ISSN: 1392-6292/ eISSN: 1648-3510

VILNIUS TECH Vilnius Gediminas Technical University

MATHEMATICAL MODELLING and ANALYSIS

2026
Volume 31
Issue 1
Pages 1–25
https://doi.org/10.3846/mma.2026.22960

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

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Article History:
- received December 19, 2024
- revised July 13, 2025
- accepted September 5, 2025

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 platforms. A system of nonlinear partial differential equations coupled with an ordinary differential equation is introduced to avoid drawbacks from other models found in the literature. These incorporated a memory effect but from a numerical standpoint, required storing all previous time steps, making them computationally expensive. This paper proposes a new numerical method to simulate such devices based on nonuniform grids and an implicit midpoint time discretization. Our main results are the second order convergence of the method for nonsmooth solutions and the scheme's stability under the assumption of quasiuniform grids and a small enough timestep.

Keywords: drug delivery; polymeric devices; Maxwell-Wiechert; numerical method; second-order convergence.

AMS Subject Classification: 35Q92; 65N06; 65N12.

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1 Introduction

In this paper, we consider the system of differential equations

$$\frac{\partial c_\ell}{\partial t}(x,t) = \nabla\cdot\big(a_\ell(c_\ell(x,t))\nabla c_\ell(x,t)\big) + \nabla\cdot\big(a_\sigma(c_\ell(x,t))\nabla\sigma\big(x,t)\big), \tag{1.1}$$

$$\frac{\partial c_d}{\partial t}(x,t) = \nabla\cdot\big(a_d(c_\ell(x,t))\nabla c_d(x,t)\big) + f(c_s(x,t),\, c_d(x,t),\, c_\ell(x,t)), \tag{1.2}$$

$$\frac{\partial c_s}{\partial t}(x,t) = -f(c_s(x,t),\, c_d(x,t),\, c_\ell(x,t)), \tag{1.3}$$

for $x \in (0, R), t \in (0, T]$. In [10], the system equations (1.1) to (1.3) were introduced with

$$\nabla\sigma(x,t) = -\int_0^t q(s,t,c_\ell(x,s),c_\ell(x,t))\nabla c_\ell(x,s)ds, \tag{1.4}$$

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, with instantaneous swelling. This differential system is complemented by the following initial and boundary conditions:

$$c_\ell(x,0) = 0, \;\; c_d(x,0) = 0, \;\; c_s(x,0) = c_{s,0}(x), \;\; x \in (0,R), \tag{1.5}$$

$$\nabla c_\ell(0,t) = 0, \;\; \nabla c_d(0,t) = 0, \;\; c_\ell(R,t) = c_{ext}, \; c_d(R,t) = 0, \;\; t \in (0,T]. \tag{1.6}$$

The authors considered therein that the drug release is a consequence of the following set of phenomena: *(i)* the solvent molecules are absorbed by the polymeric structure due to the solvent gradient concentration (solvent absorption), *(ii)* the polymeric chains relax, the structure swells and a stress gradient arises (swelling), *(iii)* the dissolution process occurs due to the contact of the solid drug with the absorbed solvent molecules (dissolution) and *(iv)* the molecules of the dissolved drug diffuse throughout the platform and continue to diffuse in the external surrounding medium (diffusion). A key aspect of this model is the interaction between fluid absorption and the polymer's mechanical response. As the fluid permeates the structure, the polymer deforms and swells, generating internal stress. This stress creates a counter-acting flux, pushing fluid from regions of high stress to regions of low stress. Consequently, the overall fluid transport is driven not only by the concentration gradient but also by this stress gradient.

While the polymer itself is initially free of solvent, the surrounding environment is not. The subsequent phenomena (solvent absorption, polymer swelling, and drug dissolution/release) are also driven by the interaction between this initially dry platform and the external solvent.

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 response to 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 [10] the authors considered that $\epsilon = g(c_\ell)$ and σ defined by the Boltzman integral $\sigma(x,t) = -\int_0^t E(t-s)\frac{\partial\epsilon}{\partial s}(x,s)ds$, where $E(\cdot)$ is the kernel function associated with the generalized Maxwell-Wiechert model, $E(t) = E_0 + \sum_{j=1}^m E_j e^{-\frac{t}{\tau_j}}$, where E_j is the Young modulus, $\tau_j = \frac{\mu_j}{E_j}$ and μ_j is the polymeric viscosity.

The initial boundary value problem (IBVP) defined by Equations (1.1)–(1.6), is based on the 3D model originally proposed in [10]. The framework is simplified here to one dimension to enable a more detailed and rigorous mathematical analysis than was feasible for the full problem. Furthermore, while the work in [10] focused on a spherical domain, this set of differential equations can be made more general and applied to any domain whose boundary is divided into two parts: one with a constant fluid concentration and one that is isolated. The original problem was studied from a numerical point of view in [4, 5] for smooth (C^4) and nonsmooth (H^3) solutions with respect to space. 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 both scenarios of smoothness. Moreover, in [4], 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 known stability relation for uniform grids $\Delta t \leq C_s h^2$. In [11] 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 Equation (1.4) leads to several challenges in the computation of the numerical approximation for the solution of the initial boundary value problem (IBVP) defined by Equations (1.1)–(1.6), 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 consider the special case of the generalized Maxwell-Wiechert model with one fluid arm. In this context, we modify the definition of stress, σ, given by Equation (1.4), to the following differential form:

$$\frac{\partial \sigma}{\partial t} + \beta \sigma = -\alpha \epsilon - \gamma \frac{\partial \epsilon}{\partial t}, \tag{1.7}$$

where $\beta = \frac{E_1}{\mu}, \alpha = \frac{E_0 E_1}{\mu}$, $\gamma = E_0 + E_1$ and μ represents the viscosity of the polymer and E_0 and E_1 are the Young's modulus (see [7]). The minus sign in Equations (1.4) and (1.7) 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 [10].

It is worth noting that Equation (1.7) can be derived directly from the Boltzmann integral representation for σ and the aforementioned linear relationship between ϵ and c_ℓ through a straightforward calculation. Conversely, integrating Equation (1.7) to obtain an explicit solution for σ and taking its gradient yields an expression analogous to Equation (1.4). 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 Equations (1.1)–(1.3) and (1.7) and

$$\nabla \sigma(0,t) = 0,\ \sigma(R,t) = \sigma_{ext}, t \in (0,T],\ \sigma(x,0) = \sigma_0(x),\ x \in (0,R). \tag{1.8}$$

We point out that in the nonlinear system of Equations (1.1)–(1.3) and (1.7), the concentration c_ℓ is defined by Equations (1.1) and (1.7) and it is included in (1.2) and (1.3). 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. To prove the stability of the numerical solution we will follow the approach considered, for instance, in [18, 19, 21, 22]. This technique imposes the uniform boundness of the numerical approximations using a discrete version of the $W^{1,\infty}(0,R)$. Regarding the unconditionally second convergence order of numerical methods for quasilinear parabolic equations, we refer the papers [17, 25] 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, we establish unconditionally second convergence order with respect to a discrete H^1-norm and no uniform bounds for the corresponding numerical approximations are required. The coupled and nonlinear nature of the system of Equations (1.1)–(1.3) and (1.7) increases its complexity. 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. Finally, 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 *a priori* error analysis conducted in this paper is not based on the usual approach introduced in [26] that was largely followed in the literature. For instance, recently, the results of [26] have been considered in [16, 27, 28, 29]. Instead, our approach is based on the error analysis for the error equations. Our results can be seen in two different perspectives. 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. As an example we mention [23] where a mixed finite element method in space is combined with a second order backward formula for a quasilinear parabolic equation is studied. However, within finite difference methods, our convergence estimates allow to conclude that the order of the global error is greater than that of the truncation error. In fact, the latter is of first order only in space with respect to norm $\|\cdot\|_\infty$, while the former is of second order in space and time. This unexpected convergence behavior is known as supraconvergence phenomenon and it was widely studied in the 80's in [8, 14, 15, 20]. More recently, we also mention the following contributions [1, 9, 24].

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. In Section 4, we illustrate the convergence properties of the method w.r.t. both h_{max} and Δt. 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 $h_i > 0, i = 1, \ldots, N$, $\sum_{i=1}^{N} h_i = R$, $h_{max} = \max_{i=1,\ldots,N} h_i \to 0$ and $h_{min} = \min_{i=1,\ldots,N} h_i \to 0$. We recall that a sequence of grids is said to be quasiuniform if there exists a constant $C > 0$, independent of h, such that $\frac{h_{max}}{h_{min}} \leq C$. 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 corresponding 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 behavior 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, defined as $\|v_h\|_{h,\infty} = \max_{i=0,\ldots,N} |v_h(x_i)|,\ v_h \in V_h$. 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 operators D_{-x} and $D_x^\star$ defined by

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

respectively. By M_h we denote the average operator

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

for $v_h \in V_h^*$. We also 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 $v_h \in V_{h,0}$,*

$$\left\|v_h\right\|_h \leq R \left\|D_{-x}v_h\right\|_+.$$

Proposition 2 [Discrete inverse inequality]. *For all $v_h \in V_{h,0}$, it holds*

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

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

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

□

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

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

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,*

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

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

Remark 1. If A is constant then 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 $v_h(t) : \overline{\Omega}_h^\star \longrightarrow \mathbb{R}$, $v_h(t)(x_i) = v_h(x_i,t), i = -1,\dots,N$. 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 $v^{(i)} : [0,T] \longrightarrow H^r(0,R)$, $i = 0,\dots,m$ are continuous, imbued with the norm $\|v\|_{C^m(H^r)} = \max_{t\in[0,T]} \left\|v(t)\right\|_{H^r(0,R)}$. In a similar fashion we 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 $\{t_m = m\Delta t,\ m = 0,\dots,M\}$. We introduce now a full discretization scheme for problem defined by Equations (1.1)–(1.3) and (1.7)–(1.8) based on an implicit midpoint integration approach in time

$$\begin{aligned} D_{-t}c_{\ell,h}^{m+1} &= D_x^\star\left(a_\ell\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{\ell,h}^{m+1/2}\right)\\ &\quad + D_x^\star\left(a_\sigma\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}\sigma_h^{m+1/2}\right), \end{aligned} \tag{3.1}$$

$$D_{-t}\sigma_h^{m+1} + \beta\sigma_h^{m+1/2} = -\alpha c_{\ell,h}^{m+1/2} - \gamma D_{-t}c_{\ell,h}^{m+1}, \tag{3.2}$$

$$D_{-t}c_{d,h}^{m+1} = D_x^\star\left(a_d\left(M_h c_{\ell,h}^{m+1/2}\right)D_{-x}c_{d,h}^{m+1/2}\right) + f_h^{m+1/2}, \tag{3.3}$$

$$D_{-t}c_{s,h}^{m+1} = -f_h^{m+1/2}, \tag{3.4}$$

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

$$c_{\ell,h}^0(x_i) = c_{\ell,0}(x_i),\ c_{d,h}^0(x_i) = 0,\ c_{s,h}^0(x_i) = c_{s,0}(x_i),\ \sigma_h^0(x_i) = \sigma_0(x_i), \tag{3.5}$$

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

$$D_{a_\mu,c}c_{\mu,h}^{j+1/2}(x_0) = 0,\ \ j = 0,\dots,M-1,\ \mu = \ell,d,\sigma, \tag{3.6}$$

$$c_{\ell,h}^j(x_N) = c_{ext},\ \ \sigma_h^j(x_N) = \sigma_{ext},\ \ c_{d,h}^j(x_N) = 0,\ \ j = 0,\dots,M. \tag{3.7}$$

In (3.1), D_{-t} denotes the backward finite difference operator in time,

$$c_{p,h}^{m+1/2} = \frac{c_{p,h}^m + c_{p,h}^{m+1}}{2},\ p=\ell,d,s,\ f_h^m = f(c_{s,h}^m, c_{d,h}^m, c_{\ell,h}^m),\ f_h^{m+1/2} = \frac{f_h^m + f_h^{m+1}}{2}.$$

Following [5], 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 constants $a_{0,\mu}, M_\mu > 0$ 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 constant $C_f > 0$ such that, for all $x, y, z, \tilde{x}, \tilde{y}, \tilde{z} \in \mathbb{R}$,

$$|(f(x,y,z) - f(\tilde{x},\tilde{y},\tilde{z})| \leq C_f \Big(|\tilde{z}||y-\tilde{y}| + \big(1+|y|\big)\big(|z-\tilde{z}| + |z||x-\tilde{x}|\big) \Big).$$

Remark 2. 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. The numerical scheme defined by Equations (3.1) and (3.4)–(3.7) 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, with a suitable midpoint time discretization scheme. Although this numerical method is defined as a finite difference scheme, this duality of point of view allows us to circumvent the typical Taylor expansion analysis to analyze the consistency and error associated with the method and use tools such as the Bramble-Hilbert lemma. In the process, we are able to prove second order convergence results using less regularity of the solutions.

3.1 Stability analysis

Let $c_{i,h}^m$, $i = d, \ell, s$, and σ_h^m, $m = 1\ldots, M$, denote fixed solutions of the discrete problem defined by Equations (3.1)–(3.7) with initial conditions $c_{i,h}^0, i = d, \ell, s$, and σ_h^0 and let $\omega_{i,h}^m = c_{i,h}^m - \tilde{c}_{i,h}^m$, $i = d, \ell, s$, $\omega_{\sigma,h}^m = \sigma_h^m - \tilde{\sigma}_h^m$, where $\tilde{c}_{i,h}^m$, $i = d, \ell, s$, $\tilde{\sigma}_h^m$ is another set of solutions of the same discrete problem with initial conditions $\tilde{c}_{i,h}^0$, $i = d, \ell, s$, and $\tilde{\sigma}_h^0$. To simplify the exposure, we introduce now two notations for $\mu = \ell, \sigma, d, s$. If $u_h, v_h, w_h \in V_h^\star$, we define $b_\mu(u_h, v_h; w_h) = \big(a_\mu(M_h w_h) D_{-x} u_h, D_{-x} v_h\big)_+$. However, if these grid functions depend on time, say, $u_h^m, v_h^m, w_h^m \in V_h^\star$, then we define $b_\mu^m(u_h, v_h; w_h) = b_\mu(u_h^m, v_h^m; w_h^m)$.

We start by stating a result that will be used to bound specific terms in the upcoming analysis.

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

$$\begin{aligned} |b_\mu(v_h, w_h; u_h) - b_\mu(\tilde{v}_h, w_h; \tilde{u}_h)| \leq {} & M_\mu \big\| D_{-x}(v_h - \tilde{v}_h) \big\|_+ \big\| D_{-x} w_h \big\|_+ \\ & + M_\mu \big\| D_{-x} v_h \big\|_{+,\infty} \big\| u_h - \tilde{u}_h \big\|_h \big\| D_{-x} w_h \big\|_+. \end{aligned}$$

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

$$\begin{aligned} b_\mu(\tilde{v}_h, w_h; \tilde{u}_h) - b_\mu(v_h, w_h; u_h) \leq {} & M_\mu \big\| D_{-x} v_h \big\|_{+,\infty} \big\| u_h - \tilde{u}_h \big\|_h \big\| D_{-x} w_h \big\|_+ \\ & - a_{0,\mu} \big\| D_{-x} w_h \big\|_+^2. \end{aligned}$$

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

$$\begin{aligned} \Big(D_{-t}\omega_{\ell,h}^{m+1}, \omega_{\ell,h}^{m+1/2} \Big)_h = {} & b_\ell^{m+1/2}(\tilde{c}_{\ell,h}, \omega_{\ell,h}; \tilde{c}_{\ell,h}) - b_\ell^{m+1/2}(c_{\ell,h}, \omega_{\ell,h}; c_{\ell,h}) \\ & + b_\sigma^{m+1/2}(\tilde{\sigma}_{\ell,h}, \omega_{\ell,h}; \tilde{c}_{\ell,h}) - b_\sigma^{m+1/2}(\sigma_{\ell,h}, \omega_{\ell,h}; c_{\ell,h}), \end{aligned}$$

$$\left(D_{-t}\omega_{d,h}^{m+1},\omega_{d,h}^{m+1/2}\right)_h = b_d^{m+1/2}(\tilde{c}_{d,h},\omega_{d,h};\tilde{c}_{\ell,h}) - b_d^{m+1/2}(c_{d,h},\omega_{d,h};c_{\ell,h}) + \left(f_h^{m+1/2} - \tilde{f}_h^{m+1/2},\omega_{d,h}^{m+1/2}\right)_h,$$

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

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

$$\begin{aligned}\frac{1}{2}D_{-t}\left\|\omega_{\ell,h}^{m+1}\right\|_h^2 \leq{}& M_\ell\left\|D_{-x}c_{\ell,h}^{m+1/2}\right\|_{+,\infty}\left\|\omega_{\ell,h}^{m+1/2}\right\|_h\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+ \\ &- a_{0,\ell}\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+^2 + M_\sigma\left\|D_{-x}\omega_{\sigma,h}^{m+1/2}\right\|_+\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+ \\ &+ M_\sigma\left\|D_{-x}\sigma_h^{m+1/2}\right\|_{+,\infty}\left\|\omega_{\ell,h}^{m+1/2}\right\|_h\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+. \end{aligned} \quad (3.8)$$

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

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

Proof. Taking each member of Equation (3.2) 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 considering 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

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

and from the latter we get

$$\begin{aligned}\gamma\left(D_{-x}D_{-t}\omega_{\sigma,h}^{m+1},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+ + \beta\gamma\left(D_{-x}\omega_{\sigma,h}^{m+1/2},D_{-x}\omega_{\ell,h}^{m+1/2}\right)_+ \\ = -\alpha\gamma\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+^2 - \frac{\gamma^2}{2}D_{-t}\left\|D_{-x}\omega_{\ell,h}^{m+1/2}\right\|_+^2.\end{aligned} \quad (3.9)$$

We conclude the proof using the identity

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

in (3.9) 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 are now able to establish an bounds for the perturbations on $c_{\ell,h}$ and σ_h.

Proposition 7. *Let $c^m_{\ell,h}$ and σ^m_h, $m = 0, \dots, M$, denote fixed solutions of the discrete problem defined by Equations (3.1), (3.2) and (3.5)–(3.7) and let $\omega^m_{\ell,h} = c^m_{\ell,h} - \tilde{c}^m_{\ell,h}$, $\omega^m_{\sigma,h} = \sigma^m_h - \tilde{\sigma}^m_h$, where $\tilde{c}^m_{\ell,h}$, $\tilde{\sigma}^m_h$ is another solution of the same discrete problem with initial conditions $\tilde{c}^0_{\ell,h}$, and $\tilde{\sigma}^0_h$. If the assumption $\mathbf{H_{diff}}$ holds, the coefficients satisfy*

$$M_\sigma + \alpha + \beta\gamma < 2\min\left(\beta, \alpha\gamma + a_{0,\ell}\right) \tag{3.10}$$

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

$$\max_m \left(\|D_{-x} c^{m+1/2}_{\ell,h}\|^2_{+,\infty}, \|D_{-x} \sigma^{m+1/2}_h\|^2_{+,\infty} \right) \leq C, \tag{3.11}$$

for some $C > 0$, independent of h and Δt, then, for all $\Delta t < \min\left\{\Delta t_0, \frac{1}{2C}\right\}$, the following inequality holds

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

for $m = 1, 2, \dots, M-1$, where $C_\ell > 0$ is a constant independent of h and Δt.

Proof. Let $\Delta t < \min\left\{\Delta t_0, \frac{1}{2C}\right\}$. Combining Equation (3.8) with Proposition 6, it follows that for all $\epsilon \neq 0$,

$$\begin{aligned} & D_{-t}\left[\|\omega^{m+1}_{\ell,h}\|^2_h + \|D_{-x}\omega^{m+1}_{\sigma,h} + \gamma D_{-x}\omega^{m+1}_{\ell,h}\|^2_+ \right] \\ & \quad + A_0 \|D_{-x}\omega^{m+1/2}_{\sigma,h}\|^2_+ + B_0(\epsilon)\|D_{-x}\omega^{m+1/2}_{\ell,h}\|^2_+ \\ & \leq \left(\frac{M^2_\ell}{\epsilon^2} \|D_{-x} c^{m+1/2}_{\ell,h}\|^2_{+,\infty} + \frac{M^2_\sigma}{\epsilon^2} \|D_{-x}\sigma^{m+1/2}_h\|^2_{+,\infty} \right) \|\omega^{m+1/2}_{\ell,h}\|^2_h, \end{aligned} \tag{3.12}$$

where $A_0 = 2\beta - M_\sigma - \alpha - \beta\gamma$ and $B_0(\epsilon) = 2\left(\alpha\gamma + a_{0,\ell} - \epsilon^2 - \frac{M_\sigma}{2} - \frac{\alpha+\beta\gamma}{2}\right)$. From (3.10), it follows that $A_0 > 0$ and we can fix ϵ such that $B_0(\epsilon) > 0$. Let

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

With this notation, (3.12) leads to

$$\begin{aligned} & (1 - \theta_\ell(c_{\ell,h}, \sigma_h)\Delta t) \left(\|\omega^{m+1}_{\ell,h}\|^2_h + \|D_{-x}\omega^{m+1}_{\sigma,h} + \gamma D_{-x}\omega^{m+1}_{\ell,h}\|^2_+ \right) \\ & \quad + \Delta t \left(A_0 \|D_{-x}\omega^{m+1/2}_{\sigma,h}\|^2_+ + B_0(\epsilon)\|D_{-x}\omega^{m+1/2}_{\ell,h}\|^2_+ \right) \\ & \leq (1 + \theta_\ell(c_{\ell,h}, \sigma_h)\Delta t) \left(\|\omega^m_{\ell,h}\|^2_h + \|D_{-x}\omega^m_{\sigma,h} + \gamma D_{-x}\omega^m_{\ell,h}\|^2_+ \right). \end{aligned} \tag{3.13}$$

From the uniform bound defined by Equation (3.11) and the inequality from (3.13), applying Lemma 1 from [13] allows to obtain

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

for some constant $C_\ell > 0$. □

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 Equations* (3.1)–(3.7) *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*

$$\max_{i=0,\ldots,M}\left\{\left\|c_{d,h}^i\right\|_{h,\infty},\left\|D_{-x}c_{d,h}^i\right\|_{h,\infty},\left\|c_{\ell,h}^i\right\|_{h,\infty},\left\|\tilde{c}_{\ell,h}^i\right\|_{h,\infty}\right\}\leq C, \qquad (3.14)$$

for some $C > 0$, independent of h and Δt, then, for all $\Delta t < \min\left\{\Delta t_0, \frac{1}{8C}\right\}$, the following inequality holds

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

for $m = 1, 2, \ldots, M-1$, where $C_{d,s} > 0$ is a constant independent of h and Δt.

Proof. We start by noting that using Equations (3.3) and (3.4) and taking into account summation by parts and the boundary conditions for $\omega_{d,h}^{m+1}$ we have

$$\Big(D_{-t}\omega_{d,h}^{m+1},\omega_{d,h}^{m+1/2}\Big)_h+\Big(D_{-t}\omega_{s,h}^{m+1},\omega_{s,h}^{m+1/2}\Big)_h=b_d^{m+1/2}(c_{d,h},\omega_{d,h};\tilde{c}_{\ell,h})$$
$$+\Big(f_h^{m+1/2}-\tilde{f}_h^{m+1/2},\omega_{d,h}^{m+1/2}-\omega_{s,h}^{m+1/2}\Big)_h-b_d^{m+1/2}(c_{d,h},\omega_{d,h};c_{\ell,h})$$
$$-\Big(a_d(M_h\tilde{c}_{\ell,h}^{m+1/2})D_{-x}\omega_{d,h}^{m+1/2},D_{-x}\omega_{d,h}^{m+1}\Big)_+. \qquad (3.15)$$

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

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

where $C_d > 0$ is a suitable constant. Through a straightforward application of assumption $\mathbf{H_f}$, it can be shown that the following holds

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

where $\tilde{C}_f > 0$ is a convenient constant and $E_{s,d}^m = \|\omega_{d,h}^m\|_h^2 + \|\omega_{s,h}^m\|_h^2$. Considering the last estimates in Equations (3.15) and (3.14), we obtain

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

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 [13] implies

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

with $C_{bound} = \exp\big(2T\alpha \max\{\frac{1}{D_0(\epsilon)}, \frac{1}{1-\alpha\Delta t}\}\big)$. □

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

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

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

Theorem 1. *Let* $c_{i,h}^m$, $i = d, s, \ell$ *and* σ_h^m, $m = 0, \dots, M$, *denote fixed solutions of the discrete problem defined by Equations* (3.1)–(3.7) *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 $\mathbf{H_{diff}}$, $\mathbf{H_f}$ and Equation (3.10) hold and there exist constants $C_{stab}, \Delta t_0 > 0$ such that, for all $\Delta t \in (0, \Delta t_0)$, the corresponding solution satisfies

$$\max_{m=0,\dots,M} \Big\{ \big\| D_{-x} c_{\ell,h}^m \big\|_{+,\infty}, \big\| D_{-x} \sigma_h^m \big\|_{+,\infty}, \\ \big\| D_{-x} c_{d,h}^m \big\|_{+,\infty}, \big\| c_{d,h}^m \big\|_{h,\infty}, \big\| c_{\ell,h}^m \big\|_{h,\infty}, \big\| \tilde{c}_{\ell,h}^m \big\|_{h,\infty} \Big\} \leq C_{stab},$$

independently of h, then there exists a constant $C > 0$, independent of h and Δt, such that, for Δt sufficiently small, the following inequality holds

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

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

Remark 4. We conclude this section remarking that the stability of Equations (3.1)–(3.7) 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 constant $C_{stab} > 0$, h and Δt independent, such that, for Δt small enough,

$$\begin{aligned} &\big\| D_{-x} c_{\ell,h}^{j+1/2} \big\|_{+,\infty}^2 \leq C_{stab}, \ \ \big\| D_{-x} \sigma_h^{j+1/2} \big\|_{+,\infty}^2 \leq C_{stab}, \\ &\big\| D_{-x} c_{d,h}^{j+1/2} \big\|_{+,\infty} \leq C_{stab}, \ \ j = 0, \dots, M-1, \ h \in \Lambda, \\ &\big\| c_{d,h}^j \big\|_{h,\infty} \leq C_{stab}, \ \big\| c_{\ell,h}^j \big\|_{h,\infty} \leq C_{stab}, \big\| \tilde{c}_{\ell,h}^j \big\|_{h,\infty} \leq C_{stab}, \ \ j = 0, \dots, N, h \in \Lambda. \end{aligned}$$

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 Equations (3.1)–(3.7). 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 Equations (1.1)–(1.3) and (1.7)) with $\epsilon = \lambda c_\ell$, Equations (1.5), (1.6) and (1.8), 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, [2, 12].

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

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

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 $V = H^3(0, T; H^2(0, R)) \cap C^0(0, T; H^3(0, R))$, and the error

$E^j_{\ell,\sigma} := \|E^j_{\ell,h}\|^2_h + \|D_{-x}\left(E^j_{\sigma,h} + \gamma E^j_{\ell,h}\right)\|^2_+$, $j = 0, \ldots, M$. 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 a solution of the problem defined by Equations* (1.1) *and* (1.5)–(1.8) *and* $c_{\ell,h}, \sigma_h \in V_h$ *denote the solution of the problem defined by Equations* (3.1),(3.2) *and* (3.5)–(3.7)*. If the assumptions* $\mathbf{H_{diff}}$ *and* (3.10) *hold then there exists a constant* $C_\ell > 0$ *such that for* Δt *small enough,*

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

for $m = 1, 2, \ldots, M-1$*, where*

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

Proof. This proof follows the reasoning behind the one of Proposition 7. We start by establishing estimates for $D_{-t}\|E_{\ell,h}\|^2_h$ and $\|D_{-x}E^{m+1/2}_{\ell,h}\|^2_+$. A straightforward, although tedious, calculation allows to show the following equalities

$$\begin{aligned}\Big(D_{-t}E^{m+1}_{\ell,h}, E^{m+1/2}_{\ell,h}\Big)_h &= \Big(\big(c'_\ell(t_{m+1/2})\big)_h, E^{m+1/2}_{\ell,h}\Big)_h - \Big(D_{-t}c^{m+1}_{\ell,h}, E^{m+1/2}_{\ell,h}\Big)_h \\ &+ \sum_{p=c_\ell,\sigma}\Big(b^{m+1/2}_p(p_h, E_{\ell,h}; c_{\ell,h}) - b^{m+1/2}_p(R_h p, E_{\ell,h}; R_h c_\ell)\Big) \\ &+ \Big(T^{m+1}_1, E^{m+1/2}_{\ell,h}\Big)_h + \sum_{p=c_\ell,\sigma}\Big(T^{m+1/2}_{1,p}, D_{-x}E^{m+1/2}_{\ell,h}\Big)_+,\end{aligned} \tag{3.16}$$

where

$$T^{m+1}_1 = R_h c'_\ell(t_{m+1/2}) - \big(c'_\ell(t_{m+1/2})\big)_h + D_{-t}R_h c_\ell(t_{m+1}) - R_h c'_\ell(t_{m+1/2}),$$

$$\begin{aligned}T^{m+1/2}_{1,p} = -\Bigg(&\Big(a_p\big(\widehat{c}_\ell(t_{m+1/2})\big) - a_p\big(M_h R_h c^{m+1/2}_\ell\big)\Big)\widehat{\frac{\partial p}{\partial x}}(t_{m+1/2}) \\ &- \Big(a_p\big(M_h R_h c^{m+1/2}_\ell\big)\Big)\Big(\widehat{\frac{\partial p}{\partial x}}(t_{m+1/2}) - D_{-x}R_h p^{m+1/2}\Big)\Bigg),\end{aligned}$$

for $p = c_\ell, \sigma$. Following the proof of Equation (3.8), it can be shown that, from (3.16), for all $\epsilon \neq 0$, we have

$$D_{-t}\|E_{\ell,h}^{m+1}\|_h^2 + (2a_{0,\ell} - 2\epsilon^2 - M_\sigma)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2 \leq \frac{1}{\epsilon^2}\sum_{p=c_\ell,\sigma}$$
$$\times\left(M_p^2\|D_{-x}R_h p^{m+1/2}\|_{+,\infty}^2\right)\|E_{\ell,h}^{m+1/2}\|_h^2 + M_\sigma\|D_{-x}E_{\sigma,h}^{m+1/2}\|_+^2$$
$$+\left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h + \sum_{p=\ell,\sigma}\left(T_{1,p}^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+, \tag{3.17}$$

where $\epsilon \neq 0$. Using the Bramble-Hilbert Lemma (see [6]) and the proof of Theorem 1 of [3], it can be shown that there exist constants $C_1, C_2 > 0$, independent of h and Δt, such that the following inequalities hold

$$\left(T_1^{m+1}, E_{\ell,h}^{m+1/2}\right)_h \leq C_1\left(h_{max}^2\left\|c_\ell'(t_{m+1/2})\right\|_{H^2(0,R)}\|D_{-x}E_{\ell,h}^{m+1/2}\|_+\right.$$
$$\left.+\Delta t^{3/2}\|c_\ell'''\|_{L_m^2(H^1)}\|E_{\ell,h}^{m+1/2}\|_h\right),$$
$$\left(T_{1,p}^{m+1/2}, D_{-x}E_{\ell,h}^{m+1/2}\right)_+ \leq C_3(p, c_\ell)\left(h_{max}^2 + \Delta t^{3/2}\right)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+,$$

for $p = c_\ell, \sigma$, with $L_m^2(H^1) = L^2(t_m, t_{m+1}; H^1(0,R))$ and

$$C_3(p, c_\ell) = C_2\left(\left\|\frac{\partial p}{\partial x}(t_{m+1/2})\right\|_{L^\infty(0,R)}\left\|c_\ell(t_{m+1/2})\right\|_{H^2(0,R)}\right.$$
$$+\left\|p(t_{m+1/2})\right\|_{H^3(0,R)} + \|p(t_m)\|_{H^2(0,R)} + \|p(t_{m+1})\|_{H^2(0,R)}$$
$$\left.+\left\|\frac{\partial p}{\partial x}(t_{m+1/2})\right\|_{L^\infty(0,R)}\|c_\ell''\|_{L_m^2(H^1)} + \left\|\left(\frac{\partial p}{\partial x}\right)''\right\|_{L_m^2(H^1)}\right).$$

Inserting the previous inequalities into (3.17) we obtain

$$D_{-t}\|E_{\ell,h}^{m+1}\|_h^2 + (2a_{0,\ell} - 3\epsilon^2 - M_\sigma)\|D_{-x}E_{\ell,h}^{m+1/2}\|_+^2$$
$$\leq \frac{1}{\epsilon^2}\sum_{p=c_\ell,\sigma}\left(M_p^2\|D_{-x}R_h p^{m+1/2}\|_{h,\infty}^2 + \frac{1}{2}\right)\|E_{\ell,h}^{m+1/2}\|_h^2$$
$$+ M_\sigma\|D_{-x}E_{\sigma,h}^{m+1/2}\|_+^2 + T_{\ell,\sigma}^{m+1/2}, \tag{3.18}$$

where, for $i = 1, \ldots, N-1$, $|T_{\ell,\sigma}^{m+1/2}(x_i)| \leq \tilde{C}_1 h_{max}^4 + \tilde{C}_2\Delta t^3$, with

$$\tilde{C}_1 = C\left(\epsilon^2\left\|c_\ell'(t_{m+1/2})\right\|_{H^2(0,R)}^2 + \sum_{p=c_\ell,\sigma}\left(\|p\|_{C^0(H^2)}\left\|c_\ell(t_{m+1/2})\right\|_{H^2(0,R)}\right.\right.$$
$$\left.\left.+\left\|p(t_{m+1/2})\right\|_{H^3(0,R)} + \|p(t_m)\|_{H^2(0,R)} + \|p(t_{m+1})\|_{H^2(0,R)}\right)^2\right),$$
$$\tilde{C}_2 = C\left(\|c_\ell'''\|_{L_m^2(H^1)}^2 + \sum_{p=c_\ell,\sigma}\left(\|p\|_{C^0(H^2)}\|c_\ell''\|_{L_m^2(H^1)} + \left\|\left(\frac{\partial p}{\partial x}\right)''\right\|_{L_m^2(H^1)}\right)^2\right),$$

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

We now focus on obtaining estimates for $\left\|D_{-x}\left(E_{\sigma,h}^{m+1} + \gamma E_{\ell,h}^{m+1}\right)\right\|_{+}^{2}$, $\left\|D_{-x}E_{\ell,h}^{m+1/2}\right\|_{+}^{2}$ and $\left\|D_{-x}E_{\sigma,h}^{m+1}\right\|_{+}^{2}$. Taking the error equation associated with Equation (3.2), a simple calculation reveals that, for $E_{\sigma,h}^{j}$ and $E_{\ell,h}^{j}$, it holds

$$D_{-t}E_{\sigma,h}^{m+1} + \beta E_{\sigma,h}^{m+1/2} = -\alpha E_{\ell,h}^{m+1/2} - \gamma D_{-x}E_{\ell,h}^{m+1} + T_{\sigma,\ell}^{m+1}, \tag{3.19}$$

where

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

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

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

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

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

where $C > 0$ denotes a suitable constant. This implies the bound

$$\begin{aligned} & \left(D_{-x}T_{\ell,\sigma}^{m+1}, \gamma D_{-x}E_{\sigma,h}^{m+1/2} + D_{-x}E_{\ell,h}^{m+1/2}\right)_{+} \\ & \leq \epsilon_2^2\left\|D_{-x}E_{\ell,h}^{m+1/2}\right\|_{+}^{2} + \epsilon_3^2\left\|D_{-x}E_{\sigma,h}^{m+1/2}\right\|_{+}^{2} + \tilde{T}_{\ell,\sigma}^{m+1}, \end{aligned} \tag{3.20}$$

with

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

and $\epsilon_i \neq 0, i = 2, 3$. Combining Equations (3.18)–(3.20) we get

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

where $B_0(\epsilon) = 2(\alpha\gamma + a_{0,\ell}) - (M_\sigma + \alpha + \beta\gamma) - 4\epsilon^2$, $A_0(\epsilon_3) = 2\beta - (M_\sigma + \alpha + \beta\gamma) - 2\epsilon_3^2$ and $2\epsilon_2^2 = \epsilon^2$.

Considering the assumption (3.10) 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 and

$$\begin{aligned}&(1-\Delta t\theta_\ell(c_\ell,\sigma))E^{m+1}_{\ell,\sigma}\\&+\Delta t\min\{A_0(\epsilon_3),B_0(\epsilon)\}\left(\left\|D_{-x}E^{m+1/2}_{\sigma,h}\right\|_+^2+\left\|D_{-x}E^{m+1/2}_{\ell,h}\right\|_+^2\right)\\ \leq&\Big(1+\Delta t\theta_\ell(c_\ell,\sigma)\Big)E^m_{\ell,\sigma}+\Delta t\left(2\tilde{T}^{m+1}_{\ell,\sigma}+T^{m+1}_{\ell,h}\right),\end{aligned} \tag{3.21}$$

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 that $\Delta t\max_{p=\ell,\sigma}\{M_p\cdot\max_{p=\ell,\sigma}\|p\|_{C^0(H^2)}\}<2\epsilon^2$ and applying a discrete Gronwall Lemma to Equation (3.21), 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 $X = X_1 \cap X_2$, where $X_1 = C^0(0,T;H^3(0,R)\cap H^1_{0,R}(0,R))\cap H^2(0,T;H^2(0,R)$ and $X_2 = H^1_{0,R}(0,R))\cap H^3(0,T;H^1_{0,R}(0,R))$.

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 a solution of the problem defined by Equations* (1.1) *and* (1.5)–(1.8) *and $c_{d,h}\in V_{h,0}$ and $c_{s,h}\in V_h$ denote the solution of the problem defined by Equations* (3.1)–(3.7)*. If $f(c_s,c_d,c_\ell)\in C^0(H^2)$ and the assumptions $\mathbf{H_{diff}}$, $\mathbf{H_f}$ and Equation* (3.10) *hold then, there exists a constant $C_{d,s}>0$, such that for Δt small enough,*

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

where $T_{err,d,s}\leq C_1h^4_{max}+C_2\Delta t^4$,

$$\begin{aligned}C_1=&\sum_{p=c_\ell,\sigma}\left(\|p\|_{C^0(H^2)}\|c_\ell\|_{C^0(H^2)}+\|p\|_{C^0(H^3)}+\|p\|_{C^1(H^2)}\right)^2\\&+\left\|f(c_s,c_d,c_\ell)\right\|^2_{C^0(H^2)}\left(\|c_d\|_{C^1(H^2)}+\|c_d\|_{C^0(H^3)}\left(\|c_\ell\|_{C^0(H^2)}+1\right)\right)^2,\\C_2=&\sum_{p=c_\ell,\sigma}\left(\|p\|_{C^0(H^2)}\|c_\ell\|_{H^2(H^1)}+\|p\|_{H^2(H^2)}\right)^2+\|p\|_{H^3(H^2)}\\&+\|c_d\|^2_{C^0(H^2)}\|c_\ell\|^2_{H^2(H^1)}+\|c_d\|^2_{H^2(H^2)}+\|c_d\|^2_{H^3(H^1)}+\|c_s\|^2_{H^3(H^1)}.\end{aligned}$$

Proof. We follow the steps of the proof of Proposition 9. We start by noticing that from Equations (3.3) and (3.4) we easily establish, for all $\epsilon\neq 0$, that

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

where

$$
\begin{aligned}
T_1 &= \left((R_h f^{m+1/2})_h - R_h f^{m+1/2}, E_{d,h}^{m+1/2}\right)_h,\\
T_2 &= \left(R_h f^{m+1/2} - f_h^{m+1/2}, E_{d,h}^{m+1/2} + E_{s,h}^{m+1/2}\right)_h,\\
T_{d,s} &\le D_1 \Delta t^{3/2} \|D_{-x} E_{d,h}^{m+1/2}\|_+ + D_2 h_{max}^2 \|D_{-x} E_{d,h}^{m+1/2}\|_+ \\
&\quad + D_3 \Delta t^{3/2} \|E_{d,h}^{m+1/2}\|_h + D_4 \Delta t^{3/2} \|E_{s,h}^{m+1/2}\|_h,
\end{aligned}
$$

with $D_1 = C_1\left(\|c_d\|_{C^0(H^2)}\|c_\ell\|_{H^2_m(H^1)} + \|c_d\|_{H^2_m(H^2)}\right)$, $D_2 = C_1(\|c_d\|_{C^1(H^2)} + \|c_d\|_{C^0(H^3)}(\|c_\ell\|_{C^0(H^2)} + 1))$, $D_3 = C_1\|c_d\|_{H^3_m(H^1)}$, $D_4 = C_1\|c_s\|_{H^3_m(H^1)}$, and $H^i_m(H^r) = H^i(t_m, t_{m+1}; H^r(0,R))$, for some constant $C_1 > 0$, 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, $|T_1| \le C_2 h_{max}^2 \|f(c_s, c_d, c_\ell)\|_{C^0(H^2)} \|D_{-x} E_{d,h}^{m+1/2}\|_+$, for some constant $C_2 > 0$, independent of h and Δt. Regarding T_2, using assumption $\mathbf{H_f}$, it holds, for all $\eta \neq 0$,

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

From Proposition 9, we know that $\|c_{\ell,h}^{m+1/2}\|_h$ is uniformly bounded, w.r.t, h and Δt, which means that there exists a constant $C_{conv,\ell} > 0$ such that $\|c_{\ell,h}^{m+1/2}\|_h^2 \le C_{conv,\ell}$.

Choosing $\epsilon^2 = \frac{a_d}{6}$ and $\eta^2 = 3\min\left\{\frac{C_f^2 R C_{conv,\ell}}{a_d}, \frac{C_f\|c_\ell\|_{C^0(H^1)}(1+\|c_d\|_{C^0(H^1)})}{2}\right\}$, it follows that

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

where

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

$$z^m = C_3 h_{max}^4\Bigg(\Big(\|c_d\|_{C^1(H^2)}+\|c_d\|_{C^0(H^3)}\big(\|c_\ell\|_{C^0(H^2)}+1\big)\Big)^2$$
$$+\|f(c_s,c_d,c_\ell)\|^2_{C^0(H^2)}\Bigg)+C_3\Delta t^3$$
$$\times\left(\|c_d\|^2_{C^0(H^2)}\|c_\ell\|^2_{H^2_m(H^1)}+\|c_d\|^2_{H^2_m(H^2)}+\|c_d\|^2_{H^3_m(H^1)}+\|c_s\|^2_{H^3_m(H^1)}\right),$$

for some constant $C_3 > 0$, 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

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

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 a solution of the problem defined by Equations* (1.1) *and* (1.5)–(1.8) *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 Eq.* (3.1)–(3.7)*. Under assumptions $f(c_s,c_d,c_\ell)\in C^0(H^2)$, $\mathbf{H_{diff}}$, $\mathbf{H_f}$ and* (3.10)*, there exists a constant $C > 0$, independent of h and Δt, such that for sufficiently small small Δt, the following inequality holds for $m = 1,\ldots,M$,*

$$\mathbb{E}_h^m \le C(h^4_{max}+\Delta t^4)\left(\sum_{p=\ell,d,s}\|E^0_{p,h}\|^2_h + \|D_{-x}E^0_{\ell,h}\|^2_+ + \|D_{-x}E^0_{\sigma,h}\|^2_+\right).$$

Remark 5. 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 presents second convergence order

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

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

As mentioned before, these upper bounds were established avoiding the approach of Wheeler [26]. 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 6. As mentioned in Section 3.1, the stability of the fluid discretization can be established showing that $\|D_{-x}c_{\ell,h}^{j+1/2}\|_{+,\infty}^2$ and $\|D_{-x}\sigma_h^{j+1/2}\|_{+,\infty}^2$, are uniformly 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

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

Using the estimate from Proposition 9, there exists a constant $C > 0$, independent of h and Δt, such that

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

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

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

we can conclude that for Δt small enough, the bound given by Equation (3.11) 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 $\|c_{p,h}^m\|_{h,\infty}$, with $p = d, s$ and $\|\tilde{c}_{\ell,h}^m\|_{h,\infty}$, under the same requirements for the grids and Δt.

Theorem 1 can now be reformulated as follows.

Theorem 3. *Under the assumptions of Theorem* 1*, 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*

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

for some constant $C > 0$.

4 Numerical simulation

This section aims to illustrate the main convergence result of this work, Theorem 2, for the fully-discrete approximation defined by Equations (3.1)–(3.7). 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 Equations (1.1) and (1.5)–(1.8) used in our numerical test solve a modified problem obtained by adding in each partial differential equation a source term

R_i, $i = \ell, d, s, \sigma$. We highlight that these solutions aim at reproducing the qualitative behavior of the system. 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-Wiechert 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 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 $c_d(x,t) = g(x,t)\,\psi(t)$, $(x,t) \in [0,R] \times [0,T]$ where

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

with $a_2(t) = a_0 - \left(\frac{t - \tilde{t}}{T}\right)^2 \cdot \mathbf{1}_{\{t \ge \tilde{t}\}}$ and $\psi(t) = 1 - \left(\frac{t - \tilde{t}}{\tilde{t}}\right)^2 \cdot \mathbf{1}_{\{t < \tilde{t}\}}$. 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

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

Finally the polymeric chains' stress is given by

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

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

The numerical method defined by Equations (3.1)–(3.7) 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 [4,5,10]), 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 $h_{max} = 9.8638 \cdot 10^{-4}$ as well as an estimated rate of convergence calculated as

$$\text{rate}_i = \frac{\log(E_{i+1}) - \log(E_i)}{\log(\Delta t_{i+1}) - \log(\Delta t_i)},$$

where E_i and E_{i+1} are two consecutive errors calculated based on the consecutive parameters Δt_i and Δt_{i+1}, respectively (a similar definition holds for h_{max}). Thus we can show computationally that the method reaches second order for $\mathbb{E}_h^m$ with respect to Δt.

Table 1. Estimated convergence rates. Fixed $h_{max} = 9.86 \cdot 10^{-4}$.

Δt	$\mathbb{E}_h^m$	Rate
$3.12 \cdot 10^{-1}$	13.95	-
$2.08 \cdot 10^{-1}$	8.15	1.32
$1.56 \cdot 10^{-1}$	4.55	2.02
$1.04 \cdot 10^{-1}$	1.74	2.37
$7.81 \cdot 10^{-2}$	$9.59 \cdot 10^{-1}$	2.07

Table 2. Estimated convergence rates. Fixed $\Delta t = 4.88 \cdot 10^{-4}$.

h_{max}	$\mathbb{E}_h^m$	Rate
$6.28 \cdot 10^{-2}$	$2.94 \cdot 10^{-1}$	-
$3.13 \cdot 10^{-2}$	$1.96 \cdot 10^{-1}$	0.58
$1.56 \cdot 10^{-2}$	$1.18 \cdot 10^{-1}$	0.73
$7.82 \cdot 10^{-3}$	$3.42 \cdot 10^{-2}$	1.78
$3.96 \cdot 10^{-3}$	$8.35 \cdot 10^{-3}$	2.07
$1.99 \cdot 10^{-3}$	$2.23 \cdot 10^{-3}$	1.91
$9.77 \cdot 10^{-4}$	$5.27 \cdot 10^{-4}$	2.02

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}.

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 $\Delta t \leq Ch_{max}$, for some constant C. Finally, we illustrate numerically the convergence rates obtained in the main result using an exact solution based on biological information.

Acknowledgements

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 Giuseppe Romanazzi and Geovan Campos was supported by FAPESP grant 2021/14713-5.

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