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EXISTENCE, UNIQUENESS AND REGULARITY FOR A DISSOLUTION-DIFFUSION MODEL

By

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Existence, uniqueness and regularity for a dissolution-diffusion model

María Emilia Castillo Pedro Morin

Abstract

We perform a mathematical analysis of a model for drug dissolution-diffusion in non erodible nor swellable devices. We deduce a model and obtain a coupled nonlinear system which contains a parabolic equation for the dissolved drug and an ordinary differential equation for the solid drug, which is assumed evenly distributed in the whole domain into microspheres which can differ in size. We analyze the existence, uniqueness, and regularity properties of the system. Existence is proved using Galerkin approximations. Uniqueness is obtained in the non-saturated case, and lack of uniqueness is shown when the initial concentration of dissolved drug is higher than the saturation density in a region. A square root function appears in the equation for the solid drug, and is responsible for the lack of uniqueness in the oversaturated case. The regularity results are sufficient for the optimal a priori error estimates of a finite element discretization of the system, which is presented in [CM].

1 Introduction

Numerous mathematical approaches have been proposed to give an adequate theoretical background to the modeling of drug release from polymeric devices [SS, SP]. The interest in this kind of systems has increased in the medical and pharmaceutical industry, because controlled drug-release (CDR) systems allow for predictable release kinetics, small fluctuations of plasma drug level, diminishing amount of toxic secondary effects, among other advantages [ECDD, BSBK].

We focus here on a model based on a diffusion equation including a continuum dissolution source described by the Noyes-Whitney equation; other models are based on a moving dissolution front separating a region of coexisting solid and dissolved drug from a region of completely dissolved drug; see [CLG] for a detailed description of other models.

Up to now, all mathematical studies have consisted in finding exact solutions for simple geometries using Fourier analysis, or simplified quasi-stationary assumptions, such as fast or slow dissolution rates (see [CG] and references therein). The goal of this article is to study the well-posedness of a dissolution-diffusion problem, modeling the kinetics of a drug inside a polymeric device, avoiding the assumption of fast or slow dissolution. We prove existence of solutions, and study uniqueness and regularity properties. An algorithm for the numerical approximation of the solutions to the problem can be found in [CM],

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where the regularity estimates obtained here are instrumental for obtaining optimal a priori error estimates.

The rest of the article is organized as follows. In Section 2 we deduce the mathematical model and prove existence of solutions in Section 3. Uniqueness of solutions is discussed in 4 where uniqueness is proved under the assumption that the initial concentration of dissolved drug is less than or equal to the maximum solubility, and the existence of multiple solutions is proved when the initial concentration of dissolved drug is above saturation. Finally, in Section 5 regularity estimates are obtained for both state variables, concentration of dissolved drug C and area of solid particles per unit volume a.

2 Mathematical Model and Weak formulation

We start this section by briefly deducing a model for drug dissolution-diffusion in a non-erodible polymeric device. We consider a model for one drug, which can be either in a solid or in a dissolved state. We assume that the solid drug is distributed in particles of equal density, evenly dispersed in the whole device, which can differ in mass and volume, but keep a spherical shape when dissolved [CLG]. We also assume that they are so small that do not affect the diffusion of the dissolved drug, which thus evolves by diffusion with constant coefficient.

Under these assumptions we can state the mathematical model on a domain $\Omega \subset \mathbb{R}^3$, occupied by the polymeric device. If C denotes the concentration of dissolved drug, following the same steps used to obtain the diffusion equation with Fick's law we arrive at the following equation:

$$\frac{\partial C}{\partial t} - D\Delta C = -\frac{\partial m}{\partial t}, \qquad x \in \Omega, \quad t > 0, \tag{2.1}$$

where D is the drug diffusion coefficient and m is the mass of solid drug per unit volume, so that $-\frac{\partial m}{\partial t}$ is the mass of solid drug being dissolved per unit volume per unit time.

Following [CLG], we use the Noyes-Whitney model for the dissolution of the microspheres, i.e., we assume that the microspheres dissolve at a rate proportional to the product of their surface area and the difference between the saturation solubility C_s and the concentration around them. If a denotes the area of the microspheres of solid drug per unit volume, this can be stated mathematically as

$$\frac{\partial m}{\partial t}(x,t) = -k_D a(x,t)(C_s - C(x,t)), \qquad x \in \Omega, \quad t > 0, \tag{2.2}$$

where k_D is the dissolution rate constant of the solid drug particles. Using relations between ratio, area and mass of a sphere and (2.2), we can rewrite (2.2) as

$$\frac{\partial a}{\partial t} = -\underbrace{\frac{4k_D\sqrt{\pi}N^{1/2}}{\rho_s}}_{\beta}\sqrt{a}(C_s - C), \qquad x \in \Omega, \quad t > 0, \tag{2.3}$$

where N represents the number of particles per unit volume and ρ_s is the intrinsic density of the solid drug particles.

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Statement of the problem. Adding initial conditions and boundary conditions of Neumann and Robin type we arrive at the following problem:

$$\begin{aligned}
\frac{\partial C}{\partial t} - D\Delta C &= k_D a(C_s - C), && \text{in } \Omega \times (0, t_F),\\
\frac{\partial a}{\partial t} &= -\beta\sqrt{a}(C_s - C), && \text{in } \Omega \times (0, t_F),\\
C(\cdot, 0) &= C^0(\cdot), && \text{in } \Omega,\\
a(\cdot, 0) &= a^0(\cdot), && \text{in } \Omega\\
D\frac{\partial C}{\partial n} &= 0, && \text{on } \Gamma_N \times (0, t_F),\\
D\frac{\partial C}{\partial n} &= k_B(C_B - C), && \text{on } \Gamma_B \times (0, t_F).
\end{aligned} \tag{2.4}$$

This problem is stated over $\Omega \subset \mathbb{R}^d$ ($d = 1, 2, 3$), which is an open, bounded and connected set with Lipschitz boundary $\Gamma = \Gamma_B \cup \Gamma_N$. Γ_B is the nontrivial part of the boundary where drug is released to the surrounding medium, and $\Gamma_N = \Gamma \backslash \Gamma_B$ is the insulated part; C_B denotes the drug concentration in the bulk medium, k_B the external mass transfer coefficient, $\frac{\partial C}{\partial n} = \nabla C \cdot n$ and n denotes the exterior unit normal to $\partial\Omega$. We assume also that

$$D, k_D, k_B, C_B \in (0, +\infty), \qquad \beta \in L^\infty(\Omega), \quad \beta \geq 0, \tag{2.5}$$

$$C^0, a^0 \in L^\infty(\Omega), \quad C^0, a^0 \geq 0. \tag{2.6}$$

Proceeding as usual, integrating by parts in Ω, we arrive at the following weak formulation of the problem.

Definition 1. *The pair (C, a) is a weak solution of (2.4) if $C \in L^2(0, t_F; H^1(\Omega))$ with $C_t \in L^2(0, t_F; H^{-1}(\Omega))$, $a \in H^1(0, t_F; L^2(\Omega))$ and for a.e. $t \in [0, t_F]$*

$$\begin{cases}
\langle C_t(t), v\rangle + \mathscr{B}[C(t), v] = k_D \displaystyle\int_\Omega a(t)(C_s - C(t))v + k_B C_B \int_{\Gamma_B} v, & \forall v \in H^1(\Omega),\\
\displaystyle\int_\Omega a_t(t) w = \int_\Omega \beta(C(t) - C_s)\sqrt{a(t)}w, & \forall w \in L^2(\Omega),\\
C(0) = C^0, \quad a(0) = a^0,
\end{cases} \tag{2.7}$$

where $\langle f, v\rangle$ stands for the evaluation of the functional $f \in H^{-1}(\Omega)$ in $v \in H^1(\Omega)$ and

$$\mathscr{B} : H^1(\Omega) \times H^1(\Omega) \to \mathbb{R}, \quad \mathscr{B}[C, v] := D\int_\Omega \nabla C \nabla v + k_B \int_{\Gamma_B} Cv.$$

The space $L^2(\Omega)$ is the space of Lebesgue measurable functions on Ω which are square integrable, $H^1(\Omega)$ denotes the usual Sobolev space of functions in $L^2(\Omega)$ with weak derivatives of first order in $L^2(\Omega)$ and $H^{-1}(\Omega)$ is the dual space of $H^1(\Omega)$. The spaces $L^p(0, t_F; X)$ denote the usual spaces of weakly measurable functions $f : [0, t_F] \to X$, such that $\int_0^{t_F} \|f(t)\|_X^p \, \mathrm{d}t < \infty$. The space $H^1(0, t_F; X)$ denotes the space of functions in $L^2(0, t_F; X)$ with weak derivative of first order in $L^2(0, t_F; X)$; see [T, Chapter 3] for details and main results.

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Remark 2. The following Friedrich inequality holds for a constant $\mathbb{C}_F$ depending on Γ_B and Ω:

$$\|v\|^2_{L^2(\Omega)} \leq \mathbb{C}_F^2 \left(\|\nabla v\|^2_{L^2(\Omega)} + \|v\|^2_{L^2(\Gamma_B)} \right), \quad \forall v \in H^1(\Omega). \tag{2.8}$$

As an immediate consequence, the bilinear form $\mathscr{B}$ is coercive and bounded, i.e., there exist positive constants $\mathbb{C}_1$, $\mathbb{C}_2$ such that, for all $v, w \in H^1(\Omega)$,

$$\mathbb{C}_1 \|v\|^2_{H^1(\Omega)} \leq \mathscr{B}[v,v] \quad \text{and} \quad \mathscr{B}[v,w] \leq \mathbb{C}_2 \|v\|_{H^1(\Omega)} \|w\|_{H^1(\Omega)}.$$

3 Building solutions

In this section we prove the existence of weak solutions to (2.4). We will do so by constructing Galerkin approximations and passing to the limit, following the main steps from [E] for the heat equation. Problems with similar features have been studied in [AV, DS]. The proofs in [AV] are based on a regularization of the non-Lipschitz term and hinge upon using powerful tools from [LSU]. The proofs from [DS] are based on an iteration at the infinite-dimensional level. These proofs do not directly apply to our problem. Our more elementary approach allows us to prove also higher regularity results and obtain an explicit formula in terms of C for the area of solid particles a.

3.1 Galerkin approximations.

We consider a sequence $\{\mathcal{T}_n\}$ of conforming and shape regular triangulations of Ω, such that $\bigcup_{T \in \mathcal{T}_n} T = \overline{\Omega}$, and $h_n := \max_{T \in \mathcal{T}_n} h_T \to 0$ when $n \to \infty$, where h_T denotes the diameter of T, which could be curved at the boundary.

We define the following finite-dimensional spaces:

$$V_n = \{v \in H^1(\Omega) : v|_T \in \mathscr{P}_1, \ \forall T \in \mathcal{T}_n\},$$

$$W_n = \{w \in L^2(\Omega) : w|_T \in \mathscr{P}_0, \ \forall T \in \mathcal{T}_n\},$$

where $\mathscr{P}_\ell$ is the space of polinomials of degree less than or equal to ℓ. We also assume that the triangulations are nested so that for all $n \in \mathbb{N}$, $V_n \subset V_{n+1}$, $W_n \subset W_{n+1}$, $\cup_{n=1}^\infty V_n$ is dense in $H^1(\Omega)$ and $\cup_{n=1}^\infty W_n$ is dense in $L^2(\Omega)$.

For a fixed $n \in \mathbb{N}$, we define the Galerkin approximations as follows: Let $C_n : [0, t_F] \to V_n$, $a_n : [0, t_F] \to W_n$ be solutions of the following system of ordinary differential equations on $[0, t_F]$,

$$(C_{n,t}, v) + \mathscr{B}[C_n, v] = k_D \int_\Omega a_n (C_s - C_n) v + k_B C_B \int_{\Gamma_B} v, \quad \forall v \in V_n \tag{3.1}$$

$$\int_\Omega a_{n,t} w = \int_\Omega \beta \left(\min\{C_n, \bar{C}_0\} - C_s \right) \Phi_n(a_n) w, \quad \forall w \in W_n \tag{3.2}$$

$$C_n(0) = C_n^0, \qquad a_n(0) = a_n^0 + \frac{2}{n^2}, \tag{3.3}$$

Hereafter $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$, $\bar{C}_0 = \max\left\{\|C^0\|_{L^\infty(\Omega)}, C_s\right\}$, C_n^0 and a_n^0 denote the $L^2(\Omega)$-projections of C^0 and a^0 on V_n and W_n, respectively. Using $\min\{C_n, \bar{C}_0\}$ instead of C_n in (3.2) permits to obtain easily a

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bound for a_n. To avoid the non-lipschitzcity of the square root, we have used Φ_n, defined by

$$\Phi_n(\alpha) = \begin{cases} \sqrt{\alpha} - \frac{1}{n}, & \text{if } \alpha > 1/n^2, \\ 0, & \text{if } \alpha \le 1/n^2. \end{cases} \tag{3.4}$$

The term $\frac{2}{n^2}$ in (3.3) allows us to find a formula to the solution a_n over each element of the triangulation using the first branch in the definition of Φ_n. This fact will help us to show the existence of two solutions when $a^0 \equiv 0$ (see Section 4.2).

Remark 3. If $C^0 \in H^1(\Omega)$ in (2.6) we could define also $C_n(0)$ as the H^1-projection of C^0 on V_n or as the Ritz projection $R_nC(0)$ of $C(0)$ which is defined by:

$$R_nC(0) \in V_n : \qquad \mathscr{B}[R_nC(0), v] = \mathscr{B}[C(0), v], \quad \forall v \in V_n. \tag{3.5}$$

The same arguments that we will use in what follows apply to both choices of $C_n(0)$, yielding analogous bounds.

Stability and global existence of Galerkin approximations. We first prove some useful stability bounds for the Galerkin approximations, and then conclude their global existence.

Proposition 4. *If (C_n, a_n) is a solution of (3.1)–(3.3) in $[0, t_F)$ for some $t_F > 0$, then the following estimates hold with constants $\mathbb{C}_4$, $\mathbb{C}_5$ independent of n and t_F:*

$$\|C_n\|^2_{L^\infty(0,t_F;L^2(\Omega))}, \mathbb{C}_4\|C_n\|^2_{L^2(0,t_F;H^1(\Omega))} \le \|C^0\|^2_{L^2(\Omega)} + \mathbb{C}_5|\Omega|t_F\|a_n\|^2_{L^\infty(0,t_F;L^\infty(\Omega))} + k_B C_B^2|\Gamma_B|t_F, \tag{3.6}$$

$$\|a_n\|_{L^\infty(0,t_F;L^\infty(\Omega))} \le \left(\|a^0\|_{L^\infty(\Omega)} + 2\right) e^{t_F} + \left(\frac{\|\beta\|^2_{L^\infty(\Omega)}}{4}\left(\bar{C}_0 - C_s\right)^2\right)(e^{t_F} - 1), \tag{3.7}$$

and

$$\|a_{n,t}\|^2_{L^2(0,t_F;L^\infty(\Omega))} \le \|a_n\|_{L^\infty(0,t_F;L^\infty(\Omega))}\|\beta\|^2_{L^\infty(\Omega)}|\Omega|^{2/3}\|\min\left\{C_n, \bar{C}_0\right\} - C_s\|^2_{L^2(0,t_F;H^1(\Omega))}. \tag{3.8}$$

Proof. Since $a_n(t) \in W_n$, $a_n(t)$ is constant over each element $T \in \mathcal{T}_n$. Then, denoting $\alpha_T(t) = a_n(t)_{|T}$, we write (3.2) as

$$\alpha_T'(t) = \Phi_n(\alpha_T(t)) ⨍_T \beta\left(\min\left\{C_n, \bar{C}_0\right\} - C_s\right) \mathrm{d}x, \quad T \in \mathcal{T}_n,\ t \in (0, t_F). \tag{3.9}$$

On the one hand, since $\alpha_T(0) \ge 2/n^2 > 0$ and $\Phi_n(\alpha) = 0$ if $\alpha \le 1/n^2$, it turns out that $\alpha_T(t) \ge 1/n^2$ for all $t \in [0, t_F)$.

On the other hand, since $\min\{C_n, \bar{C}_0\} - C_s \le \bar{C}_0 - C_s$ and $\beta(x), \Phi_n(\alpha_T(t)) \ge 0$ we get,

$$\alpha_T'(t) \le \Phi_n(\alpha_T(t)) ⨍_T \beta\left(\bar{C}_0 - C_s\right) \mathrm{d}x.$$

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Applying Cauchy-Schwarz inequality to the above expression and recalling that $0 \leq \phi_n(\alpha) \leq \sqrt{\alpha}$, we obtain,

$$\alpha_T'(t) \leq \alpha_T(t) + \frac{\|\beta\|^2_{L^\infty(\Omega)}}{4} \left(\bar{C}_0 - C_s\right)^2,$$

$$\frac{d}{dt}\left(e^{-t}\alpha_T(t)\right) = e^{-t}\left(\alpha_T{}'(t) - \alpha_T(t)\right) \leq e^{-t}\left(\frac{\|\beta\|^2_{L^\infty(\Omega)}}{4}\left(\bar{C}_0 - C_s\right)^2\right).$$

Integrating from 0 to t and multiplying by e^t we arrive at

$$\alpha_T(t) \leq \alpha_T(0)e^t + \left(\frac{\|\beta\|^2_{L^\infty(\Omega)}}{4}\left(\bar{C}_0 - C_s\right)^2\right)(e^t - 1), \tag{3.10}$$

for all t in $[0, t_F)$ and $T \in \mathcal{T}_n$. Since $\alpha_T(t) \geq 0$, $a_n(t)(x) = \alpha_T(t)$ if $x \in T$, and $\alpha_T(0) = ⨍_T a^0 + 2/n^2$ we have that

$$\|a_n\|_{L^\infty(0,t_F;L^\infty(\Omega))} \leq \left(\left\|a^0\right\|_{L^\infty(\Omega)} + 2\right)e^{t_F} + \left(\frac{\|\beta\|^2_{L^\infty(\Omega)}}{4}\left(\bar{C}_0 - C_s\right)^2\right)(e^{t_F} - 1),$$

We have thus proved the desired bound (3.7) for a_n. The argument above is based on the mere existence of C_n and not on additional assumptions of C_n. This could be done thanks to the presence of $\min\{C_n, \bar{C}_0\}$ instead of C_n in the equation for the temporal derivative of a_n.

To prove the estimate for C_n, we set $v = C_n$ in (3.1), and get

$$\frac{1}{2}\frac{d}{dt}\|C_n\|^2_{L^2(\Omega)} + \mathscr{B}[C_n, C_n] + k_D\int_\Omega a_n C_n^2 = k_D C_s \int_\Omega a_n C_n + k_B C_B \int_{\Gamma_B} C_n.$$

The definition of $\mathscr{B}[\cdot,\cdot]$ and Cauchy-Schwarz inequality yield, for any $\varepsilon > 0$,

$$\frac{1}{2}\frac{d}{dt}\|C_n\|^2_{L^2(\Omega)} + D\int_\Omega |\nabla C_n|^2 + \frac{k_B}{2}\int_{\Gamma_B} C_n^2 \leq \frac{k_D C_s}{4\varepsilon}\int_\Omega a_n^2 + \varepsilon k_D C_s \int_\Omega C_n^2 + k_B\frac{C_B^2}{2}|\Gamma_B|,$$

where we have dropped the term $k_D\int_\Omega a_n C_n^2 \geq 0$ from the left-hand side. Therefore, by Friedrich inequality (2.8),

$$\frac{1}{2}\frac{d}{dt}\|C_n\|^2_{L^2(\Omega)} + \frac{D}{2}\int_\Omega |\nabla C_n|^2 + \left[\frac{\min\left\{\frac{D}{2}, \frac{k_B}{2}\right\}}{\mathbb{C}_F^2} - \varepsilon k_D C_s\right]\int_\Omega C_n^2 \leq \frac{k_D C_s}{4\varepsilon}\int_\Omega a_n^2 + k_B\frac{C_B^2}{2}|\Gamma_B|.$$

Setting $\varepsilon = \frac{1}{2}\frac{\min\left\{\frac{D}{2},\frac{k_B}{2}\right\}}{\mathbb{C}_F^2 k_D C_s}$ so that $\mathbb{C}_3 := \frac{\min\left\{\frac{D}{2},\frac{k_B}{2}\right\}}{\mathbb{C}_F^2} - \varepsilon k_D C_s > 0$, we get

$$\frac{1}{2}\frac{d}{dt}\|C_n\|^2_{L^2(\Omega)} + \frac{D}{2}\int_\Omega |\nabla C_n|^2 + \mathbb{C}_3\int_\Omega C_n^2 \leq \frac{\mathbb{C}_F^2 k_D^2 C_s^2}{2\min\left\{\frac{D}{2},\frac{k_B}{2}\right\}}\int_\Omega a_n^2 + k_B\frac{C_B^2}{2}|\Gamma_B|.$$

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Defining $\mathbb{C}_4 := \min\{D, 2\mathbb{C}_3\}$ and $\mathbb{C}_5 = \frac{\mathbb{C}_F^2 k_D^2 C_s^2}{2\min\left\{\frac{D}{2}, \frac{k_B}{2}\right\}}$, the above inequality becomes:

$$\frac{d}{dt}\|C_n\|^2_{L^2(\Omega)} + \mathbb{C}_4\|C_n\|^2_{H^1(\Omega)} \leq \mathbb{C}_5 \int_\Omega a_n^2 + k_B C_B^2 |\Gamma_B|.$$

Integrating with respect to t, we obtain, for $t \in [0, t_F)$:

$$\|C_n(t)\|^2_{L^2(\Omega)} + \mathbb{C}_4 \int_0^t \|C_n\|^2_{H^1(\Omega)} \leq \|C_n(0)\|^2_{L^2(\Omega)} + \mathbb{C}_5 \int_0^t \int_\Omega a_n^2 + k_B C_B^2 |\Gamma_B| t.$$

In view of (3.7) and recalling that $C_n(0)$ is the L^2-projection of C^0 on V_n, the asserted estimates (3.6) follow.

Going back to (3.9) we observe

$$\begin{aligned}
|\alpha_T'(t)| &= |\Phi_n(\alpha_T(t))| \left| \fint_T \beta\left(\min\left\{C_n, \bar{C}_0\right\} - C_s\right) \mathrm{d}x \right|, \\
&\leq \sqrt{\alpha_T(t)} \|\beta\|_{L^\infty(\Omega)} |T|^{1/3} \left(\int_T |\min\{C_n(t), \bar{C}_0\} - C_s|^4 \right)^{1/4}, \\
&\leq \|a_n\|^{1/2}_{L^\infty(0,t;L^\infty(\Omega))} \|\beta\|_{L^\infty(\Omega)} |\Omega|^{1/3} \|\min\{C_n(t), \bar{C}_0\} - C_s\|_{H^1(\Omega)},
\end{aligned}$$

by Sobolev embedding theorem; and (3.8) follows. □

Existence and uniqueness of a local solution to (3.1)–(3.3) is guaranteed by standard theory for ordinary differential equations from [CL, Theorem 2.3, Chapter 1, pag 10] because the right-hand side of (3.1)–(3.3) is Lipschitz continuous. The bounds from the previous proposition, with the results on continuation of solutions from [CL, Theorem 4.1, Chapter 1, pag 15] yield global existence and uniqueness of solution to (3.1)–(3.3). We state this as follows:

Theorem 5. *Problem (3.1)–(3.3) has a unique solution (C_n, a_n) in $[0, \infty)$, for each $n \in \mathbb{N}$ and the bounds (3.6)–(3.8) hold for any $t_F > 0$.*

Having proved existence and stability bounds for (C_n, a_n) the next step consists in proving that a subsequence converges to some candidate (C, a).

3.2 Limiting process for C_n.

By Proposition 4, $\{C_n\}$ is a bounded sequence in $L^2(0, t_F; H^1(\Omega))$, which is a reflexive Banach space. Then there exists a weak convergent subsequence $\{C_{n_k}\}$, which we keep calling $\{C_n\}$, and $C \in L^2(0, t_F; H^1(\Omega))$ such that

$$C_n \rightharpoonup C \text{ in } L^2(0, t_F; H^1(\Omega)).$$

Following ideas from the proof of [T, Theorem 3.2, p. 283] we can prove that there exist $\gamma > 0$ such that $\{C_n\}$ is bounded in $H^\gamma_{[0,t_F]}(\mathbb{R}; H^1(\Omega), L^2(\Omega))$. Due to [T, Theorem 2.2, p. 274] this space is compactly embedded in $L^2(0, t_F; L^2(\Omega))$ and we thus conclude that there exists a subsequence of $\{C_n\}$ which we still call $\{C_n\}$, that converges to C in $L^2(0, t_F; L^2(\Omega))$.

Remark 6. This argument using the fractional order space $H^\gamma_{[0,t_F]}(\mathbb{R}; H^1(\Omega), L^2(\Omega))$ is necessary to prove existence in the most general case of $C^0 \in L^2(\Omega)$. It can be avoided if we assume $C^0 \in H^1(\Omega)$. In the latter, choosing $C_n(0)$ as the

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$H^1(\Omega)$-projection of C^0 into V_n, the sequences C_n, $C_{n,t}$ are uniformly bounded in $L^\infty(0,t_F;H^1(\Omega))$ and $L^2(0,t_F;L^2(\Omega))$, respectively (see Theorem 20 below). This also implies the existence of a subsequence converging strongly to C in $L^2(0,t_F;L^2(\Omega))$.

3.3 Limiting process for a_n.

The goal of this subsection is to prove the following important result.

Theorem 7. *The sequence $\{a_n\}$ has a subsequence which we still call $\{a_n\}$ that satisfies:*

$$\sqrt{a_n} \to \sqrt{a}, \quad \textit{and} \quad a_n \to a, \qquad \textit{in} \quad L^2(0,t_F;L^2(\Omega)),$$

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

$$a(t) = \left(\sqrt{a^0} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C(\tau),\bar{C}_0\right\} - C_s\right) \mathrm{d}\tau\right)_+^2.$$

Remark 8. Since $L^\infty(0,t_F;L^\infty(\Omega)) \subset L^2(0,t_F;L^2(\Omega))$ and $L^2(0,t_F;L^2(\Omega))$ is a reflexive Banach space, using (3.7) we have the existence of a subsequence of $\{a_n\}$ converging weakly to some function a. It is important to notice though, that this weak convergence does not imply $\sqrt{a_n} \rightharpoonup \sqrt{a}$, and the converse is not true either. It is sufficient to consider the example $a_n(x) = (10+\sin nx)^2$, for $x \in [0,1]$, for which $\sqrt{a_n} \rightharpoonup \tilde{a} \equiv 10$, and

$$a_n = 100 + \frac{1}{2} - \frac{\cos 2nx}{2} + 2\sin nx \rightharpoonup 100 + \frac{1}{2} \neq \tilde{a}^2.$$

In order to prove Theorem 7 we need to use other properties of $\{a_n\}$ besides weak convergence. We will show that $\{a_n\}$ converges pointwise to a and conclude the assertion by Lebesgue dominated convergence theorem, using the estimates (3.7) and (3.6).

We now prove some intermediate results and postpone the proof of Theorem 7 to the end of this section. We start analyzing the convergence of the initial data.

Proposition 9. *$\sqrt{a_n(0)} \to \sqrt{a^0}$ in $L^2(\Omega)$ when $n \to \infty$.*

Proof. Recall that $a_n(0) = a_n^0 + 2/n^2$, where a_n^0 is the $L^2(\Omega)$-projection of a^0 on W_n. Then $a_n(0) = \sum_{T\in\mathcal{T}_n} \alpha_T \chi_T + 2/n^2$ with $\alpha_T = ⨍_T a^0$. Then

$$\begin{aligned}
\int_\Omega \left(\sqrt{a_n(0)} - \sqrt{a^0}\right)^2 \mathrm{d}x &= \sum_{T\in\mathcal{T}_n} \int_T \left(\sqrt{\alpha_T + \frac{2}{n^2}} - \sqrt{a^0}\right)^2 \mathrm{d}x \\
&\le \sum_{T\in\mathcal{T}_n} \int_T \left(\alpha_T - 2\sqrt{\alpha_T}\sqrt{a^0} + a^0 + \frac{2}{n^2}\right) \mathrm{d}x \\
&\le 2\sum_{T\in\mathcal{T}_n} \int_T \sqrt{a^0}\left(\sqrt{a^0} - \sqrt{\alpha_T}\right) \mathrm{d}x + \frac{2|\Omega|}{n^2},
\end{aligned}$$

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where in the last inequality we have used that $\sum_{T\in\mathcal{T}_n}\int_T\left(\alpha_T-a^0\right)\mathrm{d}x=0$. Next we observe that $\sqrt{\alpha_T}=\frac{1}{|T|^{1/2}}\left(\int_T a^0\right)^{1/2}\geq\frac{1}{|T|}\int_T\sqrt{a^0}$, whence

$$\int_T\sqrt{a^0}\left(\sqrt{a^0}-\sqrt{\alpha_T}\right)\mathrm{d}x\leq\int_T\sqrt{a^0}\left(\sqrt{a^0}-\frac{1}{|T|}\int_T\sqrt{a^0}\right)\mathrm{d}x.$$

Consequently by Hölder and Cauchy-Schwartz inequalities

$$\begin{aligned}\int_\Omega\left(\sqrt{a_n(0)}-\sqrt{a^0}\right)^2\mathrm{d}x&\leq 2\sum_{T\in\mathcal{T}_n}\int_T\sqrt{a^0}\left(\sqrt{a^0}-\frac{1}{|T|}\int_T\sqrt{a^0}\right)\mathrm{d}x+\frac{2|\Omega|}{n^2}\\&\leq 2\left(\int_\Omega a^0\right)^{1/2}\left(\sum_{T\in\mathcal{T}_n}\int_T\left(\sqrt{a^0}-\frac{1}{|T|}\int_T\sqrt{a^0}\right)^2\mathrm{d}x\right)^{1/2}+\frac{2|\Omega|}{n^2}\\&=2\left(\int_\Omega a^0\right)^{1/2}\left(\int_\Omega\left(\sqrt{a^0}-\sum_{T\in\mathcal{T}_n}\frac{1}{|T|}\int_T\sqrt{a^0}\,\mathrm{d}y\chi_T(x)\right)^2\mathrm{d}x\right)^{1/2}+\frac{2|\Omega|}{n^2}.\end{aligned}$$

The assertion follows from the fact that $\sum_{T\in\mathcal{T}_n}\frac{1}{|T|}\int_T\sqrt{a^0}\,\mathrm{d}y\,\chi_T(x)$ is the $L^2(\Omega)$-projection of $\sqrt{a^0}$ in W_n. □

We define now $\Sigma:=\bigcup_{n\in\mathbb{N}}\bigcup_{T\in\mathcal{T}_n}\partial T$, i.e., the set of points belonging to the sides of the elements of all the triangulations of the sequence. Its Lebesgue measure is zero because it is a countable union of sets with Lebsegue measure zero. Besides, given $n\in\mathbb{N}$ fixed and $x\in\Omega\setminus\Sigma$, there exists a unique $T=T(x,n)\in\mathcal{T}_n$ such that $x\in T$. We will hereafter omit the subindex T and for a given $x\in\Omega\setminus\Sigma$, we will consider the elements T^n such that $x\in T^n\in\mathcal{T}_n$. For example, $\alpha^n(t)$ will denote $\alpha^n_{T(x,n)}(t):=a_n(t)(x)=a_n(t)_{|T(x,n)}$ where $T(x,n)$ is the only element $T\in\mathcal{T}_n$ such that $x\in T$. By Proposition 9 the sequence $\left\{\sqrt{\alpha^n(0)}\right\}_{n\in\mathbb{N}}$ is convergent, and thus $\alpha^n(0)\to\alpha^0$, as $n\to\infty$ for some $\alpha^0\in\mathbb{R}$. From (3.2) and (3.3),

$$\alpha^n(t)'=f^n(t)\Phi_n(\alpha^n(t)),\quad t>0,\quad\text{with}\quad\alpha^n(0)=\fint_T a^0+\frac{2}{n^2}>\frac{1}{n^2},$$

with Φ_n as in (3.4), and $f^n(t):=\fint_T\beta\left(\min\left\{C_n,\bar{C}_0\right\}-C_s\right)$. It is straightforward to check that the solution $\alpha^n(t)$ to this scalar IVP satisfies the following (algebraic) equation for each $t>0$:

$$\sqrt{\alpha^n(t)}=\sqrt{\alpha^n(0)}-\frac{1}{n}\log\left(\frac{\sqrt{\alpha^n(t)}-\frac{1}{n}}{\sqrt{\alpha^n(0)}-\frac{1}{n}}\right)+\frac{1}{2}\int_0^t f^n(\tau)\,\mathrm{d}\tau.\qquad(3.11)$$

For t fixed, let us call $X_n:=\sqrt{\alpha^n(t)}$ and $\ell_n:=\sqrt{\alpha^n(0)}+\frac{1}{2}\int_0^t f^n(\tau)\,\mathrm{d}\tau$, then, rewritting (3.11) in terms of X_n and ℓ_n, it reads:

$$X_n+\frac{1}{n}\log\left(\frac{X_n-\frac{1}{n}}{\sqrt{\alpha^n(0)}-\frac{1}{n}}\right)=\ell_n.\qquad(3.12)$$

The following lemma, whose proof is postponed to the end of this section, states existence and uniqueness of X_n satisfying (3.12) for each n and asserts convergence of X_n when $\ell_n\to\ell$ and $\alpha^n(0)\to\alpha^0$.

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Lemma 10. *Let $\{\ell_n\}, \{\alpha^n(0)\} \subset \mathbb{R}$ be sequences such that $\ell_n \to \ell$ and $\sqrt{\alpha^n(0)} \to \sqrt{\alpha^0}$, with $\sqrt{\alpha^n(0)} > \frac{1}{n}$. Then, for each n, there exists a unique $X_n \in \left(\frac{1}{n}, \infty\right)$ such that*

$$X_n + \frac{1}{n}\log\left(\frac{X_n - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}}\right) = \ell_n, \tag{3.13}$$

and moreover $X_n \longrightarrow \ell_+ = \begin{cases} \ell, & \text{if } \ell \geq 0, \\ 0, & \text{if } \ell < 0, \end{cases}$ *when n tends to ∞.*

Proposition 11 below states that $\ell_n := \sqrt{\alpha^n(0)} + \frac{1}{2}\int_0^t f^n(\tau)\,\mathrm{d}\tau$ converges to $\ell := \sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}\tau$ when $n \to \infty$. This allows us to prove Theorem 7.

Proof of Theorem 7. By Proposition 11 there is a subsequence $\{\ell_{n_k}\}_{k\in\mathbb{N}}$, which we keep calling $\{\ell_n\}_{n\in\mathbb{N}}$, such that $\ell_n \to \ell$ for almost all (x,t) in $\Omega \times [0, t_F]$, as $n \to \infty$. Therefore, by Lemma 10 we have that

$$\begin{aligned} X_n = \sqrt{a_n(x,t)} = \sum_{T\in\mathcal{T}_n}\sum_{i=1}^{N_W^n} \alpha_i^n(t)\chi_{T_i^n}(x) \\ \to \left(\sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}\tau\right)_+, \end{aligned}$$

for almost all (x,t) in $\Omega \times [0, t_F]$. By (3.7) and the dominated convergence theorem, we conclude that

$$\begin{aligned} \sqrt{a_n} &\to \left(\sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}\tau\right)_+, \\ \text{and} \qquad a_n &\to \left(\sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}\tau\right)_+^2 = a, \end{aligned} \tag{3.14}$$

with convergence in $L^2(0, t_F; L^2(\Omega))$. □

Proposition 11. *When $n \to \infty$,*

$$\begin{aligned} \sum_{T\in\mathcal{T}_n}\left(\sqrt{\alpha^n(0)} + \frac{1}{2}\int_0^t \fint_T \beta\left(\min\left\{C_n, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}y\,\mathrm{d}\tau\right)\chi_T(x) \\ \to \sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\left\{C, \bar{C}_0\right\} - C_s\right)\,\mathrm{d}\tau. \end{aligned}$$

in $L^2(\Omega \times [0, t_F])$.

Proof. Convergence of $\sum_{T\in\mathcal{T}_n}\sqrt{\alpha^n(0)}\chi_T$ to $\sqrt{a^0}$ in $L^2(\Omega)$, and consequently in $L^2(\Omega \times [0, t_F])$ was shown in Proposition 9.

To prove the convergence of the second term, it is sufficient to see that

$$\begin{aligned} g_n(x,t) := \sum_{T\in\mathcal{T}_n}\int_0^t \fint_T \beta(y)\min\left\{C_n(y,\tau), \bar{C}_0\right\}\,\mathrm{d}y\,\mathrm{d}\tau\chi_T(x) \\ \to \int_0^t \beta(x)\min\left\{C(x,\tau), \bar{C}_0\right\}\,\mathrm{d}\tau =: g(x,t), \end{aligned}$$

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in $L^2(\Omega \times [0, t_F])$. If we define $\mathbb{X}_n = \{v \in L^2(0, t_F; L^2(\Omega)) : v(\cdot, t) \in W_n\}$, then $\cup_{n=1}^{\infty} \mathbb{X}_n$ is dense in $L^2(0, t_F; L^2(\Omega))$. If $\mathscr{P}_n$ denotes the $L^2(\Omega \times (0, t_F))$-projection on $\mathbb{X}_n$, then $g_n(\cdot, t) = \int_0^t \mathscr{P}_n \left(\beta \min\{C_n(\cdot, \tau), \bar{C}_0\}\right) \mathrm{d}\tau$ and by Hölder inequality we obtain

$$
\begin{aligned}
&\|g_n(\cdot, t) - g(\cdot, t)\|_{L^2(\Omega)} \\
&\qquad \le t_F^{1/2} \left\| \mathscr{P}_n \left(\beta \min\left\{C_n, \bar{C}_0\right\}\right) - \beta \min\left\{C, \bar{C}_0\right\} \right\|_{L^2(\Omega \times (0, t_F))} \\
&\qquad \le t_F^{1/2} \left\| \mathscr{P}_n \left[\beta \min\left\{C_n, \bar{C}_0\right\} - \beta \min\left\{C, \bar{C}_0\right\}\right] \right\|_{L^2(\Omega \times (0, t_F))} \\
&\qquad\quad + t_F^{1/2} \left\| \mathscr{P}_n \left(\beta \min\left\{C, \bar{C}_0\right\}\right) - \beta \min\left\{C, \bar{C}_0\right\} \right\|_{L^2(\Omega \times (0, t_F))}.
\end{aligned}
$$

Since $C_n \to C$ in $L^2(0, t_F; L^2(\Omega))$ we have that $\beta \min\left\{C_n, \bar{C}_0\right\} \to \beta \min\left\{C, \bar{C}_0\right\}$ in $L^2(\Omega \times [0, t_F])$, because $\beta \in L^\infty(\Omega)$. Finally,

$$
\|g_n(\cdot, t) - g(\cdot, t)\|_{L^2(\Omega)} \to 0, \text{ as } n \to \infty, \tag{3.15}
$$

uniformly in $t \in [0, t_F]$, which readily implies that

$$
\|g_n(\cdot, t) - g(\cdot, t)\|_{L^2(0, t_F; L^2(\Omega))} \to 0, \text{ as } n \to \infty,
$$

and the assertion follows. $\square$

We end this section by proving Lemma 10, which was used in the proof of Theorem 7, the main goal of this section.

Proof of Lemma 10. The mapping $g_n : \left(\frac{1}{n}, \infty\right) \to \mathbb{R}$, defined by $g_n(x) = x + \frac{1}{n} \log\left(\frac{x - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}}\right)$ is onto $\mathbb{R}$ and also one-to-one since $g_n'(x) = 1 + \frac{1}{n} \frac{\sqrt{\alpha^n(0)} - \frac{1}{n}}{x - \frac{1}{n}} > 0$ for all $x \in \left(\frac{1}{n}, \infty\right)$. Therefore, there exists a unique X_n satisfying (3.13).

In order to show convergence of $\{X_n\}$ to ℓ_+ we consider three cases: $\ell < 0$, $\ell > 0$ and $\ell = 0$.

$\boxed{1}$ If $\ell < 0$, then there exists N_0 such that, for $n \ge N_0$, $\ell_n < \frac{\ell}{2}$ and thus

$$
\frac{1}{n} \log\left(\frac{X_n - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}}\right) = \ell_n - X_n < \frac{\ell}{2} - \frac{1}{n} < \frac{\ell}{2}, \quad \text{for } n \ge N_0.
$$

Then, $\log\left(\frac{X_n - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}}\right) < n\frac{\ell}{2}$, and thus $\frac{1}{n} < X_n < \frac{1}{n} + \left(\sqrt{\alpha^n(0)} - \frac{1}{n}\right) e^{n\frac{\ell}{2}}$ for $n \ge N_0$, which implies $X_n \to 0 = \ell_+$ (recall that $\ell < 0$).

$\boxed{2}$ If $\ell > 0$, there exists N_0 such that, for all $n \ge N_0$, $\frac{1}{n} < \frac{\ell}{2} < \ell_n < \frac{3\ell}{2}$. Using the monotonicity of g_n and analyzing separately the cases $\ell_n < \sqrt{\alpha^n(0)}$, $\ell_n = \sqrt{\alpha^n(0)}$, $\ell_n > \sqrt{\alpha^n(0)}$, one can easily prove that

$$
0 < \gamma \le \frac{X_n - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}} \le 4\ell n, \quad \forall n \ge N_0,
$$

with γ independent of n, whence

$$
X_n = \ell_n - \frac{1}{n} \log\left(\frac{X_n - \frac{1}{n}}{\sqrt{\alpha^n(0)} - \frac{1}{n}}\right) \to \ell = \ell_+, \quad \text{when } n \to \infty.
$$

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$\boxed{3}$ If $\ell = 0$, we show that $X_n \to 0$ by contradiction. Assume that $\{X_n\}$ does not converge to zero, then there exists a subsequence $\{X_{n_k}\}_{k\in\mathbb{N}}$ bounded below by a constant $\gamma > 0$. Consequently, if $\tilde{\gamma}$ denotes an upper bound for $\sqrt{\alpha^n(0)}$, it turns out that

$$0 < \frac{\gamma}{2\tilde{\gamma}} \leq \frac{\gamma - \frac{1}{n_k}}{\tilde{\gamma} - \frac{1}{n_k}} \leq \frac{X_{n_k} - \frac{1}{n_k}}{\sqrt{\alpha^{n_k}(0)} - \frac{1}{n_k}},$$

for all $k \in \mathbb{N}$ such that $n_k > 2\max\{1/\gamma, 1/\tilde{\gamma}\}$. Then,

$$\gamma \leq X_{n_k} = \ell_{n_k} - \frac{1}{n_k}\log\frac{X_{n_k} - \frac{1}{n_k}}{\sqrt{\alpha^{n_k}(0)} - \frac{1}{n_k}} \leq \ell_{n_k} - \frac{1}{n_k}\log\frac{\gamma}{2\tilde{\gamma}} \to 0, \quad \text{as } k \to \infty.$$

This is a contradiction that stems from the assumption that X_n does not converge to zero. □

3.4 Existence of a weak solution

We summarize the most relevant results until here in the following theorem.

Theorem 12. *Let (C_n, a_n), $n \in \mathbb{N}$, be solutions of (3.1)–(3.3). Then there exist $C \in L^2(0, t_F; H^1(\Omega))$, $a \in L^2(0, t_F; L^2(\Omega))$ and a subsequence of $\{(C_n, a_n)\}$ which we still call $\{(C_n, a_n)\}$ such that, as $n \to \infty$,*

$$C_n \to C \quad \text{in } L^2(0, t_F; L^2(\Omega)), \qquad C_n \rightharpoonup C \quad \text{in } L^2(0, t_F; H^1(\Omega)), \tag{3.16}$$
$$\sqrt{a_n} \to \sqrt{a} \quad \text{and} \quad a_n \to a \quad \text{in } L^2(0, t_F; L^2(\Omega)). \tag{3.17}$$

Also, the limit a can be written in terms of C as follows:

$$a(x,t) = \left(\sqrt{a^0(x)} + \frac{1}{2}\int_0^t \beta\left(\min\{C, \bar{C}_0\} - C_s\right)\,\mathrm{d}\tau\right)_+^2. \tag{3.18}$$

The goal of this section is to show that (C, a) is a weak solution to (2.4), i.e. it satisfies Definition 1. In order to pass to the limit in equation (3.1), we consider first scalar functions $\psi \in C^\infty[0, t_F]$ with $\psi(t_F) = 0$ and $v \in \cup_{n=1}^\infty V_n$, i.e., $v \in V_{n_0}$, for some n_0. We multiply (3.1) by $\psi(t)$, integrate with respect to t and integrate by parts to obtain, for $n \geq n_0$,

$$\begin{aligned} &-\int_0^{t_F} (C_n(t)\psi'(t), v)\,\mathrm{d}t - (C_n(0), v)\psi(0) \\ &\quad = -\int_0^{t_F} \mathscr{B}[C_n, v]\psi(t)\,\mathrm{d}t + k_D\int_0^{t_F} ((C_s - C_n)a_n, v)\psi(t)\,\mathrm{d}t \\ &\qquad + k_B\int_0^{t_F} (\!(C_B, v)\!)\psi(t)\,\mathrm{d}t. \end{aligned} \tag{3.19}$$

where, as before, $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$, and $(\!(\cdot,\cdot)\!)$ denotes

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the inner product in $L^2(\Gamma_B)$. From (3.16) we have, as $n \to \infty$,

$$
\begin{aligned}
\int_0^{t_F} (C_n(t)\psi'(t), v)\,\mathrm{d}t &\to \int_0^{t_F} (C(t)\psi'(t), v)\,\mathrm{d}t, \\
(C_n(0), v)\psi(0) &\to (C^0, v)\psi(0), \\
\int_0^{t_F} \mathscr{B}[C_n, v]\psi(t)\,\mathrm{d}t &\to \int_0^{t_F} \mathscr{B}[C, v]\psi(t)\,\mathrm{d}t, \\
\int_0^{t_F} (\!(C_B, v)\!)\psi(t)\,\mathrm{d}t &\to \int_0^{t_F} (\!(C_B, v)\!)\psi(t)\,\mathrm{d}t.
\end{aligned}
$$

In order to see that the interaction term $\int_0^{t_F} ((C_s - C_n)a_n, v)\psi(t)\,\mathrm{d}t$ tends to $\int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t$ we observe that, by Hölder inequality,

$$
\begin{aligned}
&\left| \int_0^{t_F} ((C_s - C_n)a_n, v)\psi(t)\,\mathrm{d}t - \int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t \right| \\
&\quad \leq \left| \int_0^{t_F} \int_\Omega ((C_s - C) - (C_s - C_n))a_n v\,\mathrm{d}x\psi(t)\,\mathrm{d}t \right| \\
&\qquad + \left| \int_0^{t_F} \int_\Omega (C_s - C)(a_n - a)v\,\mathrm{d}x\psi(t)\,\mathrm{d}t \right|, \\
&\quad \leq \|C_n - C\|_{L^2(0,t_F;L^2(\Omega))} \|a_n\|_{L^2(0,t_F;L^2(\Omega))} \|v\psi\|_{L^\infty(0,t_F;L^\infty(\Omega))} \\
&\qquad + \|C_s - C\|_{L^2(0,t_F;L^2(\Omega))} \|a_n - a\|_{L^2(0,t_F;L^2(\Omega))} \|v\psi\|_{L^\infty(0,t_F;L^\infty(\Omega))}.
\end{aligned}
$$

Consequently, $\int_0^{t_F} ((C_s - C_n)a_n, v)\psi(t)\,\mathrm{d}t \to \int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t$ as $n \to \infty$ due to (3.16) and (3.17).

Therefore, for $\psi \in C^\infty[0, t_F]$ with $\psi(t_F) = 0$ and $v \in \cup_{n=1}^\infty V_n$,

$$
\begin{aligned}
&- \int_0^{t_F} (C(t), v)\psi'(t)\,\mathrm{d}t - (C^0, v)_{L^2(\Omega)}\psi(0) \\
&\qquad = - \int_0^{t_F} \mathscr{B}[C, v]\psi(t)\,\mathrm{d}t + k_D \int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t \\
&\qquad\quad + k_B \int_0^{t_F} (\!(C_B, v)\!)\psi(t)\,\mathrm{d}t.
\end{aligned}
\tag{3.20}
$$

Since each term in (3.20) depends linearly and continuously on v, for the $H^1(\Omega)$ norm, and $\cup_{n=1}^\infty V_n$ is dense in $H^1(\Omega)$, (3.20) is valid for all $v \in H^1(\Omega)$.

Since (3.20) holds for the particular case of $\psi \in C_c^\infty(0, t_F)$, we obtain the following identity, which is valid in the distribution sense on $(0, t_F)$, for all $v \in H^1(\Omega)$:

$$
\frac{d}{dt}(C, v) = -D(\nabla C, \nabla v) - k_B(\!(C, v)\!) - k_D(aC, v) + k_D C_s(a, v) + k_B(\!(C_B, v)\!).
$$

Then, using that $H^1(\Omega)$ is reflexive, and applying Lemma 1.1 from [T, pag 250] with $X = H^{-1}(\Omega)$, we conclude that $C_t \in L^2(0, t_F; H^{-1}(\Omega))$ and C satisfies the first equation of (2.7), i.e., for all $v \in H^1(\Omega)$ and almost every $t \in [0, t_F]$:

$$
\langle C_t, v \rangle + \mathscr{B}[C, v] = k_D \int_\Omega a(C_s - C)v + k_B C_B \int_{\Gamma_B} v. \tag{3.21}
$$

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It remains to check the initial condition for C. Lemma 1.2 [T, pag. 260] enables us to assert that C agrees with a continuous function from $[0,t_F]$ to $L^2(\Omega)$. Taking $v \in H^1(\Omega)$ fixed, we multiply the above equation by $\psi \in C^\infty(0,t_F)$ with $\psi(t_F)=0$, integrate with respect to t to obtain:

$$\int_0^{t_F} \langle C_t, v\rangle\, \psi\, \mathrm{d}t = -\int_0^{t_F} \mathscr{B}[C,v]\psi(t)\,\mathrm{d}t \\ + k_D \int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t + k_B \int_0^{t_F} ((C_B, v))\psi(t)\,\mathrm{d}t.$$

Using statement (iii) from Lemma 1.1 [T, pag 250] and integrating by parts, we have:

$$-\int_0^{t_F} (C,v)\,\psi'\,\mathrm{d}t - (C(0),v)\psi(0) = -\int_0^{t_F} \mathscr{B}[C,v]\psi(t)\,\mathrm{d}t \\ + k_D \int_0^{t_F} ((C_s - C)a, v)\psi(t)\,\mathrm{d}t + k_B \int_0^{t_F} ((C_B, v))\psi(t)\,\mathrm{d}t.$$

Comparing the above equation with (3.20), we obtain $(C(0)-C^0,v)\psi(0)=0$, and thus

$$(C(0)-C^0, v) = 0, \quad \forall v \in H^1(\Omega).$$

and finally $C(0)=C^0$.

Let us see now the equation for a. From (3.2), using the convergences asserted in Theorem (12),

$$(a_t, w) = \left(\beta\left(\min\left\{C,\bar{C}_0\right\} - C_s\right)\sqrt{a_+}, w\right), \quad \forall w \in L^2(\Omega),$$

at almost every $t\in[0,t_F]$. Since a, $a_t \in L^2(0,t_F;L^2(\Omega))$, Lemma 1.1 from [T, pag 250], implies that a is a.e. equal to a continuous function in $C([0,t_F];L^2(\Omega))$. Then, evaluation of the expression (3.18) give us $a(0)=a^0$ in $L^2(\Omega)$.

Thus far, we have proved that the pair (C,a) satisfies $C\in L^2(0,t_F;H^1(\Omega))$ with $C_t \in L^2(0,t_F;H^{-1}(\Omega))$, $a\in H^1(0,t_F;L^2(\Omega))$ and a.e. $t\in[0,t_F]$ it holds

$$\begin{cases} \langle C_t, v\rangle + \mathscr{B}[C,v] = k_D \displaystyle\int_\Omega a(C_s - C)v + k_B C_B \int_{\Gamma_B} v, & \forall v \in H^1(\Omega), \\ \displaystyle\int_\Omega a_t w = \int_\Omega \beta(\min\left\{C,\bar{C}_0\right\} - C_s)\sqrt{a_+}w, & \forall w \in L^2(\Omega), \\ C(0) = C^0, \qquad a(0) = a^0. \end{cases} \tag{3.22}$$

The only difference between this system and (2.7) is the appearance of $\sqrt{a_+}$ instead of $\sqrt{a}$ and $\min\left\{C,\bar{C}_0\right\}$ instead of C in the second equation. Thus, in order to prove that (C,a) is as solution to (2.7) it is sufficient to prove that $a\geq 0$ and $C\leq \bar{C}_0$. This is the goal of the following proposition.

Proposition 13. *Let $a \in L^2(0,t_F;L^2(\Omega))$, $a_t \in L^2(0,t_F;L^2(\Omega))$ and $C \in L^2(0,t_F;H^1(\Omega))$, $C_t \in L^2(0,t_F;H^{-1}(\Omega))$ satisfy (3.22), then $a\geq 0$ and $C \leq \bar{C}_0$, so that $a_+ = a$ and $\min\{C,\bar{C}_0\} = C$ in $\Omega\times[0,t_F]$.*

Proof. $\boxed{1}$ Writing $a = a_+ - a_-$ and testing the second equation in (3.22) with $w = a_-$ we have that,

$$\int_\Omega a_t a_- = \int_\Omega \beta(\min\{C,\bar{C}_0\} - C_s)\sqrt{a_+}a_- = 0,$$

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because a_+ and a_- have disjoint supports. Besides,

$$\int_\Omega a_t a_- = \int_\Omega (a_+ - a_-)_t\, a_- = \int_\Omega (-a_-)_t\, a_- = -\frac{1}{2}\frac{d}{dt}\|a_-(t)\|^2_{L^2(\Omega)}.$$

Therefore, $\frac{1}{2}\frac{d}{dt}\|a_-(t)\|^2_{L^2(\Omega)} = 0$ and $\|a_-(t)\|^2_{L^2(\Omega)} = \|a_-(0)\|^2_{L^2(\Omega)} = \left\|a^0_-\right\|_{L^2(\Omega)} = 0$, because $a^0 \geq 0$, whence $a_- \equiv 0$ and $a \geq 0$.

$\boxed{2}$ Setting $v = \left(C - \bar{C}_0\right)_+$ in the first equation in (3.22), and taking into account that $\bar{C}_0 = \max\left\{\|C^0\|_{L^\infty(\Omega)}, C_s\right\}$ is a constant, we obtain the following equality:

$$\begin{aligned}\langle\left(C-\bar{C}_0\right)_t, \left(C-\bar{C}_0\right)_+\rangle + D\int_\Omega \left|\nabla\left(C-\bar{C}_0\right)_+\right|^2 + k_B\int_{\Gamma_B}(C-C_B)\left(C-\bar{C}_0\right)_+ \\ = \int_\Omega k_D a(C_s - C)\left(C-\bar{C}_0\right)_+,\end{aligned}$$

or equivalently

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\left\|\left(C-\bar{C}_0\right)_+\right\|^2_{L^2(\Omega)} + D\left\|\nabla\left(C-\bar{C}_0\right)_+\right\|^2_{L^2(\Omega)} + k_B\int_{\Gamma_B}(C-C_B)\left(C-\bar{C}_0\right)_+ \\ = \int_\Omega k_D a(C_s - C)\left(C-\bar{C}_0\right)_+.\end{aligned}$$

Since $C_B \leq C_s \leq \bar{C}_0$, at those points where $\left(C-\bar{C}_0\right)_+ \neq 0$ we have $C - \bar{C}_0 > 0$ and then

- $C > \bar{C}_0 \geq C_B$ yields $(C - C_B)\left(C-\bar{C}_0\right)_+ \geq 0$;
- $C > \bar{C}_0 \geq C_s$ implies $(C_s - C)\left(C-\bar{C}_0\right)_+ \leq 0$.

We thereupon conclude that

$$\frac{1}{2}\frac{d}{dt}\left\|\left(C-\bar{C}_0\right)_+\right\|^2_{L^2(\Omega)} \leq 0,$$

and thus, for all $t > 0$,

$$0 \leq \left\|\left(C(t)-\bar{C}_0\right)_+\right\|_{L^2(\Omega)} \leq \left\|\left(C(0)-\bar{C}_0\right)_+\right\|_{L^2(\Omega)} = \left\|\left(C^0-\bar{C}_0\right)_+\right\|_{L^2(\Omega)} = 0,$$

which readily implies $\bar{C}_0 - C \geq 0$ for almost every $x \in \Omega$ and $t > 0$. □

In an analogous way, one can prove that $C^0 \geq C_B$ (resp. $C^0 \geq 0$) implies that $C \geq C_B$ (resp. $C \geq 0$) for almost all $t > 0$ and almost all $x \in \Omega$.

Remark 14. It is important to notice that the same assertion of Proposition 13 holds if we assume that (C, a) is a weak solution of the original problem (2.4). More precisely, if $a \in L^2(0, t_F; L^2(\Omega))$, with $a_t \in L^2(0, t_F; L^2(\Omega))$ and $C \in L^2(0, t_F; H^1(\Omega))$, with $C_t \in L^2(0, t_F; H^{-1}(\Omega))$ satisfy (2.7), then $a \geq 0$ and $C \leq \bar{C}_0$. Also, if $C^0 \geq C_B$ (resp. $C^0 \geq 0$) then $C \geq C_B$ (resp. $C \geq 0$) for almost all $t > 0$ and almost all $x \in \Omega$.

We summarize the results obtained until here in the following theorem:

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Theorem 15 (Existence). *Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with Lipschitz boundary $\partial\Omega = \Gamma_N \cup \Gamma_B$, and D, k_D, k_B and C_B positive constants, $\beta \in L^\infty(\Omega)$, $\beta \geq 0$, $0 \leq C_B \leq C_s$, and $C^0, a^0 \in L^\infty(\Omega)$, $a^0, C^0 \geq 0$. Then there exists a weak solution of (2.4), i.e., there exists a pair (C, a) of functions with $a \in L^2(0, t_F; L^2(\Omega))$, and $C \in L^2(0, t_F; H^1(\Omega))$, satisfying Definition 1. Furthermore, the following estimates are valid:*

$$0 \leq C \leq \bar{C}_0, \quad 0 \leq a, \qquad a.e.\ (x,t) \in \Omega \times [0, t_F], \tag{3.23}$$

and we have a formula for a

$$a(t) = \left(\sqrt{a^0} + \frac{1}{2}\int_0^t \beta\,(C(\tau) - C_s)\,\mathrm{d}\tau\right)_+^2. \tag{3.24}$$

If, moreover, $C^0 \geq C_B$, then $C \geq C_B$.

4 Uniqueness

In this section we will study the uniqueness of solution to problem (2.7). We will consider two situations that only differ in an assumption on C^0 related to the concentration of maximum solubility C_s (or saturation). In the first situation, in which $C^0 \leq C_s$ in Ω we will prove uniqueness, and in the second situation, in which $C^0 > C_s$ in some region of Ω we will show that there could exist at least two solutions.

4.1 Initial concentration below saturation

Theorem 16 (Uniqueness). *If $C^0 \leq C_s$ problem (2.7) has a unique solution.*

Proof. Let (C_1, a_1) and (C_2, a_2) be solutions of (2.7). Then

$$\begin{aligned}\int_\Omega (a_1 - a_2)_t w &= \int_\Omega \beta((C_1 - C_s)\sqrt{a_1} - (C_2 - C_s)\sqrt{a_2})w \\ &= \int_\Omega \beta(C_1 - C_2)\sqrt{a_1} w + \int_\Omega \beta(C_s - C_2)(\sqrt{a_2} - \sqrt{a_1})w,\end{aligned}$$

for all $w \in L^2(\Omega)$ and almost all $t \in [0, t_F]$. Taking $w = a_1 - a_2$ we obtain:

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}\|a_1 - a_2\|^2_{L^2(\Omega)} = &\int_\Omega \beta\sqrt{a_1}(C_1 - C_2)(a_1 - a_2) \\ &+ \int_\Omega \beta(C_s - C_2)(\sqrt{a_2} - \sqrt{a_1})(a_1 - a_2).\end{aligned} \tag{4.1}$$

From the assumption, $\bar{C}_0 = \max\{\|C^0\|_{L^\infty(\Omega)}, C_s\} = C_s$, so that by Remark 14, $0 \leq C_1, C_2 \leq C_s$ a.e., and $C_s - C_2 \geq 0$. Also, as a consequence of the second equation in (2.7), $0 \leq a_1 \leq \|a^0\|_{L^\infty(\Omega)}$. Due to the monotonicity of the square root, $(\sqrt{a_2} - \sqrt{a_1})(a_1 - a_2) \leq 0$, and the second term of (4.1) is less than or equal to zero. Hence

$$\frac{d}{dt}\|a_1 - a_2\|^2_{L^2(\Omega)} \leq \int_\Omega (C_1 - C_2)^2 + \underbrace{\|a^0\|_{L^\infty(\Omega)}\|\beta\|^2_{L^\infty(\Omega)}}_{\mathbb{C}} \int_\Omega (a_1 - a_2)^2. \tag{4.2}$$

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Analogously,

$$\langle (C_1-C_2)_t, v\rangle + \mathscr{B}[C_1-C_2, v] = k_D \int_\Omega (C_s-C_2)(a_1-a_2)v - k_D \int_\Omega (C_1-C_2)a_1 v.$$

Taking $v = C_1 - C_2$ and applying [T, Lemma 1.2, Chapter 3, pag 260] we obtain:

$$\frac{1}{2}\frac{d}{dt}\|C_1 - C_2\|^2_{L^2(\Omega)} \le k_D \int_\Omega (C_s - C_2)(a_1 - a_2)(C_1 - C_2).$$

As we already observed, $0 \le C_2 \le C_s$ and thus $0 \le C_s - C_2 \le C_s$, so that

$$\frac{d}{dt}\|C_1 - C_2\|^2_{L^2(\Omega)} \le k_D^2 C_s^2 \int (C_1 - C_2)^2 + \int (a_1 - a_2)^2. \tag{4.3}$$

Adding (4.2) and (4.3) we obtain

$$\begin{aligned}\frac{d}{dt}&\left[\|a_1 - a_2\|^2_{L^2(\Omega)} + \|C_1 - C_2\|^2_{L^2(\Omega)}\right] \\ &\le \underbrace{\max\left\{1 + k_D^2 C_s^2, 1 + \mathbb{C}\right\}}_{\tilde{\mathbb{C}}} \left[\|a_1 - a_2\|^2_{L^2(\Omega)} + \|C_1 - C_2\|^2_{L^2(\Omega)}\right].\end{aligned}$$

By Gronwall inequality, for all $t \in [0, t_F]$ it holds:

$$\begin{aligned}\|(a_1 - a_2)(t)\|^2_{L^2(\Omega)} &+ \|(C_1 - C_2)(t)\|^2_{L^2(\Omega)} \\ &\le e^{\tilde{\mathbb{C}}t}\left[\|(a_1 - a_2)(0)\|^2_{L^2(\Omega)} + \|(C_1 - C_2)(0)\|^2_{L^2(\Omega)}\right],\end{aligned}$$

and taking into account that (a_1, C_1) and (a_2, C_2) coincide at $t = 0$, we obtain:

$$\|(a_1 - a_2)(t)\|^2_{L^2(\Omega)} + \|(C_1 - C_2)(t)\|^2_{L^2(\Omega)} \le 0,$$

then, $a_1(t) = a_2(t)$ and $C_1(t) = C_2(t)$ in $L^2(\Omega)$ sense for all $t \in [0, t_F]$. □

4.2 Initial concentration above saturation

In this section we show that if $C^0 > C_s$ in some region of the domain, then there could be at least two solutions of problem (2.7). Consider the situation where there exists a set of positive measure $\Omega_0 \subset \Omega$ where $C^0 > C_s + \varepsilon > C_s$, for some $\varepsilon > 0$, and $a^0 \equiv 0$ in Ω. On the one hand, the construction from Section 3 leads to a solution (C_1, a_1) of (2.7) that satisfies the following: Given a set of positive measure $\Omega_1 \subset\subset \Omega_0$, there exists $t_1 > 0$ such that

$$C_1(x,t) > C_s, \quad a_1(x,t) = \left(\frac{1}{2}\int_0^t \beta\left(C_1 - C_s\right)\, \mathrm{d}\tau\right)^2_+, \qquad x \in \Omega_1,\ 0 \le t < t_1,$$

The first claim is a consequence of the continuity of C and the second one follows from formula (3.24). As a consequence, $a_1 > 0$ in Ω_1 for $0 < t < t_1$.

On the other hand, we define $a_2 \equiv 0$ and let C_2 be the weak solution of the following classical initial/boundary problem obtained taking $a \equiv 0$ in (2.4):

$$\begin{cases} C_t - D\Delta C = 0, \text{ in } \Omega \times [0, t_F], \\ C(x, 0) = C^0(x) \text{ in } \Omega, \\ D\nabla C \cdot n = 0 \text{ on } \Gamma_N \times [0, t_F], \\ D\nabla C \cdot n = k_B(C_B - C) \text{ on } \Gamma_B \times [0, t_F]. \end{cases} \tag{4.4}$$

Then (C_2, a_2) is also a solution of (2.7), which is clearly different from (C_1, a_1).

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Remark 17. It is neccesary that $C^0 > C_s$ in some region of the domain. In the previous subsection we consider the case $C^0 \le C_s$, and we showed uniqueness of solution, regardless of the initial condition for a; with the only assumption $a^0 \ge 0$. If $C^0 \le C_s$ and $a^0 \equiv 0$, the problem (2.4) has a unique solution and it is the pair conformed by $a \equiv 0$ and C the unique solution of (4.4).

We conjecture that there could be multiple solutions when $C^0 > C_s$ in a subset of positive Lebesgue measure even if $a^0 > 0$ almost everywhere in Ω. We believe that the following situation is feasible: If a^0 is small where $C^0 < C_s$, then a will decrece and could be attain zero value in finite time in that region. At the same time, by diffusion, the concentration C could grow up in that region. Then, it could happen that at a certain time $t > 0$ there will be a region of positive measure contained in Ω, where $a(\cdot, t) = 0$ and $C(\cdot, t) > C_s$. From this point on there could be two solutions like the ones presented above.

5 Regularity

In this section we present regularity results for the solution (C, a) of problem (2.7) under the hypothesis that guarantee unique solution; from now on we assume, without stating it explicitely, that $C^0 \le C_s$, so that $\bar{C}_0 = C_s$. Theorem 15 implies that $0 \le C \le C_s$, $0 \le a \le \|a^0\|_{L^\infty(\Omega)}$ and (3.24) holds.

A similar bound holds for the Galerkin approximations a_n from Section 3. Since $\min\{C_n, C_s\} - C_s = -(C_s - C_n)_+$, the right-hand side of equation (3.9) for the time derivative of $\alpha_T^n = a_n(t)_{|T}$ is ≤ 0. Then, from the definition of $a_n(0)$ in (3.3) we conclude that,

$$\|a_n\|_{L^\infty(0,t_F;L^\infty(\Omega))} \le \|a^0\|_{L^\infty(\Omega)} + 2 =: A_0, \tag{5.1}$$

From now on we assume that the assumptions of Theorems 15 and 16 hold and (C, a) denotes the unique weak solution to (2.4). In each of the statements that follow, we only mention the additional assumptions that imply further regularity.

Proposition 18. *The time derivative of $\sqrt{a}$ exists and satisfies*

$$(\sqrt{a})_t = -\frac{1}{2}(C_s - C)\chi_{\{\sqrt{a}>0\}} \in L^2(0, t_F; L^2(\Omega)),$$

that is, $\sqrt{a} \in H^1(0, t_F; L^2(\Omega))$; also $(\sqrt{a})_t \in L^\infty(0, t_F; L^\infty(\Omega))$.

Proof. From (3.24) we have that $\sqrt{a} = \left(\sqrt{a^0} - \frac{1}{2}\int_0^t \beta(C_s - C)\,\mathrm{d}\tau\right)_+$. Since $C \in L^2(0, t_F; H^1(\Omega))$,

$$\frac{\partial}{\partial t}\sqrt{a} = -\frac{1}{2}\beta(C_s - C)\chi_{\{\sqrt{a^0} - \frac{1}{2}\int_0^t \beta(C_s - C)\,\mathrm{d}\tau > 0\}} = -\frac{1}{2}\beta(C_s - C)\chi_{\{\sqrt{a}>0\}},$$

in the weak sense in $\Omega \times (0, t_F)$, which in turn implies that $\sqrt{a} \in H^1(0, t_F; L^2(\Omega))$ and $(\sqrt{a})_t = -\frac{1}{2}(C_s - C)\chi_{\{\sqrt{a}>0\}}$. Besides, for a fixed t

$$\|(\sqrt{a})_t\|_{L^\infty(\Omega)} \le \frac{1}{2}\|\beta\|_{L^\infty(\Omega)}\|(C_s - C)\|_{L^\infty(\Omega)} \le \frac{1}{2}C_s\|\beta\|_{L^\infty(\Omega)},$$

due to Theorem 15, whence $(\sqrt{a})_t \in L^\infty(0, t_F; L^\infty(\Omega))$. □

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In the next proposition we prove that the spatial regularity of a and $\sqrt{a}$ is higher if $\sqrt{a^0}$ and β are also more regular. It is worth mentioning though, that since there are no space derivatives in the equation for a, there is no regularizing effect. On the other hand, the appearance of $\sqrt{a}$ on the right-hand side of the equation for a_t is responsible of two issues. The value of a reaches zero at finite time, and the space regularity of $\sqrt{a}$ (resp. a) cannot be higher than $H^1(\Omega)$ (resp. $H^2(\Omega)$) after that time instant.

Proposition 19. *If $\sqrt{a^0}, \beta \in L^\infty(\Omega) \cap H^1(\Omega)$, then $\sqrt{a}$, $a \in L^2(0, t_F; H^1(\Omega))$.*

Proof. From the assumption on β and the fact that $C \in L^2(0, t_F; H^1(\Omega)) \cap L^2(0, t_F; L^\infty(\Omega))$, we have $\beta\,(C_s - C) \in L^2(0, t_F; H^1(\Omega))$, and $\int_0^t \beta(C_s - C) \in L^\infty(0, t_F; H^1(\Omega))$, with $\frac{\partial}{\partial x_i} \int_0^t \beta(C_s - C) = \int_0^t \frac{\partial}{\partial x_i} (\beta(C_s - C))$. Thus, for a fixed $t \in [0, t_F]$, due to (3.24)

$$\frac{\partial}{\partial x_i}\sqrt{a} = \left(\frac{\partial}{\partial x_i}\sqrt{a^0} - \frac{1}{2}\int_0^t \frac{\partial}{\partial x_i}\left(\beta(C_s - C)(\tau)\right) \mathrm{d}\tau \right) \chi_{\{\sqrt{a}>0\}},$$

and $\sqrt{a} \in L^2(0, t_F; H^1(\Omega))$.

Since $a = (\sqrt{a})^2$ and $\sqrt{a(t)} \in L^\infty(\Omega) \cap H^1(\Omega)$, for each t, we have $\frac{\partial}{\partial x_i} a = 2\sqrt{a}\frac{\partial}{\partial x_i}\sqrt{a}$. Now, $\sqrt{a} \in L^\infty(0, t_F; L^\infty(\Omega)) \cap L^2(0, t_F; H^1(\Omega))$yields $\frac{\partial}{\partial x_i} a \in L^2(0, t_F; L^2(\Omega))$ and thus $a \in L^2(0, t_F; H^1(\Omega))$. □

Theorem 20. *If $C^0 \in H^1(\Omega)$, then*

$$C \in L^\infty(0, t_F; H^1(\Omega)), \quad C_t \in L^2(0, t_F; L^2(\Omega)),$$

and the following estimate holds

$$\begin{aligned}
\mathbb{C}_1 \|C(t)\|^2_{L^\infty(0,t_F;H^1(\Omega))},\ & \|C_t\|^2_{L^2(0,t_F;L^2(\Omega))} \\
&\le 4k_D^2 \frac{\mathbb{C}_5}{\mathbb{C}_4} A_0^4 |\Omega| t_F \\
&\quad + 4k_D^2 A_0^2 \left(\frac{k_B}{\mathbb{C}_4} C_B^2 |\Gamma_B| t_F + \frac{1}{\mathbb{C}_4} \|C^0\|^2_{H^1(\Omega)} + C_s^2 |\Omega| t_F \right) \\
&\quad + 4\mathbb{C}_2 \|C^0\|^2_{H^1(\Omega)} + 2(2\mathbb{C}_2 + \mathbb{C}_1) C_B^2 |\Omega|.
\end{aligned}$$

Proof. Let (C_n, a_n) be the solution of problem (3.1)–(3.3) with C_n^0 taken as the H^1-projection of C^0 on V_n. This choice of C_n^0 also leads to a sequence satisfying analogous bounds to those of Section 3 and to a subsequence converging to the same solution (C, a). Since C_B is constant (3.1) also reads

$$(C_{n,t}, v) + \mathscr{B}\left[(C_n - C_B), v\right] = k_D \int_\Omega a_n (C_s - C_n)\, v, \quad \forall v \in V_n.$$

Thus, testing with $v = (C_n - C_B)_t = C_{n,t}$,

$$\begin{aligned}
\|C_{n,t}\|^2 + \frac{1}{2}\frac{d}{dt}\mathscr{B}\left[C_n - C_B, C_n - C_B\right] &= k_D \int_\Omega a_n (C_s - C_n)\, C_{n,t} \\
&\le \frac{k_D^2}{2} \|a_n\|^2_{L^\infty(0,t_F;L^\infty(\Omega))} \|C_s - C_n\|^2_{L^2(\Omega)} + \frac{1}{2}\|C_{n,t}\|^2_{L^2(\Omega)}.
\end{aligned}$$

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Integrating from 0 to t, with $t \leq t_F$, using estimate (5.1) and Remark 2,

$$\begin{aligned}\int_0^t \|C_{n,t}\|^2_{L^2(\Omega)} + \mathbb{C}_1\|C_n(t) - C_B\|^2_{H^1(\Omega)} \leq 2k_D^2 A_0^2 \|C_n\|^2_{L^2(0,t;L^2(\Omega))} \\ + 2k_D^2 A_0^2 C_s^2 |\Omega| t \\ + \mathbb{C}_2 \|C_n(0) - C_B\|^2_{H^1(\Omega)}.\end{aligned}$$

Combining this with (3.6), (5.1) and the fact that $\|C_n(0)\|_{H^1(\Omega)} \leq \|C^0\|_{H^1(\Omega)}$,

$$\begin{aligned}&\int_0^t \|C_{n,t}\|^2_{L^2(\Omega)} + \frac{\mathbb{C}_1}{2}\|C_n(t)\|^2_{H^1(\Omega)} - \mathbb{C}_1 C_B^2|\Omega| \\ &\quad \leq 2k_D^2 A_0^2 \left(\frac{1}{\mathbb{C}_4}\|C^0\|^2_{H^1(\Omega)} + \frac{\mathbb{C}_5}{\mathbb{C}_4} A_0^2 |\Omega| t_F + \frac{k_B}{\mathbb{C}_4} C_B^2 |\Gamma_B| t_F \right) \\ &\quad\quad + 2k_D^2 A_0^2 C_s^2 |\Omega| t_F + 2\mathbb{C}_2\|C^0\|^2_{H^1(\Omega)} + 2\mathbb{C}_2 C_B^2|\Omega|.\end{aligned}$$

This last bound carries over to the limit as $n \to \infty$ yielding the desired assertion. $\square$

Assuming more regularity of C^0 and compatibility with the boundary conditions we can prove higher regularity of the concentration variable C.

Proposition 21. *Let $C^0 \in H^2(\Omega)$, $D\frac{\partial C^0}{\partial n} = 0$ on Γ_N, $D\frac{\partial C^0}{\partial n} = k_B(C_B - C^0)$ on Γ_B, then $C_t \in L^\infty(0, t_F; L^2(\Omega)) \cap L^2(0, t_F; H^1(\Omega))$ and $C_{tt} \in L^2(0, t_F; H^{-1}(\Omega))$.*

Proof. Let (C_n, a_n) denote the solution of problem (3.1)–(3.3) with $C_n^0 = R_N(C^0)$ taken the Ritz projection of C^0 on V_n, defined in (3.5).

As we observed in the proof of the previous proposition, for all $t \geq 0$,

$$(C_{n,t}, v) + \mathscr{B}[C_n - C_B, v] = (k_D a_n (C_s - C_n), v), \quad \forall v \in V_n. \tag{5.2}$$

At $t = 0$, using that $\mathscr{B}[C_n^0, v] = \mathscr{B}[C^0, v]$ for all $v \in V_n$,

$$(C_{n,t}(0), v) = (k_D a_n(0) (C_s - C_n(0)), v) - \mathscr{B}[C^0 - C_B, v], \quad \forall v \in V_n.$$

Since $C^0 \in H^2(\Omega)$, integration by parts and the compatibility assumption on C^0 imply

$$|\mathscr{B}(C^0 - C_B, v)| \leq D\|C^0\|_{H^2(\Omega)}\|v\|_{L^2(\Omega)}.$$

Since $\|a_n(0)\|_{L^\infty(\Omega)} \leq \|a^0\|_{L^\infty(\Omega)}$ we conclude that there exists a constant $\mathbb{C}$, depending on $\|a^0\|_{L^\infty(\Omega)}$, $\|C^0\|_{H^2(\Omega)}$ and the problem parameters D, k_D, C_s, C_B such that

$$\|C_{n,t}(0)\|_{L^2(\Omega)} \leq \mathbb{C}. \tag{5.3}$$

Taking derivatives respect to t in (5.2) and denoting with $\tilde{C}_n = C_{n,t}$ and $\tilde{a}_n = a_{n,t}$, the following equation holds:

$$(\tilde{C}_{n,t}, v) + \mathscr{B}[\tilde{C}_n, v] = k_D \int_\Omega \tilde{a}_n (C_s - C_n) v - k_D \int_\Omega a_n \tilde{C}_n v, \quad \forall v \in V_n. \tag{5.4}$$

Then

$$(\tilde{C}_{n,t}, \tilde{C}_n) + \mathscr{B}[\tilde{C}_n, \tilde{C}_n] = k_D \int_\Omega \tilde{a}_n (C_s - C_n)\tilde{C}_n - k_D \int_\Omega a_n \tilde{C}_n^2.$$

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The coercivity of the bilinear form $\mathscr{B}$ and the fact that $a_n \geq 0$, imply

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\tilde{C}_n\|^2_{L^2(\Omega)} + \mathbb{C}_1\|\tilde{C}_n\|^2_{H^1(\Omega)} \leq k_D \int_\Omega \tilde{a}_n(C_s - C_n)\tilde{C}_n.$$

Integrating with respect to time and invoking Hölder inequality,

$$\begin{aligned}&\frac{1}{2}\|\tilde{C}_n(t)\|^2_{L^2(\Omega)} + \mathbb{C}_1\int_0^t \|\tilde{C}_n\|^2_{H^1(\Omega)} \\ &\qquad \leq \frac{1}{2}\left\|\tilde{C}_n(0)\right\|^2_{L^2(\Omega)} + k_D\int_0^t\left(\int_\Omega \tilde{a}_n^2(C_s - C_n)^2\right)^{1/2}\left(\int_\Omega \tilde{C}_n^2\right)^{1/2}.\end{aligned}$$

Employing Cauchy inequality,

$$\begin{aligned}&\|\tilde{C}_n(t)\|^2_{L^2(\Omega)} + \mathbb{C}_1\int_0^t \|\tilde{C}_n\|_{H^1(\Omega)} \\ &\qquad \leq \left\|\tilde{C}_n(0)\right\|^2_{L^2(\Omega)} + \frac{k_D^2}{\mathbb{C}_1}\int_0^t\left(\int_\Omega \tilde{a}_n^2(C_s - C_n)^2\right) \\ &\qquad \leq \left\|\tilde{C}_n(0)\right\|^2_{L^2(\Omega)} + \frac{k_D^2}{\mathbb{C}_1}\|\tilde{a}_n\|^2_{L^2(0,t_F;L^\infty(\Omega))}\|C_s - C_n\|^2_{L^\infty(0,t_F;L^2(\Omega))},\end{aligned}$$

Using estimates of Proposition 4 and (5.3),

$$\|\tilde{C}_n\|^2_{L^\infty(0,t_F;L^2(\Omega))} + \mathbb{C}_4\|\tilde{C}_n\|^2_{L^2(0,t_F;H^1(\Omega))} \leq \tilde{\mathbb{C}},$$

with $\tilde{\mathbb{C}}$ a constant independent of n but solely depending on $\|C^0\|_{H^2(\Omega)}$, $\|a^0\|_{L^\infty(\Omega)}$ and problem parameters. Therefore $\{\tilde{C}_n\}$ is a bounded sequence in the reflexive space $L^2(0,t_F;H^1(\Omega))$, whence it has a subsequence converging weakly to C_t. This implies that $C_t \in L^\infty(0,t_F;L^2(\Omega)) \cap L^2(0,t_F;H^1(\Omega))$.

Proceeding as we did to prove (3.21) we arrive at

$$\langle C_{tt}, v\rangle + \mathscr{B}[C_t, v] = k_D\int_\Omega a_t(C_s - C)v - k_D\int_\Omega aC_t v, \quad \forall v \in H^1(\Omega),$$

and the proposition is proved. □

If we assume further regularity of $\partial\Omega$ and that Γ_B and Γ_N are *separated* we can prove more space regularity for C.

Theorem 22. *Assume $C^0 \in H^2(\Omega)$, and $D\frac{\partial}{\partial n}C^0 = 0$ on Γ_N, $D\frac{\partial}{\partial n}C^0 = k_B(C_B - C^0)$ on Γ_B. If $\Omega \subset \mathbb{R}^d$ has a boundary $\Gamma \in C^{1,1}$ such that $\Gamma = \Gamma_B \cup \Gamma_N$ and $\operatorname{dist}\{\Gamma_B, \Gamma_N\} > 0$, then $C \in L^\infty(0,t_F;H^2(\Omega))$.*

Remark 23. The assumption $\operatorname{dist}\{\Gamma_B, \Gamma_N\} > 0$ is only necessary for the existence of $\theta \in C^\infty(\mathbb{R}^d)$ such that $\theta|_{\Gamma_B} = 1$ and $\theta|_{\Gamma_N} = 0$. This will allow for an extension of the boundary values which will in turn permit the use of elliptic regularity to conclude the assertion of the theorem. Many commercial devices have their outer boundary releasing drug to the bulk medium, whereas they have an inner boundary touching a solid elastic core, which is insulating; this assumption is thus fulfilled in practical applications.

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Proof. By Theorem 20 we know that $C \in L^\infty(0,t_F;H^1(\Omega))$, $C_t \in L^2(0,t_F;L^2(\Omega))$ and for almost every $t\in[0,t_F]$, and every $v\in H^1(\Omega)$

$$\begin{cases} \langle C_t, v\rangle + \mathscr{B}[C,v] + k_D\int_\Omega aCv = k_D\int_\Omega aC_s v + k_B C_B \int_{\Gamma_B} v, \\ C(0) = C^0. \end{cases}$$

Let us define $f := k_D C_s a - C_t - k_D aC$. Theorem 20 implies that $f(t)\in L^2(\Omega)$ for almost every $t\in[0,t_F]$, for which $C(t)$ is a weak solution of the following (elliptic) problem:

$$\begin{cases} -D\Delta C = f, & \text{in } \Omega \\ D\dfrac{\partial C}{\partial n} = 0, & \text{on } \Gamma_N, \\ D\dfrac{\partial C}{\partial n} = -k_B(C-C_B), & \text{on } \Gamma_B. \end{cases}$$

Since $\operatorname{dist}\{\Gamma_B,\Gamma_N\} > 0$, there exists $\theta\in C^\infty(\mathbb{R}^d)$ such that $\theta|_{\Gamma_B} = 1$ and $\theta|_{\Gamma_N} = 0$. Let us define $g := -k_B(C-C_B)\theta$. Then $g(t)\in H^1(\Omega)$ for almost every $t\in[0,t_F]$ because $C(t)\in L^\infty(\Omega)\cap H^1(\Omega)$ for almost every $t\in[0,t_F]$ and $\theta\in C^\infty(\mathbb{R}^d)$.

Moreover, for almost all $t\in[0,t_F]$, $\|g\|_{H^1(\Omega)} \le \mathbb{C}\|C\|_{H^1(\Omega)} + \tilde{\mathbb{C}}$ where $\mathbb{C}$, $\tilde{\mathbb{C}}$ depend on θ, C_B and k_B. By construction, $g|_{\Gamma_B} = -k_B(C-C_B)$ and $g|_{\Gamma_N}=0$, and then $C(t)$ is weak solution to

$$\begin{cases} -D\Delta C + C = \tilde{f} := f + C, & \text{in } \Omega \\ D\dfrac{\partial C}{\partial n} = g, & \text{on } \partial\Omega. \end{cases}$$

Finally by Corollary 2.2.2.6 [Gr, pag 92], we have that $C\in H^2(\Omega)$ and

$$\begin{aligned} \|C\|_{H^2(\Omega)} &\le \tilde{\tilde{\mathbb{C}}}\left(\|f+C\|_{L^2(\Omega)} + \|g\|_{H^1(\Omega)}\right) \\ &\le \mathbb{C}\left(\|f\|_{L^2(\Omega)} + \|C\|_{L^2(\Omega)} + \mathbb{C}_1\|C\|_{H^1(\Omega)} + \tilde{\mathbb{C}}\right), \end{aligned}$$

where $\tilde{\tilde{\mathbb{C}}}$ depend on Ω and D. By Proposition 21 and Theorem 20, we have $\|C\|_{L^\infty(0,t_F;H^2(\Omega))}$ is finite. □

It is interesting to note that regularity results for this problem have a limitation due to the presence of $\sqrt{a}$. This terms implies that a vanishes in positive measure sets at finite time, and $a(t)$ does not belong to $H^3(\Omega)$ even if a_0 belongs to $H^\infty(\Omega)$.

Remark 24. A finite element method for solving (2.4) is presented in [CM]. This method consists simply in an implicit Euler time discretization of the Galerkin approximation presented in this article. Optimal a priori error estimates are obtained and presented in [CM] which depend on the regularity results presented here.

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