_u'(t)\|_h^2 + \|\nabla_h E_u(t)\|_{h,+}^2 \ &\leq C_1 \int_0^t \Big(\|E_u'(s)\|_h^2 + \|\nabla_h E_u(s)\|_{h,+}^2\Big) ds \\ &\quad + \int_0^t \tau(s) ds + \eta(t), t \in [0,T],\end{aligned} \tag{68}$$

where the error terms $\tau(t)$ and $\eta(t)$ admits the representation

$$|\tau(t)| \leq C h_{max}^4 \sum_{i=1}^N \Big(\|u^{(3)}(t)\|_{H^2(I_i)}^2 + \|u'(t)\|_{H^3(I_i)}^2 + \|p'(t)\|_{H^3(I_i)}^2 + \|p(t)\|_{H^3(I_i)}^2\Big)$$

and

$$|\eta(t)| \leq C h_{max}^4 \sum_{i=1}^N \Big(\|u^{(2)}(t)\|_{H^2(I_i)}^2 + \|u(t)\|_{H^3(I_i)}^2 + \|p(t)\|_{H^3(I_i)}^2\Big).$$

Applying the Gronwall Lemma to (68) and considering that

$$\begin{aligned}&\int_0^t \tau(s) ds + \eta(t) \leq C h_{max}^4 \Big(\|u^{(3)}\|_{L^2(0,T,H^2(\Omega))}^2 + \|u'\|_{L^2(0,T,H^3(\Omega))}^2 \\ &\quad + \|p\|_{H^1(0,T,H^3(\Omega))}^2 + \|u^{(2)}\|_{C(0,T,H^2(\Omega))}^2 + \|u'\|_{C(0,T,H^3(\Omega))}^2 + \|p\|_{C(0,T,H^3(\Omega))}^2\Big) \\ &\leq C h_{max}^4 \Big(\|u\|_{H^3(0,T,H^2(\Omega))}^2 + \|u\|_{H^1(0,T,H^3(\Omega))}^2, + \|p\|_{H^1(0,T,H^3(\Omega))}^2\Big)\end{aligned}$$

we conclude (59).

■

From Propositions 4 and 5 we finally obtain the next result for the error $E_p(t)$.

Corollary 2. *Under the assumptions of Propositions 4 and 5, there exists a positive constant C_p independent of u, p, h and t, such that*

$$\begin{aligned}\|\nabla_h E_p(t)\|_{h,+}^2 \leq C_p h_{max}^4 \Big(&\|u\|_{H^3(0,T,H^2(\Omega))}^2 \\ &+ \|u\|_{H^1(0,T,H^3(\Omega))}^2 + \|p\|_{H^1(0,T,H^3(\Omega))}^2\Big),\end{aligned} \tag{69}$$

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

In what follows we establish an estimate for $E_c(t) = R_h c(t) - c_h(t)$.

Proposition 6. *Under the assumptions of Propositions 4 and 5, if*

$$c \in C^1(0,T,H^2(\Omega)\cap H_0^1(\Omega)) \cap L^2(0,T,H^3(\Omega)\cap H_0^1(\Omega))$$

and $c_h \in C^1(0,T,W_{h,0})$, *then there exists a positive constant* C_c *independent of* c, u, p, h *and* t, *such that*

$$\begin{aligned}
&\|E_c(t)\|_h^2 + \int_0^t \|\nabla_h E_c(s)\|_{h,+}^2 ds \\
&\leq C_c h_{max}^4\Big(\|u\|^2_{H^3(0,T,H^2(\Omega))} + \|u\|^2_{H^1(0,T,H^3(\Omega))} + \|p\|^2_{H^1(0,T,H^3(\Omega))} \\
&\quad + \|c\|^2_{H^1(0,T,H^2(\Omega))} + \|c\|^2_{L^2(0,T,H^3(\Omega))} + \|c\nabla p\|^2_{L^2(0,T,H^2(\Omega))}\Big),\ t\in[0,T]. \quad (70)
\end{aligned}$$

Proof: Using the notations introduced before, it can be shown that $E_c(t)$ satisfies the following

$$\begin{aligned}
(E_c'(t),E_c(t))_h &= ((c'(t))_h,E_c(t))_h - (c_h'(t),E_c(t))_h + (c'(t)-(c'(t))_h,E_c(t))_h \\
&= -(D_h\nabla\hat{c}(t),\nabla_h E_c(t))_{h,+} + (\hat{v}(t)\hat{c}(t),\nabla_h E_c(t))_{h,+} \\
&\quad + (D_h\nabla_h c_h(t),\nabla_h E_c(t))_{h,+} - (M_h(v_h(t)c_h(t)),\nabla_h E_c(t))_{h,+} \\
&\quad + (c'(t)-(c'(t))_h,E_c(t))_h \\
&= -(D_h\nabla_h E_c(t),\nabla_h E_c(t))_{h,+} \\
&\quad + (M_h(v(t)c(t)-v_h(t)c_h(t)),\nabla_h E_c(t))_{h,+} + \sum_{i=1}^3 T_i(t),
\end{aligned}$$

where

$$T_1(t) = (c'(t)-(c'(t))_h,E_c(t))_h,$$
$$T_2(t) = (D_h(\nabla_h c(t)-\nabla\hat{c}(t),\nabla_h E_c(t))_{h,+}$$

and

$$T_3(t) = (\hat{v}(t)\hat{c}(t) - M_h(v(t)c(t)),\nabla_h E_c(t))_{h,+}.$$

We observe that we have

$$|T_1(t)| \leq Ch_{max}^4\sum_{i=1}^N \|c'(t)\|^2_{H^2(I_i)} + \epsilon_1^2\|\nabla_h E_c(t)\|^2_{h,+},$$

$$|T_2(t)| \leq Ch_{max}^4\sum_{i=1}^N \|c(t)\|^2_{H^3(I_i)} + \epsilon_2^2\|\nabla_h E_c(t)\|^2_{h,+}$$

and

$$|T_3(t)| \leq Ch_{max}^4 \sum_{i=1}^{N} \|c(t)\nabla p(t)\|_{H^2(I_i)}^2 + \epsilon_3^2 \|\nabla_h E_c(t)\|_{h,+}^2,$$

where $\epsilon_i \neq 0, i = 1, 2, 3$.

To obtain an estimate for the term $(M_h(v(t)c(t) - v_h(t)c_h(t)), \nabla_h E_c(t))_{h,+}$ we start by noting that

$$v(t)c(t) - v_h(t)c_h(t) = v(t)(c(t) - c_h(t)) + (v(t) - v_h(t))c_h(t),$$

and consequently we obtain

$$\begin{aligned}
|(M_h(v(t)c(t) - v_h(t)c_h(t)), \nabla_h E_c(t))_{h,+}| &\leq \sqrt{2}\|v(t)\|_\infty \| \|E_c(t)\|_h \|\nabla_h E_c(t)\|_{h,+} \\
&\quad + \sqrt{2}\|c_h(t)\|_\infty \| \|v(t) - v_h(t)\|_{h,+} \|\nabla_h E_c(t)\|_{h,+} \\
\leq \frac{1}{2\epsilon_4^2}\|v(t)\|_\infty^2 \| \|E_c(t)\|_h^2 &+ 2\epsilon_4^2 \|\nabla_h E_c(t)\|_{h,+}^2 \\
&\quad + \frac{1}{2\epsilon_4^2}\|c_h(t)\|_\infty^2 \| \|v(t) - v_h(t)\|_{h,+}^2.
\end{aligned}$$

We conclude that there exist two positive constants $C_i, i = 1, 2$, such that

$$\begin{aligned}
\frac{d}{dt}\|E_c(t)\|_h^2 + \|\nabla_h E_c(t)\|_{h,+} &\leq C_1 \|v(t)\|_\infty^2 \|E_c(t)\|_h^2 \\
&\quad + C_2 \|c_h(t)\|_\infty^2 \|v(t) - v_h(t)\|_{h,+}^2 + \tau(t), \quad (71)
\end{aligned}$$

where

$$|\tau(t)| \leq Ch_{max}^4 \sum_{i=1}^{N} \Big(\|c'(t)\|_{H^2(I_i)}^2 + \|c(t)\|_{H^3(I_i)}^2 + \|c(t)\nabla p(t)\|_{H^2(I_i)}^2 \Big).$$

The inequality (71) leads to

$$\begin{aligned}
\|E_c(t)\|_h^2 &+ \int_0^t e^{C_1 \int_s^t \|v(\mu)\|_\infty^2 d\mu} \|\nabla_h E_c(s)\|_{h,+}^2 ds \\
&\leq C_2 \Big(\int_0^t e^{C_1 \int_s^t \|v(\mu)\|_\infty^2 d\mu} \|c_h(s)\|_\infty^2 \|v(s) - v_h(s)\|_{h,+}^2 ds \\
&\quad + \int_0^t e^{C_1 \int_s^t \|v(\mu)\|_\infty^2 d\mu} \tau(s) ds \Big), \ t \in [0, T]. \quad (72)
\end{aligned}$$

Moreover, from Corollary 2 we have

$$\|v(t) - v_h(t)\|_{h,+} \leq Ch_{max}^4 \Big(\|u\|_{H^3(0,T,H^2(\Omega))}^2 + \|u\|_{H^1(0,T,H^3(\Omega))}^2 + \|p\|_{H^1(0,T,H^3(\Omega))}^2 \Big),$$

for $t \in [0,T]$, and then from (72) we deduce

$$\begin{aligned} &\|E_c(t)\|_h^2 + \int_0^t \|\nabla_h E_c(s)\|_{h,+}^2 ds \\ &\quad \leq C h_{max}^4 \Big(\|u\|^2_{H^3(0,T,H^2(\Omega))} + \|u\|^2_{H^1(0,T,H^3(\Omega))} + \|p\|^2_{H^1(0,T,H^3(\Omega))} \Big) \\ &\quad \int_0^t e^{C_1 \int_s^t \|v(\mu)\|_\infty^2 d\mu} \|c_h(s)\|_\infty^2 ds + C_2 \int_0^t e^{C_1 \int_s^t \|v(\mu)\|_\infty^2 d\mu} \tau(s) ds,\ t \in [0,T]. \end{aligned} \tag{73}$$

Finally, by Proposition 2, $\int_0^t \|c_h(s)\|_\infty^2 ds$ is bounded in $h \in \Lambda$ and $t \in [0,T]$, from (73) we conclude (70).

■

4. Numerical examples

The goal of this section is twofold: one, illustrate the convergence results obtained in the previous section, and second, illustrate the behavior of our system in the context of CED modeling. For the computational implementation we exploit the FDM formulation (39), (40), and (41). First we present the time discretization strategy. We remark that the theoretical analysis for this strategy could be made using the work in [7, 1] as a starting point.

In the temporal domain $[0,T]$ we define the time grid $t_m = m\Delta t$, $m = 0,\dots,M_t$, with Δt the uniform time step and $M_t \Delta t = T$. We denote by p_h^m, v_h^m, u_h^m, and c_h^m the numerical approximations for $p_h(t_m)$, $v_h(t_m)$, $u_h(t_m)$, and $c_h(t_m)$, respectively. The proposed time discretization is given by: find p_h^m, v_h^m, u_h^m, and c_h^m, such that,

$$-\nabla_h^*(A_h \nabla_h p_h^{m+1}) + \nabla_{h,c}\Big(\frac{u_h^m - u_h^{m-1}}{\Delta t}\Big) = s_h^{m+1}, \tag{74}$$

$$v_h^{m+1} = A_h D_h^* p_h^{m+1} + \frac{u_h^m - u_h^{m-1}}{\Delta t},$$

$$\frac{u_h^{m+1} - 2u_h^m + u_h^{m-1}}{\Delta t^2} = \nabla_h^*(E_{0,h} \nabla_h u_h^{m+1}) - D_h^* p_h^{m+1} + r_h^{m+1}, \tag{75}$$

and

$$\frac{c_h^{m+1} - c_h^m}{\Delta t} + \nabla_{c,h}(v_h^{m+1} c_h^{m+1}) = \nabla_h^*(D_h \nabla_h c_h^{m+1}) + f_h^{m+1}, \tag{76}$$

for $m = 0, \ldots, M_t - 1$. This is complemented with the initial conditions

$$\frac{u_h^0 - u_h^{-1}}{\Delta t} = R_h \psi,\ u_h^0 = R_H \phi,\ \text{and}\ c_h^0 = R_h c_0,\ \text{in}\ \Omega_h, \tag{77}$$

and null Dirichlet boundary conditions.

4.1. Example 1: convergence rates. Let us define the errors, $e_{h,p}^m = p_h^m - p_h(t_m)$, $e_{h,u}^m = u_h^m - u_h(t_m)$, and $e_{h,c}^m = c_h^m - c_h(t_m)$. The convergence rates are measured using the following quantities,

$$E_p = \max_{m=1,\ldots,M_t} \|e_{h,p}^m\|_{1,h}^2,$$

associated with the discretization of the pressure equation (74),

$$E_u = \max_{m=1,\ldots,M_t} \|e_{h,u}^m\|_{1,h}^2,$$

associated with the discretization of the displacement equation (75), and

$$E_c = \max_{m=1,\ldots,M_t} \|e_{h,c}^m\|_{1,h}^2.$$

associated with the discretization of the concentration equation (76). For the numerical simulation we set $\Omega = [0, 1]$, $T = 1$, and the time step $\Delta t = h_{min}^2$, which is small enough to neglect the discretization error in time. We also define the coefficient functions $A = 1 + x$, $E_0 = e^x$, and $D = 1 + 2x$. The initial conditions and the functions $s(t)$, $r(t)$, and $f(t)$ are chosen such that the exact solution of the coupled problem (1), (5) (6), (7), (8) and (9), is given by

$$\begin{aligned} p(x,t) &= e^{2t} x(1 - x), \\ u(x,t) &= e^t x \sin(\pi x), \\ c(x,t) &= e^t x(1 - \cos(2\pi x)). \end{aligned}$$

We repeatedly solve this example over non-uniform random meshes of variable size, h_{max} between 0.0176 and 0.0786. The results are given in Figure 1 where we plot, for each mesh, the logarithm of the errors E_p, E_u, and E_c versus the logarithm of h_{max}. The slope of the best fitting least square line is an estimation of the convergence rate. As can be seen the rates are close to two, confirming our theoretical analysis.

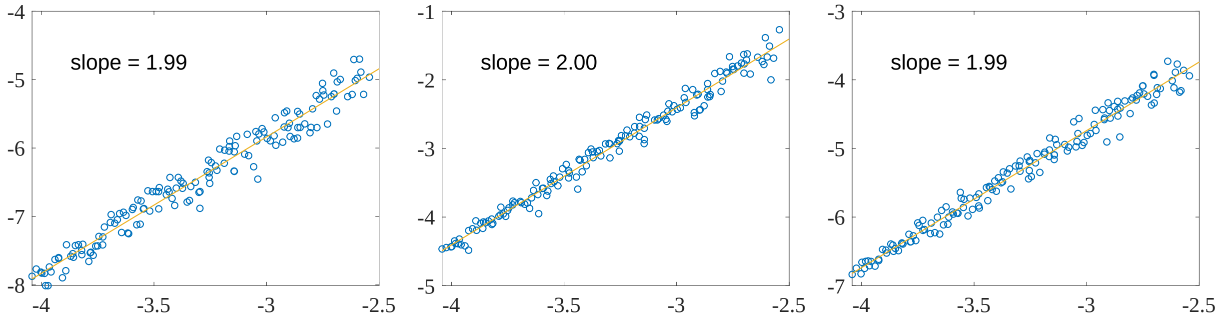

FIGURE 1. From left to right: Log-log plots of E_p, E_u, and E_c versus h_{max}. The best fitting least square line and the respective slope is also given.

Example 2: CED simulation. In this example, for simplicity, we omit physical units. We consider a CED problem where a therapeutic agent is injected in a porous-elastic media. The spatial domain is $\Omega = [0, 4]$ and we take a uniform mesh with step size 0.001. A smooth source term with an injection rate of 0.1 is assigned at the center of the domain. In particular, we set $s_h(t) = f_h(t) = q$, with $q = 0.1e^{-\frac{(x-2)^2}{0.02^2}}$. The diffusion coefficient is equal to $D = 1 \times 10^{-6}$, the permeability is equal to $K = 1 \times 0.01$, and we are considering that the viscosity is equal to $\mu = 1$. The model is complemented with null Dirichlet boundary conditions.

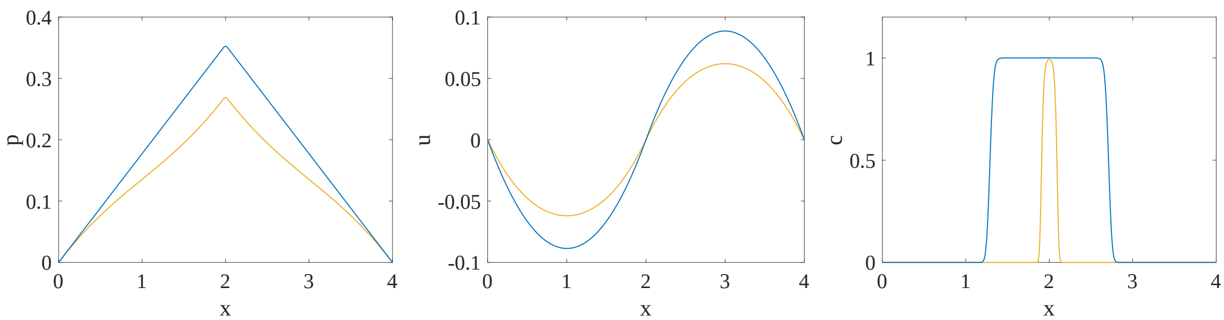

FIGURE 2. From left to right: pressure p, displacement u, and concentration c at time $T = 5$ (light brown line) and $T = 400$ (blue line), for the CED homogeneous model.

Case 1: homogeneous tissue. In this case we consider a homogeneous tissue with Young's modulus equal to $E_0 = 1$. The numerical results for $T = 50$ and $T = 400$ for pressure p, displacement u, and concentration c, are given in Figure 2. In this homogeneous scenario we expect all the quantities to be symmetric around the source center. Our numerical results show this behavior. Also expected is the maximum pressure at the center of the source. The pressure and the displacement are time dependent, but after approximately $T = 200$ they show a very small variation.

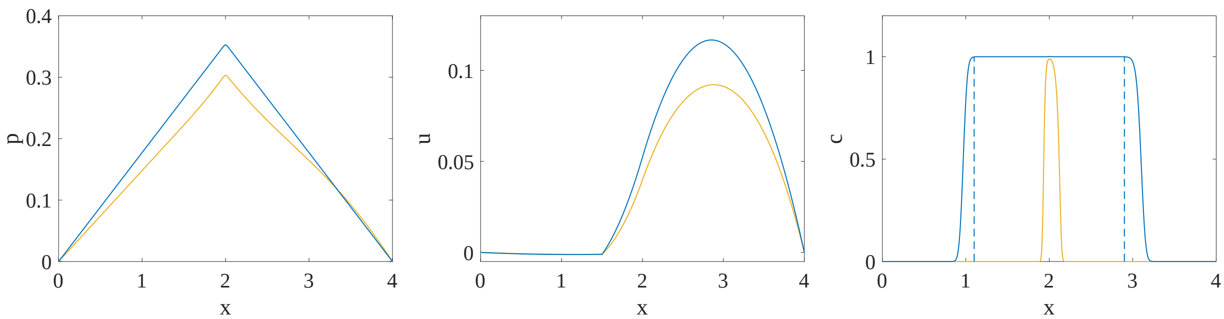

FIGURE 3. From left to right: pressure p, displacement u, and concentration c at time $T = 5$ (light brown line) and $T = 600$ (blue line), for the CED non-homogeneous model.

Case 2: non-homogeneous tissue. In this case we consider a non-homogeneous tissue. Namely, we set the Young's modulus equal to $E_0 = 100$ for $x \leq 1.5$ and equal to $E_0 = 1$ for $x > 1.5$. This scenario models a tissue with very different elastic properties, almost rigid behavior for $x \leq 1.5$ and an elastic behavior for $x > 1.5$. In this non-homogeneous scenario we expect the displacement to be close to zero in the almost rigid portion of the domain. Since we are considering constant permeability we also expect the pressure to be higher in the elastic portion, at least initially. The velocity should also be higher in the elastic portion since it depends not only on the pressure gradient but also on the displacement. Again, the displacement must be zero in the almost rigid portion. Therefore, and since the porosity is constant, we expect the therapeutic agent to spread slightly faster through the elastic portion of the domain ($x > 1.5$). The numerical results for $T = 50$ and $T = 600$ are given in Figure 3 and they show this behavior. As before the pressure and the displacement reach a steady state at approximately $T = 200$. In conclusion, the difference in the agent concentration distribution shows that displacement influences transport and highlights the importance of using porous-elastic models in CED simulation.

5. Conclusion

In this paper we study a piecewise linear FEM for a coupled system of partial differential equations. Systems of this type arise, for instance, in the mathematical modeling of porous-elastic CED. CED is a state-of-the-art technology that uses catheters to inject therapeutic agents directly into target sites like brain tissue. In this case, the evolution of the concentration of the therapeutic agent is described by the convection-diffusion equation (1) where the convective velocity v depends on ∇p and $\frac{\partial u}{\partial t}$, p is solution of the elliptic equation (5) and u is solution of the wave equation (6).

To solve numerically the differential system (1), (5) and (6) with Dirichlet boundary condition and suitable initial conditions, we proposed a fully discrete piecewise linear FEM that is equivalent to a FDM. Stability results based on energy estimates are proved for the continuous model (Proposition 1) and for the fully discrete (in space) FEM (Proposition 3).

We observe that the piecewise linear FEM approximation for the velocity v is only first order convergent. Moreover, if we look to our methods as a finite difference scheme, we observe that the truncation error is only first order convergent with respect to the norm $\|.\|_\infty$. Nevertheless, in Proposition 6 we establish that the numerical approximation for the concentration is second order convergent with respect to a discrete L^2-norm. In the proof of this result, the convergence estimates for the numerical pressure and displacement deduced in Propositions 4 and 5, respectively, have a central role.

Numerical experiments illustrate the theoretical finds in what concerns the convergence rates established for the numerical pressure, displacement and concentration. They also illustrate the behavior of a particular CED model:

- in an homogeneous tissue we observe that the pressure, displacement and therapeutic agent concentration are symmetric around the source center (Figure 2);
- in a non-homogeneous tissue, lower displacement and lower propagation of the therapeutic agent are observed in regions of higher stiffness (Figure 3).

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J.A. Ferreira
CMUC, Department of Mathematics, University of Coimbra, Coimbra, Portugal
E-mail address: ferreira@mat.uc.pt

L. Pinto
CMUC, Department of Mathematics, University of Coimbra, Coimbra, Portugal
E-mail address: luisp@mat.uc.pt

R.F. Santos
CEMAT/IST and Department of Mathematics, University of Algarve, Portugal
E-mail address: rsantos@ualg.pt