A second order method for a drug release process defined by a differential Maxwell-Wichert stress-strain relation

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November 27, 2024

Abstract

Polymeric drug delivery platforms offer promising capabilities for controlled drug release thanks to their ability to be custom-designed with specific properties. In this paper we present a model to simulate the complex interplay between solvent absorption, polymer swelling, drug release and stress development within these types of platforms. A system of nonlinear partial differential equations coupled with an ordinary differential equations is introduced to avoid drawbacks from other models found in the literature. These incorporated a memory effect to account for polymer relaxation but from a numerical point of view, required storing information from all previous time steps, making them computationally expensive. This paper proposes a new numerical method to simulate such drug delivery devices based on nonuniform grids and an implicit midpoint time discretization. Our main results are the proof of second order convergence of the method for nonsmooth solutions and the scheme's stability under the assumption of quasiuniform grids and a sufficiently small timestep. We also illustrate numerically the second order convergence result proven in the main result using solutions based on biological information.

1 Introduction

In this paper we consider the differential problem

$$\frac{\partial c_\ell}{\partial t}(x,t) = \nabla\cdot\big(a_\ell(c_\ell(x,t))\nabla c_\ell(x,t)\big) + \nabla\cdot\big(a_\sigma(c_\ell(x,t))\nabla\sigma(x,t)\big) \tag{1}$$

$$\frac{\partial c_d}{\partial t}(x,t) = \nabla\cdot\big(a_d(c_\ell(x,t))\nabla c_d(x,t)\big) + f(c_s(x,t),\, c_d(x,t),\, c_\ell(x,t)), \tag{2}$$

$$\frac{\partial c_s}{\partial t}(x,t) = -f(c_s(x,t),\, c_d(x,t),\, c_\ell(x,t)) \tag{3}$$

for $x\in(0,R), t\in(0,T]$. In [13], the system of eqs. (1) to (3) was introduced with

$$\sigma(x,t) = -\int_0^t q(s,t,c_\ell(x,s),c_\ell(x,t))\nabla c_\ell(x,s)ds, \tag{4}$$

to describe the drug release from a viscoelastic spherical polymeric structure of radius R containing a drug immersed in a spherical environment of fixed radius. This differential system is complemented by the following initial and boundary conditions:

$$c_\ell(x,0)=0, c_d(x,0)=0,\ c_s(x,0)=c_{s,0}(x),\ x\in(0,R), \tag{5}$$

$$\nabla c_\ell(0,t)=0,\ \nabla c_d(0,t)=0,\ c_\ell(R,t)=c_{ext},\ c_d(R,t)=0, t\in(0,T]. \tag{6}$$

The authors considered therein that the drug release is a consequence of the following set of phenomena:

1. the solvent molecules are absorbed by the polymeric structure due to the solvent gradient concentration (solvent absorption);
2. the polymeric chains relax, the structure swells and a pressure gradient arises (swelling);
3. the dissolution process occurs due to the contact of the solid drug with the absorbed solvent molecules (dissolution);
4. the molecules of the dissolved drug diffuse throughout the platform and continue to diffuse in the external surrounding medium (diffusion).

In this case, c_ℓ, c_s and c_d represent fluid, solid and dissolved drug concentrations, respectively, f denotes the dissolution function and σ represents the polymeric chains' stress. This stress is opposite to the solvent uptake and represents the deformation induced by the solvent concentration. In this context, the fluid flux is given by

$$J_\ell = -a_\ell(c_\ell)\nabla c_\ell - a_\sigma(c_\ell)\nabla\sigma.$$

In [13] the authors considered that $\epsilon = g(c_\ell)$ and

$$\sigma(x,t) = -\int_0^t E(t-s)\frac{\partial \epsilon}{\partial s}(x,s)ds,$$

where $E(\cdot)$ is the kernel function associated with the Maxwell-Wiechert model,

$$E(t) = E_0 + \sum_{j=1}^{m} E_j e^{-\frac{t}{\tau_j}},$$

E_j denotes the Young's modulus, $\tau_j = \frac{\mu_j}{E_j}$ (with μ_j representing the polymeric viscosity).

The initial boundary value problem (IBVP) defined by eqs. (1) to (6) was studied from a numerical point of view in [5, 6] for smooth and nonsmooth solutions. In these papers the authors propose second order approximations in space. The presence of the Neumann boundary condition at $x = 0$ lead to several challenges that were solved in these papers for for both scenarios of smoothness. Moreover, in [5], an Euler implicit-explicit numerical method combined with a uniform grid for the memory term was studied. In order to prove convergence for the solid and dissolved drug approximations it was sufficient to guarantee uniform bounds for the numerical approximation for the fluid. Such property was concluded assuming a certain quasiuniformity for the spatial grid and a stability condition similar to the well know stability relation for uniform grids $\Delta t \leq C_s h^2$. In [22] a numerical method similar to the one considered here for a diffusion equation with a memory term defined with an exponential kernel function was also studied.

The presence of the memory term in eq. (4) leads to several challenges in the computation of the numerical approximation for the solution of the initial boundary value problem (IBVP) defined by eqs. (1) to (6), if our goal is to compute second order accurate approximations for c_ℓ, c_d and c_s. In this case we should apply second order approximation quadrature rules to discretize the integral term and we need to store information for all timesteps during the release process. Moreover, the presence of the integral term replacing the stress σ makes it more difficult to construct stress estimates depending on the data of the problem.

The goal of this paper is to replace eq. (4) by

$$\frac{\partial \sigma}{\partial t} + \beta\sigma = -\alpha\epsilon - \gamma\frac{\partial \epsilon}{\partial t}, \tag{7}$$

where $\beta = \frac{E_0+E_1}{\mu}$, $\alpha = \frac{E_0 E_1}{\mu}$, $\gamma = E_0$ and μ represents the viscosity of the polymer and E_0 and E_1 are the Young's modulus (see [8]). The minus signal in eqs. (4) and (7) arises to take into account that the stress is developed by the polymeric chains as a response to the fluid entrance generating an opposite convective flux to the standard Fickian diffusion process. To simplify, we take $\epsilon = \lambda c_\ell$, instead of the nonlinear relations considered in [13, 15]. We aim to present a numerical scheme that leads to second order approximations using an implicit midpoint approach in time for the differential system defined by eqs. (1) to (3) and (7) and

$$\nabla\sigma(0,t)=0,\ \sigma(R,t)=\sigma_{ext}, t\in(0,T],\ \sigma(x,0)=\sigma_0(x),\ x\in(0,R). \tag{8}$$

We point out that in the nonlinear system of eqs. (1) to (3) and (7), the concentration c_ℓ is defined by eqs. (1) and (7) and it is included in eqs. (2) and (3). Our goal is to propose a finite difference method that can be seen as a fully discrete piecewise linear-constant finite element method following a midpoint quadrature approach that is simultaneously locally stable and unconditionally convergent with respect to a discrete version of the usual norm in $H^1(0,R)$. The key ideas and challenges to prove stability and convergence followed throughout the paper are summarized as follows:

1. Since we are dealing with nonlinear evolution problems, to conclude local stability in a numerical approximations for fluid, solid and dissolved drug concentrations and stress, respectively, $c^n_{\ell,h}, \sigma^n_h, c^n_{s,h}$ and $c^n_{d,h}$, we follow the approach considered, for instance, in [28, 29, 31, 33]. To prove stability for these numerical approximations, we need to impose their uniform boundness with respect a discrete version of the usual norms in $W^{1,\infty}(0,R)$.

2. In what concerns unconditionally second convergence order of numerical methods for quasi-linear parabolic equations, we refer the papers [27, 36] and the references therein where the convergence analysis requires the uniform boundeness of the numerical approximation with respect to a suitable norm. In our context, the problem involves nonlinear parabolic equations for the fluid c_ℓ and dissolved drug c_d concentrations coupled with ordinary differential equations for the stress σ and for the solid drug c_s. For the fluid, solid and dissolved drug concentrations and stress approximations we establish unconditionally second convergence order with respect to a discrete H^1-norm. No uniform bounds for the correspondent numerical approximations are required following our approach.

3. The fluid concentration c_ℓ and stress σ are defined by eqs. (1) and (7) and the diffusion coefficient in eq. (2), as well as the reaction terms in eqs. (2) and (3) depend on c_ℓ. These facts increase the complexity of the system eqs. (1) to (3) and (7). Furthermore, σ is defined by an ordinary differential equation and we would like to obtain for this variable a second order approximation with respect to a discrete H^1-norm. This goal is not easy to fulfill.

4. Taking into account the convergence estimates with respect to a discrete H^1-norm, we are able to verify that the uniform boundness assumptions imposed to conclude local stability hold provided that the initial approximations are in balls centered in the initial conditions of the differential problem with mesh dependent radius.

The error analysis conducted in this paper is not based on the usual approach introduced in [37] that was largely followed in the literature. For instance, recently, the results of [37] have been considered in [26, 38, 39, 40]. Instead, our approach is based on the error analysis for the error equations. Our results can bee seen in two different perspectives:

1. As mentioned before, our method can be seen as a fully discrete piecewise linear-constant finite element method and the second order estimates with respect to the discrete H^1-norm are unexpected because piecewise linear finite element method lead to a first order error estimate with respect to the usual H^1-norm. The unexpected convergence orders obtained for finite element approximations are known as superconvergent results and recently the literature has been fruitful for this type of estimates. Without being exhaustive we mention [34] where a mixed finite element method in space is combined with a second order backward formula for a quasilinear parabolic equation is studied. The author establishes that a postprocessing of the fully discrete solution allows to obtain second order in time and space with respect to the usual H^1-norm. In [11], superconvergence is shown for the

gradient approximation of the second order elliptic equation discretized by weak Galerkin finite element methods on nonuniform rectangular partitions. A mixed finite element is used to approximate a compressible miscible flow problem in porous media. A recovery technique is introduced to obtain second order approximation for Darcy's velocity. In [32], a quasilinear parabolic system coupled with an elliptic equations is numerically solved by using a bilinear finite element approach. A post-processing procedure is introduced to establish second-order error estimates with respect to the usual H^1-norm.

2. Within finite difference methods, our convergence estimates allow us to conclude that the order of the global error is greater than the order of the truncation error . In fact, the truncation error is of first order only in space with respect to norm $\|\cdot\|_\infty$, while the global error is of second order in space and time. This unexpected convergence behaviour is known as supraconvergence phenomenon and it was widely studied in the 80's of the last century in [10, 23, 24, 25, 30]. The authors and their collaborators have recent contributions in the convergence analysis of supraconvergence phenomenon of numerical methods for linear and nonlinear partial differential equations, for instance, [9, 14, 17, 18, 19, 21]. We also mention the following contributions [1, 12, 35].

The paper is organized as follows. In Section 2 we present some notations and basic results related with the finite elements scheme proposed. In Section 3 we introduce a fully discrete (in time and space) numerical method using an implicit midpoint time integrator and nonuniform grids in space. The stability of the method is established in Section 3.1 provided some suitable uniform bounds on the solution of the numerical problem. To establish such bounds, the convergence properties of the method are studied in Section 3.2. The final proof of the stability of the numerical scheme is a consequence of the convergence result. Finally, in Section 5, we present some conclusions.

2 Definitions and basic results

In this section we present the basic definitions and tools needed to provide the mathematical support for the proposed numerical method and the upcoming sections. By Λ we denote a sequence of vectors $h = (h_1, \ldots, h_N)$ such that $h_i > 0, i = 1, \ldots, N$, $\sum_{i=1}^N h_i = R$ and $h_{max} = \max_{i=1,\ldots,N} h_i \to 0$. The sequence Λ is used to introduce in $\overline{\Omega} = [0, R]$ a sequence of grids

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

Let $x_{-1} = -x_1$ and $h_0 = h_1$.

As we are dealing with Neumann boundary conditions at x_0, to discretize the boundary conditions, we introduce a fictitious point $x_{-1} = -x_1$ and the correspondent set of grids

$$\overline{\Omega}_h^\star = \overline{\Omega}_h \cup \{x_{-1}\}.$$

The numerical approximations that we compute are defined in all grid points. They will naturally belong to the space of grid functions

$$V_h^\star = \{v_h : \overline{\Omega}_h^\star \longrightarrow \mathbb{R}\}.$$

To study the behaviour of the error, as we are considering Dirichlet boundary conditions at $x = x_N$, we also introduce a new vector space

$$V_{h,0}^\star = \{v_h \in V_h^\star : v_h(x_N) = 0\}.$$

The errors for the numerical approximation for the solvent, dissolved and solid drugs concentrations will be measured on the grid points of $[0, R]$ and these errors are null at x_N. Consequently, we need to introduce

$$V_{h,0} = \{v_h \in V_h : v_h(x_N) = 0\},$$

where

$$V_h = \{w_h : \overline{\Omega}_h \longrightarrow \mathbb{R}\}.$$

The norm $\|\cdot\|_h$ used in measuring the errors is induced by the inner product

$$(u_h, v_h)_h = \frac{h_1}{2} u_h(x_0) v_h(x_0) + \sum_{i=1}^{N-1} h_{i+1/2} u_h(x_i) v_h(x_i), \quad u_h, v_h \in V_{h,0}$$

where $h_{i+1/2} = \frac{1}{2}(h_i + h_{i+1})$. Another useful norm is the discrete counterpart of the $L^\infty(0, R)$ norm

$$\|v_h\|_{h,\infty} = \max_{i=0,\ldots,N} |v_h(x_i)|, \; v_h \in V_h.$$

We also use the notation

$$(u_h, v_h)_+ = \sum_{i=1}^{N} h_i u_h(x_i) v_h(x_i), \; \|u_h\|_+ = \sqrt{(u_h, u_h)_+}$$

and

$$\|v_h\|_{+,\infty} = \max_{i=1,\ldots,N} |v_h(x_i)|$$

for grid functions defined in $x_1, \ldots, x_N$.

For $v_h \in V_h^\star$ we introduce the finite difference operators D_{-x} and $D_x^\star$ defined by

$$\begin{aligned} D_{-x} v_h(x_i) &= \frac{v_h(x_i) - v_h(x_{i-1})}{h_i}, \quad i = 1, \ldots, N, \\ D_x^\star v_h(x_i) &= \frac{v_h(x_{i+1}) - v_h(x_i)}{h_{i+1/2}}, \quad i = 0, \ldots, N-1, \end{aligned}$$

respectively. By M_h we denote the average operator

$$M_h v_h(x_i) = \frac{v_h(x_i) + v_h(x_{i-1})}{2}, \quad i = 0, \ldots, N-1,$$

for $v_h \in V_h^*$.

We introduce the following discrete version of the usual norm in $H^1(0, R)$:

$$\|u_h\|_{1,h} = \left(\|u_h\|_h^2 + \|D_{-x} u_h\|_+^2\right)^{1/2}, \; u_h \in V_{h,0}.$$

We now recall some useful result regarding these discrete operators.

Proposition 1 (Discrete Friedrichs-Poincaré inequality)**.** *For all $v_h \in V_{h,0}$,*

$$\|v_h\|_h \le R \|D_{-x} v_h\|_+$$

Proof. It is sufficient to note that, for all $u_h \in V_{h,0}$, holds the following

$$u_h(x_i) = -\sum_{j=i}^{N} h_j D_{-x} u_h(x_j), i = 0, \ldots, N-1.$$

□

Proposition 2 (Discrete inverse inequality)**.** *For all $v_h \in V_{h,0}$,*

$$\|D_{-x} v_h\|_{+,\infty} \le \frac{2}{h_{min}^{3/2}} \|v_h\|_h.$$

Proof. Given the definition of $\|\cdot\|_{+,\infty}$, there exists $k \in \{1, 2, \ldots, N\}$ such that

$$\begin{aligned}\|D_{-x}v_h\|_{+,\infty}^2 &= |D_{-x}v_h(x_k)|^2 \\ &\leq \frac{2}{h_{min}^2}\left(v_h(x_k)^2 + v_h(x_{k-1})^2\right) \\ &\leq \frac{4}{h_{min}^3}\|v_h\|_h^2.\end{aligned}$$

□

Proposition 3. *For all $v_h \in V_{h,0}$,*

$$\|v_h\|_{h,\infty} \leq \frac{\sqrt{R}}{h_{min}}\|v_h\|_h.$$

Proof. The proof follows similar steps as the one for Proposition 2. □

Proposition 4. *Let $A : \mathbb{R} \longrightarrow \mathbb{R}$, $u_h \in V_h^*$ and $v_h \in V_{h,0}$. Then*

$$\left(D_x^\star(A(M_h u_h)D_{-x}u_h), v_h\right)_h = -\left(A(M_h u_h)D_{-x}u_h, D_{-x}v_h\right)_+ - D_{A,c}u_h(x_0)v_h(x_0),$$

where

$$D_{A,c}u_h(x_0) = \frac{1}{2}\left(A(M_h u_h(x_0))D_{-x}u_h(x_0) + A(M_h u_h(x_1))D_{-x}u_h(x_1)\right).$$

Remark 1. For the particular case, A is constant, we have $D_{A,c}u_h(x_0) = AD_c u_h(x_0)$.

To simplify the presentation of the numerical methods that we study in what follows, we consider the following notation: if $v_h : \overline{\Omega}_h^\star \times [0,T] \longrightarrow \mathbb{R}$, by $v_h(t)$ we represent the following grid function $v_h(t) : \overline{\Omega}_h^\star \longrightarrow \mathbb{R}$, $v_h(t)(x_i) = v_h(x_i, t), i = -1, \ldots, N$. By $v_h'(t)$ we represent its time derivative. For grid functions v_h defined in others grid sets the definition is similar. Finally, we introduce the notation $C^m(H^r) = C^m([0,T]; H^r(0,R))$ for the space of functions $v : [0,T] \longrightarrow H^r(0,R)$ such that $v^{(i)} : [0,T] \longrightarrow H^r(0,R)$, $i = 0, \ldots, m$ are continuous, imbued with the norm

$$\|v\|_{C^m(H^r)} = \max_{t\in[0,T]} \|v(t)\|_{H^r(0,R)}.$$

We also introduce the simplified notation $H^i(H^r)$ for the Bochner space $H^i(0,T; H^r(0,R))$, $i, k \geq 0$.

3 Fully discrete approximation

Let $M \in \mathbb{N}$ and $\Delta t = \frac{T}{M}$. We consider in $[0,T]$ the uniform time grid $\{t_m = m\Delta t,\ m = 0, \ldots, M\}$. We introduce now a full discretization scheme for problem defined by eqs. (1) to (3) and (5) to (8) based on an implicit midpoint integration approach in time

$$\begin{aligned}D_{-t}c_{\ell,h}^{m+1} &= D_x^\star\left(a_\ell\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{\ell,h}^{m+1/2}\right) \\ &\quad + D_x^\star\left(a_\sigma\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}\sigma_h^{m+1/2}\right), \qquad (9)\\ D_{-t}\sigma_h^{m+1} + \beta\sigma_h^{m+1/2} &= -\alpha c_{\ell,h}^{m+1/2} - \gamma D_{-t}c_{\ell,h}^{m+1}, \qquad (10)\\ D_{-t}c_{d,h}^{m+1} &= D_x^\star\left(a_d\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{d,h}^{m+1/2}\right) + f_h^{m+1/2} \qquad (11)\\ D_{-t}c_{s,h}^{m+1} &= -f_h^{m+1/2}, \qquad (12)\end{aligned}$$

in $\overline{\Omega}_h \backslash \{x_N\}$ and $m = 0, 1, \ldots, M-1$. with

$$c^0_{\ell,h}(x_i) = c_{\ell,0}(x_i), \tag{13}$$
$$c^0_{d,h}(x_i) = 0, \tag{14}$$
$$c^0_{s,h}(x_i) = c_{s,0}(x_i), \tag{15}$$
$$\sigma^0_h(x_i) = \sigma_0(x_i), \tag{16}$$

for $i = 0, \ldots, N-1$, and

$$D_{a_\ell,c} c^{j+1/2}_{\ell,h}(x_0) = D_{a_d,c} c^{j+1/2}_{d,h}(x_0) = D_{a_\sigma,c} \sigma^{j+1/2}_h(x_0) = 0,\ j = 0, \ldots, M-1, \tag{17}$$
$$c^j_{\ell,h}(x_N) = c_{ext}, \tag{18}$$
$$\sigma^j_h(x_N) = \sigma_{ext}, \tag{19}$$
$$c^j_{d,h}(x_N) = 0, j = 0, \ldots, M. \tag{20}$$

In eq. (9), D_{-t} denotes the backward finite difference operator in time, $c^{m+1/2}_{p,h} = \frac{1}{2}(c^m_{p,h} + c^{m+1}_{p,h})$ for $p = \ell, d, s$, $f^m_h = f(c^m_{s,h}, c^m_{d,h}, c^m_{\ell,h})$ and $f^{m+1/2}_h = \frac{1}{2}(f^m_h + f^{m+1}_h)$. Following [6], throughout this paper we always assume that:

($\mathbf{H_{diff}}$) for $\mu = \ell, d, \sigma$, $a_\mu : \mathbb{R} \longrightarrow \mathbb{R}$ is differentiable, its derivative is bounded and there exist positive constants $a_{0,\mu}$ and M_μ such that

$$0 < a_{0,\mu} \leq a_\mu(x) \leq M_\mu,\ |a'_\mu(x)| \leq M_\mu, \quad \text{for all } x \in \mathbb{R};$$

($\mathbf{H_f}$) there exists a positive constant C_f such that

$$|(f(x, y, z) - f(\tilde{x}, \tilde{y}, \tilde{z})| \leq C_f \left(|\tilde{z}||y - \tilde{y}| + (1 + |y|)\left(|z - \tilde{z}| + |z||x - \tilde{x}|\right)\right),$$

for all $x, y, z, \tilde{x}, \tilde{y}, \tilde{z} \in \mathbb{R}$.

Remark 2. We remark that the last condition generalizes the condition that holds for the particular dissolution function $f(c_s, c_d, c_\ell) = \hat{H}(c_s)K(C_{sol} - c_d)c_\ell$, where $\hat{H}$ is a smooth approximation of the Heaviside function $H(c_s)$, C_{sol} is the solubility limit of the drug and K is the dissolution rate.

Remark 3. We observe that the numerical scheme defined by eqs. (9), (12), (13), (16), (17) and (20) can be seen as a fully discrete piecewise finite element method: piecewise linear for c_ℓ, σ, c_d and piecewise constant for c_s. In fact, the weak problem that leads to the last finite difference scheme can be write as follows: for $t \in (0, T]$, compute $c_\ell(t), \sigma(t), \in H^1(\Omega)$, $c_s(t) \in L^2(0, R)$, such that $c_\ell(R, t) = c_{\ell,ext}$, $\sigma(R, t) = \sigma_{ext}$, $c_d(R, t) = 0$ and

$$\begin{aligned}
&(c'_\ell(t), \omega_\ell) = -(a_\ell(c_\ell(t))\nabla c_\ell(t), \nabla\omega_\ell) - (a_\sigma(\sigma(t))\nabla\sigma(t), \nabla\omega_\ell), && \forall\omega_\ell \in H^1_{R,0}(0, R),\\
&(\sigma'(t), \omega_\sigma) = -\beta(\sigma(t), \omega_\sigma) - \alpha(c_\ell(t), \omega_\sigma) - \gamma(c'_\ell(t), \omega_\sigma), && \forall\omega_\sigma \in L^2(0, R),\\
&(c'_d(t), \omega_d) = -(a_d(c_\ell(t))\nabla c_d(t), \nabla\omega_d) + (f(t), \omega_d), && \forall\omega_d \in H^1_{R,0}(0, R),\\
&(c'_s(t), \omega_s) = -(f(t), \omega_s), && \forall\omega_s \in L^2(0, R),
\end{aligned} \tag{21}$$

with the initial conditions defined by eqs. (13) and (16)) imposed in the L^2 sense. In (21) the following notations were used: $H^1_{R,0}(0, R) = \{\omega \in H^1(0, R) : \omega(R) = 0\}$ and $f(t) = f(c_s(t), c_d(t), c_\ell(t))$.

The semi-discrete piecewise linear-constant finite element method reads as follows: for $t \in (0, T]$, compute $P_h c_{\ell,h}(t), P_h\sigma_h(t), P_h c_{d,h}(t) \in H^1(0, R)$ such that $c_{\ell,h}(x_N, t) = c_{\ell,ext}$, $\sigma_h(x_N, t) = 0$ and $Q_h c_{s,h}(t) \in L^2(0, R)$, such that

$$\begin{aligned}
(P_h c'_{\ell,h}(t), P_h\omega_{\ell,h}) &= -(a_\ell(P_h c_{\ell,h}(t))\nabla P_h c_{\ell,h}(t), \nabla P_h\omega_{\ell,h})\\
&\quad - (a_\sigma(P_h\sigma_h(t))\nabla P_h\sigma_h(t), \nabla P_h\omega_\ell)\\
(P_h\sigma'_h(t), Q_h\omega_{\sigma,h}) &= -\beta(P_h\sigma_h(t), Q_h\omega_{\sigma,h}) - \alpha(P_h c_{\ell,h}(t), Q_h\omega_{\sigma,h}) - \gamma(P_h c'_{\ell,h}(t), Q_h\omega_{\sigma,h}),\\
(P_h c'_{d,h}(t), P_h\omega_{d,h}) &= -(a_d(P_h c_{\ell,h}(t))\nabla P_h c_{d,h}(t), \nabla P_h\omega_{d,h}) + (f_{P,h}(t), P_h\omega_{d,h}),\\
(Q_h c'_{s,h}(t), Q_h\omega_{s,h}) &= -(f_h(t), Q_h\omega_{s,h}),
\end{aligned} \tag{22}$$

for all $\omega_{\ell,h}, \omega_{d,h}, \omega_{s,h}, \omega_{\sigma,h} \in V_{h,0}$ with the initial conditions

$$c_{\ell,h}(x_i, 0) = c_{\ell,0}(x_i), \tag{23}$$

$$c_{d,h}(x_i, 0) = 0, \tag{24}$$

$$c_{s,h}(x_i, 0) = c_{s,0}(x_i), \tag{25}$$

$$\sigma_h(x_i, 0) = \sigma_0(x_i), \tag{26}$$

for $i = 0, \dots, N-1$. In (22) the following notations were used: for $u_h \in V_{h,0}$, $P_h u_h$ denotes the usual piecewise linear polynomial interpolator of u_h, $Q_h u_h$ represents the piecewise constant polynomial interpolator of u_h, that is, for $i = 0, \dots, N-1$, and for $x \in [x_i, x_{i+1})$, $Q_h u_h(x) = u_h(x_i)$ and $f_{P,h}(t) = f(Q_h c_{s,h}(t), P_h c_{d,h}(t), P_h c_{\ell,h}(t))$.

This leads to the final fully discrete piecewise linear-constant finite element method: for $t \in (0, T]$, compute $c_{\ell,h}(t), P_h\sigma_h(t), P_h c_d(t), c_{s,h}(t) \in V_{h,0}$ such that $c_{\ell,h}(x_N, t) = c_{\ell,ext}$, $\sigma_h(x_N, t) = 0$, and

$$\begin{aligned}
(c'_{\ell,h}(t), \omega_{\ell,h})_h &= -(a_\ell(M_h c_{\ell,h}(t)) D_{-x} c_{\ell,h}(t), D_{-x}\omega_{\ell,h})_+ \\
&\quad - (a_\sigma(M_h\sigma_h(t)) D_{-x}\sigma_h(t), D_{-x}\omega_\ell)_+, \\
(\sigma'_h(t)\omega_{\sigma,h})_h &= -\beta(\sigma_h(t), \omega_{\sigma,h})_h - \alpha(c_{\ell,h}(t), \omega_{\sigma,h})_h - \gamma(c'_{\ell,h}(t), \omega_{\sigma,h})_h, \\
(c'_{d,h}(t), \omega_{d,h})_h &= -(a_d(M_h c_{\ell,h}(t)) D_{-x} c_{d,h}(t), D_{-x}\omega_{d,h}) + (f_h(t), \omega_{d,h}), \\
(c'_{s,h}(t), \omega_{s,h})_h &= -(f_h(t), \omega_{s,h})_h,
\end{aligned} \tag{27}$$

for all $\omega_{\ell,h}, \omega_{d,h}, \omega_{s,h}, \omega_{\sigma,h} \in V_{h,0}$, subjected to the initial conditions defined by eqs. (23) and (26)). In (27) we adopted the notation $f_h(t) = f(c_{s,h}(t), c_{d,h}(t), c_{\ell,h}(t))$.

Finally, a suitable time integration scheme for (27) leads to: for $m = 0, \dots, M-1$, compute $c^m_{\ell,h}, \sigma^m_h, c^m_{d,h}, c^m_{s,h} \in V_{h,0}$ such that $c^m_{\ell,h}(x_N) = c_{\ell,ext}, \sigma^m_h(x_N) = 0,$ and

$$\begin{aligned}
(D_{-t}c^{m+1}_{\ell,h}, \omega_{\ell,h})_h &= -(a_\ell(M_h c^{m+1/2}_{\ell,h}) D_{-x} c^{m+1/2}_{\ell,h}, D_{-x}\omega_{\ell,h})_+ \\
&\quad - (a_\sigma(M_h\sigma^{m+1/2}_h) D_{-x}\sigma^{m+1/2}_h, D_{-x}\omega_\ell)_+, \\
(D_{-t}\sigma^{m+1}_h), \omega_{\sigma,h})_h &= -\beta(\sigma^{m+1/2}_h, \omega_{\sigma,h})_h - \alpha(c^{m+1/2}_{\ell,h}, \omega_{\sigma,h})_h - \gamma(D_{-t}c^{m+1}_{\ell,h}, \omega_{\sigma,h})_h, \\
(D_{-t}c^{m+1}_{d,h}, \omega_{d,h})_h &= -(a_d(M_h c^{m+1/2}_{\ell,h}) D_{-x} c^{m+1/2}_{d,h}, D_{-x}\omega_{d,h}) + (f^{m+1/2}_h, \omega_{d,h}), \\
(D_{-t}c^{m+1}_{s,h}, \omega_{s,h})_h &= -(f^{m+1/2}_h, \omega_{s,h})_h,
\end{aligned} \tag{28}$$

for all $\omega_{\ell,h}, \omega_{d,h}, \omega_{s,h}, \omega_{\sigma,h} \in V_{h,0}$, complemented the initial conditions defined by eqs. (13) and (16), leading to (9)-(20).

3.1 Stability analysis

Let $c^m_{i,h}$, $i = d, \ell, s$, and σ^m_h, $m = 1 \dots, M$ denote fixed solutions of the discrete problem defined by equations eqs. (9) to (20) with initial conditions $c^0_{i,h}, i = d, \ell, s$, and σ^0_h and let $\omega^m_{i,h} = c^m_{i,h} - \tilde{c}^m_{i,h}$, $i = d, \ell, s$, $\omega^m_{\sigma,h} = \sigma^m_h - \tilde{\sigma}^m_h$, where $\tilde{c}^m_{i,h}$, $i = d, \ell, s$, $\tilde{\sigma}^m_h$ is another set of solutions of the same discrete problem with initial conditions $\tilde{c}^0_{i,h}$, $i = d, \ell, s$, and $\tilde{\sigma}^0_h$. We start by stating a result that will be used to bound specific terms in the upcoming analysis.

Proposition 5. *Let $u_h, v_h, \tilde{u}_h, \tilde{v}_h \in V^\star_h$ such that $u_h - \tilde{u}_h \in V^\star_{h,0}$ and $w_h \in V_{h,0}$. If $a_\mu : \mathbb{R} \longrightarrow \mathbb{R}$ satisfies $\mathbf{H}_{\mathbf{diff}}$ then*

$$\begin{aligned}
|\left(a_\mu\left(M_h u_h\right) D_{-x} v_h - a_\mu\left(M_h \tilde{u}_h\right) D_{-x}\tilde{v}_h, D_{-x} w_h\right)_+| &\le M_\mu \|D_{-x}(v_h - \tilde{v}_h)\|_+ \|D_{-x} w_h\|_+ \\
&\quad + M_\mu \|D_{-x} v_h\|_{+,\infty} \|u_h - \tilde{u}_h\|_h \|D_{-x} w_h\|_+
\end{aligned}$$

Moreover, if $w_h = v_h - \tilde{v}_h$ then

$$\begin{aligned}
&\left(a_\mu\left(M_h \tilde{u}_h\right) D_{-x}\tilde{v}_h - a_\mu\left(M_h u_h\right) D_{-x} v_h, D_{-x} w_h\right)_+ \\
&\qquad \le M_\mu \|D_{-x} v_h\|_{+,\infty} \|u_h - \tilde{u}_h\|_h \|D_{-x} w_h\|_+ - a_{0,\mu} \|D_{-x} w_h\|^2_+
\end{aligned}$$

We are now able to establish upper bounds for a perturbation of the numerical solution. Indeed, considering Proposition 4, it can be shown that

$$
\begin{aligned}
\left(D_{-t}\omega_{\ell,h}^{m+1},\omega_{\ell,h}^{m+1/2}\right)_h = &-\left(a_\ell\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{\ell,h}^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+\\
&+\left(a_\ell\left(M_h\tilde{c}_{\ell,h}^{m+1/2}\right)D_{-x}\tilde{c}_{\ell,h}^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+\\
&-\left(a_\sigma\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}\sigma_h^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+\\
&+\left(a_\sigma\left(M_h\tilde{c}_{\ell,h}^{m+1/2}\right)D_{-x}\tilde{\sigma}_h^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+
\end{aligned}
$$

$$
\begin{aligned}
\left(D_{-t}\omega_{d,h}^{m+1},\omega_{d,h}^{m+1/2}\right)_h = &-\left(a_d\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{d,h}^{m+1/2},D_{-x}\omega_{d,h}^{m+1/2}\right)_+\\
&+\left(a_d\left(M_h\tilde{c}_{\ell,h}^{m+1/2}\right)D_{-x}\tilde{c}_{d,h}^{m+1/2},D_{-x}\omega_{d,h}^{m+1/2}\right)_+\\
&+\left(\left(f_h^{m+1/2}-\tilde{f}_h^{m+1/2}\right),\omega_{d,h}^{m+1/2}\right)_h,
\end{aligned}
$$

and

$$
\left(D_{-t}\omega_{s,h}^{m+1},\omega_{s,h}^{m+1/2}\right)_h = -\left(\left(f_h^{m+1/2}-\tilde{f}_h^{m+1/2}\right),\omega_{s,h}^{m+1/2}\right)_h.
$$

We now focus on equation (3.1). Using Proposition 5, it is straightforward to show that

$$
\begin{aligned}
\frac{1}{2}D_{-t}\|\omega_{\ell,h}^{m+1}\|_h^2 \le\ & M_\ell\|D_{-x}c_{\ell,h}^{m+1/2}\|_{+,\infty}\|\omega_{\ell,h}^{m+1/2}\|_h\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+ - a_{0,\ell}\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2\\
&+M_\sigma\|D_{-x}\sigma_h^{m+1/2}\|_{+,\infty}\|\omega_{\ell,h}^{m+1/2}\|_h\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+\\
&+M_\sigma\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+.
\end{aligned}
\tag{29}
$$

Remark 4. From the expressions in the previous inequality, in order to obtain an upper bound for $\|\omega_{\ell,h}^{m+1}\|_h$, we need to determine an upper bound for $\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+$.

With this in mind, we start by proving the following result.

Proposition 6. *Under the previous assumptions, $\omega_{\sigma,h}^{m+1}$ and $\omega_{\ell,h}^{m+1}$ satisfy*

$$
\begin{aligned}
\frac{1}{2}D_{-t}\left[\|D_{-x}\left(\omega_{\sigma,h}^{m+1}+\gamma\omega_{\ell,h}^{m+1}\right)\|_+^2\right]+\beta\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+^2+\alpha\gamma\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2&\\
=-(\alpha+\beta\gamma)\left(D_{-x}\omega_{\ell,h}^{m+1/2},D_{-x}\omega_{\sigma,h}^{m+1/2}\right)_+&.
\end{aligned}
$$

Proof. Taking each member of eq. (10) and applying the operator D_{-x}, we derive

$$
D_{-x}D_{-t}\omega_{\sigma,h}^{m+1}+\beta D_{-x}\omega_{\sigma,h}^{m+1/2}=-\alpha D_{-x}\omega_{\ell,h}^{m+1/2}-\gamma D_{-x}D_{-t}\omega_{\ell,h}^{m+1}.
$$

We now apply the discrete inner product $(\cdot,\cdot)_+$ to each member of the previous equation considereing two different elements: $D_{-x}\omega_{\sigma,h}^{m+1/2}$ and $D_{-x}\omega_{\ell,h}^{m+1/2}$. From the former, we obtain

$$
\begin{aligned}
\frac{1}{2}D_{-t}\|D_{-x}\omega_{\sigma,h}^{m+1}\|_+^2+\beta\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+^2 = &-\alpha\left(D_{-x}\omega_{\ell,h}^{m+1/2},D_{-x}\omega_{\sigma,h}^{m+1/2}\right)_+\\
&-\gamma\left(D_{-x}D_{-t}\omega_{\ell,h}^{m+1},D_{-x}\omega_{\sigma,h}^{m+1/2}\right)_+
\end{aligned}
$$

and from the latter we get

$$
\begin{aligned}
\gamma\left(D_{-x}D_{-t}\omega_{\sigma,h}^{m+1},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+ +\beta\gamma\left(D_{-x}\omega_{\sigma,h}^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+&\\
=-\alpha\gamma\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2-\frac{\gamma^2}{2}D_{-t}\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2&.
\end{aligned}
\tag{30}
$$

Now, using the identity

$$D_{-t}\left(D_{-x}\omega_{\sigma,h}^{m+1}, D_{-x}\omega_{\ell,h}^{m+1}\right)_+ = \left(D_{-x}D_{-t}\omega_{\sigma,h}^{m+1}, D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+ + \left(D_{-x}D_{-t}\omega_{\ell,h}^{m+1}, D_{-x}\omega_{\sigma,h}^{m+1/2}\right)_+$$

in eq. (30) and replacing the common term, $\gamma\left(D_{-x}D_{-t}\omega_{\ell,h}^{m+1}, D_{-x}\omega_{\sigma,h}^{m+1/2}\right)_+$, we conclude the proof. □

We are now able to establish an upper bound for the perturbations on $c_{\ell,h}$ and σ_h.

Proposition 7. *Let $c_{\ell,h}^m$ and σ_h^m, $m = 0,\dots,M$ denote fixed solutions of the discrete problem defined by eqs. (9), (10), (13) and (16) to (19) and let $\omega_{\ell,h}^m = c_{\ell,h}^m - \tilde{c}_{\ell,h}^m$, $\omega_{\sigma,h}^m = \sigma_h^m - \tilde{\sigma}_h^m$, where $\tilde{c}_{\ell,h}^m$, $\tilde{\sigma}_h^m$ is another solution of the same discrete problem with initial conditions $\tilde{c}_{\ell,h}^0$, and $\tilde{\sigma}_h^0$. If the assumption $\mathbf{H_{diff}}$ holds, the coefficients satisfy*

$$M_\sigma + \alpha + \beta\gamma < 2\min\left(\beta, \alpha\gamma + a_{0,\ell}\right) \tag{31}$$

and there exists $\Delta t_0 > 0$ such that, for all $\Delta t \in (0, \Delta t_0)$, the corresponding solution satisfies

$$\max_m \left(\|D_{-x}c_{\ell,h}^{m+1/2}\|_{+,\infty}^2, \|D_{-x}\sigma_h^{m+1/2}\|_{+,\infty}^2\right) \le C \tag{32}$$

for some positive C, independent of h and Δt, then, for all $\Delta t < \min\left\{\Delta t_0, \frac{1}{2C}\right\}$, the following inequality holds

$$\begin{aligned}\|\omega_{\ell,h}^m\|_h^2 + \|D_{-x}\omega_{\sigma,h}^m + \gamma D_{-x}\omega_{\ell,h}^m\|_+^2 + \Delta t\sum_{i=0}^{m-1}\left[\|D_{-x}\omega_{\sigma,h}^{i+1/2}\|_+^2 + \|D_{-x}\omega_{\ell,h}^{i+1/2}\|_+^2\right] \\ \le C_\ell\left(\|\omega_{\ell,h}^0\|_h^2 + \|D_{-x}\omega_{\sigma,h}^0\|_+^2 + \|D_{-x}\omega_{\ell,h}^0\|_+^2\right).\end{aligned}$$

for $m = 1, 2, \dots, M-1$, where C_ℓ is a positive constant independent of h and Δt.

Proof. Let $\Delta t < \min\left\{\Delta t_0, \frac{1}{2C}\right\}$. Combining eq. (29) with Proposition 6, it follows that for all $\epsilon \neq 0$,

$$\begin{aligned}D_{-t}\left[\|\omega_{\ell,h}^{m+1}\|_h^2 + \|D_{-x}\omega_{\sigma,h}^{m+1} + \gamma D_{-x}\omega_{\ell,h}^{m+1}\|_+^2\right] \\ +A_0\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+^2 + B_0(\epsilon)\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2 \\ \le \left(\frac{M_\ell^2}{\epsilon^2}\|D_{-x}c_{\ell,h}^{m+1/2}\|_{+,\infty}^2 + \frac{M_\sigma^2}{\epsilon^2}\|D_{-x}\sigma_h^{m+1/2}\|_{+,\infty}^2\right)\|\omega_{\ell,h}^{m+1/2}\|_h^2\end{aligned} \tag{33}$$

where

$$A_0 = 2\left(\beta - \frac{M_\sigma}{2} - \frac{\alpha+\beta\gamma}{2}\right)$$

and

$$B_0(\epsilon) = 2\left(\alpha\gamma + a_{0,\ell} - \epsilon^2 - \frac{M_\sigma}{2} - \frac{\alpha+\beta\gamma}{2}\right).$$

From eq. (31), it follows that $A_0 > 0$ and we can fix ϵ such that $B_0(\epsilon) > 0$. Let

$$\theta_\ell(c_{\ell,h},\sigma_h) = \frac{1}{\epsilon^2}\max_{\mu=\ell,\sigma} M_\mu^2 \cdot \max_{j=0,\dots,N-1}\left\{\|D_{-x}c_{\ell,h}^{j+1/2}\|_{+,\infty}^2, \|D_{-x}\sigma_h^{j+1/2}\|_{+,\infty}^2\right\}.$$

With this notation, eq. (33) leads to

$$\begin{aligned}(1-\theta_\ell(c_{\ell,h},\sigma_h)\Delta t)\left(\|\omega_{\ell,h}^{m+1}\|_h^2 + \|D_{-x}\omega_{\sigma,h}^{m+1} + \gamma D_{-x}\omega_{\ell,h}^{m+1}\|_+^2\right) \\ +\Delta t\left(A_0\|D_{-x}\omega_{\sigma,h}^{m+1/2}\|_+^2 + B_0(\epsilon)\|D_{-x}\omega_{\ell,h}^{m+1/2}\|_+^2\right) \\ \le (1+\theta_\ell(c_{\ell,h},\sigma_h)\Delta t)\left(\|\omega_{\ell,h}^m\|_h^2 + \|D_{-x}\omega_{\sigma,h}^m + \gamma D_{-x}\omega_{\ell,h}^m\|_+^2\right).\end{aligned} \tag{34}$$

From the uniform bound defined by eq. (32) and the inequality from eq. (34), applying Lemma 1 from [19] allows to obtain

$$\begin{aligned}\|\omega_{\ell,h}^m\|_h^2 + \|D_{-x}\omega_{\sigma,h}^m + \gamma D_{-x}\omega_{\ell,h}^m\|_+^2 + \Delta t \sum_{i=0}^{m-1} \left[\|D_{-x}\omega_{\sigma,h}^{i+1/2}\|_+^2 + \|D_{-x}\omega_{\ell,h}^{i+1/2}\|_+^2\right] \\ \leq C_\ell(1 + C\,\Delta t)\left(\|\omega_{\ell,h}^0\|_h^2 + \|D_{-x}\omega_{\sigma,h}^0\|_+^2 + \|D_{-x}\omega_{\ell,h}^0\|_+^2\right).\end{aligned} \tag{35}$$

where

$$C_\ell = 2\max\{1,\gamma^2\}\exp\left(C\,T\,\max\left\{\frac{1}{A_0}, \frac{1}{B_0(\epsilon)}, \frac{1}{1 - C\min\left\{\Delta t_0, \frac{1}{2C}\right\}}\right\}\right).$$

□

We have already dealt with calculating upper bounds for suitable norms involving the perturbations of $c_{\ell,h}$ and σ_h. We now turn our attention to the perturbations of the dissolved and solid approximations, i.e., $\omega_{d,h}$ and $\omega_{s,h}$. Employing a similar technique, we can prove the following result.

Proposition 8. *Let $c_{i,h}^m$, $i = d, s, \ell$ and σ_h^m, $m = 0, \ldots, M$ denote fixed solutions of the discrete problem defined by eqs. (9) to (20) and let $\omega_{i,h}^m = c_{i,h}^m - \tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\omega_{\sigma,h}^m = \sigma_h^m - \tilde{\sigma}_h^m$, where $\tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\tilde{\sigma}_h^m$ is another solution of the same discrete problem. If the assumptions $\mathbf{H_{diff}}$ and $\mathbf{H_f}$ hold and there exists $\Delta t_0 > 0$ such that, for all $\Delta t \in (0, \Delta t_0)$, the corresponding solution satisfies*

$$\max_{i=0,\ldots,M}\left\{\|c_{d,h}^i\|_{h,\infty}, \|D_{-x}c_{d,h}^i\|_{h,\infty}, \|c_{\ell,h}^i\|_{h,\infty}, \|\tilde{c}_{\ell,h}^i\|_{h,\infty}\right\} \leq C \tag{36}$$

for some positive C, independent of h and Δt, then, for all $\Delta t < \min\left\{\Delta t_0, \frac{1}{8C}\right\}$, the following inequality holds

$$\|\omega_{d,h}^m\|_h^2 + \|\omega_{s,h}^m\|_h^2 + \Delta t \sum_{i=0}^{m-1} \|D_{-x}\omega_{d,h}^{j+1/2}\|_+^2 \leq C_{d,s}\left(\|\omega_{d,h}^0\|_h^2 + \|\omega_{s,h}^0\|_h^2 + \Delta t \sum_{j=0}^{m} \|\omega_{\ell,h}^i\|_h^2\right), \tag{37}$$

for $m = 1, 2, \ldots, M-1$, where $C_{d,s}$ is a positive constant independent of h and Δt.

Proof. We start by noting that using eqs. (11) and (12) and taking into account summation by parts and the boundary conditions for $\omega_{d,h}^{m+1}$ we have

$$\begin{aligned}\left(D_{-t}\omega_{d,h}^{m+1}, \omega_{d,h}^{m+1/2}\right)_h + \left(D_{-t}\omega_{s,h}^{m+1}, \omega_{s,h}^{m+1/2}\right)_h \\ = -\left(\left(a_d\left(M_h c_{\ell,h}^{m+1/2}\right) - a_d\left(M_h \tilde{c}_{\ell,h}^{m+1/2}\right)\right) D_{-x}c_{d,h}^{m+1/2}, D_{-x}\omega_{d,h}^{m+1/2}\right)_+ \\ - \left(a_d(M_h\tilde{c}_{\ell,h}^{m+1/2}) D_{-x}\omega_{d,h}^{m+1/2}, D_{-x}\omega_{d,h}^{m+1}\right)_+ \\ + \left(f_h^{m+1/2} - \tilde{f}_h^{m+1/2}, \omega_{d,h}^{m+1/2} - \omega_{s,h}^{m+1/2}\right)_h.\end{aligned} \tag{38}$$

Considering the assumptions on the coefficient functions, using Proposition 5, for all $\epsilon \neq 0$, we have

$$\begin{aligned}-\left(\left(a_d\left(M_h c_{\ell,h}^{m+1/2}\right) - a_d\left(M_h\tilde{c}_{\ell,h}^{m+1/2}\right)\right) D_{-x}c_{d,h}^{m+1/2}, D_{-x}\omega_{d,h}^{m+1/2}\right)_+ \\ \leq \frac{\epsilon^2}{2}\|D_{-x}\omega_{d,h}^{m+1/2}\|_+^2 + C_d\frac{M_d^2}{4\epsilon^2}\max_{j=0,\ldots,N-1}\|D_{-x}c_{d,h}^{j+1/2}\|_{+,\infty}^2 \cdot \left(\|\omega_{\ell,h}^{m+1}\|_h^2 + \|\omega_{\ell,h}^m\|_h^2\right)\end{aligned}$$

and

$$-\left(a_d\left(M_h\tilde{c}_{\ell,h}^{m+1/2}\right) D_{-x}\omega_{d,h}^{m+1/2}, D_{-x}\omega_{d,h}^{m+1}\right)_+ \leq -a_{0,d}\|D_{-x}\omega_{d,h}^{m+1/2}\|_+^2,$$

where C_d is a suitable positive constant. Through a straightforward application of assumption $\mathbf{H_f}$, it can be shown that the following holds

$$\begin{aligned}&\left(f_h^{m+1/2} - \tilde{f}_h^{m+1/2}, \omega_{d,h}^{m+1/2} - \omega_{s,h}^{m+1/2}\right)_h \\ &\qquad \le C_f \max_{i=0,\ldots,N} \left\{\|c_{d,h}^i\|_{h,\infty}, \|c_{\ell,h}^i\|_{h,\infty}, \|\tilde{c}_{\ell,h}^i\|_{h,\infty}\right\} \left(E_{s,d}^{m+1} + E_{s,d}^m\right) \\ &\qquad\qquad + \tilde{C}_f \max_{i=0,\ldots,N} \left(1 + \|c_{d,h}^i\|_{h,\infty}\right)^2 \left(\|\omega_{\ell,h}^{m+1}\|_h + \|\omega_{\ell,h}^m\|_h^2\right),\end{aligned}$$

where $\tilde{C}_f$ is a convenient positive constants and

$$E_{s,d}^m = \|\omega_{d,h}^m\|_h^2 + \|\omega_{s,h}^m\|_h^2.$$

Considering the last estimates in eq. (38) and eq. (36), we obtain

$$(1 - \alpha\Delta t)\, E_{s,d}^{m+1} + 2(a_{0,d} - \epsilon^2)\|D_{-x}\omega_{d,h}^{m+1/2}\|_+^2 \le (1 + \alpha\Delta t)\, E_{s,d}^m + \Delta t z^m. \tag{39}$$

where $\alpha = 4C_f C$, $\beta = 2\tilde{C}_f(1+C)^2 + C_{d,1}\frac{M_d^2}{4\epsilon^2}$ and $z^m = \beta\left(\|\omega_{\ell,h}^{m+1}\|_h^2 + \|\omega_{\ell,h}^m\|_h^2\right)$. Choosing $\epsilon \neq 0$ such that $D_0(\epsilon) = 2(a_{0,d} - \epsilon^2) > 0$, Lemma 1 from [19] implies

$$\begin{aligned}&\|\omega_{d,h}^m\|_h^2 + \|\omega_{s,h}^m\|_h^2 + \Delta t \sum_{i=0}^{m-1} \|D_{-x}\omega_{d,h}^{i+1/2}\|_+^2 \\ &\qquad \le \left((1 + \alpha\Delta t)\left(\|\omega_{d,h}^0\|_h^2 + \|\omega_{s,h}^0\|_h^2\right) + 2\,\beta\Delta t \sum_{i=0}^{m} \|\omega_{\ell,h}^i\|_h\right) \cdot \\ &\qquad\qquad \cdot \exp\left(2T\alpha \max\left\{\frac{1}{D_0(\epsilon)}, \frac{1}{1-\alpha\Delta t}\right\}\right).\end{aligned}$$

□

The combination of Propositions 7 and 8 leads to our first main result. Let

$$\begin{aligned}\mathbb{E}_{\ell,\sigma,d,s}^m = &\|\omega_{\ell,h}^m\|_h^2 + \|\omega_{d,h}^m\|_h^2 + \|\omega_{s,h}^m\|_h^2 + \|D_{-x}\omega_{\sigma,h}^m + \gamma D_{-x}\omega_{\ell,h}^m\|_+^2 \\ &+ \Delta t \sum_{i=0}^{m-1} \left[\|D_{-x}\omega_{\sigma,h}^{i+1/2}\|_+^2 + \|D_{-x}\omega_{\ell,h}^{i+1/2}\|_+^2 + \|D_{-x}\omega_{d,h}^{i+1/2}\|_+^2\right]\end{aligned}$$

for $m = 1, \ldots, M$.

Theorem 1. *Let $c_{i,h}^m$, $i = d, s, \ell$ and σ_h^m, $m = 0, \ldots, M$ denote fixed solutions of the discrete problem defined by eqs. (9) to (20) and let $\omega_{i,h}^m = c_{i,h}^m - \tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\omega_{\sigma,h}^m = \sigma_h^m - \tilde{\sigma}_h^m$, where $\tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\tilde{\sigma}_h^m$ is another solution of the same discrete problem. If the assumptions $\mathbf{H_{diff}}$ and $\mathbf{H_f}$ hold, the coefficients satisfy eq. (31) and there exist positive constants C_{stab} and Δt_0 such that, for all $\Delta t \in (0, \Delta t_0)$, the corresponding solution satisfies*

$$\max_{m=0,\ldots,M} \left\{\|D_{-x}c_{\ell,h}^m\|_{+,\infty}, \|D_{-x}\sigma_h^m\|_{+,\infty}, \|D_{-x}c_{d,h}^m\|_{+,\infty}, \|c_{d,h}^m\|_{h,\infty}, \|c_{\ell,h}^m\|_{h,\infty}, \|\tilde{c}_{\ell,h}^m\|_{h,\infty}\right\} \le C_{stab} \tag{40}$$

independently of h, then there exists a positive constant C, independent of h and Δt, such that, for Δt sufficiently small, the following inequality holds

$$\mathbb{E}_{\ell,\sigma,d,s}^m \le C\left(\|\omega_{\ell,h}^0\|_h^2 + \|D_{-x}\omega_{\sigma,h}^0\|_+^2 + \|D_{-x}\omega_{\ell,h}^0\|_+^2 + \|\omega_{d,h}^0\|_h^2 + \|\omega_{s,h}^0\|_h^2\right) \tag{41}$$

for $m = 1, 2, \ldots, M-1$.

Remark 5. We conclude this section remarking that the stability of eqs. (9) to (20) in $c_{i,h}^j, i = d, s, \ell, \sigma_h^j, j = 0, \dots, M$, is concluded from Theorem 1 provided that there exists a positive constant C_{stab}, h and Δt independent, such that, for Δt small enough,

$$\|D_{-x} c_{\ell,h}^{j+1/2}\|_{+,\infty}^2 \leq C_{stab}, \, \|D_{-x} \sigma_h^{j+1/2}\|_{+,\infty}^2 \leq C_{stab}, \|D_{-x} c_{d,h}^{j+1/2}\|_{+,\infty} \leq C_{stab},$$

$j = 0, \dots, M-1, h \in \Lambda$, and

$$\|c_{d,h}^j\|_{h,\infty} \leq C_{stab}, \, \|c_{\ell,h}^j\|_{h,\infty} \leq C_{stab}, \|\tilde{c}_{\ell,h}^j\|_{h,\infty} \leq C_{stab},$$

for $j = 0, \dots, N, h \in \Lambda$.

3.2 Convergence analysis

Let $c_{i,h}^m$, $i = d, \ell, s$, and σ_h^m, $m = 1, \dots, M$ denote fixed solutions of the discrete problem defined by eqs. (9) to (20) . Let $E_{i,h}^j = R_h c_i(t_j) - c_{i,h}^j, i = d, \ell, s$, $E_{\sigma,h}^j = R_h \sigma(t_j) - \sigma_h^j$, for $j = 0, \dots, N$, be the discretization errors, where $c_i, i = d, \ell, s, \sigma$ represent the solution of the initial boundary value problem defined by eqs. (1) to (3) and (7)) with $\epsilon = \lambda c_\ell$, eqs. (5), (6) and (8), and $R_h : C([0, R]) \longrightarrow V_h$ denotes the standard restriction operator to the grid functions defined on Ω_h.

To establish error estimates we use the approach introduced in [3] for elliptic problems and largely followed by the authors and their collaborators in, for instance, [4, 20, 22, 2] for non-Fickian diffusion problems and [18, 14, 17, 21, 16] for coupled problems.

Let $g \in C([0, R])$. We introduce $(g)_h \in V_h$ defined by

$$\begin{aligned}
(g)_h(x_0) &= \frac{2}{h_1} \int_{x_0}^{x_{1/2}} g(x) dx, \\
(g)_h(x_i) &= \frac{1}{h_{i+1/2}} \int_{x_{i-1/2}}^{x_{i+1/2}} g(x) dx, i = 1, \dots, N-1, \\
(g)_h(x_N) &= \frac{2}{h_N} \int_{x_{N-1/2}}^{x_N} g(x) dx
\end{aligned}$$

and $\hat{g} : V_h \backslash \{x_0\} \longrightarrow \mathbb{R}$ defined by $\hat{g}(x_i) = R_h g(x_{i-1/2})$, $i = 1, \dots, N$. We also define the space

$$V = H^3(0, T; H^2(0, R)) \cap C^0(0, T; H^3(0, R)) \tag{42}$$

$$E_{\ell,\sigma}^j := \|E_{\ell,h}^j\|_h^2 + \|D_{-x}\left(E_{\sigma,h}^j + \gamma E_{\ell,h}^j\right)\|_+^2, \, j = 0, \dots, M.$$

The first result on convergence, estimating the error for approximations $c_{\ell,h}$ and σ_h, is as follows.

Proposition 9. *Let $c_\ell, \sigma \in V$ denote solutions of the problem defined by eqs.* (1) *and* (5) *to* (8) *and $c_{\ell,h}, \sigma_h \in V_h$ denote the solution of the problem defined by eqs.* (9), (10), (13) *and* (16) *to* (19). *If the assumption* $\mathbf{H_{diff}}$ *holds and the coefficients satisfy eq.* (31) *then, there exists a positive constant C_ℓ such that for Δt small enough,*

$$E_{\ell,\sigma}^m + \Delta t \sum_{j=0}^{m-1} \sum_{p=\ell,\sigma} \|D_{-x} E_{p,h}^{j+1/2}\|_+^2 \leq C_\ell \Big(\|E_{\ell,h}^0\|_h^2 + \|D_{-x} E_{\sigma,h}^0\|_+^2 + \|D_{-x} E_{\ell,h}^0\|_+^2 + T_{er,\ell} \Big),$$

for $m = 1, 2, \dots, M-1$, where

$$\begin{aligned}
T_{er,\ell} \leq h_{max}^4 &\left(\sum_{p=c_\ell,\sigma} \Big(\|p\|_{C^0(H^2)} \|c_\ell\|_{C^0(H^2)} + \|p\|_{C^0(H^3)} + \|p\|_{C^1(H^2)} \Big)^2 \right) \\
&+ \Delta t^4 \left(\sum_{p=c_\ell,\sigma} \Big(\|p\|_{C^0(H^2)} \|c_\ell\|_{H^2(H^1)} + \|p\|_{H^2(H^2)} \Big)^2 + \|p\|_{H^3(H^2)} \right).
\end{aligned}$$

Proof. This proof follows the reasoning behind the one of Proposition 7.

1. Estimates for $D_{-t}\|E_{\ell,h}\|_h^2$ and $\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2$:
   A straightforward, although tedious, calculation allows to show the following equalities

$$
\begin{aligned}
\left(D_{-t}E_{\ell,h}^{m+1}, E_{\ell,h}^{m+1/2}\right)_h &= \left(\left(c'_\ell(t_{m+1/2})\right)_h, E_{\ell,h}^{m+1/2}\right)_h - \left(D_{-t}c_{\ell,h}^{m+1}, E_{\ell,h}^{m+1/2}\right)_h \\
&\quad + \left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h \\
&= \sum_{p=c_\ell,\sigma}\left(a_p\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}p_h^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+ \\
&\quad - \sum_{p=c_\ell,\sigma}\left(a_p\left(M_hR_hc_\ell^{m+1/2}\right)D_{-x}R_hp^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+ \\
&\quad + \sum_{p=c_\ell,\sigma}\left(T_{1,p}^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+ + \left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h +
\end{aligned}
\tag{43}
$$

   where

$$
T_1^{m+1} = \left(R_hc'_\ell(t_{m+1/2}) - \left(c'_\ell(t_{m+1/2})\right)_h\right) + \left(D_{-t}R_hc_\ell(t_{m+1}) - R_hc'_\ell(t_{m+1/2})\right)
$$

   and

$$
\begin{aligned}
T_{1,p}^{m+1/2} = -\Bigg(&\left(a_p\left(\widehat{c}_\ell(t_{m+1/2})\right) - a_p\left(M_hR_hc_\ell^{m+1/2}\right)\right)\widehat{\frac{\partial p}{\partial x}}(t_{m+1/2}) \\
&- \left(a_p\left(M_hR_hc_\ell^{m+1/2}\right)\right)\left(\widehat{\frac{\partial p}{\partial x}}(t_{m+1/2}) - D_{-x}R_hp^{m+1/2}\right)\Bigg),
\end{aligned}
$$

   for $p = c_\ell, \sigma$. Following the proof of eq. (29), it can be shown that, from eq. (43), for all $\epsilon \neq 0$, we have

$$
\begin{aligned}
& D_{-t}\|E_{\ell,h}^{m+1}\|_h^2 + (2a_{0,\ell} - 2\epsilon^2 - M_\sigma)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2 \\
&\quad \leq \frac{1}{\epsilon^2}\sum_{p=c_\ell,\sigma}\left(M_p^2\|D_{-x}R_hp^{m+1/2}\|_{+,\infty}^2\right)\|E_{\ell,h}^{m+1/2}\|_h^2 \\
&+M_\sigma\|D_{-x}E_{\sigma,h}^{m+1/2}\|_+^2 + \left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h + \sum_{p=\ell,\sigma}\left(T_{1,p}^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+,
\end{aligned}
\tag{44}
$$

   where $\epsilon \neq 0$. Using the Bramble-Hilbert Lemma, see [7], and the proof of Theorem 1 of [3], it can be shown that there exist positive constants C_1, C_2, independent of h and Δt, such that the following inequalities hold

$$
\begin{aligned}
\left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h \leq C_1\Big(&h_{max}^2\|c'_\ell(t_{m+1/2})\|_{H^2(0,R)}\|D_{-x}E_{\ell,h}^{m+1/2}\|_+ \\
&+\Delta t^{3/2}\|c'''_\ell\|_{L^2(t_m,t_{m+1};H^1(0,R))}\|E_{\ell,h}^{m+1/2}\|_h\Big),
\end{aligned}
\tag{45}
$$

$$
\begin{aligned}
\left(T_{1,p}^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+ \leq C_2h_{max}^2\Bigg(&\left\|\frac{\partial p}{\partial x}(t_{m+1/2})\right\|_{L^\infty(0,R)}\|c_\ell(t_{m+1/2})\|_{H^2(0,R)} \\
&+ \|p(t_{m+1/2})\|_{H^3(0,R)} + \|p(t_m)\|_{H^2(0,R)} \\
&+ \|p(t_{m+1})\|_{H^2(0,R)}\Bigg)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+ \\
&+ C_2\Delta t^{3/2}\Bigg(\left\|\frac{\partial p}{\partial x}(t_{m+1/2})\right\|_{L^\infty(0,R)}\|c''_\ell\|_{L^2(t_m,t_{m+1};H^1(0,R))} \\
&+ \left\|\left(\frac{\partial p}{\partial x}\right)''\right\|_{L^2(t_m,t_{m+1};H^1(0,R))}\Bigg)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+
\end{aligned}
\tag{46}
$$

for $p = c_\ell, \sigma$. Inserting eqs. (45) and (46) into eq. (44) we obtain

$$\begin{aligned} D_{-t}\|E_{\ell,h}^{m+1}\|_h^2 + (2a_{0,\ell} - 3\epsilon^2 - M_\sigma)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2 \\ \leq \frac{1}{\epsilon^2}\sum_{p=c_\ell,\sigma}\left(M_p^2\|D_{-x}R_h p^{m+1/2}\|_{h,\infty}^2 + \frac{1}{2}\right)\|E_{\ell,h}^{m+1/2}\|_h^2 + M_\sigma\|D_{-x}E_{\sigma,h}^{m+1/2}\|_+^2 + T_{\ell,\sigma}^{m+1/2} \end{aligned} \tag{47}$$

where, for $i = 1, \ldots, N-1$,

$$\begin{aligned} |T_{\ell,\sigma}^{m+1/2}(x_i)| \leq Ch_{max}^4 \Bigg(&\epsilon^2 \left\|c_\ell'(t_{m+1/2})\right\|_{H^2(0,R)}^2 \\ &+ \sum_{p=c_\ell,\sigma}\Big(\|p\|_{C^0(H^2)}\left\|c_\ell(t_{m+1/2})\right\|_{H^2(0,R)} \\ &\qquad + \left\|p(t_{m+1/2})\right\|_{H^3(0,R)} + \|p(t_m)\|_{H^2(0,R)} + \|p(t_{m+1})\|_{H^2(0,R)}\Big)^2\Bigg) \\ &+ C\Delta t^3\Bigg(\left\|c_\ell'''\right\|_{L^2(t_m,t_{m+1};H^1(0,R))}^2 \\ &+ \sum_{p=c_\ell,\sigma}\left(\|p\|_{C^0(H^2)}\left\|c_\ell''\right\|_{L^2(t_m,t_{m+1};H^1(0,R))} + \left\|\left(\frac{\partial p}{\partial x}\right)''\right\|_{L^2(t_m,t_{m+1};H^1(0,R))}\right)^2\Bigg) \end{aligned}$$

for some $\epsilon \neq 0$, and $C > 0$, independent of Δt and h.

2. Estimates for $\left\|D_{-x}\left(E_{\sigma,h}^{m+1} + \gamma E_{\ell,h}^{m+1}\right)\right\|_+^2$, $\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2$ and $\|D_{-x}E_{\sigma,h}^{m+1}\|_+^2$:

We now focus to the error equation associated with eq. (10). A simple calculation reveals that, for $E_{\sigma,h}^j$ and $E_{\ell,h}^j$, it holds

$$D_{-t}E_{\sigma,h}^{m+1} + \beta E_{\sigma,h}^{m+1/2} = -\alpha E_{\ell,h}^{m+1/2} - \gamma D_{-x}E_{\ell,h}^{m+1} + T_{\sigma,\ell}^{m+1},$$

where

$$\begin{aligned} T_{\sigma,\ell}^{m+1} = &\left(D_{-t}R_h\sigma(t_{m+1}) - R_h\sigma'(t_{m+1/2})\right) - \gamma\left(R_h c_\ell'(t_{m+1/2}) - D_{-t}R_h c_\ell(t_{m+1})\right) \\ &- \alpha\left(R_h c_\ell(t_{m+1/2}) - c_\ell^{m+1/2}\right) - \beta\left(R_h\sigma(t_{m+1/2}) - \sigma^{m+1/2}\right). \end{aligned}$$

Following the proof of Proposition 6, it can be shown that

$$\begin{aligned} \frac{1}{2}D_{-t}\left\|D_{-x}\left(E_{\sigma,h}^{m+1} + \gamma E_{\ell,h}^{m+1}\right)\right\|_+^2 + \beta\|D_{-x}E_{\sigma,h}^{m+1}\|_+^2 + \alpha\gamma\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2 \\ = -(\alpha + \beta\gamma)\left(D_{-x}E_{\ell,h}^{m+1/2}, D_{-x}E_{\sigma,h}^{m+1/2}\right)_+ \\ + \left(D_{-x}T_{\ell,\sigma}^{m+1}, D_{-x}\left(E_{\sigma,h}^{m+1/2} + \gamma E_{\ell,h}^{m+1/2}\right)\right)_+ \end{aligned} \tag{48}$$

Using again the Bramble-Hilbert Lemma ([7]), it can be established for $i = 1, \ldots, N$, $m = 0, \ldots, M-1$ that

$$|D_{-x}T_{\sigma,\ell}^{m+1}(x_i)| \leq C\Delta t^{3/2}\sum_{p=c_\ell,\sigma}\left(\sum_{k=2}^{3}\left\|p^{(k)}\right\|_{L^2(t_m,t_{m+1};H^2(0,R))}\right), \tag{49}$$

where C denotes a suitable positive constant. This implies the bound

$$\begin{aligned} \left(D_{-x}T_{\ell,\sigma}^{m+1}, \gamma D_{-x}E_{\sigma,h}^{m+1/2} + D_{-x}E_{\ell,h}^{m+1/2}\right)_+ \leq \epsilon_2^2\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2 \\ + \epsilon_3^2\|D_{-x}E_{\sigma,h}^{m+1/2}\|_+^2 + \tilde{T}_{\ell,\sigma}^{m+1}, \end{aligned} \tag{50}$$

with

$$\tilde{T}_{\ell,\sigma}^{m+1} \leq C\Delta t^3\sum_{p=c_\ell,\sigma}\left(\sum_{k=2}^{3}\left\|p^{(k)}\right\|_{L^2(t_m,t_{m+1};H^2(0,R))}\right)$$

and $\epsilon_i \neq 0, i = 2, 3$.

Combining eqs. (47), (48) and (50) we get

$$
\begin{aligned}
D_{-t}\Big[\big\|E_{\ell,h}^{m+1}\big\|_h^2 &+ \big\|D_{-x}E_{\sigma,h}^{m+1/2}+\gamma D_{-x}E_{\ell,h}^{m+1/2}\big\|_+^2\Big] \\
&+ A_0(\epsilon_3)\big\|D_{-x}E_{\sigma,h}^{m+1/2}\big\|_+^2 + B_0(\epsilon)\big\|D_{-x}E_{\ell,h}^{m+1/2}\big\|_+^2 \\
&\leq \frac{1}{\epsilon^2}\sum_{p=c_\ell,\sigma}\left(M_p^2\big\|D_{-x}R_h p^{m+1/2}\big\|_{+,\infty}^2+\frac{1}{2}\right)\big\|E_{\ell,h}^{m+1/2}\big\|_h^2 + 2\tilde{T}_{\ell,\sigma}^{m+1} + T_{\ell,h}^{m+1},
\end{aligned}
$$

where $2\epsilon_2^2=\epsilon^2$,

$$A_0(\epsilon_3)=2\left(\beta-\frac{M_\sigma}{2}-\frac{\alpha+\beta\gamma}{2}-\epsilon_3^2\right)$$

and

$$B_0(\epsilon)=2\left(\alpha\gamma+a_{0,\ell}-\frac{M_\sigma}{2}-\frac{\alpha+\beta\gamma}{2}-2\epsilon^2\right).$$

Considering the assumption (31) on the coefficients $\alpha,\beta,\gamma,a_{0,\ell}$ and M_σ, we conclude the existence the coefficients $\epsilon,\epsilon_3\neq 0$ such that $A_0(\epsilon_3),B_0(\epsilon)$ are positive such that

$$
\begin{aligned}
(1-\Delta t\theta_\ell(c_\ell,\sigma))E_{\ell,\sigma}^{m+1} &+ \Delta t\min\{A_0(\epsilon_3),B_0(\epsilon)\}\left(\big\|D_{-x}E_{\sigma,h}^{m+1/2}\big\|_+^2+\big\|D_{-x}E_{\ell,h}^{m+1/2}\big\|_+^2\right) \\
&\leq \Big(1+\Delta t\theta_\ell(c_\ell,\sigma)\Big)E_{\ell,\sigma}^m + \Delta t\left(2\tilde{T}_{\ell,\sigma}^{m+1}+T_{\ell,h}^{m+1}\right),
\end{aligned}
\tag{51}
$$

where

$$\theta_\ell(c_\ell,\sigma)=\frac{1}{2\epsilon^2}\max_{p=\ell,\sigma}M_p\cdot\max_{p=\ell,\sigma}\|p\|_{C^0(H^2)}.$$

Assuming

$$\Delta t<\frac{2\epsilon^2}{\max_{p=\ell,\sigma}M_p\cdot\max_{p=\ell,\sigma}\|p\|_{C^0(H^2)}}$$

and applying a discrete Gronwall Lemma to eq. (51), we conclude the proof. □

We finally turn our attention to the error associated with the concentration of solid and dissolved drugs, c_d and c_s. Let

$$X=C^0(0,T;H^3(0,R)\cap H_{0,R}^1(0,R))\cap H^2(0,T;H^2(0,R)\cap H_{0,R}^1(0,R))\cap H^3(0,T;H_{0,R}^1(0,R)).$$

Proposition 10. *Let $c_\ell,\sigma\in V$, $c_d\in X$ and $c_s\in H^3(0,T;H^1(0,R))$ denote solutions of the problem defined by eqs. (1) and (5) to (8) and $c_{d,h}\in V_{h,0}$ and $c_{s,h}\in V_h$ denote the solution of the problem defined by eqs. (9) to (20). If $f(c_s,c_d,c_\ell)\in C^0(H^2)$, the assumption $\mathbf{H_{diff}}$ and $\mathbf{H_f}$ hold, and the coefficients satisfy eq. (31) then, there exists a positive constant $C_{d,s}$, such that for Δt small enough,*

$$\big\|E_{d,h}^m\big\|_h^2+\big\|E_{s,h}^m\big\|_h^2+\Delta t\sum_{j=0}^{m-1}\big\|D_{-x}E_{d,h}^{j+1/2}\big\|_+^2\leq C_{d,s}\Big(\|E_{d,h}^0\|_h^2+\|E_{s,h}^0\|_h^2+T_{er,d,s}\Big),$$

where

$$
\begin{aligned}
T_{err,d,s}\leq h_{max}^4\Bigg(&\sum_{p=c_\ell,\sigma}\Big(\|p\|_{C^0(H^2)}\|c_\ell\|_{C^0(H^2)} \\
&+\|p\|_{C^0(H^3)}+\|p\|_{C^1(H^2)}\Big)^2+\|f(c_s,c_d,c_\ell)\|_{C^0(H^2)}^2 \\
&+\Big(\|c_d\|_{C^1(H^2)}+\|c_d\|_{C^0(H^3)}\Big(\|c_\ell\|_{C^0(H^2)}+1\Big)\Big)^2\Bigg) \\
+\Delta t^4\Bigg(&\sum_{p=c_\ell,\sigma}\Big(\|p\|_{C^0(H^2)}\|c_\ell\|_{H^2(H^1)}+\|p\|_{H^2(H^2)}\Big)^2 \\
&+\|p\|_{H^3(H^2)}+\|c_d\|_{C^0(H^2)}^2\|c_\ell\|_{H^2(H^1)}^2+\|c_d\|_{H^2(H^2)}^2 \\
&+\|c_d\|_{H^3(H^1)}^2+\|c_s\|_{H^3(H^1)}^2\Bigg).
\end{aligned}
$$

Proof. We follow the steps of the proof of Proposition 9. We start by noticing that from eqs. (11) and (12) we easily establish, for all $\epsilon \neq 0$, that

$$\frac{1}{2}D_{-t}\left(\left\|E_{d,h}^{m+1}\right\|_h^2 + \left\|E_{s,h}^{m+1}\right\|_h^2\right) + \left(a_{0,d} - \frac{\epsilon^2}{2}\right)\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+^2$$
$$\leq \frac{M_d^2}{2\epsilon^2}\left\|c_d\right\|_{C^0(H^2)}^2\left\|E_{\ell,h}^{m+1/2}\right\|_h^2 + T_1 + T_2 + +T_{d,s}$$

where

$$T_1 = \left((R_h f^{m+1/2})_h - R_h f^{m+1/2}, E_{d,h}^{m+1/2}\right)_h$$
$$T_2 = \left(R_h f^{m+1/2} - f_h^{m+1/2}, E_{d,h}^{m+1/2} + E_{s,h}^{m+1/2}\right)_h$$

$$\begin{aligned}T_{d,s} \leq C_1 \Big(& h_{max}^2 \left(\|c_d\|_{C^1(H^2)} + \|c_d\|_{C^0(H^3)}\left(\|c_\ell\|_{C^0(H^2)} + 1\right)\right)\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+ \\ & +\Delta t^{3/2}\left(\|c_d\|_{C^0(H^2)}\|c_\ell\|_{H^2(t_m,t_{m+1};H^1(0,R))} + \|c_d\|_{H^2(t_m,t_{m+1};H^2(0,R))}\right)\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+ \\ & +\Delta t^{3/2}\left(\|c_d\|_{H^3(t_m,t_{m+1};H^1(0,R))}\left\|E_{d,h}^{m+1/2}\right\|_h + \|c_s\|_{H^3(t_m,t_{m+1};H^1(0,R))}\left\|E_{s,h}^{m+1/2}\right\|_h\right)\Big)\end{aligned}$$

for some positive constant C_1, independent of h and Δt. Both terms T_1 and T_2 can be bound using the Bramble-Hilbert Lemma. For T_1 we get

$$|T_1| \leq C_2 h_{max}^2 \|f(c_s, c_d, c_\ell)\|_{C^0(H^2)}\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+$$

for some positive constant C_2, independent of h and Δt.

Regarding T_2, using assumption $\mathbf{H_f}$, it holds, for all $\eta \neq 0$,

$$\begin{aligned}|T_2| \leq & \frac{\left(C_f(1 + \|c_d\|_{C^0(H^1)})\right)^2}{\eta^2}\left\|E_{\ell,h}^{m+1/2}\right\|_h^2 \\ & + \left(\frac{\eta^2}{2} + \frac{C_f^2 R\left\|c_{\ell,h}^{m+1/2}\right\|_h^2}{2\epsilon^2} + \frac{C_f\|c_\ell\|_{C^0(H^1)}(1 + \|c_d\|_{C^0(H^1)})}{2}\right)\left\|E_{d,h}^{m+1/2}\right\|_h^2 \\ & + \left(\frac{\eta^2}{2} + \frac{C_f^2 R\left\|c_{\ell,h}^{m+1/2}\right\|_h^2}{2\epsilon^2} + \frac{3C_f\|c_\ell\|_{C^0(H^1)}(1 + \|c_d\|_{C^0(H^1)})}{2}\right)\left\|E_{s,h}^{m+1/2}\right\|_h^2 \\ & + \epsilon^2\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+^2\end{aligned}$$

From Proposition 9, we know that $\left\|c_{\ell,h}^{m+1/2}\right\|_h$ is uniformly bounded, w.r.t, h and Δt, which means that there exists a positive constant $C_{conv,\ell}$ such that

$$\left\|c_{\ell,h}^{m+1/2}\right\|_h^2 \leq C_{conv,\ell}.$$

Choosing $\epsilon^2 = \frac{a_d}{6}$ and

$$\eta^2 = 3 \cdot \min\left\{\frac{C_f^2 R C_{conv,\ell}}{a_d}, \frac{C_f\|c_\ell\|_{C^0(H^1)}(1 + \|c_d\|_{C^0(H^1)})}{2}\right\},$$

it follows that

$$(1 - \alpha\Delta t)\left(\left\|E_{d,h}^{m+1}\right\|_h^2 + \left\|E_{s,h}^{m+1}\right\|_h^2\right) + \Delta t a_{0,d}\left\|D_{-x}E_{d,h}^{m+1/2}\right\|_+^2$$
$$\leq 2\Delta t\left((1 + \|c_d\|)^2 + \frac{M_d^2}{2\epsilon^2}\|c_d\|_{C^0(H^2)}^2\right)\left\|E_{\ell,h}^{m+1/2}\right\|_h^2$$
$$(1 + \alpha\Delta t)\left(\left\|E_{d,h}^m\right\|_h^2 + \left\|E_{s,h}^m\right\|_h^2\right) + \Delta t z^m$$

where

$$\alpha = 2\max\left\{\frac{3C_f^2 R C_{conv,\ell}}{a_d}, \frac{3C_f \|c_\ell\|_{C^0(H^1)}\left(1+\|c_d\|_{C^0(H^1)}\right)}{2}\right\}$$

and

$$\begin{aligned}
z^m = {} & C_3 h_{max}^4 \left(\left(\|c_d\|_{C^1(H^2)} + \|c_d\|_{C^0(H^3)}\left(\|c_\ell\|_{C^0(H^2)}+1\right)\right)^2 \right.\\
& \left. + \|f(c_s,c_d,c_\ell)\|^2_{C^0(H^2)}\right)\\
& + C_3\Delta t^3\left(\|c_d\|^2_{C^0(H^2)}\|c_\ell\|^2_{H^2(t_m,t_{m+1};H^1(0,R))} + \|c_d\|^2_{H^2(t_m,t_{m+1};H^2(0,R))}\right)\\
& + C_3\Delta t^3\left(\|c_d\|^2_{H^3(t_m,t_{m+1};H^1(0,R))} + \|c_s\|^2_{H^3(t_m,t_{m+1};H^1(0,R))}\right)
\end{aligned}$$

for some positive constant C_3, independent of h and Δt. Assuming $\Delta t < \frac{1}{\alpha}$, we finally conclude the proof. □

We can now state our final convergence result for the error

$$\mathbb{E}_h^m = \sum_{p=\ell,d,s} \|E_{p,h}^m\|_h^2 + \|D_{-x}\left(E_{\sigma,h}^m + \gamma E_{\ell,h}^m\right)\|_+^2 + \Delta t \sum_{j=0}^{m-1}\sum_{p=\ell,\sigma,d} \|D_{-x}E_{p,h}^{j+1/2}\|_+^2$$

Theorem 2. *Let $c_\ell, \sigma \in V$, $c_d \in X$ and $c_s \in H^3(0,T;H^1(0,R))$ denote solutions of the problem defined by eqs. (1) and (5) to (8) and $c_{d,h} \in V_{h,0}$ and $c_{\ell,h}, \sigma_h, c_{s,h} \in V_h$ denote the solution of the problem defined by eqs. (9) to (20). If $f(c_s,c_d,c_\ell) \in C^0(H^2)$, the assumption $\mathbf{H_{diff}}$ and $\mathbf{H_f}$ hold and the coefficients satisfy eq. (31) then, there exists a positive constant C, independent of h and Δt, such that for Δt small enough,*

$$\mathbb{E}_h^m \le C(h_{max}^4 + \Delta t^4),\ m = 1,\dots,M.$$

Remark 6. Let us suppose that the initial errors are null. In this case Theorem 2 establishes that the fully discrete piecewise linear-constant finite element method (28) presents second convergence order

$$\|E_{\ell,h}^m\|_h^2 + \|E_{\sigma,h}^m + \gamma E_{\ell,h}^m\|_{1,h}^2 + \Delta t\sum_{j=0}^{m-1}\sum_{p=\ell,\sigma}\|E_{p,h}^{j+1/2}\|_{1,h}^2 \le C\big(h_{max}^4 + \Delta t^4\big),$$

$$\sum_{p=d,s}\|E_{p,h}^m\|_h^2 + \Delta t\sum_{j=0}^{m-1}\|E_{d,h}^{j+1/2}\|_{1,h}^2 \le C\big(h_{max}^4 + \Delta t^4\big).$$

As mentioned before, these upper bounds were established avoiding the approach of Wheeler [37]. Furthermore, as the fully-discrete Galerkin method is obtained considering linear piecewise approximation for c_ℓ, σ and c_d, the second convergence order with respect to the norm $\|.\|_{1,h}$ which can be seen as a discrete version of the usual H^1-norm.

Remark 7. As mentioned in Section 3.1, the stability of the fluid discretization can be established showing that $\|D_{-x}c_{\ell,h}^{j+1/2}\|^2_{+,\infty}$ and $\|D_{-x}\sigma_h^{j+1/2}\|^2_{+,\infty}$, are uniformelly bounded, w.r.t. h and Δt. Let $c_{\ell,h}^0, \sigma_h^0$ be such that

$$\|E_{\ell,h}^0\|_h \le Ch_{max}^2, \quad \|D_{-x}E_{\ell,h}^0\|_+ \le Ch_{max}^2, \quad \|D_{-x}E_{\sigma,h}^0\|_+ \le Ch_{max}^2.$$

From Proposition 2 it follows that

$$\begin{aligned}
\|D_{-x}c_{\ell,h}^{j+1/2}\|^2_{+,\infty} &\le 2\|D_{-x}E_{\ell,h}^{j+1/2}\|^2_{+,\infty} + 2\|D_{-x}R_h c_\ell^{j+1/2}\|^2_{+,\infty}\\
&\le \frac{8}{h_{min}^3}\|E_{\ell,h}^{m+1/2}\|_h^2 + 2\|c_\ell\|^2_{C^0(H^2)}.
\end{aligned}$$

Using the estimate from Proposition 9, there exists a positive constant C, independent of h and Δt, such that

$$\left\|D_{-x}c_{\ell,h}^{j+1/2}\right\|_{+,\infty}^2 \leq C\frac{h_{max}^4+\Delta t^4}{h_{min}^4} + 2\left\|c_\ell\right\|_{C^0(H^2)}^2.$$

Therefore, under the assumption of the grids being quasiuniform, the stability condition $\frac{\Delta t}{h_{max}} \leq \tilde{C}$, for some constant $\tilde{C}$ and that we choose our perturbations in a ball centered around the numerical solution and with radius such that

$$\left\|\omega_{\ell,h}^0\right\|_h^2 + \left\|D_{-x}\omega_{\sigma,h}^0\right\|_+^2 + \left\|D_{-x}\omega_{\ell,h}^0\right\|_+^2 + \|\omega_{d,h}^0\|_h^2 + \|\omega_{s,h}^0\|_h^2 \leq Ch_{max}^4,$$

we can conclude that for Δt small enough, the bound given by eq. (32) holds and the stability is ensured in the mentioned sense. Regarding the stability of the scheme w.r.t. $c_{d,h}$ and $c_{s,h}$, using Proposition 3, similar uniform bounds can be obtained for $\left\|c_{p,h}^m\right\|_{h,\infty}$, with $p = d, s$ and $\left\|\tilde{c}_{\ell,h}^m\right\|_{h,\infty}$, under the same requirements for the grids and Δt.

Theorem 1 can now be reformulated as follows.

Theorem 3. *Let $c_{i,h}^m$, $i = d, s, \ell$ and σ_h^m, $m = 0, \ldots, M$ denote fixed solutions of the discrete problem defined by eqs. (9) to (20). If the grid is quasiuniform, the assumptions $\mathbf{H_{diff}}$ and $\mathbf{H_f}$ hold and the coefficients satisfy eq. (31) then for Δt sufficiently small, the numerical method is stable, provided the perturbations $\omega_{i,h}^m = c_{i,h}^m - \tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\omega_{\sigma,h}^m = \sigma_h^m - \tilde{\sigma}_h^m$, where $\tilde{c}_{i,h}^m$, $i = d, s, \ell$ and $\tilde{\sigma}_h^m$ satisfy the same discrete problem with perturbed initial data and*

$$\left\|\omega_{\ell,h}^0\right\|_h^2 + \left\|D_{-x}\omega_{\sigma,h}^0\right\|_+^2 + \left\|D_{-x}\omega_{\ell,h}^0\right\|_+^2 + \|\omega_{d,h}^0\|_h^2 + \|\omega_{s,h}^0\|_h^2 \leq Ch_{max}^4,$$

for some positive constant C.

4 Numerical simulation

This section aims to illustrate the main convergence result of this work, Theorem 2, for the fully-discrete approximation defined by eqs. (9) to (20). The theoretical solutions $c_\ell, \sigma \in V$, $c_d \in X$ and $c_s \in H^3(0,T; H^1(0,R))$ of eqs. (1) and (5) to (8) used in our numerical test solve a modified problem obtained by adding in each partial differential equation a source term R_i, $i = \ell,\, d,\, s, \sigma$.

In our test we run the simulation in the time interval $[0,T]$ with $T = 5\ s$ and in the space interval $[0,R]$ with $R = 1\ mm$ representing the radius of Maxwell-Wichert polymeric platform with Young modules $E_0 = E_1 = 1\ Pa$, viscosity $\mu = 10^6\ Pa\cdot s$, and relaxation time $\tau = \frac{\mu}{E_1} = 10^6\ s$.

The solvent concentration c_ℓ used is defined by

$$c_\ell(x,t) = e^{-\frac{t}{15}}\tilde{c}(x) + \phi(t),\ (x,t) \in [0,R]\times[0,T]$$

with $\phi(t) = c_{ext}(1 - e^{-\frac{t}{15}})$ and

$$\tilde{c}(x) = \left(1 - \frac{1}{m}\right)(c_{ext}-1)\frac{x^2}{R^2} + \frac{c_{ext}-1}{m} + \frac{|ax-R|^{p+1} + a\,R^p(p+1)(x-R)}{(aR-R)^{p+1}},$$

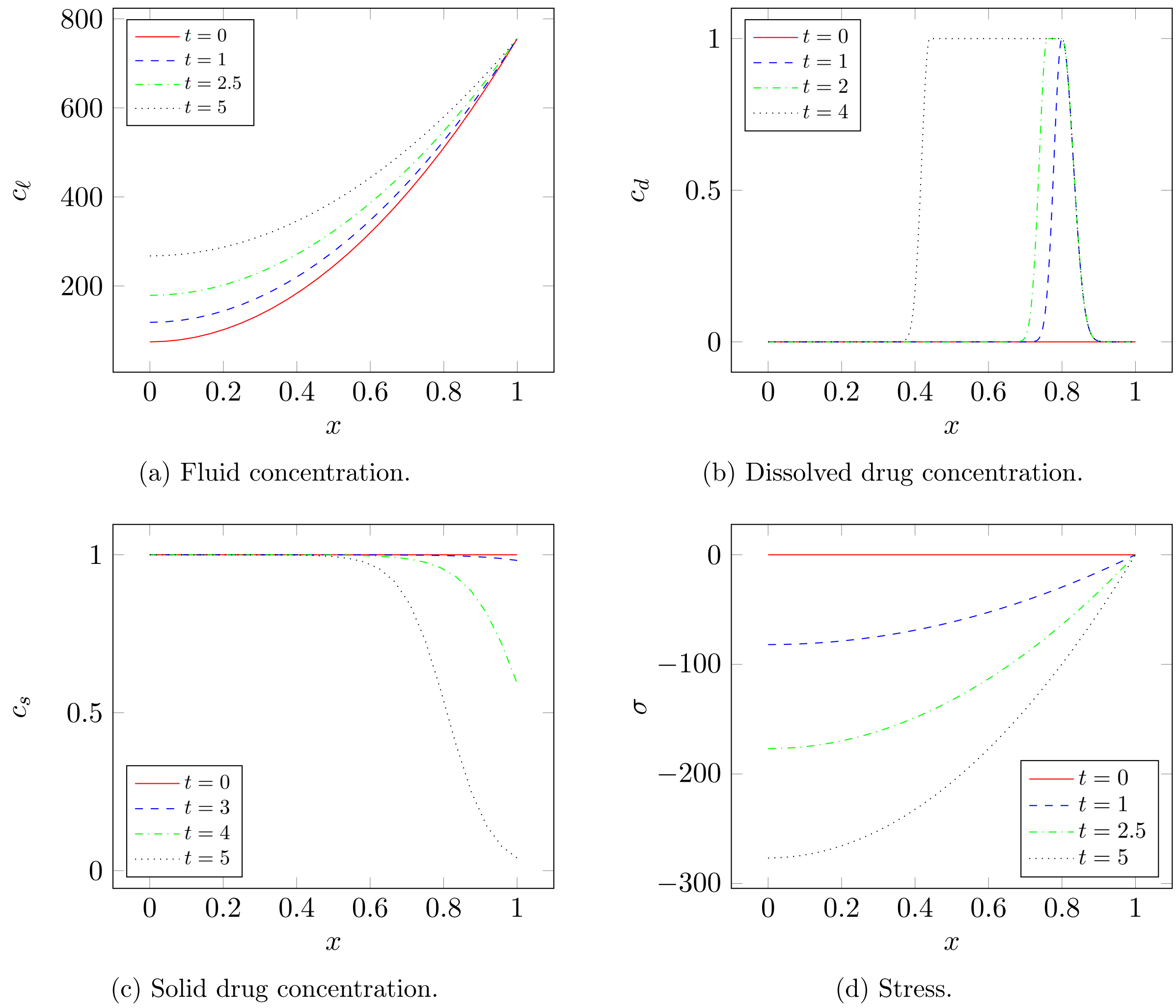
where $c_{ext} = 755.74\ kg/m^3$ is the exterior solvent concentration, $a = 3$, $m = 10$ and $p = 1.7$. Note that $x = \frac{R}{a}$ is a critical point that guarantees that $c_\ell(\cdot,t) \in H^3(0,R)$ (and not in $C^3(0,R)$), in order to satisfy the hypothesis of Theorem 2.

We also define

$$c_d(x,t) = g(x,t)\,\psi(t),\ (x,t) \in [0,R]\times[0,T] \tag{52}$$

where

$$g(x,t) = \begin{cases} \exp\left(-\frac{(x-a_2(t))^2+|x-a_2(t)|^{p+1}}{10^{-3}}\right) & if \quad 0 \leq x \leq a_2(t) \\ 1 & if \quad a_2(t) < x < a_0 \\ \exp\left(-\frac{(x-a_0)^2+|x-a_0|^{p+1}}{2\cdot10^{-3}}\right) & if \quad a_0 \leq x \leq R, \end{cases}$$



(a) Fluid concentration.

(b) Dissolved drug concentration.

(c) Solid drug concentration.

(d) Stress.

Figure 1: Plot of the analytical solutions for different instances of $t \in [0, T]$.

with

$$a_2(t) = \begin{cases} a_0 & if \quad 0 \leq t < \tilde{t} \\ a_0 - \left(\dfrac{t - \tilde{t}}{T}\right)^2 & if \quad \tilde{t} \leq t \leq T \end{cases}$$

and

$$\psi(t) = \begin{cases} 1 - \left(\dfrac{t - \tilde{t}}{\tilde{t}}\right)^2 & if \quad 0 \leq t < \tilde{t} \\ 1 & if \quad \tilde{t} \leq t \leq T. \end{cases}$$

We remark that $c_d(\cdot, t)$ is in $H^3(0, R)$ but not in $C^3(0, R)$.

The solid drug concentration solution used in our simulation is

$$c_s(x, t) = \left(1 + \frac{t}{5 \times 10^{-5}}\; e^{-10\left(\frac{10}{4} - \frac{tx}{3}\right)}\right)^{-1}, \; (x, t) \in [0, R] \times [0, T]. \tag{53}$$

Finally the polymeric chains' stress is given by

$$\sigma(x, t) = (c_\ell(x, t) - c_{ext})\xi(t), \; (x, t) \in [0, R] \times [0, T] \tag{54}$$

where

$$\xi(t) = E_0\left(1 - e^{-\frac{t}{15}}\right) + \left(\frac{E_1 \tau}{\tau - 15}\right)\left(1 - e^{-t\left(\frac{1}{15} - \frac{1}{\tau}\right)}\right).$$

Profile plots of c_ℓ, c_d, c_s, σ are given in Figure 1 for different values of t. The numerical method defined by eqs. (9) to (20) is implemented with initial conditions given by $c_\ell(x, 0), c_d(x, 0), c_s(x, 0)$.

Based on real biological information, see [5, 6, 13], we use the coefficient functions $a_\ell(c_\ell)$, $a_d(c_\ell)$, $a_\sigma(c_\ell)$ defined as follows

$$a_\ell(c_\ell) = D_{\ell e}\ e^{-\beta_\ell\left(1-\frac{c_\ell}{c_{ext}}\right)}, \quad a_d(c_\ell) = D_{de}\ e^{-\beta_d\left(1-\frac{c_\ell}{c_{ext}}\right)}, \quad a_\sigma(c_\ell) = \frac{R^2}{8\tilde{\mu}} c_\ell,$$

with $D_{\ell e} = 3.74 \cdot 10^{-9}\, m^2 s^{-1}$, $D_{de} = 2.72 \cdot 10^{-10}\, m^2 s^{-1}$, $\beta_\ell = 0.8$, $\beta_d = 0.5$, $\tilde{\mu} = 10^6\ Pa \cdot s$. These choices yield a nonlinear numerical problem in $c_{\ell,h}$ that is solved iteratively by Newton's method to get an approximation of $c_{\ell,h}$ at each time step. In Table 1 we show the errors calculated versus different values for Δt at time $T = 5\ s$ in a fixed grid with $h_{max} = 9.8638 \cdot 10^{-4}$. Thus we can show computationally that the method reaches second order for $\mathbb{E}_h^m$ with respect to Δt.

Δt	$\mathbb{E}_h^m$	Rate
$3.1250 \cdot 10^{-1}$	13.9571	-
$2.0833 \cdot 10^{-1}$	8.1536	1.3262
$1.5625 \cdot 10^{-1}$	4.5565	2.0227
$1.0416 \cdot 10^{-1}$	1.7421	2.3713
$7.8125 \cdot 10^{-2}$	$9.5928 \cdot 10^{-1}$	2.0740

Table 1: Estimated convergence rates for fixed $h_{max} = 9.8638 \cdot 10^{-4}$ and varying Δt.

In Table 2 we plot the numerical errors versus different values for h_{max} using a fixed $\Delta t = 4.8828 \cdot 10^4$ in each grid. The results illustrate computationally that $\mathbb{E}_h^m$ is of second order with respect to h_{max}.

h_{max}	$\mathbb{E}_h^m$	Rate
$6.2801 \cdot 10^{-2}$	$2.9494 \cdot 10^{-1}$	-
$3.1362 \cdot 10^{-2}$	$1.9660 \cdot 10^{-1}$	0.5840
$1.5639 \cdot 10^{-2}$	$1.1810 \cdot 10^{-1}$	0.7324
$7.8246 \cdot 10^{-3}$	$3.4207 \cdot 10^{-2}$	1.7892
$3.9635 \cdot 10^{-3}$	$8.3530 \cdot 10^{-3}$	2.0728
$1.9932 \cdot 10^{-3}$	$2.2342 \cdot 10^{-3}$	1.9184
$9.7753 \cdot 10^{-4}$	$5.2751 \cdot 10^{-4}$	2.0260

Table 2: Estimated convergence rates for fixed $\Delta t = 4.8828 \cdot 10^{-4}$ and varying h_{max}.

5 Conclusions

In this paper we present a model to simulate the complex interplay between solvent absorption, polymer swelling, drug release, and stress development within polymeric drug delivery platforms. A Maxwell-Wiechert model has been incorporated to capture the memory effect arising from polymer relaxation. To avoid the drawbacks of using an integral representation for the stress, we replace such memory term with a new differential equation. From a numerical standpoint, this leads to eliminating the need to store information from all previous time steps.

The main goal of this manuscript is to propose a fully discrete numerical scheme for the aforementioned system of differential equations, and subsequent stability and convergence analysis. Being a nonlinear system of differential equations, stability needs careful attention. Our main results are: (i) the stability of the numerical method provided suitable uniform bounds for the numerical solution and its perturbation and (ii) second order, in space and time, convergence for nonsmooth solutions, with no restriction on the grids. The bounds needed to ensure stability are derived from our main convergence theorem and are valid if the grid is quasiuniform and the timestep satisfies a relation of the type $\Delta t \leq C h_{max}$, for some constant C. Finally, we illustrate numerically the convergence rates obtained in the main result using an exact solution based on biological information.

Acknowledgment

This work was partially supported by the Centre for Mathematics of the University of Coimbra (funded by the Portuguese Government through FCT/MCTES, DOI 10.54499/UIDB/00324/2020). The work of G. Romanazzi and G.C.M. Campos was supported by FAPESP grant 2021/14713-5.

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