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A nonlinear model for marble sulphation including surface rugosity and mechanical damage

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ABSTRACT

Here we propose and analyze a mathematical model that aims to describe the marble sulphation process occurring in a given material. The model accounts for rugosity as well as for damaging effects. This model is characterized by some technical difficulties that seem hard to overcome from a theoretical viewpoint. Therefore, we introduce some physically reasonable modifications in order to establish the existence of a suitable notion of solution on a given time interval. Numerical simulations are presented and discussed, also in view of further research.

1. Introduction

Predicting the behavior of monumental stones under weathering and other damage phenomena is a difficult and greatly relevant problem for people working in the field of conservation and restoration of cultural heritage. Several factors contribute to this kind of processes, which are eventually the results of the interaction of various mechanisms, including chemical reactions and mechanically induced stresses, see for instance [1–4].

During the last twenty years advanced mathematical models have been proposed to describe some of these damage phenomena, with a specific focus on chemical aggression. In [5,6], a family of models was introduced to describe the aggression mechanisms due to sulphur dioxide (SO_2), which reacts with calcium carbonate

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of stones to produce, after a possibly complicated chain of reaction, an external layer of gypsum ($CaSO_4$), which is more liable to deteriorate. Other phenomena, as the effect of high permeability, swelling and the effects of humidity, were considered in [7,8]. These models were analyzed in depth in [9–12], where some analytical results were established, also with respect to the qualitative behavior of the materials.

In [13], we studied the same basic sulphation model of [5], but introducing a new coupling between bulk and surface evolution equations to include the effects of surface rugosity, i.e. the local microscopic variation of a surface with respect to a flat configuration.

In the present paper we are going to perform another step in building an effective damage theory of stones, by coupling the chemical effect considered by the model in [13] with elastic damage due to mechanical stress introduced in [14], partially inspired by the results in [15]. For a first attempt to consider a coupling between chemical and mechanical phenomena see also [16], where the alternative Barenblatt–Kachanov framework was considered.

To be more specific, here we consider a monument made of a calcium carbonate stone, located in a smooth bounded domain $\Omega \subseteq \mathbb{R}^3$, with boundary Γ, and subjected to a degradation process during a time interval $(0,T)$, for any given $T>0$. To describe this phenomenon, we introduce the following variables: s is the SO_2 porous concentration inside the material, c stands for the local density of $CaCO_3$, $\mathbf{u}$ accounts for (small) elastic displacements, and χ is a damage parameter. On the boundary Γ we model the rugosity through a variable r (see [13] for more details).

Let us focus on the new unknown χ, which can be interpreted as a macroscopic measure of the state of damage of the material (see [14,15]). More precisely, referring to the phase transition theory (in solids), χ stands for the local proportion of the unbroken bonds at the microscopic level. This means that

- $\chi = 1$ represents completely undamaged material;
- $\chi = 0$ represents completely damaged material;
- $\chi \in (0,1)$ represents intermediate cases.

It is known that damage may be viewed as the losing of stiffness of the material, so that we are assuming that the stiffness matrix degenerates (for the complete damage model) once χ vanishes somewhere.

Let us now introduce some other meaningful physical quantities needed to model the phenomenon. We denote by $\phi(c,\chi)$ the porosity of the material, which depends on the state of the microscopic cohesion as well as on c. We also assume that the diffusion coefficient for the gradient of χ may depend on both χ and c and we denote it by $a(\chi,c)$. The function $w(c,\chi)$ is a cohesive function forcing χ towards 1 and decreasing as $\chi \searrow 0$ and as c decreases (i.e. we suppose that gypsum is less cohesive than marble). The stiffness of the material is assumed degenerating once $\chi = 0$ and equal to χ^2. Following [15], we also take a scalar displacement u for the sake of simplicity. Then a possible model reads as follows

Problem P. Find (s,c,r,χ,u) such that

$$
\begin{aligned}
&\partial_t(\phi(c,\chi)s) - \mathrm{div}\,(\phi(c,\chi)\nabla s) = -\phi(c,\chi)sc, \ \text{ in } \Omega\times(0,T),\\
&\phi(c,\chi)\partial_n s = -\nu(r)(s-s_e), \ \text{ on } \Gamma\times(0,T),\\
&\partial_t c = -\phi(c,\chi)cs, \ \text{ in } \Omega\times(0,T),\\
&\partial_t r + \partial I_{[0,+\infty)}(r) + \Psi'(r) + G(r,c,s,\chi) \ni F, \quad \text{on } \Gamma\times(0,T),\\
&\partial_t\chi - \mathrm{div}\,(a(c,\chi)\nabla\chi) + \partial I_{[0,1]}(\chi) \ni W(\chi,c) - \chi k(c)|\nabla u|^2, \ \text{ in } \Omega\times(0,T),\\
&\partial_n\chi = 0, \quad \text{on } \Gamma\times(0,T),\\
&-\mathrm{div}\,(\chi^2 k(c)\nabla u) = f, \quad \text{in } \Omega\times(0,T),\\
&u = u_\Gamma, \quad \text{on } \Gamma\times(0,T),\\
&s(0)=s_0,\ c(0)=c_0,\ \chi(0)=\chi_0, \quad \text{in } \Omega, \qquad r(0)=r_0, \quad \text{on } \Gamma,
\end{aligned}
$$

where s_e, Ψ, F, f, u_γ, s_0, c_0, χ_0 are given functions and the following relations hold:

$$0 \le c_0(x) \le C_0,\ 0 \le s_0(x) \le S_0,\ \forall x \in \Omega, \tag{1.1}$$

$$r_0 \ge 0,\ \text{on } \Gamma, \quad 0 \le s_e \le S_0,\ \text{on } \Gamma, \tag{1.2}$$

$$0 \le \chi_0(x) \le 1,\ \forall x \in \Omega, \quad \partial_n \chi_0 = 0,\ \text{on } \Gamma, \tag{1.3}$$

$$\phi(c,\chi) = (A + Bc)(1 + \chi_0 - \chi) := \phi_1(c)\phi_2(\chi), \tag{1.4}$$

$$A > 0,\ A + BC_0 > 0,\ B \le (S_0)^{-1}, \tag{1.5}$$

$$a(c,\chi) = (\gamma c + \delta)(\chi + 1),\ \text{with } \gamma\sigma + \delta \ge \gamma_1 > 0, \forall \sigma \in [0, C_0], \tag{1.6}$$

$$k(c) = \alpha c + \beta, \quad \alpha \ge 0, \beta > 0, \tag{1.7}$$

$$W(\chi, c) = \eta c(1 - \chi), \quad \eta > 0, \tag{1.8}$$

$$\nu(\cdot) \ge 0,\ \text{in } \mathbb{R}, \tag{1.9}$$

$$\phi(c_0, \chi_0)\partial_n s_0 = -\nu(r_0)(s_0 - s_e),\ \text{on } \Gamma. \tag{1.10}$$

The function G accounts for the effects of c, s and χ on the rugosity r and satisfies $G(r, 0, s, \chi) = G(r, c, 0, \chi) = 0$. A tentative expression for a function G depending on $\phi_1(c)$ is given in [13, Eq.(5.2)], when G does not depend on χ. The function Ψ is sufficiently smooth and represents a non-monotone potential depending on r. The function F takes into account possible external actions responsible for the formation of rugosity on the boundary, like, for instance, wind, rain or temperature variations, while f stands for the volume forces acting on the body. The existence of a solution to the full problem P seems hard to establish for the following reasons: the too strong dependence of ϕ on χ and of G on its variables and, more importantly, the degeneracy of the stationary equation for u. In the latter case, we observe that the regularity we can obtain for χ seems too low to proceed using known techniques. Therefore we introduce some physically reasonable modifications that allow us to establish the existence of a (weak) solution.

First of all, we replace χ by its time relaxation as follows. Let us take $h > 0$ fixed and introduce $k_h(t) = \frac{1}{h}e^{-t/h}$. Hence, we consider

$$\hat{\chi}(t) = (k_h * \chi)(t) + hk_h(t)\chi_0 = \int_0^t k_h(t-s)\chi(s)\,ds + hk_h(t)\chi_0. \tag{1.11}$$

Remark 1.1. The choice of the variable $\hat{\chi}$ in the porosity ϕ and the diffusion coefficient a corresponds to introduce a time relaxation on the phase variable χ.

Indeed, we could introduce $\hat{\chi}$ as the solution of the initial value problem

$$h\partial_t\hat{\chi} + \hat{\chi} = \chi, \quad \hat{\chi}(0) = \chi_0.$$

We point out that (cf. (1.11))

$$\hat{\chi}(t) \le 1 + \chi_0 - e^{-T/h}, \quad \forall t \in [0, T].$$

Thus, we deduce that

$$1 + \chi_0 - \hat{\chi}(t) \ge e^{-T/h} > 0.$$

Moreover, from (1.4) we can infer that for $c \in [0, C_0]$ there holds

$$\phi(c, \hat{\chi}) \ge \min\{A + BC_0, Ae^{-T/h}\} = m > 0. \tag{1.12}$$

Concerning G we require that it acts as a suitable weak–strong continuous operator with respect to its variables (see (2.10) below). In the equation for u we add the term $\varepsilon|\nabla u|^2\nabla u$ for some fixed $\varepsilon > 0$. Thanks to this penalization of the energy functional, we can handle the degeneracy as well as to have a sufficiently smooth right hand-side in the evolution equation for χ (cf. [15] where a quadratic penalization suffices). Once we prove the existence of a solution, we shall also analyze what happens when ε goes to 0 along the lines of [15]. Summing up, we consider the following regularized problem

Problem P_ε. Find (s, c, r, χ, u) such that

$$
\begin{aligned}
&\partial_t(\phi(c,\hat{\chi})s) - \text{div }(\phi(c,\hat{\chi})\nabla s) = -\phi(c,\hat{\chi})sc, \quad \text{in } \Omega \times (0,T),\\
&\phi(c,\hat{\chi})\partial_n s = -\nu(r)(s - s_e), \quad \text{on } \Gamma \times (0,T),\\
&\partial_t c = -\phi(c,\hat{\chi})cs, \quad \text{in } \Omega \times (0,T),\\
&\partial_t r + \partial I_{[0,+\infty)}(r) + \Psi'(r) + G(r,c,s,\chi) \ni F, \quad \text{on } \Gamma \times (0,T),\\
&\partial_t \chi - \text{div }(a(c,\hat{\chi})\nabla\chi) + \partial I_{[0,1]}(\chi) \ni W(\chi,c) - \chi k(c)|\nabla u|^2, \quad \text{in } \Omega \times (0,T),\\
&\partial_n \chi = 0, \quad \text{on } \Gamma \times (0,T),\\
&-\text{ div }(\varepsilon|\nabla u|^2\nabla u + \chi^2 k(c)\nabla u) = f, \quad \text{in } \Omega \times (0,T),\\
&u = u_\Gamma, \quad \text{on } \Gamma \times (0,T),\\
&s(0) = s_0,\ \ c(0) = c_0,\ \ \chi(0) = \chi_0, \quad \text{in } \Omega, \qquad r(0) = r_0, \quad \text{on } \Gamma.
\end{aligned}
$$

Our main theoretical result is the existence of a suitable notion of solution to problem P_ε. Then we discuss the limit case $\varepsilon \searrow 0$ and we propose and investigate some numerical simulations.

The plan of the paper is as follows. In the next section we report our main assumptions, we define a suitable notion of solution for problem P_ε and we state our main result. Section 3 is devoted to the time discretization of problem P_ε, by giving a full proof of the existence of these solutions and their uniform bounds. To pass to the limit with respect to the time step, we introduce a standard time interpolation of the discrete solution, to reformulate the problem in a continuum time setting (see Section 3.4). In Section 4, we pass into the limit as the time step $\tau \to 0$ and we find a solution to problem P_ε. What happens as ε goes to 0 is discussed in Section 5. There, making some restrictions, we show that the limit problem has a solution which is weaker than the previous one since a Radon measure (defect measure) appears on the right-hand side of the equation for χ (cf. [15] and below). Finally, in Section 6, some numerical tests are proposed to understand the analytical difficulties given by the lack of regularity of the damage function χ compared with its time relaxation $\hat{\chi}$.

Observe that in the equation for χ the mutual interaction between chemical and mechanical degradation is taken into account as well as the behavior of the nonlinear term $\chi|\nabla u|^2$. Actually, according to [15], the so-called internal stress $\sqrt{\chi}\nabla u$ is a good descriptor of the internal behavior of the material. The lack of strong convergence for such a term when ε goes to 0 yields a supplementary term, called defect measure, on the right-hand side of the equation for χ, which corresponds to the emergence of a full damage, namely a set where $\chi = 0$. The localization of this set was analyzed in the case of a pure damage system (see [15]). In our more complicated case this is a possible subject of future investigations.

2. Assumptions and main theorem

In this section we introduce additional assumptions on the data and we formulate the main theorem giving first a rigorous definition of a solution to Problem P_ε.

In addition to the relations (1.1)–(1.10) we consider the following regularity assumptions on the data

$$c_0, s_0 \in H^2(\Omega), \tag{2.1}$$

$$r_0 \in L^2(\Gamma), \quad W(r_0) \in L^1(\Gamma), \tag{2.2}$$

$$s_e \in H^{1/2}(\Gamma), \tag{2.3}$$

$$u_\Gamma \in W^{3/4,4}(\Gamma), \tag{2.4}$$
$$\chi_0 \in H^2(\Omega), \tag{2.5}$$
$$\Psi \in W^{2,\infty}(\mathbb{R}), \tag{2.6}$$
$$F \in L^2(0,T;L^2(\Gamma)), \tag{2.7}$$
$$f \in L^\infty(0,T;L^2(\Omega)), \tag{2.8}$$
$$\nu \in W^{1,\infty}(\mathbb{R}). \tag{2.9}$$

On the account of the above assumptions, note that some inequalities and identities in (1.1)–(1.10) must now be understood almost everywhere.

As far as the function G we suppose

$$\begin{aligned} &G : L^\infty(0,T;L^2(\Gamma))^4 \to L^\infty(0,T;L^2(\Gamma)),\\ &\|G(\mathbf{v})\|_{L^\infty(0,T;L^2(\Gamma))} \le C_G \|\mathbf{v}\|_{L^\infty(0,T;L^2(\Gamma))^4},\\ &\forall\, \mathbf{v}_n \rightharpoonup \mathbf{v} \text{ in } L^2(0,T;L^2(\Gamma))^4 \Rightarrow G(\mathbf{v}_n) \to G(\mathbf{v}) \text{ in } L^2(0,T;L^2(\Gamma)). \end{aligned} \tag{2.10}$$

Remark 2.1. For an analysis on functions G with a regularizing effect on the boundary see for instance the friction models in [17].

Let us denote by $\tilde{u}_\Gamma$ the harmonic extension u_Γ to Ω. We can now formulate our rigorous notion of solution to problem P_ε, namely,

Definition 2.2. $(s, c, r, \chi, \zeta, u)$ is called a solution to problem P_ε if

$$s \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad s \in [0, S_0], \text{ a.e. in } \Omega \times (0,T), \tag{2.11}$$
$$c \in W^{1,\infty}(0,T;L^\infty(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad c \in [0, C_0], \text{ a.e. in } \Omega \times (0,T), \tag{2.12}$$
$$r \in H^1(0,T;L^2(\Gamma)), \quad r \ge 0, \quad \text{a.e. on } \Gamma \times (0,T), \tag{2.13}$$
$$\chi \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad \chi \in [0,1], \text{ a.e. in } \Omega \times (0,T), \tag{2.14}$$
$$\zeta \in L^2(0,T;L^2(\Omega)), \tag{2.15}$$
$$u \in L^\infty(0,T;W^{1,4}(\Omega)), \tag{2.16}$$
$$\begin{aligned} &\int_\Omega \partial_t(\phi(c,\hat{\chi})s)v + \int_\Omega \phi(c,\hat{\chi})\nabla s \cdot \nabla v + \int_\Gamma \nu(r)(s - s_e)v\\ &= -\int_\Omega \phi(c,\hat{\chi})scv, \quad \forall\, v \in H^1(\Omega), \text{ a.e. in } (0,T), \end{aligned} \tag{2.17}$$
$$\partial_t c = -\phi(c,\hat{\chi})cs, \quad \text{a.e. in } \Omega \times (0,T), \tag{2.18}$$
$$\partial_t r + \xi + \Psi'(r) + G(r,c,s,\chi) = F, \quad \xi \in \partial I_{[0,+\infty)}(r), \quad \text{a.e. on } \Gamma \times (0,T), \tag{2.19}$$
$$\begin{aligned} &\int_\Omega \partial_t \chi w + \int_\Omega a(c,\hat{\chi})\nabla\chi \cdot \nabla w + \int_\Omega \zeta w\\ &= \int_\Omega (W(\chi,c) - \chi k(c)|\nabla u|^2)w, \quad \forall\, w \in H^1(\Omega), \quad \text{a.e. in } (0,T), \end{aligned} \tag{2.20}$$
$$\zeta \in \partial I_{[0,1]}(\chi), \quad \text{a.e. on } \Omega \times (0,T), \tag{2.21}$$
$$\begin{aligned} &\int_\Omega (\varepsilon|\nabla u|^2\nabla u + \chi^2 k(c)\nabla u) \cdot \nabla(z - \tilde{u}_\Gamma) = \int_\Omega f(z - \tilde{u}_\Gamma),\\ &\forall\, z \in W^{1,4}(\Omega) \text{ s.t. } z - \tilde{u}_\Gamma \in W^{1,4}_0(\Omega), \quad \text{a.e. in } (0,T), \end{aligned} \tag{2.22}$$
$$s(0) = s_0, \;\; c(0) = c_0, \;\; \chi(0) = \chi_0, \quad \text{a.e. in } \Omega, \qquad r(0) = r_0, \quad \text{a.e. on } \Gamma. \tag{2.23}$$

Our existence result is given by

Theorem 2.3. *Let (1.1)–(1.10) and (2.1)–(2.10) hold. Then problem P_ε has a solution in the sense of Definition 2.2.*

Remark 2.4. In the simplified model [13] damage is not considered, that is, only equations related to the variables s, c, r are analyzed. For the corresponding initial and boundary value problem we proved the existence of a global solution. We take this opportunity to correct a mistake done in [13, 3.3], namely, in (3.25) the Gronwall lemma should be preliminarily used to handle the first and the sixth term on the left-hand side of (3.25).

The proof of Theorem 2.3 is split into two sections. Section 3 is devoted to introduce a time discretization scheme and obtain a number of suitable a priori estimates. These estimates are then used in Section 4 to pass to the limit with respect to the time step and conclude the proof.

3. Time discretization of P_ε

Here and in the following sections, the dependence on ε of the solutions to Problem P_ε and to its discretized version will be omitted for the sake of simplicity.

We introduce $\tau = \frac{T}{N}$, for $N \in \mathbb{N}\setminus\{0\}$ so that we have a partition of $[0,T]$ given by $t_n = n\tau$, $n = 0,\dots,N$.

We first define the discretized convolution by setting

$$\hat{\chi}_0 = \chi_0, \quad \hat{\chi}_i = \tau \sum_{j=1}^{i} (k_h)_{i-j+1}\chi_j + h\chi_0 (k_h)_i, \quad i = 1,\dots,N, \tag{3.1}$$

where $(k_h)_i$ is an approximation of the kernel k_h given by $(k_h)_i = \frac{1}{h} e^{-(i\tau)/h}$. Then, recalling (2.7) and (2.8), we set

$$F_i(\tau) = \frac{1}{\tau}\int_{(i-1)\tau}^{i\tau} F(t)dt, \tag{3.2}$$

and

$$f_i(\tau) = \frac{1}{\tau}\int_{(i-1)\tau}^{i\tau} f(t)dt.$$

Observe that $F_i \in L^2(\Gamma)$ and $f_i \in L^2(\Omega)$ for $i = 1,\dots,N$.

3.1. *Problem P_ε^N*

The discretized version of P_ε can be written as follows.

Problem P_ε^N. Find vectors

$$(s_1,\dots,s_N) \in H^2(\Omega)^N \tag{3.3}$$

$$(c_1,\dots,c_N) \in H^2(\Omega)^N \tag{3.4}$$

$$(r_1,\dots,r_N) \in L^2(\Gamma)^N \tag{3.5}$$

$$(\chi_1,\dots,\chi_N) \in H^1(\Omega)^N \tag{3.6}$$

$$(u_1,\dots,u_N) \in W^{1,4}(\Omega)^N \tag{3.7}$$

such that, for $i = 1,\dots,N$,

$$\chi_i \in [0,1], \quad r_i \geq 0, \quad c_i \in [0, C_0], \quad s_i \in [0, S_0], \tag{3.8}$$

$$\frac{\phi(c_i,\hat{\chi}_i)s_i-\phi(c_{i-1},\hat{\chi}_{i-1})s_{i-1}}{\tau}-\text{div }(\phi(c_{i-1},\hat{\chi}_{i-1})\nabla s_i) \tag{3.9}$$
$$=-\phi(c_{i-1},\hat{\chi}_{i-1})s_{i-1}c_i, \quad \text{a.e. in } \Omega,$$
$$\phi(c_{i-1},\hat{\chi}_{i-1})\partial_n s_i=-\nu(r_i)(s_i-s_e), \quad \text{a.e. on } \Gamma, \tag{3.10}$$
$$\frac{c_i-c_{i-1}}{\tau}=-\phi(c_{i-1},\hat{\chi}_{i-1})c_i s_{i-1}, \quad \text{a.e. in } \Omega, \tag{3.11}$$
$$\frac{r_i-r_{i-1}}{\tau}+\xi_i+\Psi'(r_i)+G(r_{i-1},c_{i-1},s_{i-1},\chi_{i-1})=F_i, \tag{3.12}$$
$$\xi_i\in\partial I_{[0,+\infty)}(r_i), \quad \text{a.e. on } \Gamma,$$
$$\frac{\chi_i-\chi_{i-1}}{\tau}-\text{div }(a(c_{i-1},\hat{\chi}_{i-1})\nabla\chi_i)+\zeta_i=W(\chi_{i-1},c_{i-1})-\chi_i k(c_{i-1})|\nabla u_i|^2, \tag{3.13}$$
$$\zeta_i\in\partial I_{[0,1]}(\chi_i), \quad \text{a.e. in } \Omega,$$
$$\partial_n\chi_i=0, \quad \text{a.e. on } \Gamma, \tag{3.14}$$
$$-\text{div }(\varepsilon|\nabla u_i|^2\nabla u_i+\chi_i^2 k(c_{i-1})\nabla u_i)=f_i, \quad \text{a.e. in } \Omega, \tag{3.15}$$
$$u_i=u_\Gamma, \quad \text{a.e. on } \Gamma, \tag{3.16}$$

where (s_0,c_0,r_0,χ_0) satisfies (2.1), (2.2), and (2.5).

3.2. Existence of a discrete solution

We proceed by induction on i. Thus, we suppose to know

$$(s_j,c_j,r_j,\chi_j,u_j)\in H^2(\Omega)\times H^2(\Omega)\times L^2(\Gamma)\times H^2(\Omega)\times W^{1,4}(\Omega), \tag{3.17}$$
$$\chi_j\in[0,1], \quad r_j\geq 0, \tag{3.18}$$
$$c_j\in[0,C_0], \quad s_j\in[0,S_0], \tag{3.19}$$

for $j=0,\dots,i-1$. Then we observe that we also know $\hat{\chi}_j$ for $j=0,\dots,i-1$ (see (3.1)). We now look for $(s_i,c_i,r_i,\chi_i,u_i)\in H^2(\Omega)\times H^2(\Omega)\times L^2(\Gamma)\times H^1(\Omega)\times W^{1,4}(\Omega)$ solving (3.8)–(3.16). Note that, since χ_0 and c_0 are given, then u_0 can be introduced as the unique solution to the boundary value problem (see also (1.7))

$$-\text{div }(\varepsilon|\nabla u_0|^2\nabla u_0+\beta\chi_0^2\nabla u_0)=f_0, \text{ a.e. in } \Omega \quad \text{and} \quad u_0=u_\Gamma, \text{ a.e. on } \Gamma.$$

Step 1. Thanks to (3.11) we get $c_i\in H^2(\Omega)$ from

$$c_i\left(\frac{1}{\tau}+\phi(c_{i-1},\hat{\chi}_{i-1})s_{i-1}\right)=\frac{1}{\tau}c_{i-1}. \tag{3.20}$$

Moreover, $c_i\in[0,C_0]$ for any i, since by induction it follows from (3.20) that $c_i\geq 0$ and consequently that $c_i\leq c_{i-1}$. In addition, we can infer from (3.11) that, independently of i,

$$\frac{1}{\tau}\|c_i-c_{i-1}\|_{L^\infty(\Omega)}\leq C. \tag{3.21}$$

Step 2. Let us rewrite (3.12) as follows

$$(Id+\tau\partial W)(r_i)+\tau\Psi'(r_i)\ni r_{i-1}-\tau G(r_{i-1},c_{i-1},s_{i-1},\chi_{i-1})+\tau F_i. \tag{3.22}$$

Using [18, Corollary 2.7] and exploiting the fact that Ψ' is Lipschitz, we get the existence and uniqueness of the solution $r_i\in L^2(\Gamma)$ and $r_i\geq 0$.

Step 3. We now substitute the obtained solution r_i in (3.10) as well as $\hat{\chi}_i$ and c_i in (3.9). Thus, we can solve

$$\phi(c_i,\hat{\chi}_i)s_i - \tau\text{div}\,(\phi(c_{i-1},\hat{\chi}_{i-1})\nabla s_i) = -\tau\phi(c_{i-1},\hat{\chi}_{i-1})s_{i-1}c_i + \phi(c_{i-1},\hat{\chi}_{i-1})s_{i-1} \tag{3.23}$$

equipped with the resulting boundary condition (3.10). Using Lax–Milgram theorem and standard results for elliptic equations, we get that there exists a unique solution $s_i \in H^2(\Omega)$. Moreover, we observe that letting τ sufficiently small, the right hand side of (3.23) turns out to be non negative by induction (see also (1.4)–(1.5)). The positivity of s_i can be proved by a maximum principle argument (it is a standard matter testing the equation by $-(s_i)^-$). Then, we prove that $z_i = s_i - S_0 \le 0$. To this aim we test the following equation

$$\phi(c_i,\hat{\chi}_i)z_i - \tau\text{div}\,(\phi(c_{i-1},\hat{\chi}_{i-1})\nabla z_i) = -\tau\phi(c_{i-1},\hat{\chi}_{i-1})z_{i-1}c_i + \phi(c_{i-1},\hat{\chi}_{i-1})z_{i-1} \tag{3.24}$$

by $(s_i - S_0)^+$. Due to the fact that the right hand side is non-positive by induction (indeed $z_{i-1} \le 0$ once $s_{i-1} \le S_0$) and the fact that the boundary condition turns out to be (see (1.2), (1.9), and (3.10))

$$\phi(c_{i-1},\hat{\chi}_{i-1})\partial_n z_i + \nu(r_i)z_i = -\nu(r_i)(S_0 - s_e), \tag{3.25}$$

we eventually deduce the result and thus $s_i \in [0, S_0]$.

Step 4. Here we aim to solve (3.13)–(3.16) once c_i, r_i, s_i are known. Due to the fact that the two equations are coupled by implicit contributions, we use a fixed point argument.

Suppose $\chi_i = \bar{\chi}_i$ is given in (3.15) and such that

$$\bar{\chi}_i \in L^2(\Omega), \quad \bar{\chi}_i \in [0,1], \text{ a.e. in } \Omega. \tag{3.26}$$

Then standard arguments entail that there exists a unique solution $u_i \in W^{1,4}(\Omega)$ to the resulting equation equipped with (3.16) (see also (2.8)). Thus we can define a map by setting

$$u_i = \mathcal{T}_1(\bar{\chi}_i). \tag{3.27}$$

Recalling that $\tilde{u}_\Gamma$ denotes the harmonic extension of u_Γ, if we test (3.15) by $u_i - \tilde{u}_\Gamma$ then we obtain

$$\begin{aligned}
&\varepsilon\int_\Omega |\nabla u_i|^4 + \int_\Omega \hat{\chi}_i^2 k(c_{i-1})|\nabla u_i|^2 \\
&= \int_\Omega f_i(u_i - \tilde{u}_\Gamma) + \varepsilon\int_\Omega |\nabla u_i|^2 \nabla u_i \nabla \tilde{u}_\Gamma + \int_\Omega \hat{\chi}_i^2 k(c_{i-1})\nabla u_i \nabla \tilde{u}_\Gamma.
\end{aligned}$$

Then, by Young's inequality, we deduce (this estimate holds for any i)

$$\|\nabla u_i\|_{L^4(\Omega)} \le C. \tag{3.28}$$

Note in particular that $\nabla \tilde{u}_{\Gamma_i}$ is bounded in L^2 and that c_{i-1} is uniformly bounded. Observe that C depends on $\varepsilon > 0$.

We can now consider (3.13) with $u_i = \mathcal{T}_1(\bar{\chi}_i)$ and look for a solution to

$$\chi_i - \tau\text{div}\,(a(c_{i-1},\hat{\chi}_{i-1})\nabla\chi_i) + \tau\zeta_i + \tau\chi_i k(c_{i-1})|\nabla u_i|^2 = \chi_{i-1} + \tau W(\chi_{i-1}, c_{i-1}), \tag{3.29}$$

subject to (3.14).

Note that the operator $\tau(\partial I_{[0,1]} + k(c_{i-1})|\nabla u_i|^2 Id)$ is a maximal monotone graph, so that standard results ensure the existence and uniqueness of a solution $\chi_i := \mathcal{T}_2(u_i) \in H^1(\Omega)$. Moreover, it follows that $\chi_i \in [0,1]$

almost everywhere in Ω. In particular, if we test (3.29) by χ_i, exploiting the monotonicity of $\partial I_{[0,1]}$, we find

$$\frac{1}{2}\int_\Omega |\chi_i|^2 + \tau\int_\Omega a(\chi_{i-1},c_{i-1})|\nabla\chi_i|^2 + \int_\Omega \chi_i^2 k(c_{i-1})|\nabla u_i|^2 \\ \leq c(1+\int_\Omega |W(\chi_{i-1},c_{i-1})|^2) \leq c. \tag{3.30}$$

So that we have

$$\|\chi_i\|_{H^1(\Omega)} \leq c. \tag{3.31}$$

Testing (3.29) by ζ_i, using monotonicity arguments and (1.6), we (formally) obtain (see, for instance, [18] for a rigorous justification)

$$\int_\Omega \chi_i\zeta_i \geq 0, \quad \int_\Omega a(\chi_{i-1},c_{i-1})\nabla\chi_i\nabla\zeta_i \geq 0, \quad -\int_\Omega \chi_i k(c_{i-1})\zeta_i|\nabla u_i|^2 \leq 0.$$

Thus, by Young's inequality we finally get

$$\|\zeta_i\|_{L^2(\Omega)} \leq c. \tag{3.32}$$

Moreover, on account of the boundedness of $\chi_i|\nabla u_i|^2$ in $L^2(\Omega)$ (see (3.28) and (3.31)), by comparison in (3.29) we deduce that $-\mathrm{div}\,(a(\chi_{i-1},c_{i-1})\nabla\chi_i)$ is bounded in $(H^1(\Omega))^*$.

We now investigate the properties of the operator $\mathcal{T}(\bar{\chi}_i) = \mathcal{T}_2(\mathcal{T}_1(\bar{\chi}_i))$. We first point out that (3.31) (see also (3.26) and (3.28)) implies that $\mathcal{T}$ is a compact operator in $L^2(\Omega)$. Let us prove that $\mathcal{T}$ is also a continuous operator. Take $\bar{\chi}_{in} \to \bar{\chi}_i$ in $L^2(\Omega)$. Then, by (3.28), the Poincaré inequality and weak compactness results, we infer, up to a (not relabeled) subsequence, that

$$u_{in} := \mathcal{T}_1(\bar{\chi}_{in}) \to u_i \quad \text{weakly in } W^{1,4}(\Omega). \tag{3.33}$$

In addition, we can test Eq. (3.15) written for $\bar{\chi}_{in}$ and u_{in} by $u_{in} - \tilde{u}_\Gamma$. This gives

$$\varepsilon^{1/4}\|\nabla u_{in}\|_{L^4(\Omega)} + \|\bar{\chi}_{in}^2\nabla u_{in}\|_{L^2(\Omega)} \leq c, \tag{3.34}$$

for c independent of n. Hence, after observing that, at least for some subsequence, $\bar{\chi}_{in} \to \bar{\chi}_i$ in $L^s(\Omega)$, for all $s < +\infty$, we find that $\bar{\chi}_{in}$ strongly converges in $L^2(\Omega)$. Thus for some subsequence it also converges almost everywhere in Ω and it is uniformly bounded. On account of this, exploiting (3.33) and (3.34), we can identify the weak limit

$$(\bar{\chi}_{in})\nabla u_{in} \to (\bar{\chi}_i)\nabla u_i \quad \text{weakly in } L^2(\Omega). \tag{3.35}$$

On the other hand, using lower semicontinuity, we find $u_{in} \to u_i$ in $W^{1,4}(\Omega)$. Indeed we know that

$$|\nabla u_{in}|^2\nabla u_{in} \to \mu_i \quad \text{weakly in} (W^{1,4}(\Omega))^*$$

and we can pass to the (weak) limit in Eq. (3.15) written for n. Then, we test it by $u_{in} - \tilde{u}_\Gamma$ and exploit the above weak convergence and lower semicontinuity results. This yields

$$\limsup_{n\to+\infty} \varepsilon\int_\Omega |\nabla u_{in}|^4 \\ \leq -\liminf_{n\to+\infty}\Big(\int_\Omega \bar{\chi}_{in}^2 k(c_{i-1})|\nabla u_{in}|^2 - \int_\Omega f_i(u_{in}-\tilde{u}_\Gamma) \\ -\varepsilon\int_\Omega |\nabla u_{in}|^2\nabla u_{in}\nabla\tilde{u}_\Gamma - \int_\Omega \hat{\chi}_{in}^2 k(c_{i-1})\nabla u_{in}\nabla\tilde{u}_\Gamma\Big) \\ \leq \varepsilon\int_\Omega \mu_i\nabla u_i, \tag{3.36}$$

where we have used the (weak) limit equation. Consequently, by (3.36) we can infer that $\mu_i = |\nabla u_i|^2 \nabla u_i$ and $\int_\Omega |\nabla u_{in}|^4 \to \int_\Omega |\nabla u_i|^4$, so that

$$u_{in} \to u_i \quad \text{in } W^{1,4}(\Omega). \tag{3.37}$$

Writing (3.29) at step n, by (3.31) and (3.32) we deduce (at least for some subsequence)

$$\chi_{in} \to \chi_i \quad \text{strongly in } L^2(\Omega), \tag{3.38}$$

$$\chi_{in} \to \chi_i \quad \text{weakly in } H^1(\Omega), \tag{3.39}$$

$$\zeta_{in} \to \chi_i \quad \text{weakly in } L^2(\Omega). \tag{3.40}$$

On the other hand, by semicontinuity, we can identify $\zeta_i \in \partial I_{[0,1]}(\chi_i)$. Moreover, we get

$$\chi_{in}|\nabla u_{in}|^2 \to \eta \quad \text{weakly in } L^2(\Omega), \tag{3.41}$$

where we identify $\eta = \chi_i|\nabla u_i|^2$ due to the fact that we can extract a subsequence converging almost everywhere in Ω, exploiting (3.37) and (3.38). Thus, we can pass to the limit also in (3.29) as $n \to +\infty$ and identify $\chi_i = \mathcal{T}_2(u_i)$ and thus $\chi_i = \mathcal{T}(\bar{\chi}_i)$. By means of the Schaeffer Theorem, we can ensure the existence of a discrete solution for any i, once τ is fixed.

3.3. Uniform bounds for the discrete solution

We already obtained some bounds which hold for any $i \in \mathbb{N}$. Indeed, from (3.21) we deduce

$$\|c_i\|_{L^\infty(\Omega)} + \left\| \frac{c_i - c_{i-1}}{\tau} \right\|_{L^\infty(\Omega)} \leq C. \tag{3.42}$$

On the other hand, we can rewrite (3.28) in terms of the solution

$$\|u_i\|_{W^{1,4}(\Omega)} \leq C. \tag{3.43}$$

Moreover, due to the definition of $\partial I_{[0,1]}$, we know that $\chi_i \in [0,1]$ almost every where in Ω, for any i.

3.3.1. First estimate

We test (3.12) by r_i. Recalling that $\int_\Gamma \xi_i r_i \geq 0$, we have

$$\begin{aligned} &\frac{1}{2\tau}\int_\Gamma (|r_i|^2 - |r_{i-1}|^2 + |r_i - r_{i-1}|^2) \\ &\leq \int_\Gamma (|\Psi'(r_i)| + |G(r_{i-1}, s_{i-1}, c_{i-1}, \chi_{i-1})| + |F_i|)|r_i|. \end{aligned} \tag{3.44}$$

Then, summing up for $i = 1, \ldots, N$, multiplying by τ and using Young's inequality, we deduce

$$\begin{aligned} &\frac{1}{2}\|r_N\|^2_{L^2(\Gamma)} + \frac{1}{2}\sum_{i=1}^N \int_\Gamma |r_i - r_{i-1}|^2 \\ &\leq \frac{1}{2}\|r_0\|^2_{L^2(\Gamma)} + \frac{1}{4}\|r_N\|^2_{L^2(\Gamma)} \\ &+ \tau^2 \left(\|\Psi'(r_N)\|^2_{L^2(\Gamma)} + \|G(r_{N-1}, s_{N-1}, c_{N-1}, \chi_{N-1})\|^2_{L^2(\Gamma)} + \|F_N\|^2_{L^2(\Gamma)} \right) \\ &+ \tau \sum_{i=1}^{N-1} \left(\|\Psi'(r_i)\|_{L^2(\Gamma)} + \|G(r_{i-1}, s_{i-1}, c_{i-1}, \chi_{i-1})\|_{L^2(\Gamma)} + \|F_i\|_{L^2(\Gamma)} \right) \|r_i\|_{L^2(\Gamma)}. \end{aligned} \tag{3.45}$$

Thus, thanks to the Young inequality, we get for any i

$$\|r_i\|^2_{L^2(\Gamma)} \le C. \tag{3.46}$$

We now test (3.12) by $\frac{r_i - r_{i-1}}{\tau}$. This yields (see (2.6) and (2.7))

$$\begin{aligned} &\int_\Gamma \left|\frac{r_i - r_{i-1}}{\tau}\right|^2 \le \int_\Gamma (|\Psi'(r_i)| + |G(r_i)|)\left|\frac{r_i - r_{i-1}}{\tau}\right| + \int_\Gamma |F_i|\left|\frac{r_i - r_{i-1}}{\tau}\right| \\ &\le \frac{1}{2}\int_\Gamma \left|\frac{r_i - r_{i-1}}{\tau}\right|^2 + C(1 + \int_\Gamma |F_i|^2), \end{aligned} \tag{3.47}$$

where C depends in particular on $\|\Psi'\|_{L^\infty}$ and C_G in (2.10). Here we have also used the fact that by monotonicity we can infer

$$\int_\Gamma \xi_i(r_i - r_{i-1}) \ge 0. \tag{3.48}$$

Summing up (3.47) for $i = 1, \dots, N$, multiplying by τ and recalling (3.2), (2.6) and (2.7), we get

$$\tau \sum_{i=1}^N \left\|\frac{r_i - r_{i-1}}{\tau}\right\|^2_{L^2(\Gamma)} \le C. \tag{3.49}$$

3.3.2. Second estimate

We test (3.9) by s_i. Recalling [19, Proof of Lemma 4.3], observe that there holds

$$\begin{aligned} &\frac{1}{\tau}\int_\Omega \frac{1}{2}\phi(c_i, \hat{\chi}_i)|s_i|^2 - \frac{1}{2}\phi(c_{i-1}, \hat{\chi}_{i-1})|s_{i-1}|^2 \\ &+ \frac{1}{\tau}\int_\Omega \frac{1}{2}\phi(c_{i-1}, \hat{\chi}_{i-1})|s_i - s_{i-1}|^2 + \int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla s_i|^2 \\ &= -\int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1}) s_{i-1} c_i s_i - \frac{1}{\tau}\int_\Omega \frac{1}{2}(\phi(c_i, \hat{\chi}_i) - \phi(c_{i-1}, \hat{\chi}_{i-1}))|s_i|^2 \\ &= -\int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1}) s_{i-1} c_i s_i - \frac{1}{\tau}\int_\Omega B(c_i - c_{i-1})\phi_2(\hat{\chi}_i)|s_i|^2 \\ &- \frac{1}{\tau}\int_\Omega \phi_1(c_{i-1})(\hat{\chi}_i - \hat{\chi}_{i-1})|s_i|^2. \end{aligned} \tag{3.50}$$

On the other hand, we have

$$\begin{aligned} &(\hat{\chi}_i - \hat{\chi}_{i-1}) = \tau(k_h)_1\chi_i + h\chi_0((k_h)_i - (k_h)_{i-1}) \\ &= \frac{\tau}{h}e^{-\frac{i\tau}{h}}\chi_i + \chi_0(e^{-\frac{i\tau}{h}} - e^{-\frac{(i-1)\tau}{h}}). \end{aligned} \tag{3.51}$$

Then, using the mean value theorem, we get

$$|\hat{\chi}_i - \hat{\chi}_{i-1}| \le \tau C. \tag{3.52}$$

Summing up for $i = 1, \dots, N$, multiplying by τ, using (1.4), (3.42), (3.51), (3.52), and the uniform bound on χ_i, we obtain, exploiting Young's inequality,

$$\begin{aligned} &\int_\Omega \frac{1}{2}(\phi(c_N, \hat{\chi}_N)|s_N|^2 - \frac{1}{2}\phi(c_0, \hat{\chi}_0)|s_0|^2) + \sum_{i=1}^N \int_\Omega \frac{1}{2}\phi(c_{i-1}, \hat{\chi}_{i-1})|s_i - s_{i-1}|^2 \\ &+ \tau\sum_{i=1}^N \int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla s_i|^2 + \tau\sum_{i=1}^N \int_\Gamma \nu(r_i)|s_i|^2 \end{aligned} \tag{3.53}$$

$$
\begin{aligned}
&\leq \tau \sum_{i=1}^{N} \int_{\Omega} |\phi(c_{i-1}, \hat{\chi}_{i-1}) s_{i-1} c_i s_i| + C\tau \sum_{i=1}^{N} \int_{\Omega} |\frac{c_i - c_{i-1}}{\tau} \|\phi_2(\hat{\chi}_i)\| s_i|^2 \\
&+ \tau C \sum_{i=1}^{N} \int_{\Omega} |\phi_1(c_{i-1})| |s_i|^2 + \tau \sum_{i=1}^{N} \int_{\Gamma} \nu(r_i) s_i s_e \\
&\leq C\tau \left(\sum_{i=1}^{N} \int_{\Omega} |s_i|^2 + \sum_{i=1}^{N} \int_{\Gamma} \nu(r_i) |s_e|^2 \right) + \frac{\tau}{2} \sum_{i=1}^{N} \int_{\Gamma} \nu(r_i) |s_i|^2.
\end{aligned}
$$

Thus, at least for τ sufficiently small, we infer that

$$
\begin{aligned}
&\int_{\Omega} |s_N|^2 + \sum_{i=1}^{N} \int_{\Omega} |s_i - s_{i-1}|^2 + \tau \sum_{i=1}^{N} \int_{\Omega} |\nabla s_i|^2 + \tau \sum_{i=1}^{N} \int_{\Gamma} |s_i|^2 \\
&\leq C \left(1 + \tau \sum_{i=1}^{N-1} \int_{\Omega} |s_i|^2 \right)
\end{aligned}
\tag{3.54}
$$

and the discrete Gronwall Lemma entails

$$
\|s_i\|_{L^2(\Omega)}^2 + \tau \sum_{i=1}^{N} \|\nabla s_i\|_{L^2(\Omega)}^2 \leq C. \tag{3.55}
$$

3.3.3. Third estimate

We want to test (3.9) by $\frac{s_i - s_{i-1}}{\tau}$. We show the computations term by term. From the first one in the left hand-side we get

$$
\begin{aligned}
&\int_{\Omega} \frac{\phi(c_i, \hat{\chi}_i) s_i - \phi(c_{i-1}, \hat{\chi}_{i-1}) s_{i-1}}{\tau} \left(\frac{s_i - s_{i-1}}{\tau} \right) \\
&= \int_{\Omega} \phi(c_i, \hat{\chi}_i) \left| \frac{s_i - s_{i-1}}{\tau} \right|^2 + \int_{\Omega} (\phi(c_i, \hat{\chi}_i) - \phi(c_{i-1}, \hat{\chi}_{i-1})) \frac{s_{i-1}}{\tau} \left(\frac{s_i - s_{i-1}}{\tau} \right) \\
&= \int_{\Omega} \phi(c_i, \hat{\chi}_i) \left| \frac{s_i - s_{i-1}}{\tau} \right|^2 + \int_{\Omega} B(c_i - c_{i-1}) \phi_2(\hat{\chi}_i) \frac{s_{i-1}}{\tau} \left(\frac{s_i - s_{i-1}}{\tau} \right) \\
&+ \int_{\Omega} \phi_1(c_{i-1}) (\hat{\chi}_i - \hat{\chi}_{i-1}) \frac{s_{i-1}}{\tau} \left(\frac{s_i - s_{i-1}}{\tau} \right).
\end{aligned}
\tag{3.56}
$$

Considering the diffusion term we obtain (see [19, Proof of Lemma 4.3])

$$
\begin{aligned}
&\int_{\Omega} \phi(c_{i-1}, \hat{\chi}_{i-1}) \nabla s_i \nabla \left(\frac{s_i - s_{i-1}}{\tau} \right) \\
&= \int_{\Omega} \phi(c_{i-1}, \hat{\chi}_{i-1}) \frac{1}{2\tau} (|\nabla s_i|^2 - |\nabla s_{i-1}|^2 + |\nabla (s_i - s_{i-1})|^2) \\
&= \frac{1}{2\tau} \int_{\Omega} (\phi(c_i, \hat{\chi}_i) |\nabla s_i|^2 - \phi(c_{i-1}, \hat{\chi}_{i-1}) |\nabla s_{i-1}|^2) \\
&- \frac{1}{2\tau} \int_{\Omega} (\phi(c_i, \hat{\chi}_i) - \phi(c_{i-1}, \hat{\chi}_{i-1})) |\nabla s_i|^2 \\
&+ \frac{1}{2\tau} \int_{\Omega} \phi(c_{i-1}, \hat{\chi}_{i-1}) |\nabla (s_i - s_{i-1})|^2
\end{aligned}
\tag{3.57}
$$

and the contribution of the boundary term is

$$\begin{aligned}
&\int_\Gamma \nu(r_i)(s_i - s_e)\left(\frac{s_i - s_{i-1}}{\tau}\right) \\
&= \int_\Gamma \nu(r_i)(s_i - s_e)\left(\frac{(s_i - s_e) - (s_{i-1} - s_e)}{\tau}\right) \\
&= \int_\Gamma \nu(r_i)\frac{1}{2\tau}(|s_i - s_e|^2 - |s_{i-1} - s_e|^2 + |s_i - s_{i-1}|^2) \\
&= \frac{1}{2\tau}\int_\Gamma (\nu(r_i)|s_i - s_e|^2 - \nu(r_{i-1})|s_{i-1} - s_e|^2) \\
&- \frac{1}{2\tau}\int_\Gamma (\nu(r_i) - \nu(r_{i-1}))|s_{i-1} - s_e|^2 + \frac{1}{2\tau}\int_\Gamma \nu(r_i)|s_i - s_{i-1}|^2.
\end{aligned} \tag{3.58}$$

Combining (3.56)–(3.58), we find

$$\begin{aligned}
&\int_\Omega \phi(c_i, \hat{\chi}_i)\left|\frac{s_i - s_{i-1}}{\tau}\right|^2 + \frac{1}{2\tau}\int_\Omega (\phi(c_i, \hat{\chi}_i)|\nabla s_i|^2 - \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla s_{i-1}|^2) \\
&+ \frac{1}{2\tau}\int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla(s_i - s_{i-1})|^2 \\
&+ \frac{1}{2\tau}\int_\Gamma (\nu(r_i)|s_i - s_e|^2 - \nu(r_{i-1})|s_{i-1} - s_e|^2) + \frac{1}{2\tau}\int_\Gamma \nu(r_i)|s_i - s_{i-1}|^2 \\
&= -\int_\Omega B(c_i - c_{i-1})\phi_2(\hat{\chi}_i)\frac{s_{i-1}}{\tau}\left(\frac{s_i - s_{i-1}}{\tau}\right) \\
&- \int_\Omega \phi_1(c_{i-1})(\hat{\chi}_i - \hat{\chi}_{i-1})\frac{s_{i-1}}{\tau}\left(\frac{s_i - s_{i-1}}{\tau}\right) \\
&+ \frac{1}{2\tau}\int_\Omega (\phi(c_i, \hat{\chi}_i) - \phi(c_{i-1}, \hat{\chi}_{i-1}))|\nabla s_i|^2 + \frac{1}{2\tau}\int_\Gamma (\nu(r_i) - \nu(r_{i-1}))|s_{i-1} - s_e|^2 \\
&- \int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})c_{i-1}s_{i-1}\left(\frac{s_i - s_{i-1}}{\tau}\right).
\end{aligned} \tag{3.59}$$

Then, adding the left hand side of (3.59) for $i = 1, \ldots, N$, multiplying by τ, using (1.12), (3.51), and Young's inequality, we deduce the estimate from below

$$\begin{aligned}
&\tau m \sum_{i=1}^N \int_\Omega \left|\frac{s_i - s_{i-1}}{\tau}\right|^2 + \frac{1}{2}m\int_\Omega |\nabla s_N|^2 - \frac{1}{2}\int_\Omega (\phi(c_0, \hat{\chi}_0))|\nabla s_0|^2 \\
&+ \frac{1}{2}\sum_{i=1}^N \int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla(s_i - s_{i-1})|^2 \\
&+ \frac{1}{2}\int_\Gamma \nu(r_N)|s_N - s_e|^2 - \frac{1}{2}\int_\Gamma (\nu(r_0))|s_0 - s_e|^2 + \frac{1}{2}\sum_{i=1}^N \int_\Gamma \nu(r_i)|s_i - s_{i-1}|^2 \\
&\le \tau \sum_{i=1}^N \int_\Omega \phi(c_i, \hat{\chi}_i)\left|\frac{s_i - s_{i-1}}{\tau}\right|^2 + \frac{1}{2}\int_\Omega (\phi(c_N, \hat{\chi}_N))|\nabla s_N|^2 - \frac{1}{2}\int_\Omega (\phi(c_0, \hat{\chi}_0)stmip)|\nabla s_0|^2 \\
&+ \frac{1}{2}\sum_{i=1}^N \int_\Omega \phi(c_{i-1}, \hat{\chi}_{i-1})|\nabla(s_i - s_{i-1})|^2 \\
&+ \frac{1}{2}\int_\Gamma (\nu(r_N))|s_N - s_e|^2 - \frac{1}{2}\int_\Gamma (\nu(r_0))|s_0 - s_e|^2 + \frac{1}{2}\sum_{i=1}^N \int_\Gamma \nu(r_i)|s_i - s_{i-1}|^2.
\end{aligned} \tag{3.60}$$

Adding now the right hand side of (3.59) for $i = 1, \dots, N$, multiplying by τ, and arguing as above, we infer that it is bounded by

$$\begin{aligned} &\tau \frac{m}{2} \sum_{i=1}^{N} \int_{\Omega} \left| \frac{s_i - s_{i-1}}{\tau} \right|^2 + C\tau \sum_{i=1}^{N} \left(\int_{\Omega} \left| \frac{c_i - c_{i-1}}{\tau} \right|^2 |s_{i-1}|^2 + \int_{\Omega} |s_{i-1}|^2 \right) \\ &+ C\tau \sum_{i=1}^{N} \int_{\Omega} \left(\left| \frac{c_i - c_{i-1}}{\tau} \right| + 1 \right) |\nabla s_i|^2 + \frac{1}{2}\tau \sum_{i=1}^{N} \int_{\Gamma} \|\nu'\|_{L^\infty} \left| \frac{r_i - r_{i-1}}{\tau} \right| |s_{i-1} - s_e|^2. \end{aligned} \tag{3.61}$$

Here we have used the mean value theorem and the following inequality

$$|\phi(c_i, \hat{\chi}_i) - \phi(c_{i-1}, \hat{\chi}_{i-1})| \le C(|c_i - c_{i-1}| + \tau). \tag{3.62}$$

Concerning the last term on the right hand side of (3.61), we have (see (3.49))

$$\begin{aligned} &\frac{\tau}{2} \sum_{i=1}^{N} \int_{\Gamma} \|\nu'\|_{L^\infty} \left| \frac{r_i - r_{i-1}}{\tau} \right| |s_{i-1} - s_e|^2 \\ &\le \frac{\tau}{2} \sum_{i=1}^{N} \|\nu'\|_{L^\infty} \left\| \frac{r_i - r_{i-1}}{\tau} \right\|_{L^2(\Gamma)} \|s_{i-1} - s_e\|^2_{L^4(\Gamma)} \\ &= \frac{\tau}{2} \|\nu'\|_{L^\infty} \left\| \frac{r_1 - r_0}{\tau} \right\|_{L^2(\Gamma)} \|s_0 - s_e\|^2_{L^4(\Gamma)} \\ &+ \frac{\tau}{2} \sum_{i=1}^{N-1} \|\nu'\|_{L^\infty} \left\| \frac{r_{i+1} - r_i}{\tau} \right\|_{L^2(\Gamma)} \|s_i - s_e\|^2_{L^4(\Gamma)}. \end{aligned} \tag{3.63}$$

On account of (3.60) and (3.61), using Sobolev embeddings and trace theorems, and exploiting (3.21), (3.49), (3.55), we infer that

$$\begin{aligned} &\tau \sum_{i=1}^{N} \left\| \frac{s_i - s_{i-1}}{\tau} \right\|^2_{L^2(\Omega)} + \|s_N\|^2_{H^1(\Omega)} \\ &\le C \left(1 + \tau \sum_{i=1}^{N-1} \left(1 + \left\| \frac{c_i - c_{i-1}}{\tau} \right\|_{L^\infty(\Omega)} + \left\| \frac{r_{i+1} - r_i}{\tau} \right\|_{L^2(\Gamma)} \right) \|s_i\|^2_{H^1(\Omega)} \right), \end{aligned} \tag{3.64}$$

so that the discrete Gronwall Lemma yields

$$\tau \sum_{i=1}^{N} \left\| \frac{s_i - s_{i-1}}{\tau} \right\|^2_{L^2(\Omega)} + \|s_i\|^2_{H^1(\Omega)} \le C. \tag{3.65}$$

In addition, a comparison in (3.11) gives

$$\|c_i\|_{H^1(\Omega)} \le C. \tag{3.66}$$

3.3.4. Fourth estimate

We test (3.13) by $\frac{\chi_i - \chi_{i-1}}{\tau}$. Recalling that $\int_\Omega \zeta_i (\chi_i - \chi_{i-1}) \ge 0$, we obtain

$$\begin{aligned} &\int_{\Omega} \left| \frac{\chi_i - \chi_{i-1}}{\tau} \right|^2 + \frac{1}{2\tau} \int_{\Omega} a(c_{i-1}, \hat{\chi}_{i-1}) (|\nabla \chi_i|^2 - |\nabla \chi_{i-1}|^2 + |\nabla(\chi_i - \chi_{i-1})|^2) \\ &\le \int_{\Omega} |W(\chi_{i-1}, c_{i-1})| \left| \frac{\chi_i - \chi_{i-1}}{\tau} \right| + \int_{\Omega} |\chi_i k(c_i)| |\nabla u_i|^2 \left| \frac{\chi_i - \chi_{i-1}}{\tau} \right|. \end{aligned} \tag{3.67}$$

We now multiply by τ, sum for $i = 1, \dots, N$, and use Young's inequality. Thus, we get

$$\begin{aligned}
&\frac{\tau}{2}\sum_{i=1}^{N}\int_{\Omega}\left|\frac{\chi_i-\chi_{i-1}}{\tau}\right|^2+\frac{1}{2}\int_{\Omega}a(c_N,\hat{\chi}_N)(|\nabla\chi_N|^2-\frac{1}{2}\int_{\Omega}a(c_0,\chi_0)|\nabla\chi_0|^2 \\
&+\tau\sum_{i=1}^{N}\int_{\Omega}a(c_{i-1},\hat{\chi}_{i-1})|\nabla(\chi_i-\chi_{i-1})|^2) \\
&\le\frac{\tau}{2}\sum_{i=1}^{N}\int_{\Omega}\left(|W(\chi_{i-1},c_{i-1})|^2+|\chi_i k(c_i)|^2|\nabla u_i|^4\right) \\
&+\tau\sum_{i=1}^{N}\frac{1}{2\tau}\int_{\Omega}(a(c_i,\hat{\chi}_i)-a(c_{i-1},\hat{\chi}_{i-1}))|\nabla\chi_i|^2 \\
&\le\frac{\tau}{2}\sum_{i=1}^{N}\int_{\Omega}\left(|W(\chi_{i-1},c_{i-1})|^2+|\chi_i k(c_i)|^2|\nabla u_i|^4\right) \\
&+\frac{\tau}{2}\sum_{i=1}^{N}C\left(\left|\frac{c_i-c_{i-1}}{\tau}\right|+1\right)|\nabla\chi_i|^2.
\end{aligned} \tag{3.68}$$

Here, we have used (1.6) and the fact that (see (3.51) and (3.62))

$$|a(c_i,\hat{\chi}_i)-a(c_{i-1},\hat{\chi}_{i-1})|\le C(|c_i-c_{i-1}|+\tau). \tag{3.69}$$

Therefore, taking τ sufficiently small, using (1.6), (3.8), (3.42), and (3.43), we infer

$$\begin{aligned}
&\tau\sum_{i=1}^{N}\int_{\Omega}\left|\frac{\chi_i-\chi_{i-1}}{\tau}\right|^2+\int_{\Omega}|\nabla\chi_N|^2+\tau\sum_{i=1}^{N}\int_{\Omega}|\nabla(\chi_i-\chi_{i-1})|^2 \\
&\le C\left(1+\tau\sum_{i=1}^{N-1}|\nabla\chi_i|^2\right),
\end{aligned} \tag{3.70}$$

where $C > 0$ also depends on ε, and the discrete Gronwall Lemma yields

$$\tau\sum_{i=1}^{N}\left\|\frac{\chi_i-\chi_{i-1}}{\tau}\right\|^2_{L^2(\Omega)}+\|\nabla\chi_i\|^2_{L^2(\Omega)}\le C. \tag{3.71}$$

We now (formally) test (3.13) by ζ_i. Exploiting the monotonicity of the subdifferential and (1.6), we deduce that

$$\int_{\Omega}-\mathrm{div}\,(a(c_{i-1},\hat{\chi}_{i-1})\nabla\chi_i)\zeta_i\ge 0.$$

We recall that this argument can be made rigorous by using the Yosida approximation of $\partial I_{[0,1]}$ (see, for instance, [20, 2.2.4]). Arguing as we did for (3.71), we then find

$$\tau\sum_{i=1}^{N}\|\zeta_i\|^2_{L^2(\Omega)}\le C. \tag{3.72}$$

3.4. The interpolation system

Let $(v_i)_{i=0,1,\dots,N}$ be a given vector. We will use the following notation for the related interpolation functions defined on $[0,T]$ (recall that $\tau = T/N$)

$$\bar{v}_\tau(t) = v_i, \tag{3.73}$$

$$\tilde{v}_\tau(t) = v_{i-1}, \tag{3.74}$$

$$v_\tau(0) = v_0, \quad v_\tau(t) = \gamma_i(t)v_i + (1-\gamma_i(t))v_{i-1}, \quad \gamma_i(t) = \frac{t-(i-1)\tau}{\tau}, \tag{3.75}$$

for $t \in ((i-1)\tau, i\tau]$ and $i = 1,\dots,N$. Recalling the discrete system (3.9)–(3.16), we formulate the corresponding continuous version on $[0,T]$

$$\partial_t(\phi(c_\tau,\hat{\chi}_\tau)s_\tau) - \operatorname{div}\,(\phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\nabla\bar{s}_\tau) = -\phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\tilde{s}_\tau\bar{c}_\tau, \quad \text{a.e. in } \Omega\times(0,T), \tag{3.76}$$

$$\phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\partial_n\bar{s}_\tau = -\nu(\bar{r}_\tau)(\bar{s}_\tau - s_e), \quad \text{a.e. on } \Gamma\times(0,T), \tag{3.77}$$

$$\partial_t c_\tau = -\phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\bar{c}_\tau\tilde{s}_\tau, \quad \text{a.e. in } \Omega\times(0,T), \tag{3.78}$$

$$\partial_t r_\tau + \bar{\xi}_\tau + \Psi'(\tilde{r}_\tau) + G(\tilde{r}_\tau,\tilde{c}_\tau,\tilde{s}_\tau,\tilde{\chi}_\tau) = F_\tau, \tag{3.79}$$

$$\bar{\xi}_\tau \in \partial I_{[0,+\infty)}(\bar{r}_\tau), \quad \text{a.e. on } \Gamma\times(0,T),$$

$$\partial_t\chi_\tau - \operatorname{div}\,(a(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\nabla\bar{\chi}_\tau) + \bar{\zeta}_\tau, \tag{3.80}$$

$$= W(\tilde{\chi}_\tau,\tilde{c}_\tau) - \bar{\chi}_\tau k(\tilde{c}_\tau)|\nabla\bar{u}_\tau|^2, \text{ a.e. in } \Omega\times(0,T), \quad \bar{\zeta}_\tau \in \partial I_{[0,1]}(\bar{\chi}_\tau),$$

$$\partial_n\bar{\chi}_\tau = 0, \quad \text{a.e. on } \Gamma\times(0,T), \tag{3.81}$$

$$-\operatorname{div}\,(\varepsilon|\nabla\bar{u}_\tau|^2\nabla\bar{u}_\tau + \bar{\chi}_\tau^2 k(\tilde{c}_\tau)\nabla\bar{u}_\tau) = f_\tau, \quad \text{a.e. in } \Omega\times(0,T), \tag{3.82}$$

$$\bar{u}_\tau = u_\Gamma, \quad \text{a.e. on } \Gamma\times(0,T), \tag{3.83}$$

$$s_\tau(0) = s_0,\ c_\tau(0) = c_0,\ \chi_\tau(0) = \chi_0, \quad \text{a.e. in } \Omega, \qquad r_\tau(0) = r_0, \quad \text{a.e. on } \Gamma. \tag{3.84}$$

Observe that the following estimates hold (see (3.42), (3.43), (3.66), (3.49), (3.65), (3.71))

$$\|s_\tau\|_{H^1(0,T;L^2(\Omega))\cap L^\infty(0,T;H^1(\Omega))} + \|\bar{s}_\tau\|_{L^\infty(0,T;H^1(\Omega))} + \|\tilde{s}_\tau\|_{L^\infty(0,T;H^1(\Omega))} \le C, \tag{3.85}$$

$$\|c_\tau\|_{W^{1,\infty}(0,T;L^\infty(\Omega))\cap L^\infty(0,T;H^1(\Omega))} + \|\bar{c}_\tau\|_{L^\infty(0,T;L^\infty(\Omega))\cap L^\infty(0,T;H^1(\Omega))} \tag{3.86}$$

$$+ \|\tilde{c}_\tau\|_{L^\infty(0,T;L^\infty(\Omega))\cap L^\infty(0,T;H^1(\Omega))} \le C,$$

$$\|r_\tau\|_{H^1(0;T;L^2(\Gamma))} + \|\bar{r}_\tau\|_{L^\infty(0,T;L^2(\Gamma))} + \|\tilde{r}_\tau\|_{L^\infty(0,T;L^2(\Gamma))} \le C, \tag{3.87}$$

$$\|\bar{u}_\tau\|_{L^\infty(0,T;W^{1,4}(\Omega))} \le C, \tag{3.88}$$

$$\|\bar{\chi}_\tau\|_{L^\infty(0,T;L^\infty(\Omega))\cap L^\infty(0,T;H^1(\Omega))} + \|\tilde{\chi}_\tau\|_{L^\infty(0,T;L^\infty(\Omega))\cap L^\infty(0,T;H^1(\Omega))} \le C, \tag{3.89}$$

$$\|\chi_\tau\|_{H^1(0,T;L^2(\Omega))\cap L^\infty(0,T;H^1(\Omega))} \le C. \tag{3.90}$$

Moreover, we get (see (3.8), (3.73), (3.90))

$$\|\chi_\tau\|_{L^\infty(0,T;L^\infty(\Omega))} \le C, \tag{3.91}$$

and, by comparison in (3.79), it follows that

$$\|\bar{\xi}_\tau\|_{L^2(0,T;L^2(\Gamma))} \le C. \tag{3.92}$$

Observe also that (see (3.72))

$$\|\bar{\zeta}_\tau\|_{L^2(0,T;L^2(\Omega))} \le C. \tag{3.93}$$

On the other hand, (3.51) entails

$$\|\hat{\chi}_\tau\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} + \|\tilde{\hat{\chi}}_\tau\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \le C. \tag{3.94}$$

Note that the generic $C > 0$ also depends on ε. Then, arguing as in [21, (4.36)] we deduce that

$$\|s_\tau - \bar{s}_\tau\|_{L^2(0,T;L^2(\Omega))} + \|s_\tau - \tilde{s}_\tau\|_{L^2(0,T;L^2(\Omega))} \le C\sqrt{\tau}, \tag{3.95}$$

$$\|\chi_\tau - \bar{\chi}_\tau\|_{L^2(0,T;L^2(\Omega))} + \|\chi_\tau - \tilde{\chi}_\tau\|_{L^2(0,T;L^2(\Omega))} \le C\sqrt{\tau}, \tag{3.96}$$

$$\|c_\tau - \bar{c}_\tau\|_{L^\infty(0,T;L^2(\Omega))} + \|c_\tau - \tilde{c}_\tau\|_{L^\infty(0,T;L^2(\Omega))} \le C\tau, \tag{3.97}$$

$$\|r_\tau - \bar{r}_\tau\|_{L^\infty(0,T;L^2(\Gamma))} + \|r_\tau - \tilde{r}_\tau\|_{L^\infty(0,T;L^2(\Gamma))} \le C\tau. \tag{3.98}$$

Using now weak–strong compactness results, passing to the limit as $\tau \searrow 0$, up to subsequences, we find $(s, \chi, c, r, u, \xi, \zeta)$ such that

$$s_\tau \rightharpoonup^* s \quad \text{in } H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{3.99}$$

$$\bar{s}_\tau \rightharpoonup^* s \quad \text{in } L^\infty(0,T;H^1(\Omega)), \quad \tilde{s}_\tau \rightharpoonup^* s \quad \text{in } L^\infty(0,T;H^1(\Omega)), \tag{3.100}$$

$$s_\tau \to s \quad \text{in } C^0([0,T];L^q(\Omega)), \quad 2 \le q < 6, \tag{3.101}$$

$$\chi_\tau \rightharpoonup^* \chi \quad \text{in } H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{3.102}$$

$$\bar{\chi}_\tau \rightharpoonup^* \chi, \; \tilde{\chi}_\tau \rightharpoonup^* \chi \quad \text{in } L^\infty(0,T;H^1(\Omega)), \tag{3.103}$$

$$\chi_\tau \to \chi \quad \text{in } C^0([0,T];L^p(\Omega)), \quad 2 \le p < +\infty, \tag{3.104}$$

$$c_\tau \rightharpoonup^* c \quad \text{in } W^{1,\infty}(0,T;L^\infty(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{3.105}$$

$$\bar{c}_\tau \rightharpoonup^* c, \; \tilde{c}_\tau \rightharpoonup^* c \quad \text{in } L^\infty(0,T;L^\infty(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \tag{3.106}$$

$$c_\tau \to c \quad \text{in } C^0([0,T];L^p(\Omega)), \quad 2 \le p < +\infty, \tag{3.107}$$

$$r_\tau \rightharpoonup r \quad \text{in } H^1(0,T;L^2(\Gamma)), \tag{3.108}$$

$$\bar{r}_\tau \rightharpoonup^* r, \; \tilde{r}_\tau \rightharpoonup^* r \quad \text{in } L^\infty(0,T;L^2(\Gamma)), \tag{3.109}$$

$$\bar{u}_\tau \rightharpoonup^* u \quad \text{in } L^\infty(0,T;W^{1,4}(\Omega)), \tag{3.110}$$

$$\bar{\xi}_\tau \rightharpoonup \xi \quad \text{in } L^2(0,T;L^2(\Gamma)), \tag{3.111}$$

$$\bar{\zeta}_\tau \rightharpoonup \zeta \quad \text{in } L^2(0,T;L^2(\Omega)). \tag{3.112}$$

Observe now that there hold

$$\tilde{c}_\tau \to c \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad \bar{c}_\tau \to c \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad 2 \le p < +\infty, \tag{3.113}$$

as $\tau \searrow 0$. Indeed, recalling (3.8), on account of (3.86), (3.97) and (3.107), we obtain

$$\begin{aligned} \int_\Omega |\tilde{c}_\tau - c|^p &\le C\Big(\int_\Omega |\tilde{c}_\tau - c_\tau|^p + \int_\Omega |c_\tau - c|^p\Big) \\ &\le C\Big(\int_\Omega |\tilde{c}_\tau - c_\tau|^{p-2}|\tilde{c}_\tau - c_\tau|^p + \int_\Omega |c_\tau - c|^p\Big) \\ &\le C\Big(\int_\Omega |\tilde{c}_\tau - c_\tau|^2 + \int_\Omega |c_\tau - c|^p\Big) \end{aligned} \tag{3.114}$$

and the right hand side tends to zero as $\tau \searrow 0$. The same calculations can be performed for $\bar{c}_\tau$. Analogously, by means of (3.89), (3.90), (3.91), (3.96), (3.104), we find

$$\tilde{\chi}_\tau \to \chi \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad \bar{\chi}_\tau \to \chi \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad 2 \le p < +\infty. \tag{3.115}$$

In addition, recalling (3.104), we deduce the following

$$\hat{\chi}_\tau \to \hat{\chi} \quad \text{in } C^0([0,T];L^q(\Omega)), \quad 2 \le q < 6. \tag{3.116}$$

In order to prove the strong convergence of r_τ we show that for any sequence $\tau_m \to 0$, $m \to +\infty$, then $r_m := r_{\tau_m}$ defines a Cauchy sequence.

To this aim, using (3.79) we deduce the identity

$$\begin{aligned}&\int_0^t\int_\Gamma \partial_t(r_m-r_n)(r_m-r_n)+\int_0^t\int_\Gamma(\bar{\xi}_m-\bar{\xi}_n)(r_m-r_n)\\&=-\int_0^t\int_\Gamma(\Psi'(\tilde{r}_m)-\Psi'(\tilde{r}_n))(r_m-r_n)\\&-\int_0^t\int_\Gamma(G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n))(r_m-r_n),\end{aligned} \tag{3.117}$$

which entails

$$\begin{aligned}&\frac{1}{2}\int_0^t\frac{d}{dt}\|r_m-r_n\|^2_{L^2(\Gamma)}\le\int_0^t\int_\Gamma|\Psi'(\tilde{r}_m)-\Psi'(\tilde{r}_n)||r_m-r_n|\\&+\int_0^t\int_\Gamma|G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n)||r_m-r_n|.\end{aligned} \tag{3.118}$$

Integrating (3.118) in time and recalling (2.6), we get

$$\begin{aligned}&\frac{1}{2}\|(r_m-r_n)(t)\|^2_{L^2(\Gamma)}\le C\int_0^t\int_\Gamma|\tilde{r}_m-\tilde{r}_n||r_m-r_n|\\&+\int_0^t\int_\Gamma|G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n)||r_m-r_n|\\&\le C\int_0^t\int_\Gamma[(|\tilde{r}_m-r_m|+|\tilde{r}_n-r_n|)|r_m-r_n|+|r_m-r_n|^2]\\&+\int_0^t\|G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n)\|^2_{L^2(\Gamma)}+\int_0^t\|r_m-r_n\|^2_{L^2(\Gamma)}\\&\le C\int_0^t[\|\tilde{r}_m-r_m\|^2_{L^2(\Gamma)}+\|\tilde{r}_n-r_n\|^2_{L^2(\Gamma)}]\\&+\int_0^t\|G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n)\|^2_{L^2(\Gamma)}+\int_0^t\|r_m-r_n\|^2_{L^2(\Gamma)}.\end{aligned} \tag{3.119}$$

Thus an application of Gronwall's Lemma gives

$$\begin{aligned}&\|(r_m-r_n)\|^2_{L^\infty(0,T;L^2(\Gamma))}\le C\Big(\|\tilde{r}_m-r_m\|^2_{L^\infty(0,T;L^2(\Gamma))}+\|\tilde{r}_n-r_n\|^2_{L^\infty(0,T;L^2(\Gamma))}\\&+\|G(\tilde{r}_m,\tilde{c}_m,\tilde{s}_m,\tilde{\chi}_m)-G(\tilde{r}_n,\tilde{c}_n,\tilde{s}_n,\tilde{\chi}_n)\|^2_{L^\infty(0,T;L^2(\Gamma))}\Big).\end{aligned} \tag{3.120}$$

Hence, on account of (2.10), (3.98), (3.100), (3.103), (3.106), and (3.109), we deduce that r_τ is strongly convergent in $L^\infty(0,T;L^2(\Gamma))$. Finally, combining this result again with (3.98) we can conclude that

$$\bar{r}_\tau\to r \quad \text{in } L^\infty(0,T;L^2(\Gamma)),\qquad \tilde{r}_\tau\to r\quad \text{in } L^\infty(0,T;L^2(\Gamma)). \tag{3.121}$$

4. Proof of Theorem 2.3

Here we pass to the limit as $\tau\to 0$ along a suitable subsequence in a convenient reformulation of (3.76)–(3.84). The goal is to show that (s,χ,c,r,u,ξ,ζ), which already satisfies (2.11)–(2.16), solves (2.17)–(2.23). Recalling (1.11), (1.4), and (1.6), we first observe that (3.104), (3.107), and (3.113) imply

$$\begin{aligned}&\phi(c_\tau,\hat{\chi}_\tau)\to\phi(c,\hat{\chi})\quad \text{in } C^0([0,T];L^p(\Omega)),\\&\phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\to\phi(c,\hat{\chi})\quad \text{in } L^\infty(0,T;L^p(\Omega)),\\&a(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\to a(c,\hat{\chi})\quad \text{in } L^\infty(0,T;L^p(\Omega)),\end{aligned} \tag{4.1}$$

where $2 \le p < +\infty$. Let us multiply (3.76) on $\Omega \times (0,T)$ by the test function

$$v(x,t) = \varphi(t)\psi(x), \quad \varphi \in C^\infty([0,T]) : \varphi(T) = 0, \quad \psi \in W^{1,p}(\Omega),\ p > 2.$$

On account of (3.77), we get

$$\begin{aligned} &-\int_0^T\int_\Omega \phi(c_\tau,\hat{\chi}_\tau)s_\tau\partial_t v + \int_0^T\int_\Omega \phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\nabla\bar{s}_\tau\cdot\nabla v \\ &= -\int_0^T\int_\Omega \phi(\tilde{c}_\tau,\tilde{\hat{\chi}}_\tau)\tilde{s}_\tau\bar{c}_\tau v + \int_\Omega \phi(c_\tau,\hat{\chi}_\tau)(0)s_\tau(0)\varphi(0)\psi - \int_0^T\int_\Gamma \nu(\bar{r}_\tau)(\bar{s}_\tau - s_e)v. \end{aligned} \tag{4.2}$$

By means of (3.100), (3.101), (3.113), (3.121), and (4.1), we obtain (see also (2.9))

$$\begin{aligned} &-\int_0^T\int_\Omega \phi(c,\hat{\chi})s\partial_t v + \int_0^T\int_\Omega \phi(c,\hat{\chi})\nabla s\cdot\nabla v \\ &= -\int_0^T\int_\Omega \phi(c,\hat{\chi})scv + \int_\Omega \phi(c,\hat{\chi})(0)s(0)\varphi(0)\psi - \int_0^T\int_\Gamma \nu(r)(s - s_e)v. \end{aligned} \tag{4.3}$$

Thus recalling (2.11)–(2.12) and using a density argument we recover (2.17).

Concerning (3.78), exploiting (3.100), (3.105), (3.113), and (4.1), we easily deduce (2.18). On the other hand, on account of (2.6), (2.7), (2.10), (3.108), (3.111), (3.121), and using a well known result of maximal monotone operator theory (see, e.g., [20, Prop.2.2(iv)]), from (3.79) we deduce (2.19). Let us now multiply (3.82) by $z - \tilde{u}_\Gamma \in W_0^{1,4}(\Omega)$, with $z \in W^{1,4}(\Omega)$. This gives

$$\int_\Omega \varepsilon|\nabla\bar{u}_\tau|^2\nabla\bar{u}_\tau\cdot\nabla(z-\tilde{u}_\Gamma) + \int_\Omega \bar{\chi}_\tau^2 k(\tilde{c}_\tau)\nabla\bar{u}_\tau\cdot\nabla(z-\tilde{u}_\Gamma) = \int_\Omega f_\tau(z-\tilde{u}_\Gamma). \tag{4.4}$$

Observe that, due to (3.110) and (3.88), we have

$$|\nabla\bar{u}_\tau|^2\nabla\bar{u}_\tau \rightharpoonup^* \eta \quad \text{in } L^\infty(0,T;L^{4/3}(\Omega)). \tag{4.5}$$

On the other hand, thanks to (3.96) and (3.115), we get

$$\bar{\chi}_\tau^2 \to \chi^2 \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad 2 \le p < +\infty \tag{4.6}$$

and, owing to (1.7) and (3.113), we deduce

$$k(\tilde{c}_\tau) \to k(c) \quad \text{in } L^\infty(0,T;L^p(\Omega)), \quad 2 \le p < +\infty. \tag{4.7}$$

Hence, from (4.4) we obtain (recalling again (3.110))

$$\int_\Omega \varepsilon\eta\cdot\nabla(z-\tilde{u}_\Gamma) + \int_\Omega \chi^2 k(c)\nabla u\cdot\nabla(z-\tilde{u}_\Gamma) = \int_\Omega f(z-\tilde{u}_\Gamma). \tag{4.8}$$

To identify η we use a well-known argument (see, e.g., [22]). Indeed, first let us take $z = \bar{u}_\tau$ in (4.4). This yields

$$\begin{aligned} \int_\Omega \varepsilon|\nabla\bar{u}_\tau|^4 &= -\int_\Omega \bar{\chi}_\tau^2 k(\tilde{c}_\tau)|\nabla\bar{u}_\tau|^2 \\ &+ \int_\Omega \bar{\chi}_\tau^2 k(\tilde{c}_\tau)\nabla\bar{u}_\tau\cdot\nabla\tilde{u}_\Gamma - \int_\Omega \varepsilon|\nabla\bar{u}_\tau|^2\nabla\bar{u}_\tau\cdot\nabla\tilde{u}_\Gamma + \int_\Omega f_\tau(\bar{u}_\tau - \tilde{u}_\Gamma). \end{aligned} \tag{4.9}$$

Thus we get (cf. (4.5))

$$\limsup_{\tau\to 0}\int_\Omega \varepsilon|\nabla\bar{u}_\tau|^4 \leq -\liminf_{\tau\to 0}\int_\Omega \bar{\chi}_\tau^2 k(\tilde{c}_\tau)|\nabla\bar{u}_\tau|^2 + \int_\Omega \chi^2 k(c)\nabla u\cdot\nabla\tilde{u}_\Gamma - \int_\Omega \varepsilon\eta\cdot\nabla\tilde{u}_\Gamma + \int_\Omega f(u-\tilde{u}_\Gamma). \tag{4.10}$$

Observe now that

$$\bar{\chi}_\tau\sqrt{k(\tilde{c}_\tau)}\nabla\bar{u}_\tau \rightharpoonup z \quad \text{in } L^2(\Omega)$$

and, using strong and weak convergence, we get

$$z = \chi\sqrt{k(c)}\nabla u.$$

Therefore we have

$$\int_\Omega \chi^2 k(c)|\nabla u|^2 \leq \liminf_{\tau\to 0}\int_\Omega \bar{\chi}_\tau^2 k(\tilde{c}_\tau)|\nabla\bar{u}_\tau|^2,$$

so that from (4.10) we deduce

$$\limsup_{\tau\to 0}\int_\Omega \varepsilon|\nabla\bar{u}_\tau|^4 \leq -\int_\Omega \chi^2 k(c)|\nabla u|^2 + \int_\Omega \chi^2 k(c)\nabla u\cdot\nabla\tilde{u}_\Gamma - \int_\Omega \varepsilon\eta\cdot\nabla\tilde{u}_\Gamma + \int_\Omega f(u-\tilde{u}_\Gamma). \tag{4.11}$$

Then, recalling (4.8), we infer

$$\limsup_{\tau\to 0}\int_\Omega \varepsilon|\nabla\bar{u}_\tau|^4 \leq -\int_\Omega \chi^2 k(c)\nabla u\cdot\nabla(u-\tilde{u}_\Gamma) - \int_\Omega \varepsilon\eta\cdot\nabla\tilde{u}_\Gamma + \int_\Omega f(u-\tilde{u}_\Gamma) = \int_\Omega \varepsilon\eta\cdot\nabla u. \tag{4.12}$$

As a consequence, using a monotonicity argument (see, for instance, [22]), we obtain (see (4.5))

$$|\nabla\bar{u}_\tau|^2\nabla\bar{u}_\tau \rightharpoonup^* |\nabla u|^2\nabla u \quad \text{in } L^\infty(0,T;L^{4/3}(\Omega)). \tag{4.13}$$

In addition, we deduce (see, e..g., [18])

$$\nabla\bar{u}_\tau \to \nabla u \quad \text{in } L^4((0,T)\times\Omega). \tag{4.14}$$

Finally, let us write the weak formulation of (3.80) and (3.81), namely,

$$\int_0^t\int_\Omega \partial_t\chi_\tau v + \int_0^t\int_\Omega a(\tilde{c}_\tau,\tilde{\bar{\chi}}_\tau)\nabla\bar{\chi}_\tau\cdot\nabla v + \int_0^t\int_\Omega \bar{\zeta}_\tau v = \int_0^t\int_\Omega w(\tilde{\chi}_\tau,\tilde{c}_\tau)v - \int_0^t\int_\Omega \bar{\chi}_\tau k(\tilde{c}_\tau)|\nabla\bar{u}_\tau|^2 v, \tag{4.15}$$

for any $v\in W^{1,p}(\Omega)$ with $p>2$.

In the first and second term of the left-hand side of (4.15), we pass to the limit thanks to (3.90) and (3.102) and thanks to (3.89) and (4.1), respectively. Similarly, by means of (1.8), (3.113), and (3.115), we pass to the limit in the first term of the right-hand side. On the right-hand side of (4.15), we pass to the limit in the second term making use of (3.104), (4.7), (4.14). To identify the weak limit of $\bar{\zeta}_\tau$ we use (3.112) and (3.115) and standard monotonicity arguments (see, for instance, [18]). Then, using a density argument, we recover (2.22). Initial conditions (2.23) clearly hold (see (3.84)).

5. Letting ε go to 0

The goal of this section is to show that there exists a suitable solution to the problem without penalization in the displacement equation (i.e. $\varepsilon = 0$). We are able to prove this result under some restrictions, namely, we need to suppose $f \equiv 0$ and $\tilde{u}_\Gamma \equiv 0$ and let $a(\cdot,\cdot)$ be a positive constant (see, however, Remark 5.5 below). In order to make the argument rigorous we add a viscosity term in the equation for u, namely, $-\sigma \Delta \partial_t u$ for some given $\sigma > 0$. This can be viewed as a (quasi-static) viscoelastic modification of the elasticity equation. The existence of a solution for the corresponding initial and boundary value problem $P_{\varepsilon,\sigma}$ can be proven arguing as for problem P_ε. Then we proceed to find a priori bounds which are independent of ε and σ. One could let σ go to zero first and showing that a solution to P_ε satisfies the uniform a priori bounds needed to pass to the limit as $\varepsilon \searrow 0$ along a suitable subsequence. However, just for the sake of simplicity, here we take $\sigma = \varepsilon$.

Therefore, let us consider the following modification of problem P_ε.

Problem $P_\varepsilon^\star$. Find (s, c, r, χ, u) such that

$$
\begin{aligned}
&\partial_t(\phi(c,\hat{\chi})s) - \operatorname{div}\,(\phi(c,\hat{\chi})\nabla s) = -\phi(c,\hat{\chi})sc, \quad \text{in } \Omega \times (0,T),\\
&\phi(c,\hat{\chi})\partial_n s = -\nu(r)(s - s_e), \quad \text{on } \Gamma \times (0,T),\\
&\partial_t c = -\phi(c,\hat{\chi})cs, \quad \text{in } \Omega \times (0,T),\\
&\partial_t r + \partial I_{[0,+\infty)}(r) + \Psi'(r) + G(r,c,s,\chi) \ni F, \quad \text{on } \Gamma \times (0,T),\\
&\partial_t \chi - \operatorname{div}\,(a(c,\hat{\chi})\nabla\chi) + \partial I_{[0,1]}(\chi) \ni W(\chi,c) - \chi k(c)|\nabla u|^2, \quad \text{in } \Omega \times (0,T),\\
&\partial_n \chi = 0, \quad \text{on } \Gamma \times (0,T),\\
&-\operatorname{div}\,(-\varepsilon\nabla\partial_t u + \varepsilon|\nabla u|^2\nabla u + \chi^2 k(c)\nabla u) = 0, \quad \text{in } \Omega \times (0,T),\\
&u = 0, \quad \text{on } \Gamma \times (0,T),\\
&s(0) = s_0,\ c(0) = c_0,\ \chi(0) = \chi_0, \quad \text{in } \Omega, \qquad r(0) = r_0, \quad \text{on } \Gamma.
\end{aligned}
$$

We then define a weak solution to Problem $P_\varepsilon^\star$ as follows

Definition 5.1. We call $(s, c, r, \chi, \zeta, u)$ a solution to problem $P_\varepsilon^\star$ if

$$s \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad s \in [0,S_0], \quad \text{a.e. in } \Omega \times (0,T), \tag{5.1}$$

$$c \in W^{1,\infty}(0,T;L^\infty(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad c \in [0,C_0], \quad \text{a.e. in } \Omega \times (0,T), \tag{5.2}$$

$$r \in H^1(0,T;L^2(\Gamma)), \quad r \geq 0, \quad \text{a.e. on } \Gamma \times (0,T), \tag{5.3}$$

$$\chi \in H^1(0,T;H^1(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad \chi \in [0,1], \quad \text{a.e. in } \Omega \times (0,T), \tag{5.4}$$

$$\zeta \in L^2(0,T;L^2(\Omega)), \tag{5.5}$$

$$u \in L^\infty(0,T;W_0^{1,4}(\Omega)) \cap H^1(0,T;H_0^1(\Omega)), \tag{5.6}$$

and

$$
\begin{aligned}
&\int_\Omega \partial_t(\phi(c,\hat{\chi})s)v + \int_\Omega \phi(c,\hat{\chi})\nabla s \cdot \nabla v + \int_\Gamma \nu(r)(s - s_e)v \\
&= -\int_\Omega \phi(c,\hat{\chi})scv, \quad \forall\, v \in H^1(\Omega), \quad \text{a.e. in } (0,T),
\end{aligned} \tag{5.7}
$$

$$\partial_t c = -\phi(c,\hat{\chi})cs, \quad \text{a.e. in } \Omega \times (0,T), \tag{5.8}$$

$$\partial_t r + \xi + \Psi'(r) + G(r,c,s,\chi) = F, \quad \xi \in \partial I_{[0,+\infty)}(r), \quad \text{a.e. on } \Gamma \times (0,T), \tag{5.9}$$

$$\int_\Omega \partial_t \chi w + \int_\Omega a(c,\hat{\chi})\nabla\chi\cdot\nabla w + \int_\Omega \zeta w \tag{5.10}$$
$$= \int_\Omega (W(\chi,c) - \chi k(c)|\nabla u|^2)w, \quad \forall\, w \in H^1(\Omega), \quad \text{a.e. in } (0,T),$$
$$\zeta \in \partial I_{[0,1]}(\chi), \quad \text{a.e. on } \Omega\times(0,T), \tag{5.11}$$
$$\int_\Omega (\varepsilon\nabla\partial_t u + \varepsilon|\nabla u|^2\nabla u + \chi^2 k(c)\nabla u)\cdot\nabla z = 0, \tag{5.12}$$
$$\forall\, z \in W^{1,4}_0(\Omega), \quad \text{a.e. in } (0,T),$$
$$s(0) = s_0,\ c(0) = c_0,\ \chi(0) = \chi_0,\ u(0) = u_{0\varepsilon}, \quad \text{a.e. in } \Omega, \tag{5.13}$$
$$r(0) = r_0, \quad \text{a.e. on } \Gamma. \tag{5.14}$$

The technique used to prove Theorem 2.3 can be easily adapted in this case. More precisely, we can establish the following

Theorem 5.2. *Let (1.1)–(1.10) and (2.1)–(2.10) hold. Suppose, in addition, that*

$$u_0 \in W^{1,4}_{0\varepsilon}(\Omega) \quad s.t.\ \sqrt{\varepsilon}\|u_{0\varepsilon}\|_{W^{1,4}(\Omega)} + \|\chi_0^2 k(c_0)\nabla u_{0\varepsilon}\|_{L^2(\Omega)} \le C, \tag{5.15}$$

where $C > 0$ is independent of ε. Then problem $P^\star_\varepsilon$ has a solution in the sense of Definition 5.1.

The main result of this section is

Theorem 5.3. *Let the assumptions of Theorem 5.2 hold and let $a(\cdot,\cdot) = 1$. Then there exists a suitable subsequence $\{\varepsilon_n\}_{n\in\mathbb{N}}$ converging to 0 such that a sequence of solutions $(s_{\varepsilon_n}, c_{\varepsilon_n}, r_{\varepsilon_n}, \chi_{\varepsilon_n}, \zeta_{\varepsilon_n})$ to $P^\star_\varepsilon$ converges to (s, c, r, χ, ζ) satisfying*

$$s \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad s \in [0,S_0], \quad a.e.\ in\ \Omega\times(0,T), \tag{5.16}$$
$$c \in W^{1,\infty}(0,T;L^\infty(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad c \in [0,C_0], \quad a.e.\ in\ \Omega\times(0,T), \tag{5.17}$$
$$r \in H^1(0,T;L^2(\Gamma)), \quad r \ge 0, \quad a.e.\ on\ \Gamma\times(0,T), \tag{5.18}$$
$$\chi \in H^1(0,T;H^1(\Omega)) \cap L^\infty(0,T;H^1(\Omega)), \quad \chi \in [0,1], \quad a.e.\ in\ \Omega\times(0,T), \tag{5.19}$$
$$\zeta \in L^2(0,T;L^2(\Omega)), \tag{5.20}$$
$$\int_\Omega \partial_t(\phi(c,\hat{\chi})s)v + \int_\Omega \phi(c,\hat{\chi})\nabla s\cdot\nabla v + \int_\Gamma \nu(r)(s-s_e)v \tag{5.21}$$
$$= -\int_\Omega \phi(c,\hat{\chi})scv, \quad \forall\, v \in H^1(\Omega), \quad a.e.\ in\ (0,T),$$
$$\partial_t c = -\phi(c,\hat{\chi})cs, \quad a.e.\ in\ \Omega\times(0,T), \tag{5.22}$$
$$\partial_t r + \xi + \Psi'(r) + G(r,c,s,\chi) = F, \quad \xi \in \partial I_{[0,+\infty)}(r), \quad a.e.\ on\ \Gamma\times(0,T), \tag{5.23}$$
$$\int_\Omega \partial_t\chi w + \int_\Omega \nabla\chi\cdot\nabla w + \int_\Omega \zeta w \tag{5.24}$$
$$= \int_\Omega (W(\chi,c) - \varsigma\cdot\varsigma)w - \int_\Omega w\,d\mu, \quad \forall\, w \in C^\infty_c(\Omega), \quad a.e.\ in\ (0,T),$$
$$\zeta \in \partial I_{[0,1]}(\chi), \quad a.e.\ on\ \Omega\times(0,T), \tag{5.25}$$
$$\int_\Omega \chi^{3/2}\sqrt{k(c)}\varsigma\cdot\nabla z = 0, \quad \forall\, z \in H^1_0(\Omega), \quad a.e.\ in\ (0,T), \tag{5.26}$$
$$s(0) = s_0,\ c(0) = c_0,\ \chi(0) = \chi_0, \quad a.e.\ in\ \Omega, \tag{5.27}$$
$$r(0) = r_0, \quad a.e.\ on\ \Gamma. \tag{5.28}$$

Here μ is a (positive) Radon measure and ς is the $L^2(0,T;(L^2(\Omega))^3)$-weak limit of $\{\sqrt{\chi_{\varepsilon_n} k(c_{\varepsilon_n})}\nabla u_{\varepsilon_n}\}_{n\in\mathbb{N}}$.

Remark 5.4. Theorem 5.2 does not require that f and $\tilde{u}_\Gamma$ vanish. In Theorem 5.3 one may relax the restrictions by assuming that f and $\tilde{u}_\Gamma$ suitably go to 0 as ε goes to 0.

Proof. Let $(s, c, r, \chi, \zeta, u)$ be a solution to $P^\star_\varepsilon$ (we omit its dependence on ε for the sake of simplicity). The first step is to show that this solution satisfies some a priori estimates which are uniform with respect to ε. From now on $C > 0$ stands for a generic constant which is independent of ε.

Observe that the a priori bounds on s, c and χ (see (5.1)–(5.2) and (5.4)) are satisfied and they are independent of ε. These bounds, on account of (1.11) and (5.8), entail

$$\|\hat{\chi}\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \le C, \quad \|c\|_{W^{1,\infty}(0,T;L^\infty(\Omega))} \le C. \tag{5.29}$$

Moreover, recalling (5.9) and using again a result from maximal monotone operator theory (see, e.g., [18, Theo.3.6]), we also have

$$\|r\|_{H^1(0,T;L^2(\Gamma))} \le C. \tag{5.30}$$

Take now $v = s$ in (2.17). This gives

$$\int_\Omega \partial_t(\phi(c,\hat{\chi})s)s + \int_\Omega \phi(c,\hat{\chi})|\nabla s|^2 + \int_\Gamma \nu(r)s^2 = \int_\Gamma \nu(r)s_e s - \int_\Omega \phi(c,\hat{\chi})s^2 c. \tag{5.31}$$

Observe that

$$\int_\Omega \partial_t(\phi(c,\hat{\chi})s)s = \frac{1}{2}\frac{d}{dt}\int_\Omega \phi(c,\hat{\chi})s^2 - \int_\Omega (\phi_1(c,\hat{\chi})\partial_t c + \phi_2(c,\hat{\chi})\partial_t\hat{\chi})s^2. \tag{5.32}$$

Here ϕ_j, $j = 1, 2$, are the first partial derivatives of $\phi(\cdot,\cdot)$. Thus, integrating in time (5.31) and using (5.32), we get

$$\begin{aligned} &\frac{1}{2}\int_\Omega \phi(c,\hat{\chi})s^2 + \int_0^t\int_\Omega \phi(c,\hat{\chi})|\nabla s|^2 + \int_\Gamma \nu(r)s^2 \\ &= \frac{1}{2}\int_\Omega \phi(c_0,\hat{\chi}_0)s_0^2 + \int_0^t\int_\Gamma \nu(r)s_e s - \int_\Omega \phi(c,\hat{\chi})s^2 c \\ &+ \int_0^t\int_\Omega (\phi_1(c,\hat{\chi})\partial_t c + \phi_2(c,\hat{\chi})\partial_t\hat{\chi})s^2. \end{aligned} \tag{5.33}$$

Recalling (1.4) and (2.9), thanks to (5.29) and to Young's inequality and Gronwall's lemma we get

$$\|s\|_{H^1(0,T;L^2(\Omega))\cap L^\infty(0,T;H^1(\Omega))} \le C. \tag{5.34}$$

As we pointed out at the beginning of this proof, we already have a uniform bound in $H^1(0,T;L^2(\Omega))$.

Consider (5.10) and observe that holds almost everywhere in $\Omega \times (0,T)$, namely

$$\partial_t\chi - \Delta\chi = -\zeta + W(\chi, c) - \chi k(c)|\nabla u|^2.$$

This can be viewed as a linear parabolic equation with an L^2 source and an H^1 initial datum satisfying a homogeneous Neumann boundary conditions. Therefore the following identity holds (which can be formally obtained multiplying by $\partial_t\chi$ and integrating in space and time)

$$\int_0^t\int_\Omega |\partial_t\chi|^2+\frac{1}{2}\int_\Omega |\nabla\chi|^2 \\ =\frac{1}{2}\int_\Omega |\nabla\chi_0|^2-\int_0^t\int_\Omega \zeta\partial_t\chi+\int_0^t\int_\Omega (W(\chi,c)-\chi k(c)|\nabla u|^2)\partial_t\chi. \tag{5.35}$$

We can now take $z=\partial_t u$ in (5.12). This entails

$$\int_\Omega \varepsilon|\nabla\partial_t u|^2+\frac{d}{dt}\int_\Omega \frac{\varepsilon}{4}|\nabla u|^4+\int_\Omega \chi^2 k(c)\nabla u\cdot\nabla\partial_t u=0, \tag{5.36}$$

so that

$$\int_\Omega \chi^2 k(c)\nabla u\cdot\nabla\partial_t u=\frac{1}{2}\frac{d}{dt}\int_\Omega \chi^2 k(c)|\nabla u|^2-\frac{1}{2}\int_\Omega \partial_t\left[\chi^2 k(c)\right]|\nabla u|^2, \tag{5.37}$$

but

$$\int_\Omega \partial_t\left[\chi^2 k(c)\right]|\nabla u|^2=\int_\Omega \left[2\chi k(c)\partial_t\chi+\chi^2 k'(c)\partial_t c\right]|\nabla u|^2. \tag{5.38}$$

Thus, thanks to (5.8), we deduce (see also (1.7))

$$\int_\Omega \partial_t\left[\chi^2 k(c)\right]|\nabla u|^2=\int_\Omega \left[2\chi k(c)\partial_t\chi-\alpha\chi^2\phi(c,\hat\chi)cs\right]|\nabla u|^2. \tag{5.39}$$

We now integrate (5.36) in time, taking (5.37) and (5.39) into account. This gives

$$\int_0^t\int_\Omega \varepsilon|\nabla\partial_t u|^2+\int_\Omega \frac{\varepsilon}{4}|\nabla u|^4+\int_\Omega \chi^2 k(c)|\nabla u|^2+\int_0^t\int_\Omega \left[\frac{\alpha}{2}\chi^2\phi(c,\hat\chi)cs\right]|\nabla u|^2 \\ =\int_\Omega \frac{\varepsilon}{4}|\nabla u_{0\varepsilon}|^4+\int_\Omega \chi_0^2 k(c_0)|\nabla u_{0\varepsilon}|^2+\int_0^t\int_\Omega \chi k(c)\partial_t\chi|\nabla u|^2. \tag{5.40}$$

Adding (5.35) and (5.40) together, we obtain

$$\int_0^t\int_\Omega |\partial_t\chi|^2+\frac{1}{2}\int_\Omega |\nabla\chi|^2 \\ +\int_0^t\int_\Omega \varepsilon|\nabla\partial_t u|^2+\int_\Omega \frac{\varepsilon}{4}|\nabla u|^4 \\ +\int_\Omega \chi^2 k(c)|\nabla u|^2+\int_0^t\int_\Omega \left[\frac{\alpha}{2}\chi^2\phi(c,\hat\chi)cs\right]|\nabla u|^2 \\ =\frac{1}{2}\int_\Omega |\nabla\chi_0|^2+\int_\Omega \frac{\varepsilon}{4}|\nabla u_{0\varepsilon}|^4+\int_\Omega \chi_0^2 k(c_0)|\nabla u_{0\varepsilon}|^2 \\ -\int_0^t\int_\Omega \zeta\partial_t\chi+\int_0^t\int_\Omega W(\chi,c)\partial_t\chi. \tag{5.41}$$

Thus the following inequality holds (see (5.11) and (5.15))

$$\int_0^t\int_\Omega \left[|\partial_t\chi|^2+\varepsilon|\nabla\partial_t\chi|^2\right]+\frac{1}{2}\int_\Omega |\nabla\chi|^2 \\ +\int_0^t\int_\Omega \varepsilon|\nabla\partial_t u|^2+\int_\Omega \frac{\varepsilon}{4}|\nabla u|^4+\int_\Omega \chi^2 k(c)|\nabla u|^2 \\ \le C+\int_0^t\int_\Omega W(\chi,c)\partial_t\chi. \tag{5.42}$$

Then, using (5.29) and Gronwall's inequality, we deduce

$$\begin{aligned}&\|\chi\|_{H^1(0,T;L^2(\Omega))\cap L^\infty(0,T;H^1(\Omega))}+\sqrt{\varepsilon}\|\nabla\partial_t u\|_{L^2(0,T;(L^2(\Omega))^3)}\\&+\sqrt{\varepsilon}\|\nabla u\|^2_{L^\infty(0,T;(L^4(\Omega))^3)}+\|\chi\sqrt{k(c)}\nabla u\|_{L^\infty(0,T;(L^2(\Omega))^3)}\le C.\end{aligned} \tag{5.43}$$

Finally, integrating in time (5.8) and taking the gradient of both sides, we find

$$\nabla c(t)=\nabla c_0-\int_0^t\nabla\left[\phi(c,\hat{\chi})cs\right]d\tau. \tag{5.44}$$

Multiplying (5.44) by $\nabla c(t)$ and integrating over Ω, thanks to (5.34) and (5.43), we infer

$$\|\nabla c\|_{L^\infty(0,T;(L^2(\Omega))^3)}\le C,$$

so that

$$\|c\|_{L^\infty(0,T;H^1(\Omega))}\le C. \tag{5.45}$$

Arguing now as in [15, 4.2-3], we obtain

$$\|\zeta\|_{L^2(0,T;L^2(\Omega))}\le C, \tag{5.46}$$

$$\|\sqrt{\chi k(c)}\nabla u\|_{L^2(0,T;L^2(\Omega)^3)}\le C. \tag{5.47}$$

We now have all the ingredients to find a suitable subsequence $\{\varepsilon_n\}_{n\in\mathbb{N}}$ converging to 0 such that $(s_{\varepsilon_n},c_{\varepsilon_n},r_{\varepsilon_n},\chi_{\varepsilon_n},\zeta_{\varepsilon_n})$ converges, as dictated by the above a priori estimates, to (s,c,r,χ,ζ) satisfying (5.16)–(5.20). Moreover, arguing as in the proof of Theorem 2.3 (see 3.4 and Section 4) and using the arguments devised in [15, 4.4], we can prove that (s,c,r,χ,ζ) satisfies (5.21)–(5.28). Let us detail the latter argument. Indeed, up to subsequences, we have that

$$\sqrt{\chi_{\varepsilon_n}k(c_{\varepsilon_n})}\nabla u_{\varepsilon_n}\rightharpoonup\varsigma\ \text{ in }\ L^2(0,T;(L^2(\Omega))^3).$$

Thus, on account of the strong convergences of $\{\chi_{\varepsilon_n}\}_{n\in\mathbb{N}}$ and $\{c_{\varepsilon_n}\}_{n\in\mathbb{N}}$, we obtain

$$\chi_{\varepsilon_n}k(c_{\varepsilon_n})\nabla u_{\varepsilon_n}\rightharpoonup\chi^{3/2}\sqrt{k(c)}\varsigma\ \text{ in }\ L^2(0,T;(L^2(\Omega))^3).$$

Also, recalling [15, 4.4], we find a positive Radon measure (defect measure) μ such that, in the sense of measures,

$$\chi_{\varepsilon_n}k(c_{\varepsilon_n})|\nabla u_{\varepsilon_n}|^2\rightharpoonup\varsigma\cdot\varsigma+\mu.$$

Finally, observing that

$$\varepsilon_n\nabla u_{\varepsilon_n}\to 0\ \text{ in }\ L^2(0,T;(L^2(\Omega))^3),$$

we have all the ingredients to recover (5.24) and (5.26). For the other equations we can proceed in a standard way. ■

Remark 5.5. Observe that, if $a(\cdot,\cdot)$ is given by (1.6) then the second term in (5.35) can be (formally) treated as follows

$$\begin{aligned}\int_\Omega a(c,\hat{\chi})\nabla\chi\cdot\nabla\partial_t\chi&=\frac{1}{2}\int_\Omega a(c,\hat{\chi})\frac{d}{dt}|\nabla\chi|^2\\&=\frac{1}{2}\frac{d}{dt}\int_\Omega a(c,\hat{\chi})|\nabla\chi|^2-\int_\Omega\left[a_1(c,\hat{\chi})\partial_t c+a_2(c,\hat{\chi})\partial_t\hat{\chi}\right]|\nabla\chi|^2.\end{aligned}$$

Here a_j, $j=1,2$, are the first partial derivatives of $a(\cdot,\cdot)$. Therefore, on account of (5.29), we get

$$\begin{aligned}\int_0^t\int_\Omega a(c,\hat{\chi})\nabla\chi\cdot\nabla\partial_t\chi&=\frac{1}{2}\int_\Omega a(c,\hat{\chi})|\nabla\chi(t)|^2-\frac{1}{2}\int_\Omega a(c_0,\hat{\chi}_0)|\nabla\chi_0|^2\\&\le C\int_0^t\int_\Omega|\nabla\chi|^2.\end{aligned}$$

Therefore, one can argue as above.

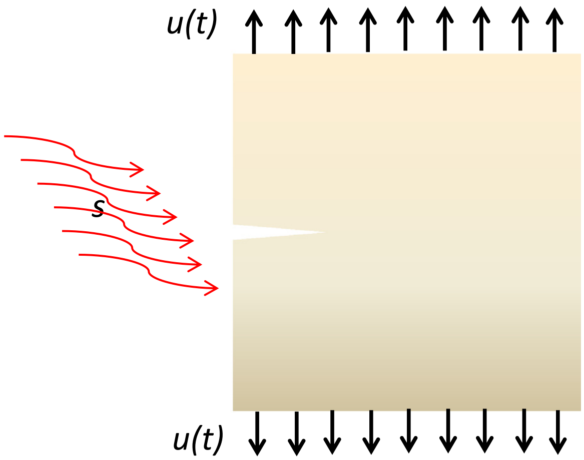


Fig. 1. Notched square marble prism in plane strain condition under tension and attached by pollution.

6. Numerical simulations

In this section some numerical simulations are performed with the aim to illustrate the capability of the proposed approach. In particular, our attention is focused on estimating the influence of considering $\hat{\chi}$ defined in (1.11) instead of χ and to validate the convergence result of (3.41). For this purpose, a simplified version of problem P is considered in order to limit the numerical difficulties. In particular, the rugosity r is kept constant so its equation is not taken into account. We recall that the influence of rugosity has been deeply investigated in [13]. Moreover, $\partial_t \chi$ is neglected and $a(\cdot,\cdot)$ is assumed to be independent of the damage.

Then, the corresponding system of equations is numerically solved in an uncoupled fashion. More precisely, at each time step the chemistry equations are solved with a fully implicit finite elements scheme for s and c, keeping χ fixed. Subsequently, the mechanical equilibrium and damage evolution are obtained with an alternate minimization algorithm which, in short, consists in solving a sequence of minimization sub-problems for u at fixed χ and for χ at fixed u. The time is discretized in n constant time intervals. For the numerical simulations, a specific code have been developed using FEniCS, an open-source finite-element computing platform for solving partial differential equations, which leans on PETSc [23], a suite of data structures and routines for scalable (parallel) solutions, and TAO [24], a toolkit for advanced optimization problems which includes the GPCG algorithm.

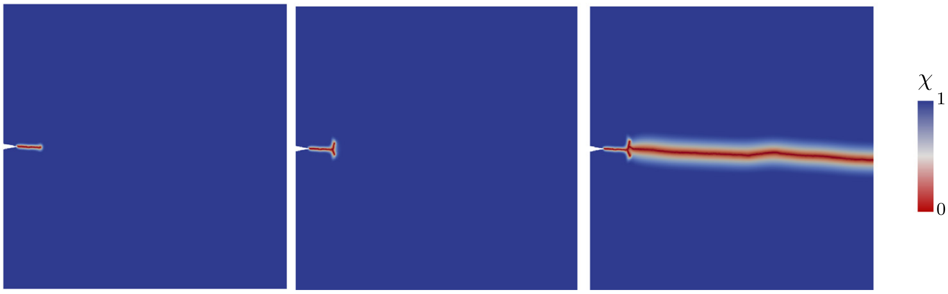
A two-dimensional notched square specimen of marble Ω of sides L is considered. The notch simulates a superficial imperfection of the solid. The setup is reported in Fig. 1. The domain is invested by a polluted air flow along the left vertical boundary and along the notch whereas the other faces are isolated. The distribution of the pollutant SO_2 is constant with a concentration equal to s_0. Moreover, the material is homogeneous so that the initial calcite concentration is c_0, whilst the initial concentration of SO_2 within the solid is null.

A time dependent vertical displacement is applied on the horizontal bases according to Fig. 1 whereas the remaining portion of the boundary is unconstrained and stress free. The main idea is to applied a load to a portion of material that has been affected by the sulphation process.

We consider a representative solid with $L = 1\,\text{mm}$ and a notch deep equal to $0.05\,\text{mm}$. We restrict the analysis to the case of an isotropic material in plane strain condition. Thus, the term $k(c)$ is strictly correlated to the fourth order elasticity tensor $\mathbb{C} = 2\mu\mathbb{I} + \lambda\mathbf{I}\otimes\mathbf{I}$, being μ and λ the Lamé coefficients depending on the elastic modulus E and the Poisson coefficient ν, $\mathbb{I}$ the fourth-order identity tensor and $\mathbf{I}$ the second-order identity tensor.

Table 1
Values of the adopted coefficients in the computation.

	E (MPa)	ν	w (MPa)	A	B	a	b
Marble	50 000	0.2	0.002	0.1	0.1	0.04	0.01
Gypsum	7000	0.2	0.0001157				



(a) $t = 0.72$ s (b) $t = 0.7295$ s (c) $t > 0.734$ s (d)

Fig. 2. Damage evolution for $t \in \{0.72, 0.7295, > 0.734\}$..

A unitary time interval is considered divided into 2000 time steps. The applied vertical displacement assumes the following load history

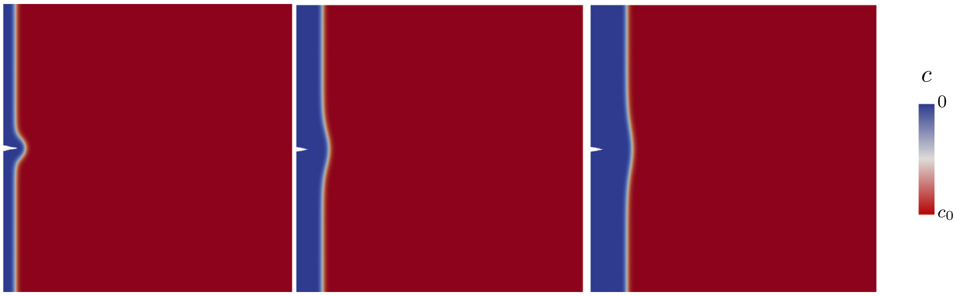
$$\begin{cases} u(t) = 0 \text{ for } t < 0.715\,, \\ u(t) = \bar{u} * (t - 0.715) \text{ for } 0.715 \le t < 0.735\,, \\ u(t) = 0.02 * \bar{u} \text{ for } 0.735 \le t \le 1\,. \end{cases} \tag{6.1}$$

with $\bar{u} = 7.5 \times 10^{-2}$ mm/s. The adopted material constants are listed in Table 1. The domain is decomposed with an unstructured triangular linear finite elements with mesh size $h = 0.0025$ mm.

The evolution of s, c and χ is illustrated through color maps plotted at different time steps in Figs. 2–6. The sulphation process, reported in Fig. 3 at different time steps, initially evolve in an almost homogeneous way despite the presence of the notch. In fact, the transition front presents a smooth profile similar to the external border of the solid. Accordingly, the concentration of SO_2 plotted in Fig. 5, follows the sulphation profile within the solid. The process is damage free as long as the mechanical action is not applied. During the displacement application a fracture initiates at the notch tip and propagates brutally up to the sulphation front as illustrated in Fig. 2a. Now the sulphation process changes completely. The SO_2 quickly penetrates the damaged area see Fig. 6 and at the same time this material portion begins its transformation into gypsum. The fracture bifurcates at the sulphation front as clearly outlined in Fig. 2b. Initially, there is stable propagation in the direction parallel to the transition zone. Subsequently, the propagation, as can be seen in Fig. 2c, becomes brutal and involves the entire specimen. The size of the diffusion zones of these fractures are different. The initial crack presents a very thin transition zone that increases as the crack reaches the sulphation front. The transition is wider as fracture reaches the pristine material fully composed by marble.

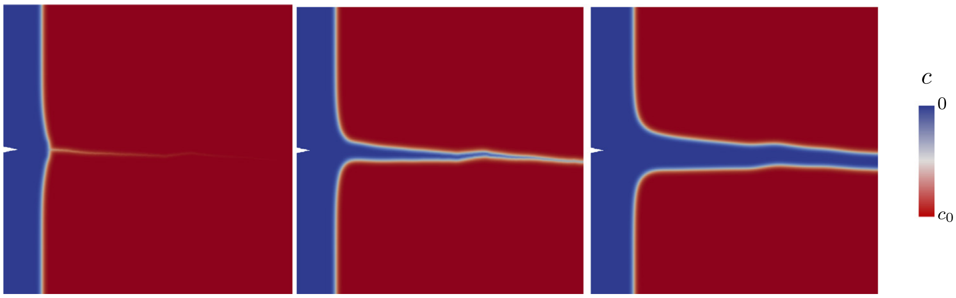
The mutual interaction between chemical process and mechanical degradation is evident. In fact, fractures propagate in the zones affected by the chemical reaction and at the same time s penetrates in the damaged zones as clearly shown in Figs. 4, 6 thus inducing the transformation of marble into gypsum in the cracked areas.

Subsequently, the solutions obtained with $\hat{\chi}$ and χ are compared. The term $\hat{\chi}$ of (1.11) is approximated through a fourth degree Newton–Cotes numerical integration scheme. The solution in term of c and s along a line crossing the fracture placed at $x_1 = 0.3$ (assuming a reference system with origin in the lower left corner of the domain) is plotted in Fig. 7 for several subsequent steps once crack has occurred. The behavior of c is only delayed in considering $\hat{\chi}$ instead of χ. This phenomenon is the one expected by observing Eq. (2.18)



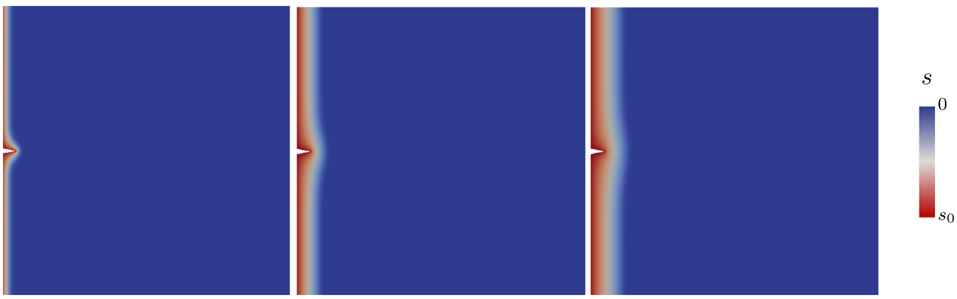
(a) $t = 0.05$ s (b) $t = 0.3$ s (c) $t = 0.72$ s (d)

Fig. 3. Evolution of c for $t \in \{0.05, 0.3, 0.72\}$.



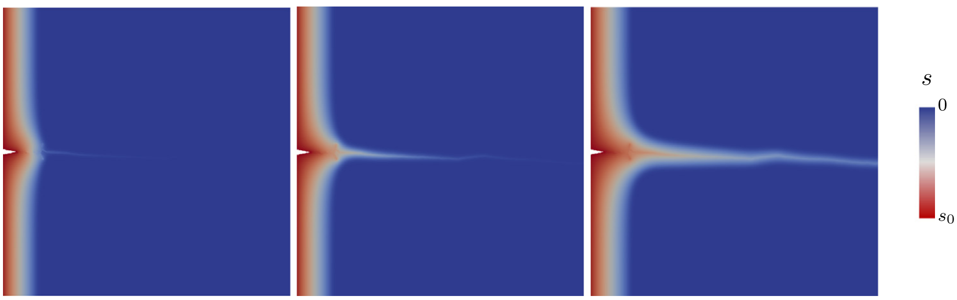
(a) $t = 0.74$ s (b) $t = 0.8$ s (c) $t = 1$ s (d)

Fig. 4. Evolution of c for $t \in \{0.74, 0.8, 1\}$.



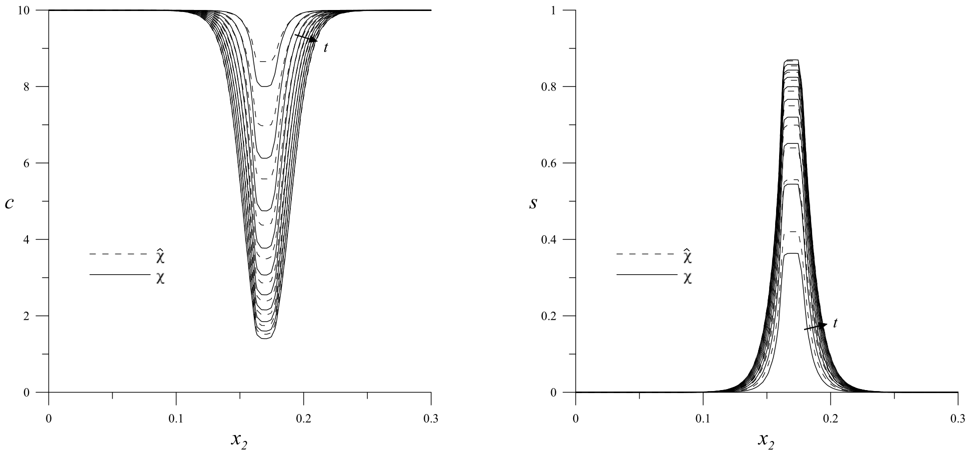
(a) $t = 0.05$ s (b) $t = 0.3$ s (c) $t = 0.72$ s (d)

Fig. 5. Evolution of concentration of SO_2 for $t \in \{0.05, 0.3, 0.72\}$.



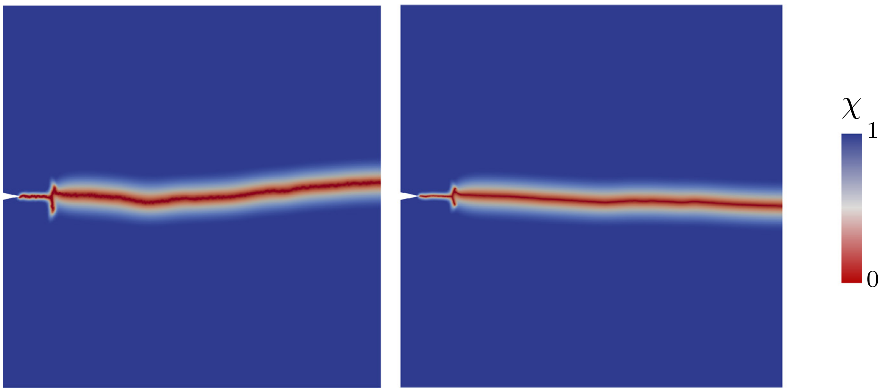
(a) $t = 0.74$ s (b) $t = 0.8$ s (c) $t = 1$ s (d)

Fig. 6. Evolution of concentration of SO_2 for $t \in \{0.74, 0.8, 1\}$.



(a) c (b) s

Fig. 7. Evolution of c and s of χ and $\hat{\chi}$ across the fracture locate at $x_1 = 0.3$ mm.



(a) $h = 0.005$ mm (b) $h = 0.00125$ mm (c)

Fig. 8. Map of χ after complete rupture for $h \in \{0.005, 0.00125\}$ mm.

that governs the evolution of c. The situation is much more intricate in case the evolution of s is considered. In fact, the reaction diffusion Eq. (2.18) permits to have both a delay and an acceleration of the solution with $\hat{\chi}$ compared to the one obtained with only χ. It should be underlined the fact that the difference of the two solutions is extremely limited and additional spatial regularity is not appreciable by the adoption of $\hat{\chi}$ instead of χ demonstrating that its introduction is for pure mathematical purpose.

Finally, the attention is focused on the convergence result (3.41). The problem has been solved adopting two additional mesh sizes with $h \in \{0.005, 0.00125\}$ mm. The two damage paths obtained with the different meshes are reported in Fig. 8 and are qualitatively similar to the one of Fig. 2c. Subsequently, the term $\chi|\nabla u|^2$ is calculated as a post-processing task and illustrated in Fig. 9 for the three cases $h \in \{0.005, 0.0025, 0.00125\}$. In particular, the maps of Fig. 9 outline that non-negligible values are visible only in the fully damaged portion of the solid regardless of the adopted mesh. This aspect is much more evident if the value $\chi|\nabla u|^2$ is plotted across the fracture located at $x_1 = 0.1$ mm as in Fig. 10. The spatial distribution of $\chi|\nabla u|^2$ is similar to a step function with a value that increases as the mesh size decreases.

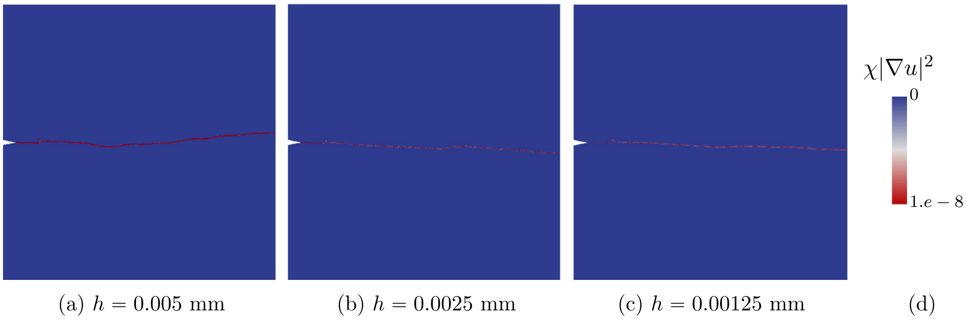


Fig. 9. Map of $\chi|\nabla u|^2$ after complete rupture for $h \in \{0.005, 0.0025, 0.00125\}$ mm.

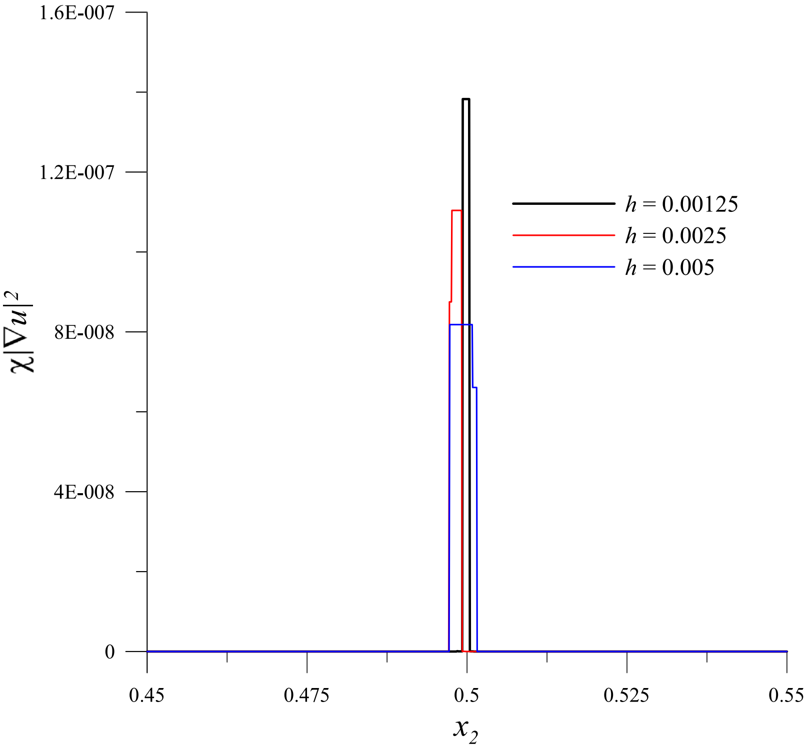


Fig. 10. Term $\chi|\nabla u|^2$ calculated along a line located at $x_1 = 0.1$ mm for three mesh refinements $h \in \{0.005, 0.0025, 0.00125\}$.

7. Conclusions and future work

In this work a model for marble sulphation process taking mechanical damage and surface rugosity into account is proposed and analyzed theoretically and numerically. More precisely, some existence results are given and simple numerical simulations are presented to illustrate specific features of the solution. From the theoretical viewpoint, it would be interesting, though challenging, to characterize in some rigorous way the regions where complete damage appears (in this direction see, for instance, [15, Sec.5]). Speaking of applications, at the present stage, the model is meant to be used in the analysis of a real work of art. To this end two natural developments are possible. Firstly, an extensive experimental campaign has to be performed in order to fit the parameters of the proposed model. Secondly, suitable numerical techniques have to be studied and implemented in order to simulate and reproduce the main phenomena described by the models. Due to the high-nonlinear and non-convex nature of problems, ad hoc algorithms should be developed. In particular, properties of consistency, stability, convergence, and, possibly, error estimates should be investigated. The numerical finite element parallel implementation should include mesh adaptive strategy to reduce computation time and increase precision in the process zones.

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Appendix

Discrete Gronwall Lemma (see [25, Prop.2.2.1]) Let $a = t_0 < t_1 < \cdots < t_M = b$ be a partition of $[a, b]$, and suppose that ϕ and ψ are non-negative step functions, with values ϕ_k and ψ_k, respectively, on the intervals $[t_{k-1}, t_k)$, $k = 1, \ldots, M$. Suppose that, for some fixed $p \geq 1$, there exists $\sigma \geq 0$ such that the following inequality holds for $k = 1, \ldots, M$,

$$\phi_k^p \leq \sigma^p + \int_a^{t_{k-1}} \psi\phi \, dt = \sigma^p + \sum_{m=1}^{k-1} \psi_m \phi_m (t_m - t_{m-1}).$$

Then, the following bounds are valid

$$\phi^{p-1}(t) \leq \sigma^{p-1} + \left(1 - \frac{1}{p}\right) \int_a^t \psi(\tau)\, d\tau, \quad a < t < b,\, p > 1, \tag{A.1}$$

$$\phi(t) \leq \sigma \exp\left(\int_a^t \psi(\tau)\, d\tau\right), \quad a < t < b,\, p = 1. \tag{A.2}$$

In particular, we have

$$\phi_k^{p-1} \leq \sigma^{p-1} + \left(1 - \frac{1}{p}\right) \sum_{m=1}^{k-1} \psi_m (t_m - t_{m-1}), \quad p > 1, \tag{A.3}$$

$$\phi_k \leq \sigma \exp\left(\sum_{m=1}^{k-1} \psi_m (t_m - t_{m-1})\right), \quad p = 1, \tag{A.4}$$

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

Gronwall Lemma (see [26, Thm.2.1]) Let $g(t) \in C^0([0, T])$ a non-negative function fulfilling, for any $t \in [0, T]$,

$$\begin{aligned} g^2(t) \leq g_0^2 &+ 2\int_0^t \|g\|_{C^0([0,\tau])} h(\tau)\, d\tau + \int_0^t \|g\|^2_{C^0([0,\tau])} \lambda(\tau)\, d\tau \\ &+ \left(\int_0^t \|g\|_{C^0([0,\tau])} \mu(\tau)\, d\tau\right)^2 + c\|g\|^2_{C^0([0,t])}, \end{aligned} \tag{A.5}$$

where $g_0 \geq 0$, h, λ, and μ are non-negative functions belonging to $L^1(0, T)$, and c is a positive constant such that $c < 1$. Then, there exists a constant C (possibly depending on λ, μ, c, T, but not on g, g_0, h, and t) such that

$$g(t) \leq C\left(g_0 + \int_0^T h(\tau)\, d\tau\right), \qquad \forall\, t \in [0, T].$$

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