Thermomechanics of demageable materials under diffusion: modeling and analysis

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Abstract. We propose a thermodynamically consistent general-purpose model describing diffusion of a solute or a fluid in a solid undergoing possible phase transformations and damage, beside possible visco-inelastic processes. Also heat generation/consumption/transfer is considered. Damage is modelled as rate-independent. The applications include metal-hydrogen systems with metal/hydride phase transformation, poroelastic rocks, structural and ferro/para-magnetic phase transformation, water and heat transport in concrete, and, if diffusion is neglected, plasticity with damage and viscoelasticity, etc. For the ensuing system of partial differential equations and inclusions, we prove existence of solutions by a carefully devised semi-implicit approximation scheme of the fractional-step type.

Mathematics Subject Classification (2000). 35K55, 35Q74, 74A15, 74R20, 74N10, 74F10, 76S99, 80A17, 80A20.

Keywords. visco-elastic porous solids, incomplete damage, diffusion driven by chemical-potential gradient, phase transformations, poroelastic materials, plasticity, swelling, creep, quasilinear parabolic systems, time-discretisation, a-priori estimates, convergence.

1. Introduction

This paper addresses damage processes in visco-elastic materials undergoing various diffusion or inelastic processes with the goal to develop a general, multi-purpose model with wide application range and covering, in particular, several particular models occuring in the literature in a unifying way.

We use the concept of internal variables, here specifically damage d and a phase-field χ. For the damage phenomenon, we consider the simplest scalar concept and therefore introduce an additional scalar variable d, which we regard as an additional microscopic kinematical descriptor. This phase-field may, however, involve a lot of components, interpreted e.g. as content of a solute or a fluid, plastic strain, porosity, viscous strain causing creep, etc. The primary fields in our model will be:

- displacement $\boldsymbol{u} : [0, T] \times \Omega \to \mathbb{R}^3$,
- phase field $\chi : [0, T] \times \Omega \to K \subset \mathbb{R}^N$,
- concentration $c : [0, T] \times \Omega \to \mathbb{R}^+$,
- damage variable $d : [0, T] \times \Omega \to [0, 1]$,
- temperature $\theta : [0, T] \times \Omega \to \mathbb{R}^+$,

where $\Omega \subset \mathbb{R}^3$ is a considered domain occupied by the solid body, $T > 0$ is a fixed time horizon. We work in the small-strain approximation and we assume that the linear strain has the following form:

$$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \boldsymbol{E} + \mathbb{E}\chi, \tag{1.1}$$

where $\boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}(\nabla \boldsymbol{u})^\top + \frac{1}{2}\nabla \boldsymbol{u}$ is the total linear strain, $\boldsymbol{E}$ is its elastic part, and $\mathbb{E}\chi$ is its anelastic part dependent linearly on the phase field χ. Here $\mathbb{E}$ is a third-order tensor, which we think as the mapping of $\mathbb{R}^N$ into $\mathbb{R}^{3\times 3}$ defined by $(\mathbb{E}\chi)_{ij} = \mathbb{E}_{ijk}\chi_k$. Using the above decomposition we can cover the concept that the free

This research has been supported by GA ČR through the projects 201/10/0357 "Modern mathematical and computational models for inelastic processes in solids", 13-18652S "Computational modeling of damage and transport processes in quasi-brittle materials", 14-15264S "Experimentally justified multiscale modelling of shape memory alloys", by the CENTEM project no. CZ.1.05/21.00/03.0088 (cofounded from ERDF within the OP RDI programme, MŠMT ČR) at New Technologies Research Centre (Univ. of West Bohemia, Plzeň), and by INdAM-GNFM through projects "Mathematical Modeling of Morphing Processes" and "Mathematical Modeling of Shape Changes in Soft Tissues".

energy as well as the dissipation energy are let to depend on the elastic strain $\boldsymbol{E}$ rather than the total strain $\boldsymbol{\varepsilon}(\boldsymbol{u})$. For a more general ansatz see Remark s 2.3 and 3.5 below.

The main difficulty is the combination of thermo-visco-(in)elastic-diffusive model with damage. As always, some simplifications are necessary mainly for analytical reasons. In particular, beside the mentioned small-strain concept, we admit only an incomplete damage. Furthermore, we perform analysis on a special ansatz, see (3.4) below. In particular, among other approximations, we neglect thermal expansion effects, direct coupling between concentration and strain (see Remark 5.7 below), direct coupling between concentration and damage, and coupling between damage and temperature. We also neglect cross-effects between dissipation in χ and d, cf. (3.1a), as well as the cross-effects in the transport processes, i.e. the Soret/Peltier effects. On the other hand, in case of a multi-component diffusant (when c would be vector valued) some cross effect could simply be modelled by a nondiagonal $\mathbf{M}$ in (3.1b). Let us emphasize that the complete damage would bring serious mathematical difficulties; in the isothermal case it has been addressed in [23] using a formulation by a time-dependent domain.

Typical application of damage in engineering models assumes that this destruction process is activated, irreversible, and much faster than the time scale of the other internal processes or than external loading. This is reflected by the dissipation potential being nonsmooth at zero rate, not everywhere finite, and homogeneous degree 1, cf. (3.3) below and [12, 34, 52, 53], and also [13]. This also substantially distinguishes between the character and the subsequent treatment of the damage d and of the phase field χ which otherwise occur in a lot of places in a position of an overall internal variable (χ, d) if $\mathbb{E}$ in (1.1) would just ignore the component d and thus one could simply merge (2.1b) with (2.1d), or (3.7b) with (3.7d), etc., similarly like e.g. in [41]. There are many variants of models which combined diffusion and elasticity under damage in literature, some of them only isothermal and regularizing damage by rate-dependent terms like [5] and/or involving a gradient term for the concentration of diffusant leading to a diffusion equation of Cahn-Hilliard type [5, 23], and of course very many other models not considering damage, like [41, 40].

The main analytical result here is the proof of existence of weak solutions of the initial-boundary-value problem for the thermodynamical system. To this goal, a rather constructive method is used which yields a conceptual algorithm that may serve for designing efficient numerical strategy after a suitable spatial discretisation (not performed here, however).

It should be emphasized that there are several important differences from [50]: the elastic strain (instead of the total strain) is systematically used also for dissipative processes and the internal variables are split into two sets, both subjected to a substantially different treatment and allow for qualification of the free energy ψ well fitted to damage. On top of it, the mathematical treatment of the heat-transfer equation is simplified like in by holding the formulation in terms of the couple temperature-enthalpy (instead of mere temperature).

The paper is organized as follows: In Section 2 we formulate the general model and briefly outline the underlying physics, referring mainly to the previous work [50]. Then, in Section 3 we present a menagerie of various specific examples illustrating a wide range of applications. Eventually, in Section 4 summarizes the main existence result, whose proof is performed in Section 5.

Thorough the whole article, we use the convention that small italics stands for scalar, small and capital bold stand, respectively, for elements of $\mathbb{R}^3$ and elements of $\mathbb{R}^{3\times3}$. We shall occasionally use Greek letters to denote elements of $\mathbb{R}^N$, where N is the number of internal variables incorporated in the phase field χ. Consistent with this rule is our usage of the letter σ to denote the conjugate variable of χ, instead of stress.For the reader's convenience we summarize in the following table the symbols mostly used in the rest of this paper

$\boldsymbol{u}$ displacement,	$\boldsymbol{\varepsilon}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla\boldsymbol{u} + \nabla\boldsymbol{u}^\top\right)$ small-strain tensor,
χ phase field,	ψ free energy,
c concentration of diffusant,	θ temperature,
d damage variable,	η entropy,
$\boldsymbol{S}$ stress,	μ chemical potential,
$\boldsymbol{f}$ bulk force,	$\mathbf{h}$ flux of diffusant,
$\boldsymbol{f}_\mathrm{s}$ surface force,	h bulk supply of diffusant (eventually set to 0),
σ internal microforce associated to χ,	h_s surface supply of diffusant,
$\boldsymbol{\Sigma}$ microstress,	$\boldsymbol{q}$ heat flux,
γ, g bulk microforces (eventually set to 0),	q bulk heat supply (eventually set to 0).
e internal energy,	

2. The general model: balance laws and dissipation inequality

The model derivation follows quite closely that of [50]. In order to derive a system of partial differential equations governing the evolution of the primary fields, we adopt the point of view of [19]. The balance equations are considered as:

$$\varrho\ddot{\boldsymbol{u}} - \mathrm{div}\,\boldsymbol{S} = \boldsymbol{f}, \qquad \text{(Force balance)} \tag{2.1a}$$

$$\sigma - \mathrm{div}\,\boldsymbol{\Sigma} = \gamma, \qquad \text{(Microscopic balance for phase field)} \tag{2.1b}$$

$$\dot{c} + \mathrm{div}\,\mathbf{h} = h, \qquad \text{(Solute balance)} \tag{2.1c}$$

$$s - \mathrm{div}\,\boldsymbol{s} = g. \qquad \text{(Microscopic balance for damage)} \tag{2.1d}$$

The second and the fourth equations involve systems of microscopic forces (σ, s) and microscopic stresses $(\Sigma, \boldsymbol{s})$ that perform work, respectively, on $(\dot{\chi}, \dot{d})$ and $(\nabla\dot{\chi}, \nabla\dot{d})$. Consistent with this interpretation is the expression of the internal power expenditure that appears on the right-hand side of the energy equation:

$$\begin{aligned}\dot{e} + \mathrm{div}\,\mathbf{q} = q + \boldsymbol{S}{:}\boldsymbol{\varepsilon}(\dot{\boldsymbol{u}}) + \sigma\cdot\dot{\chi}\\ + \boldsymbol{\Sigma}{:}\nabla\dot{\chi} + s\dot{d} + \boldsymbol{s}\cdot\nabla\dot{d} + \mu\dot{c} - \mathbf{h}{\cdot}\nabla\mu, \qquad \text{(Energy balance)}\end{aligned} \tag{2.1e}$$

where also the energetic contribution from the diffusion of a chemical species is accounted for by the last two terms. The choice of constitutive prescriptions, which we shall make into is guided by the dissipation inequality:

$$\dot{\psi} + \eta\dot{\theta} - \mu\dot{c} \le \boldsymbol{S}{:}\boldsymbol{\varepsilon}(\dot{\boldsymbol{u}}) + \sigma{\cdot}\dot{\chi} + \boldsymbol{\Sigma}{:}\nabla\dot{\chi} + s\dot{d} + \boldsymbol{s}{\cdot}\nabla\dot{d} - \mathbf{h}\cdot\nabla\mu - \frac{1}{\theta}\mathbf{q}{\cdot}\nabla\theta,$$

where $\psi = e - \eta\theta$ is the free energy. The dissipation inequality can be rewritten by exploiting the decomposition (1.1):

$$\dot{\psi} + s\dot{\theta} - \mu\dot{c} \le \boldsymbol{S}{:}\dot{\boldsymbol{E}} + (\sigma + \boldsymbol{S}{:}\mathbb{E})\cdot\dot{\chi} + \boldsymbol{\Sigma}{:}\nabla\dot{\chi} + s\dot{d} + \boldsymbol{s}\cdot\nabla\dot{d} - \mathbf{h}\cdot\nabla\mu - \frac{1}{\theta}\mathbf{q}\cdot\nabla\theta. \tag{2.2}$$

By using standard arguments, one can show that the free energy is ruled by a constitutive equation of the following type:

$$\psi = \varphi(\boldsymbol{E}, \chi, c, d, \theta, \nabla\chi, \nabla d). \tag{2.3}$$

Moreover, if entropy η does depend on the same list of variables, then necessarily

$$\eta = -\partial_\theta\varphi(\boldsymbol{E}, \chi, c, d, \theta, \nabla\chi, \nabla d). \tag{2.4}$$

The dissipation inequality can be rendered in a more compact form by defining:

$$\boldsymbol{S}_{\rm d} = \boldsymbol{S} - \partial_{\boldsymbol{E}}\varphi, \tag{2.5a}$$

$$\sigma_{\rm d} = \sigma + \boldsymbol{S}{:}\mathbb{E} - \partial_\chi\varphi, \tag{2.5b}$$

$$\boldsymbol{\Sigma}_{\rm d} = \boldsymbol{\Sigma} - \partial_{\nabla\chi}\varphi, \tag{2.5c}$$

$$s_{\rm d} = s - \partial_d\varphi, \tag{2.5d}$$

$$\boldsymbol{s}_{\rm d} = \boldsymbol{s} - \partial_{\nabla d}\varphi, \tag{2.5e}$$

$$\mu_{\rm d} = \mu - \partial_c\varphi. \tag{2.5f}$$

In (2.5b), $\boldsymbol{S}{:}\mathbb{E}$ means the vector $\sum_{i,j=1}^3 \boldsymbol{S}_{ij}\mathbb{E}_{ijk}$. With that splitting, one indeed obtains the *reduced dissipation inequality*

$$0 \le \boldsymbol{S}_{\rm d} : \dot{\boldsymbol{E}} + \sigma_{\rm d}\cdot\dot{\chi} + \boldsymbol{\Sigma}_{\rm d}{:}\nabla\dot{\chi} + s_{\rm d}\dot{d} + \boldsymbol{s}_{\rm d}\cdot\nabla\dot{d} + \dot{c}\mu_{\rm d} - \mathbf{h}\cdot\nabla\mu - \frac{1}{\theta}\boldsymbol{q}\cdot\nabla\theta. \tag{2.6}$$

Remark 2.1 (*Rheology of the model).* From (2.5a), we can see that the total mechanical stress is $\boldsymbol{S} = \partial_{\boldsymbol{E}}\varphi + \boldsymbol{S}_{\rm d}$, in what follows considered as $\boldsymbol{S} = \partial_{\boldsymbol{E}}\varphi + \mathbb{D}\dot{\boldsymbol{E}}$, cf. (3.1a). This is the classical Kelvin-Voigt rheological model. Through the internal parameters contained possibly in χ, we can easily combine it to get some more complicated solid-type rheological models as Jeffreys' material or a so-called 4-parameter solid etc.

Remark 2.2 (*An alternative understanding).* In the expression of the free energy we could alternatively use as state variables the total strain $\boldsymbol{\varepsilon}(\boldsymbol{u})$ in place of the elastic strain In particular, the mechanical energy in (3.4) could be written as $\varphi_{\rm ME}(\boldsymbol{\varepsilon}(\boldsymbol{u}){-}\mathbb{E}\chi, d)$, which would highlight the different roles played by χ and d; note that, in this case, the term $\mathbf{S} : \mathbb{E}$ in (2.5b) would be incorporated in $\partial_\chi\varphi$, and thus (2.5b) would be replaced by $\sigma_{\rm d} = \sigma - \partial_\chi\varphi$. This is ultimately the reason why we can afford viscous dissipation for χ and not for d. Note that then $\partial_{\boldsymbol{\varepsilon}}\varphi$, which is standardly understood as the elastic part of the stress tensor, is indeed equal to $\partial_{\boldsymbol{E}}\varphi$

we used in (2.5a). On the other hand, $-\partial_\chi\varphi$, which is standardly understood as the driving force for evolution of χ, is what is $\boldsymbol{S}:\mathbb{E}-\partial_\chi\varphi$ in (2.5b).

Remark 2.3 (*Difficulties with nonlinear ansatz*). One can attempt to generalize the linear term $\mathbb{E}\chi$ in (1.1) but a strong nonlinear dependence may affect the semi-convexity assumption (4.1i) below. To better clarify this last point, assume that we replace the decomposition (1.1) with $\boldsymbol{\varepsilon}(\boldsymbol{u})=\boldsymbol{E}+\boldsymbol{E}_{\rm tr}(\chi)$, where $\boldsymbol{E}_{\rm tr}$ is now a non-linear function. Suppose also that the mechanical energy has the simple form $\varphi_{_{\rm ME}}(\boldsymbol{E})=\frac12\mathbb{C}\boldsymbol{E}:\boldsymbol{E}$. Then, the energy functional pertaining to $\boldsymbol{u}$ and χ would be

$$(\boldsymbol{u},\chi)\mapsto\int_\Omega\frac12\mathbb{C}(\boldsymbol{\varepsilon}(\boldsymbol{u})-\boldsymbol{E}_{\rm tr}(\chi)):(\boldsymbol{\varepsilon}(\boldsymbol{u})-\boldsymbol{E}_{\rm tr}(\chi))\,{\rm d}x \tag{2.7}$$

but a simple calculation shows that if the function $\boldsymbol{E}_{\rm tr}$ is non-linear, then the integrand in (2.7) cannot be convex (and not even semiconvex) with respect to the variables $\boldsymbol{\varepsilon}(\boldsymbol{u})$ and χ.

3. Specialization and examples

The system of partial differential equations governing the evolution of the primary fields is obtained by combining the balance equations (2.1) with appropriate constitutive prescriptions for the dissipative parts of the auxiliary fields, consistent with the reduced dissipation inequality (2.6). We make the following choice:

$$\boldsymbol{S}_{\rm d}=\mathbb{D}\dot{\boldsymbol{E}},\qquad \sigma_{\rm d}\in\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi),\qquad s_{\rm d}\in\partial_{\dot d}\xi(\chi,\dot d), \tag{3.1a}$$

$$\boldsymbol{q}=-\mathbf{K}(\boldsymbol{E},\chi,d,c,\theta)\nabla\theta,\qquad \mathbf{h}=-\mathbf{M}(\boldsymbol{E},\chi,d,c,\theta)\nabla\mu, \tag{3.1b}$$

$$\boldsymbol{\Sigma}_{\rm d}=0,\qquad \boldsymbol{s}_{\rm d}=0,\qquad \mu_{\rm d}=0. \tag{3.1c}$$

We also set to null bulk sources in (2.1), except for the force balance (2.1a), that is:

$$\gamma=0,\qquad h=0,\qquad g=0,\qquad q=0. \tag{3.2}$$

Here ζ and ξ are (possibly non-smooth) dissipation potentials, both $\zeta(\boldsymbol{E},\chi,d,\cdot)$ and $\xi(\chi,\cdot)$ being convex and possibly nonsmooth at 0. More specifically, $\xi(\chi,\cdot)$ is assumed convex positively homogeneous degree-1, so it is always nonsmooth at 0. Assuming irreversible (i.e. unidirectional) damage, ξ will be in the form

$$\xi(\chi,\dot d)=\begin{cases}\alpha(\chi)|\dot d| & \text{if } \dot d\le0\\ \infty & \text{otherwise}\end{cases} \tag{3.3}$$

with $\alpha:\mathbb{R}^N\to\mathbb{R}^+$ denoting a phenomenological fracture-toughness coefficient, meaning the specific energy in J/m^3 need (and dissipated) by accomplishing the damage. As we shall see later, the degree-1 homogeneity of the dissipation potential ξ in $\dot d$ has the consequence that $\dot d$ will be a measure in general. On the other hand, neither $\boldsymbol{E}$ nor d are continuous. Thus, α in (3.3) cannot be made to depend on $\boldsymbol{E}$ and d neither on θ but, on the other hand, its dependence on d is legitimate because we will have a regularity of d at disposal, cf. (5.34d) below.

The involvement of non-trivial dissipative terms $\sigma_{\rm d}$ and $s_{\rm d}$ is essential. In fact, the non-smooth and unbounded dissipation potential for d allows us to incorporate the fenomenology of irreversibility of damage and its character to be an activated process. Moreover, we benefit from the dissipative term for χ to control the terms containing $\dot\chi$ and on the right-hand side of the heat equation, which would anyway be present because of an adiabatic coupling. Moreover, the specification of a non-trivial viscous stress in the first of (3.1a) which leads to Kelvin-Voigt-type visco-elastic rheological models as mentioned in Remark 2.1 is needed to handle inertia, otherwise it can be neglected, cf. Remark 5.8 below. Clearly, we may also include non-trivial viscous-like contributions $\boldsymbol{\Sigma}_{\rm d}$ and $\mathbf{s}_{\rm d}$ in the stress-like terms under divergence in the balance equations (2.1c,d). Including these contributions would not significantly extend the range of applications of our treatment and would make all notation heavier (moreover they would make our analysis more trivial to some extent, as far as the equation governing χ). Similar considerations hold for a dissipative contribution to chemical potential.

To facilitate the mathematical analysis of (2.1) with (2.5) and (3.1), we must restrict the generality of the free energy(2.3). In particular:

1. If θ and $\boldsymbol{E}$ would generally be coupled in (2.3), in general a concept of nonsimple material would be needed to have a control on $\nabla\boldsymbol{E}$, cf. [45]. An exception would be if θ would appear linearly, i.e. a term like $\theta\varphi(\boldsymbol{E})$, which then would not contribute to the heat capacity, cf. e.g. [50].

2. If c and $\boldsymbol{E}$ would generally be coupled in (2.3), then the chemical potential $\mu = \partial_c\varphi$ from (2.5f) with (3.1c) would depend on $\boldsymbol{E}$ and again the estimate (5.21) of ∇c would need a control of $\nabla\boldsymbol{E}$, i.e. the concept of nonsimple materials. Some alternative option would be introduce a gradient of c into the free energy, i.e. capillarity concept, see also Rem 5.7 below.
3. If d and θ would be coupled in (2.3), than the adiabatic heat term $\partial^2_{c\theta}\varphi(....,\theta)\dot{d}$ would occur but $\dot{d}$ is a measure and θ tends typically to jump exactly at the points where $\dot{d}$ concentrates, and such term analytically would not be well defined.
4. If c and θ would generally be coupled in (2.3), the adiabatic heat term $\partial^2_{c\theta}\varphi\dot{c}$ would occur in the right-hand side of the heat-transfer equation, cf. (3.7e) below, but we will not have any estimate on $\dot{c}$ except the "dual" estimate (5.34c) below, so this term would not be controlled as a measure.
5. If c and d would generally be coupled in (2.3), we would see a term $\partial_d\varphi_{\rm CH}(\chi,d,c)\dot{d}$ in (5.75). However, the term $\partial_d\varphi_{\rm CH}(\chi,d,c)$ would be not continuous, because of the aforementioned lack of continuity of c, and hence its combination with the measure $\dot{d}$ would not be well defined.

These five requirements led us to make the following partly decoupled ansatz for the free energy (2.3), distinguishing mechanical, chemical, and thermal parts in the sense:

$$\psi = \underbrace{\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + \varphi_{\rm CH}(\chi,c) + \varphi_{\rm TH}(\chi,\theta)}_{=:\,\varphi_{\rm TOT}(\boldsymbol{E},\chi,c,d,\theta)} + \frac{1}{2}\kappa_1|\nabla\chi|^2 + \frac{1}{2}\kappa_2|\nabla d|^2 + \delta_K(\chi) + \delta_{[0,1]}(d). \tag{3.4}$$

Here K is a convex set where values of χ are assumed to lie, while d is valued at $[0,1]$, and δ stands for the indicator function, i.e. $\delta_K(\cdot)$ is equal to 0 on K and $+\infty$ otherwise and similarly for $\delta_{[0,1]}(\cdot)$. The consequence of the decoupling (3.4) is that the *internal energy*, defined by Gibbs' relation $e = \psi - \theta\eta$ and occurring already in (2.1e), can be written as:

$$e = e_{\rm TH}(\chi,\theta) + \underbrace{\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + \varphi_{\rm CH}(\chi,c)}_{=:\,\varphi_{\rm ME/CH}(\boldsymbol{E},\chi,c,d)} + \frac{1}{2}\kappa_1|\nabla\chi|^2 + \frac{1}{2}\kappa_2|\nabla d|^2 + \delta_K(\chi) + \delta_{[0,1]}(d), \tag{3.5}$$

where the thermal part of the internal energy is

$$e_{\rm TH}(\chi,\theta) = \varphi_{\rm TH}(\chi,\theta) - \theta\partial_\theta\varphi_{\rm TH}(\chi,\theta). \tag{3.6}$$

Altogether, from (2.1) with (2.5), (3.1), and (3.4), we obtain the following system:

$$\varrho\ddot{\boldsymbol{u}} - {\rm div}\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + \mathbb{D}\dot{\boldsymbol{E}}\big) = \boldsymbol{f} \qquad \text{with } \boldsymbol{E} = \boldsymbol{\varepsilon}(\boldsymbol{u}) - \mathbb{E}\chi, \tag{3.7a}$$

$$\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi) - \kappa_1\Delta\chi + \partial_\chi\varphi_{\rm TOT}(\boldsymbol{E},\chi,c,d,\theta) - \mathbb{E}^\top{:}(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + \mathbb{D}\dot{\boldsymbol{E}}) + \sigma_{\rm r} \ni 0 \qquad \text{with } \sigma_{\rm r} \in \partial\delta_K(\chi), \tag{3.7b}$$

$$\dot{c} - {\rm div}\big(\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu\big) = 0 \qquad \text{with } \mu = \partial_c\varphi_{\rm CH}(\chi,c), \tag{3.7c}$$

$$\partial_{\dot d}\xi(\chi,\dot d) - \kappa_2\Delta d + \partial_d\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + s_{\rm r} \ni 0 \qquad \text{with } s_{\rm r} \in \partial\delta_{[0,1]}(d), \tag{3.7d}$$

$$\dot{w} - {\rm div}(\mathbf{K}(\boldsymbol{E},\chi,c,d,\theta)\nabla\theta) = \partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\cdot\dot\chi + \partial_\chi\varphi_{\rm TH}(\chi,\theta)\cdot\dot\chi + \mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}} - \alpha(\chi)\dot{d} + \mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu{\cdot}\nabla\mu \qquad \text{with } \ w = e_{\rm TH}(\chi,\theta). \tag{3.7e}$$

Note that $\zeta(\boldsymbol{E},\chi,c,d,\theta,\cdot)$ is possibly nonmooth so that $\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)$ may be multi-valued, but anyhow we assume in (4.1n) below that the term $\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\cdot\dot\chi$ appearing in the right-hand side of (3.7e) and also in (4.10f) below is well-defined. This occurs e.g. if $\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)$ has a form $a(\boldsymbol{E},\chi,c,d,\theta)|\dot\chi| + b(\boldsymbol{E},\chi,c,d,\theta)|\dot\chi|^2$ with some $a,b \geq 0$. We complete (3.7) with the following boundary condition:

$$\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d) + \mathbb{D}\dot{\boldsymbol{E}}\big)\mathbf{n} = \boldsymbol{f}_{\rm s}, \tag{3.8a}$$

$$\nabla\chi\cdot\mathbf{n} = 0, \tag{3.8b}$$

$$\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu\cdot\mathbf{n} = h_{\rm s}, \tag{3.8c}$$

$$\nabla d\cdot\mathbf{n} = 0, \tag{3.8d}$$

$$\mathbf{K}(\boldsymbol{E},\chi,c,d,\theta)\nabla\theta\cdot\mathbf{n} = q_{\rm s} \tag{3.8e}$$

to be valid on the boundary Γ of Ω. Using the convention like $\boldsymbol{u}(\cdot,t) =: \boldsymbol{u}(t)$, we complete the system by the initial conditions:

$$\boldsymbol{u}(0) = \boldsymbol{u}_0, \qquad \dot{\boldsymbol{u}}(0) = \boldsymbol{v}_0, \qquad \chi(0) = \chi_0, \qquad c(0) = c_0, \qquad d(0) = d_0, \qquad w(0) = w_0 := \varphi_{\rm TH}(\chi_0,\theta_0). \tag{3.9}$$

The above formulated model is very general and can be understood as truly multi-purpose. As some important examples from very diverse physically well justified models, let us mention the following:

Example 3.1 (*Metal/hydride phase transformation).* Some metals or intermetallics allows for relatively easy diffusion of hydrogen and undergo a transformation into hydrides accompanied by markable volume changes (even up to 30%), cf. [29]. Several continuum models have been proposed, accompanied by their analytical study [3, 4, 8, 50]. Such big volume variation then often cause damage. In this case, we have $N = 1$ and the (scalar-valued) phase field χ stands for the volume fraction related to the metal/hydride transformation, while the variable c is the hydrogen concentration. The free energy can be considered as

$$\varphi_{\rm TOT}(\boldsymbol{E},\chi,c,d,\theta) = \underbrace{\frac{1}{2}\mathbb{C}(d)\boldsymbol{E}{:}\boldsymbol{E}}_{=:\,\varphi_{\rm ME}} + \underbrace{\frac{k}{2}\big|a(\chi){-}c\big|^2 + \phi_1(c)}_{=:\,\varphi_{\rm CH}} + \underbrace{\phi_2(\chi,\theta)}_{=:\,\varphi_{\rm TH}} \tag{3.10}$$

where $k > 0$ is a (typically large) coefficient and $a(\chi)$ a function that maps values of phase field into values of concentration, which reflects the fact that different phases typically manifest themselves at different concentrations. As marked, (3.10) is consistent with our splitting ansatz (3.4). Without damage but considering still thermal expansion, this model has been treated in [50]. Thus, the present paper generalizes [50] towards this important damage phenomenon. In particular we may take $a(\chi) = \chi$. In this case, χ is somehow related to the concept of *nonlocal species concentration*, a concept introduced in [54] to handle the difficulties related to the numerical solution of the Cahn-Hilliard equation and further elaborated in [10], where the extra field (here χ) is called *micromorphic concentration.* As $\partial^2_{cc}\varphi_{\rm CH}(\chi,c) = k + \phi_1''(c)$, the uniform convexity in c requires just a semi-convexity of ϕ_1 if one admits k large. Moreover, the physically relevant non-negativity of c can then be ensured by taking for ϕ_2 a function having a controlled singularity at zero ϕ_1. An example may be the coarse-grain chemical free energy obtained from regular solution theory:

$$\phi_2(\chi,\theta) = \phi_3(\theta) + A\theta(\chi\log(\chi) + (1{-}\chi)\log(1{-}\chi)) + B\chi(1{-}\chi), \tag{3.11}$$

with A and B positive constants, cf. [24]. Of course, due to the large strains sometimes involved in the hydration phase transformation, developing the model in the small-strain setting might be debatable. For a model coupling diffusion and damage in the large setting, we refer to [11].

Example 3.2 (*Poroelastic rocks).* Geophysical models of lithospheres in short time scale (less that 1 mil. yrs) counts small strains. Typical phenomena to capture are damage, plasticity (considered here rate-dependent), and water propagation through porous rocks, cf. e.g. [57]. The phase field is then composed from plastic strain $\pi_{\rm pl}$ and porosity ϖ, while c is the water concentration, cf. e.g. [20, 21, 31]. The free energy is considered as $\psi = \frac{1}{2}\lambda(\varpi,d)({\rm tr}\,\boldsymbol{E})^2 + G(\varpi,d)|\boldsymbol{E}|^2 + \frac{1}{2}M(\varpi,d)|\beta{\rm tr}\,\boldsymbol{E}{-}c{+}\varpi|^2 + c_{\rm v}\theta({\rm ln}\theta{-}1)$ with $\boldsymbol{E} = \boldsymbol{\varepsilon}(\boldsymbol{u}) - \pi_{\rm pl}$ and with λ and μ the first Lamé coefficient, G the shear modulus (also called the second Lamé coefficient and denoted by μ which here denotes, however, the chemical potential) M the Biot modulus, and β the Biot coefficient. The chemical potential μ and the Nernst-Plack equation (3.7c) play the role of a pressure and of the Darcy equation. This however does not directly fit with the splitting (3.4) because c and $\boldsymbol{E}$ are directly coupled unless the Biot modulus or the Biot coefficient would be zero. To make it consistent with (3.4), similarly as in Example 3.1 we again distinguish between the water concentration c and the water content γ; in fact, [20, 21, 31] speak about water content, although consider the water flow governed by the Darcy equation like if it would be a water concentration. Therefore, we consider the augmented phase field as $\chi = (\pi_{\rm pl},\varpi,\gamma)$ and then the free energy as

$$\varphi_{\rm TOT}(\boldsymbol{E},\varpi,\gamma,c,d,\theta) = \underbrace{\frac{1}{2}\lambda(\varpi,d)({\rm tr}\,\boldsymbol{E})^2 + G(\varpi,d)|\boldsymbol{E}|^2 + \frac{1}{2}M(\varpi,d)|\beta{\rm tr}\,\boldsymbol{E}{-}\gamma{+}\varpi|^2}_{=:\,\varphi_{\rm ME}}$$
$$+ \underbrace{\frac{1}{2}k|\gamma-c|^2}_{=:\,\varphi_{\rm CH}} + \underbrace{c_{\rm v}\theta({\rm ln}\theta{-}1)}_{=:\,\varphi_{\rm TH}} \qquad \text{with} \quad \boldsymbol{E} = \boldsymbol{\varepsilon}(\boldsymbol{u}) - \pi_{\rm pl}. \tag{3.12}$$

Clearly, (1.1) now uses $\mathbb{E}\chi = \mathbb{E}(\pi_{\rm pl},\varpi,\gamma) := \pi_{\rm pl}$. In fact, typically considered ϖ-dependence of the Biot modulus M is affine (cf. [20, 31]) which would make the functional $\varpi \mapsto \psi$ non-convex (and even equi-semiconvexity (4.1i) below cannot be expected, which would make technical troubles in using time discretisation below). Yet, (4.1i) does not necessarilly mean M or G or λ to be constant. On the other hand, a small modification complying with the growth/coercivity restriction (4.1d) made in what follows is needed for facilitating the analysis, cf. Remark 4.3 below. However, [20, 21, 31] in fact (although not explicitly) consider cross-effects in dissipation of damage and porosity, which here has to be neglected here otherwise it would require coupling of (5.1) and (5.2) and stronger separate semi-convexity qualification likely not compatible with (3.12), and moreover damage was considered reversible, which is important in particular for longer-time scale processes in rocks. Also, [20, 21, 31] consider a phenomenological flow rule for $\pi_{\rm pl}$ not governed directly from the free energy.

Example 3.3 (*Magnetic and hydride transformations in intermetallics).* Some intermetallic compouds exposed to hydrogen (or deuterium) exhibit not only metal/hydride phase transformations as mentioned above but also a dramatic structural trasformation analogous to the martensitic ferro-to-para magnetic transformation, both mutually coupled. This is the case of Uranium- or rare-earth-based alloys, cf. [22, 25]. Experiments show that hydrogenation implies a substantial increase of the magnetic ordering temperature and noticeable increase of specific heat, cf. e.g. [15, 26]. There does not seem any models for it in mathematical literature to exist, however. The structural cubic-to-cubic phase transformation in particular single-crystal grains is similar e.g. to cubic-to-tetragonal so-called martensitic transformation which may also exhibit magnetic phase transformation in intermetalics like NiMnGa. Here, densely packed cubic configuration is typically paramagnetic (because electron orbits of particular atoms over-cover each other) while sparsely packed cubic configuration is typically ferromagnetic) in analog with cubic austenite and tetragonal martensite in NiMnGa. Counting this analogy, one can assembly a model from already existing particular models for the martensitic transformation of the Souza-Aurichio type as e.g. in [1, 27], for the ferro-to-para magnetic transformation as in [36] in combination (and ignoring gyromagnetic effects) as in [46], and for the metal/hydride transformation under diffusion as above in (3.10). When considering the magnetic variation slow and thus neglecting all induced electrical effects and when neglecting also the self-induced demagnetising field, one can consider the (vector-valued) phase field $\chi=(\lambda,m)$ composed from the volume fraction λ related to the metal/hydride transformation and m the magnetization vector. Magnetization hysteresis effects due to magnetic-domain pinning effects can be accounted for through the nonsmooth potential ζ, cf. [37, 38, 47, 51]. Again, damage is an important phenomenon which can even pulverize such materials due to markable volume changes during the cubic-to-cubic structural transformation. Combining [46, 48, 50], the free energy can be considered as

$$\begin{aligned}\varphi_{\rm TOT}(\boldsymbol{E},\chi,c,d,\theta)&=\frac12\mathbb{C}(d)\boldsymbol{E}{:}\boldsymbol{E}+\frac k2\big|a(\lambda)-c\big|^2+\phi_1(c)+\phi_2(\theta)+\frac{a_0}{2}(\theta-\theta_{\rm c})|m|^2+\frac{b_0}{4}|m|^4+\alpha_1(\theta)\lambda\\&=\underbrace{\frac12\mathbb{C}(d)\boldsymbol{E}{:}\boldsymbol{E}+\frac{b_0}{4}|m|^4}_{=:\,\varphi_{\rm ME}}+\underbrace{\frac k2\big|a(\lambda)-c\big|^2+\phi_1(c)}_{=:\,\varphi_{\rm CH}}+\underbrace{\phi_2(\theta)+\frac{a_0}{2}(\theta-\theta_{\rm c})|m|^2+\alpha_1(\theta)\lambda}_{=:\,\varphi_{\rm TH}}\end{aligned}\tag{3.13}$$

and with $\theta_{\rm c}>0$ the Curie temperature above which the ferromagnetic phase does not exists, a_0, $b_0>0$, and α_1 is the temperature-dependent latent-heat density of the medium. Now $\frac{\kappa_1}{2}|\nabla\chi|^2$ occurring in (3.4) involves also $\frac{\kappa_1}{2}|\nabla m|^2$ which is called an exchange energy in magnetism. Further considerations may go beyond the ansatz in Section 2 by involving global effects through a demagnetising field as in [36, Remark 11] or dynamical electromagnetic effects including Joule heating through the Maxwell system possibly in an eddy-current approximation as in [46].

Example 3.4 (*Water and heat propagation in concrete).* An important application in civil engineering is water/vapor and heat transport in concrete undergoing damage and creep. The creep strain is most influenced by the moisture and temperature distribution. The model would be quite similar to (3.12) although some microscopical mechanisms behind the free energy and some dissipation mechanism are different. In particular, c would be again intrepreted as water concentration and μ as pressure. Moreover, the decomposition (1.1) would be adapted to the form considered in models of concrete that take into account creep, shrinkage and thermal strains [2, 17], namely, $\boldsymbol{\varepsilon}(\boldsymbol{u})=\boldsymbol{E}+\boldsymbol{E}_{\rm cr}+\boldsymbol{E}_{\rm sh}+\boldsymbol{E}_{\rm th}$, where $\boldsymbol{E}_{\rm cr}$ would be the creep strain, $\boldsymbol{E}_{\rm sh}$ is the shrinkage strain caused by change of moisture, and $\boldsymbol{E}_{\rm th}$ would be the thermal strain. Of course, since direct coupling with c and θ is not included in our analysis, we would resort to a penalization like in (3.10) for c and a similar one for θ, cf. Remark 3.5 below. Furthermore, in this case the constraint $\chi\in K$ would be dropped, that is, we would set $K=\mathbb{R}^N$. Moreover, the dissipation potential ζ would be smooth at $\dot\pi_{\rm pl}=0$ because, in contrast to plasticity, the creep is typically not an activated processes. Also the ageing mechanisms are play a role, influencing the activation threshold α of damage. There is a lot of phenomenological models in literature, although typically not based on rational thermomechanics to be directly fitted in the framework (3.7); cf. e.g. [28].

Remark 3.5 (*A general treatment of swelling or thermal expansion).* Some models would rather need, instead of (1.1), a more general form

$$\boldsymbol{\varepsilon}(\boldsymbol{u})=\boldsymbol{E}+\mathbb{E}\chi+s(c)\mathbb{E}_{\rm sw}+r(\theta)\mathbb{E}_{\rm ex}\tag{3.14}$$

with some $\mathbb{E}_{\rm sw}$ and $\mathbb{E}_{\rm ex}$ swelling and thermal-expansion tensors and some (possibly even nonlinear) mappings $s,r:\mathbb{R}\to\mathbb{R}$ modelling swelling or thermal expansion effects, respectively. Thermal expansion would influence also the entropy: in fact, (2.4) is no longer valid and, in the spirit of Remark 2.2, we should rather consider

$\varphi_{\rm ME}(\varepsilon(\boldsymbol{u}){-}\mathbb{E}\chi{-}r(\theta)\mathbb{E}_{\rm ex},\chi,d)$ which gives an additional contribution $r(\theta)'\mathbb{E}_{\rm ex}^\top\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\varepsilon(\boldsymbol{u}){-}\mathbb{E}\chi{-}r(\theta)\mathbb{E}_{\rm ex},\chi,d)$ to the enthalpy and also a corresponding contribution to the heat capacity $-\theta\partial^2_{\theta\theta}\psi$. Additional troubles have already been mentioned in Remark 2.3. To fit such more general situations to our ansatz, we can little modify the particular problem by introducing additional phase-field variables, say χ_1 and χ_2, and augment appropriately the free-energy parts $\varphi_{\rm CH}$ or $\varphi_{\rm TH}$. More specifically, $\varphi_{\rm CH}$ can be augmented by $\frac12k|s^{-1}(\chi_1){-}c|^2$ or $\varphi_{\rm TH}$ by $\frac12k|r^{-1}(\chi_2){-}\theta|^2-\frac12k\theta^2$. In fact, we already used the former term in (3.10), (3.12), and (3.13), too. Considering a presumably large constant k makes χ_1 mostly nearly equal to $s(c)$ and χ_2 nearly equal to $r(\theta)$ and, instead of (3.14), we then take

$$\varepsilon(\boldsymbol{u})=\boldsymbol{E}+\mathbb{E}\chi+\chi_1\mathbb{E}_{\rm sw}+\chi_2\mathbb{E}_{\rm ex}, \tag{3.15}$$

which complies with (1.1). Note that the positive definiteness $\partial^2_{cc}\varphi_{\rm CH}$ is kept and the heat capacity $-\theta\partial^2_{\theta\theta}\varphi_{\rm TH}(\chi,\theta)$ is not affected by this modification. The energy balance (2.1e) is then affected through non-thermal terms, which exhibits similar modelling effects but makes the analysis easier.

Example 3.6 (*Damage by freezing water).* Application of thermal expansion discussed in Remark 3.5 can be modelling a very common phenomenon that water propagating in porous medium expands during water-ice phase transformation and may cause damage. This happens e.g. in concrete or in poroelastic rocks discussed above. Other occurrence is in polymer membranes in fuel cells [58], etc. The thermal expansion is now (approximately) proportional to the overall amount of ice, i.e. $c\lambda$ where c is the water concentration and λ the volume fraction of ice versus liquid water. Naturally, $\lambda=\lambda(\theta)$. Like in Remark 3.5, we consider rather the linear splitting $\varepsilon(\boldsymbol{u})=\boldsymbol{E}+\beta\mathbb{E}_{\rm ex}$ with β and γ new phase-field variables which are expectedly close to $\lambda(\theta)c$ and c, respectively. This can be achieved e.g. by adding terms like $\frac12k|\theta-\lambda^{-1}(\beta/\gamma)|^2-\frac12k\theta^2+\frac12k|\gamma-c|^2$ to $\varphi_{\rm TH}+\varphi_{\rm CH}$. As ice practically cannot move, the mobility of water $\mathbf{M}=\mathbf{M}(\theta)$ falls to very small values if θ is below freezing point $\theta_{\rm F}$. The heat capacity $c_{\rm v}(\gamma,\theta)=-\theta\partial^2_{\theta\theta}\varphi_{\rm TH}(\gamma,\theta)$ also depends also on the water content γ and, moreover, may contain a Dirac distribution supported at the freezing point, i.e. $c_{\rm v}(\chi,\theta)=c_{{\rm v},0}+\gamma L\delta_{\theta_{\rm F}}(\theta)$ with L the latent heat of the water/ice phase transition. This is called the Stefan problem, cf. e.g. [42, 56], and then the upper bound C in the first condition in (4.1f) and also in (4.7) is ∞ and the graph of $\vartheta(\chi,\cdot)$ from (4.6) below has a horizontal segment of the length γL at the height $\theta_{\rm F}$. Some arguments we use below must be then slightly generalized as such $\vartheta(\chi,\cdot)$ with now $\chi=(\beta,\gamma)$ is not invertible and smooth; important, (5.28) and the corresponding $\nabla\theta$-estimate holds for such generalization, too. In fact, λ should better depend on the enthalpy w rather than on temperature θ, cf. also Definition 4.1 below, but anyhow a fine reqularization of the Stefan problem seems needed to overcome singular character of this problem.

Remark 3.7 (*Other applications).* Beside, there are a lot of applications without considering any diffusion or without any damage, i.e. c or d is void (not used). For example magnetostriction in magnetic shape-memory alloys as in [46] with no damage and no diffusion, or plasticity in metals with damage but no diffusion, and or a combination of inelastic processes with some more complex rhelogies involving additional internal variables in χ as eg. Jeffreys' model involving a creep strain, i.e. it combines the Maxwell rheology (responsible for creep) with the Kelvin-Voigt one, etc., cf. also Remark 2.1.

Remark 3.8 (*Some restrictions).* Within our approach, we cannot unfortunately handle the dependence of the coefficients in the gradient terms, i.e. of κ_2 and κ_1, on damage d or on χ, which would be natural in some application. This dependence would give rise the higher-order L^1-type terms in (4.10b) and (4.10d) which would destroy the regularity (5.34d) below without which also (5.74) could not be proved.

4. Data qualification, weak formulation, and the main result

Beside the standard notation for the Lebesgue L^p-space, we will use $W^{k,p}$ for Sobolev spaces whose k-th derivatives are in L^p-spaces, the abbreviation $H^k=W^{k,2}$. We consider a fixed time interval $I=[0,T]$ and we denote by $L^p(I;X)$ the standard Bocher space of Bochner-measurable mappings $I\to X$ with X a Banach space. Also, $W^{k,p}(I;X)$ denotes the Banach space of mappings from $L^p(I;X)$ whose k-th distributional derivative in time is also in $L^p(I;X)$. Also, $C(I;X)$ and $C_{\rm weak}(I;X)$ will denote the Banach space of continuous and weakly continuous mappings $I\to X$, respectively. Moreover, we denote by ${\rm BV}(I;X)$ the Banach space of the mappings $I\to X$ that have bounded variation on I, and by ${\rm B}(I;X)$ the space of Bochner measurable, everywhere defined, and bounded mappings $I\to X$. By ${\rm Meas}(I;X)$ we denote the space of X-valued measures on I.

Let us collect our main assumptions on the data:

$$\Omega\subset\mathbb{R}^3\ \text{ is a bounded domain with }\ \Gamma:=\partial\Omega\in C^2, \tag{4.1a}$$

$$\varphi_{\rm ME}\in C^2(\mathbb{R}^N{\times}\mathbb{R}{\times}\mathbb{R}^{3\times3}),\qquad \varphi_{\rm CH}\in C^2(\mathbb{R}^N{\times}\mathbb{R}),\qquad \varphi_{\rm TH}\in C^2(\mathbb{R}^N{\times}\mathbb{R}^+),\tag{4.1b}$$

$$\mathbf{M}\in C(\mathbb{R}^{3\times3}{\times}\mathbb{R}^N{\times}\mathbb{R}{\times}\mathbb{R}{\times}\mathbb{R}),\qquad \mathbf{K}\in C(\mathbb{R}^{3\times3}{\times}\mathbb{R}^N{\times}\mathbb{R}{\times}\mathbb{R}{\times}\mathbb{R}).\tag{4.1c}$$

$$\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\ge\epsilon|\boldsymbol{E}|^2-C,\quad |\partial_{(\boldsymbol{E},\chi)}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)|\le C(1+|\boldsymbol{E}|),\tag{4.1d}$$

$$|\partial_\chi\varphi_{\rm CH}(\chi,c)|\le C(1+|c|^3),\tag{4.1e}$$

$$0<\epsilon\le-\theta\partial^2_{\theta\theta}\varphi_{\rm TH}(\chi,\theta)\le C\quad\text{ and }\quad \big|\partial_\chi\varphi_{\rm TH}(\chi,\theta)-\theta\partial^2_{\chi\theta}\varphi_{\rm TH}(\chi,\theta)\big|\le C.\tag{4.1f}$$

$$\varphi_{\rm CH}(\chi,c)\ge\epsilon c^2-C,\tag{4.1g}$$

$$\boldsymbol{E}\mapsto\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\ \text{ is strongly convex uniformly with respect to } \chi \text{ and } d,\tag{4.1h}$$

$$(\boldsymbol{E},\chi)\mapsto\varphi_{\rm ME}(\boldsymbol{E},\chi,d)+M|\chi|^2\ \text{ is convex for } M \text{ sufficiently large},\tag{4.1i}$$

$$c\mapsto\varphi_{\rm CH}(\chi,c),\ \text{is strongly convex uniformly with respect to } \chi,\tag{4.1j}$$

$$\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\ \text{ and }\ \mathbf{K}(\boldsymbol{E},\chi,c,d,\theta)\ \text{ are uniformly positive definite and bounded},\tag{4.1k}$$

$$\exists C>0,\ \epsilon>0:\quad |\partial_c\varphi_{\rm CH}(\chi,c)|\le C+\epsilon\varphi_{\rm CH}(\chi,c),\tag{4.1l}$$

$$\zeta(\boldsymbol{E},\chi,c,d,\theta,\cdot):\mathbb{R}^N\to\mathbb{R}^+\ \text{ is convex and }\ \exists\epsilon>0:\ \ \epsilon|\dot\chi|^2\le\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\le\frac{1+|\dot\chi|^2}{\epsilon},\tag{4.1m}$$

$$\dot\chi\mapsto\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi){\cdot}\dot\chi:\mathbb{R}^N\to\mathbb{R}^+\ \text{ is single-valued and strictly convex, while}\tag{4.1n}$$

$$\xi\ \text{ satisfies (3.3) with }\ \alpha:\mathbb{R}^N\to\mathbb{R}^+\ \text{ smooth and}$$
$$\text{bounded together with its second gradient and }\ \inf\alpha(\mathbb{R}^N)>0,\tag{4.1o}$$

$$|\partial^2_{\chi c}\varphi_{\rm CH}(\chi,c)|\le C,\tag{4.1p}$$

$$|\partial_\chi\varphi_{\rm TH}(\chi,\theta)|\le C\sqrt{1+\varphi_{\rm ME/CH}(\boldsymbol{E},\chi,c,d)+e_{\rm TH}(\chi,\theta)},\ \text{ and}\tag{4.1q}$$

$$\big|\partial_\chi e_{\rm TH}(\chi,\theta)\big|\le C\sqrt{1+e_{\rm TH}(\chi,\theta)}.\tag{4.1r}$$

Then, we add the qualification of the initial data:

$$\boldsymbol{u}_0{\in}H^1(\Omega;\mathbb{R}^3),\ \ \boldsymbol{v}_0{\in}L^2(\Omega;\mathbb{R}^3),\ \ c_0{\in}H^1(\Omega),\ \ \chi_0{\in}H^1(\Omega;\mathbb{R}^N),\ \ d_0{\in}H^1(\Omega),\ \ w_0{\in}L^1(\Omega),\tag{4.2a}$$

$$d_0{\in}[0,1],\quad \chi_0{\in}K,\quad w_0\ge0\quad\text{a.e. in }\Omega,\quad\text{and}\tag{4.2b}$$

$$\int_\Omega\varphi_{\rm ME}(\boldsymbol{E}_0,\chi_0,d_0)+\frac{\kappa_2}{2}|\nabla d_0|^2\,{\rm d}x$$
$$\le\int_\Omega\Big(\varphi_{\rm ME}(\boldsymbol{E}_0,\chi_0,\widetilde d)+\frac{\kappa_2}{2}|\nabla\widetilde d|^2+\alpha(\chi(t))(\widetilde d{-}d_0)\Big){\rm d}x\quad\forall\widetilde d{\in}H^1(\Omega),\ 0\le\widetilde d\le d_0\ \text{a.e. on }\Omega,\tag{4.2c}$$

with $\boldsymbol{E}_0=\boldsymbol{\varepsilon}(\boldsymbol{u}_0)-\mathbb{E}\chi_0$, and the qualification of the outer mechanical, chemical, and thermal loading:

$$\boldsymbol{f}{\in}L^2(Q;\mathbb{R}^3),\quad \boldsymbol{f}_{\rm s}{\in}L^2(\Sigma;\mathbb{R}^3),\quad q_{\rm s}{\in}L^1(\Sigma),\quad h_{\rm s}{\in}L^2(\Sigma)\ \text{ with } q_{\rm s}\ge0 \text{ and } h_{\rm s}\ge0 \text{ a.e. on }\Sigma,\tag{4.3}$$

where we used the abbreviation $Q=(0,T)\times\Omega$ and $\Sigma=(0,T)\times\Gamma$ for a fixed time horizon $T>0$. Later, $\bar Q$ will denote the closure of Q.

The uniform strong convexity means e.g. in (4.1h) that

$$\exists\epsilon>0\ \forall(\boldsymbol{E},\tilde{\boldsymbol{E}},\chi,d){\in}\mathbb{R}^{3\times3}{\times}\mathbb{R}^{3\times3}{\times}K{\times}[0,1]:\quad \big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\tilde{\boldsymbol{E}}\tilde{\boldsymbol{E}},\chi,d)-\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\big):(\tilde{\boldsymbol{E}}{-}\boldsymbol{E})\ge\epsilon|\tilde{\boldsymbol{E}}{-}\boldsymbol{E}|^2.\tag{4.4}$$

Analogous meaning has also (4.1l). The statament (4.1k) is as usual understood that there exists $\epsilon>0$ such that, for all $\boldsymbol{v}\in\mathbb{R}^3$ and $(\boldsymbol{E},\chi,c,d,\theta)\in\mathbb{R}^{3\times3}\times K\times[0,1]\times\mathbb{R}\times\mathbb{R}^+$, it holds $\epsilon|\boldsymbol{v}|^2\le\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\boldsymbol{v}\cdot\boldsymbol{v}\le|\boldsymbol{v}|^2/\epsilon$ and $\epsilon|\boldsymbol{v}|^2\le\mathbf{K}(\boldsymbol{E},\chi,c,d,\theta)\boldsymbol{v}\cdot\boldsymbol{v}\le|\boldsymbol{v}|^2/\epsilon$. In (4.1q)–(4.1r), we understand that $\varphi_{\rm ME/CH}\ge0$ and $e_{\rm TH}\ge0$, as we always can without loss of generality. The qualification (4.2c) represents a semi-stability of the initial damage profile; the adjective "semi" refers to that $\boldsymbol{E}_0$ and χ_0 are fixed on both the left- and the right-hand sides of (4.2c).

Let us briefly comment the main aspects of the above assumptions:

1. The smoothness of $\partial\Omega$ is here needed to ensure H^2 regularity of the solutions of the elliptic problems considered in Lemma 5.4 below (see in particular the regularized equation (5.36)), where we shall prove L^2 regularity of $\Delta\chi$ (see (5.34d)). To this aim, we note that the second growth assumption in (4.1d) and assumption (4.1e) on $\partial_\chi\varphi_{\rm ME/CH}$, together with assumption (4.1m) on ζ facilitates this estimate.
2. In principle we could admit a general p-growth/coercivity with $p\le2$ in (4.1d). However, we cannot handle $p>2$. The main reason is the integrability of terms in (5.76) and, if $\varrho>0$, also the duality in (5.55). For simplicity, we confine ourselves to $p=2$ only, without restricting substantially possible applications.

3. Assumptions (4.1k) are needed to have coercivity in the diffusion and the heat-conduction equation.
4. It follows from the first condition in (4.1f) that the thermal part of the internal energy $e_{\rm TH}$ defined in (3.6) is continuously differentiable, and satisfies:
$$0<\epsilon\le\partial_\theta e_{\rm TH}(\chi,\theta)\le C. \tag{4.5}$$
Hence, the function $\theta\mapsto e_{\rm TH}(\chi,\theta)$ is invertible for all χ and its inverse is continuously differentiable. Thus, there exists a function $\vartheta\in C^1(\mathbb{R}^N\times\mathbb{R}^+;\mathbb{R}^+)$ such that
$$e_{\rm TH}(\chi,\vartheta(\chi,w))=w \tag{4.6}$$
$$0<1/C\le\partial_w\vartheta(\chi,w)\le 1/\epsilon \tag{4.7}$$
with ϵ and C referring to (4.5). Moreover, we observe that the second condition in (4.1f) entails that
$$|\partial_\chi\vartheta(\chi,w)|\le C. \tag{4.8}$$
5. The semi-stability of the initial damage (4.2c) is needed for the energy conservation which, in turn, is vitally needed for the convergence in the heat equation, cf. Step 9 in the proof of Proposition 5.5.

We can now state the weak formulation of the initial-boundary-value problem (3.7)–(3.9). As for the damage part, we use the concept of the so-called energetic solution devised by Mielke and Theil [35], based on the energy (in)equality and the so-called stability, cf. (4.10d) below, and further employed in the thermodynamical concept in [43]. This formulation is essentially equivalent to the conventional weak formulation but excludes time derivatives of rate-independent variables, i.e. here the damage d.

Definition 4.1. Given initial conditions (4.2) and the bulk and boundary data (4.3), the seven-tuple $(\boldsymbol{u},\chi,c,d,\theta,\mu,w)$ with
$$\boldsymbol{u}\in L^\infty(I;W^{1,p}(\Omega;\mathbb{R}^3))\cap H^1(I;H^1(\Omega;\mathbb{R}^3)), \tag{4.9a}$$
$$\chi\in C_{\rm weak}(I;H^1(\Omega;\mathbb{R}^N))\cap H^1(I;L^2(\Omega;\mathbb{R}^N))\cap C(\bar{Q};\mathbb{R}^N), \tag{4.9b}$$
$$c\in L^\infty(I;L^2(\Omega)), \tag{4.9c}$$
$$d\in {\rm B}(I;H^1(\Omega))\cap {\rm BV}(I;L^1(\Omega)),\quad d\ge 0 \text{ a.e. on } Q, \tag{4.9d}$$
$$\theta\in L^r(I;W^{1,r}(\Omega))\qquad\text{for any } r\in[1,5/4), \tag{4.9e}$$
$$\mu\in L^\infty(I;H^1(\Omega)), \tag{4.9f}$$
$$w\in L^\infty(I;L^1(\Omega)) \tag{4.9g}$$
is called a weak solution to the initial-boundary-value problem (3.7)–(3.9) if
$$\int_Q(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)+\mathbb{D}\dot{\boldsymbol{E}}){:}\boldsymbol{\varepsilon}(\boldsymbol{z})-\varrho\dot{\boldsymbol{u}}{\cdot}\dot{\boldsymbol{z}}\,{\rm d}x\,{\rm d}t=\int_Q\boldsymbol{f}{\cdot}\boldsymbol{z}\,{\rm d}x\,{\rm d}t+\int_\Sigma\boldsymbol{f}_{\rm s}{\cdot}\boldsymbol{z}\,{\rm d}S\,{\rm d}t+\int_\Omega\boldsymbol{v}_0{\cdot}\boldsymbol{z}(0)\,{\rm d}x$$
$$\forall\boldsymbol{z}\in L^2(I;H^1(\Omega;\mathbb{R}^3))\cap H^1(I;L^2(\Omega;\mathbb{R}^3)),\ \boldsymbol{z}(T)=0, \tag{4.10a}$$
$$\int_Q\zeta(\boldsymbol{E},\chi,c,d,\theta,z)+\big(\partial_\chi\varphi_{\rm TOT}(\boldsymbol{E},\chi,c,d,\theta)-\mathbb{E}^\top{:}(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)+\mathbb{D}\dot{\boldsymbol{E}})+\sigma_{\rm r}\big){\cdot}(z-\dot\chi)+\kappa_1\nabla\chi{:}\nabla z\,{\rm d}x\,{\rm d}t$$
$$+\int_\Omega\frac{\kappa_1}{2}\big|\nabla\chi_0\big|^2{\rm d}x\ge\int_Q\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\,{\rm d}x\,{\rm d}t+\int_\Omega\frac{\kappa_1}{2}\big|\nabla\chi(T)\big|^2{\rm d}x\quad\forall z\in L^2(I;H^1(\Omega;\mathbb{R}^M)), \tag{4.10b}$$
$$\int_Q\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu\cdot\nabla z-c\dot z\,{\rm d}x\,{\rm d}t=\int_\Sigma h_{\rm s}z\,{\rm d}S\,{\rm d}t+\int_\Omega c_0z(0){\rm d}x\qquad\forall z\in H^1(Q),\ z(T)=0, \tag{4.10c}$$
$$\int_\Omega\varphi_{\rm ME}(\boldsymbol{E}(t),\chi(t),d(t))+\frac{\kappa_2}{2}|\nabla d(t)|^2\,{\rm d}x\le\int_\Omega\Big(\varphi_{\rm ME}(\boldsymbol{E}(t),\chi(t),\widetilde{d})+\frac{\kappa_2}{2}|\nabla\widetilde{d}|^2$$
$$+\alpha(\chi(t))(\widetilde{d}-d(t))\Big){\rm d}x\qquad\forall t\in I\ \forall\widetilde{d}\in H^1(\Omega),\ 0\le\widetilde{d}\le d(t)\text{ on }\Omega, \tag{4.10d}$$
$$\int_Q\mathbf{K}(\boldsymbol{E},\chi,c,d,\theta)\nabla\theta\cdot\nabla z-w\dot z\,{\rm d}x\,{\rm d}t=\int_\Omega\big(w_0+\alpha(\chi_0)d_0\big)z(0)\,{\rm d}x+\int_\Sigma q_{\rm s}z\,{\rm d}S\,{\rm d}t$$
$$+\int_Q\Big(\big(\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)+\partial_\chi\varphi_{\rm TH}(\chi,\theta)+\alpha'(\chi)d\big){\cdot}\dot\chi+\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu{\cdot}\nabla\mu$$
$$+\mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}}\Big)z+\alpha(\chi)d\dot z\,{\rm d}x\,{\rm d}t\qquad\forall z\in W^{1,\infty}(Q),\quad z(T)=0, \tag{4.10e}$$
$$\mathscr{E}_{\rm MC}(T)+\int_\Omega\alpha(\chi(T))d(T)\,{\rm d}x+\int_Q\Big(\mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}}+\big(\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)+\partial_\chi\varphi_{\rm TH}(\chi,\theta)+\alpha'(\chi)d\big){\cdot}\dot\chi$$

$$+\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu\cdot\nabla\mu\Big)\,\mathrm{d}x\mathrm{d}t = \mathscr{E}_{\rm MC}(0)+\int_\Omega\alpha(\chi_0)d_0\,\mathrm{d}x+\int_Q \boldsymbol{f}\cdot\dot{\boldsymbol{u}}\,\mathrm{d}x\mathrm{d}t+\int_\Sigma \boldsymbol{f}_{\rm s}\cdot\dot{\boldsymbol{u}}+q_{\rm s}+\mu h_{\rm s}\,\mathrm{d}S\mathrm{d}t \tag{4.10f}$$

where $\boldsymbol{E}\in H^1(I;L^2(\Omega;\mathbb{R}^{3\times3}_{\rm sym}))$, μ and w from (4.9f,g), and $\sigma_{\rm r}\in L^2(Q;\mathbb{R}^N)$, satisfy

$$\boldsymbol{E}=\boldsymbol{\varepsilon}(\boldsymbol{u})-\mathbb{E}\chi, \qquad \mu=\partial_c\varphi_{\rm CH}(\chi,c), \qquad w=e_{\rm TH}(\chi,\theta), \qquad \sigma_{\rm r}\in\partial\delta_K(\chi) \tag{4.10g}$$

a.e. in Q and where the energy occurred in (4.10f) at time $t=0$ and $t=T$ is:

$$\mathscr{E}_{\rm MC}(t):=\int_\Omega \varphi_{\rm ME/CH}(\boldsymbol{E}(t),\chi(t),d(t),c(t))+\frac{\varrho}{2}\big|\dot{\boldsymbol{u}}(t)\big|^2+\frac{\kappa_1}{2}\big|\nabla\chi(t)\big|^2+\frac{\kappa_2}{2}\big|\nabla d(t)\big|^2\,\mathrm{d}x,$$

where $\varphi_{\rm ME/CH}$ is defined in (3.5). Eventually, the remaining three initial conditions holds:

$$\boldsymbol{u}(0)=\boldsymbol{u}_0, \qquad \chi(0)=\chi_0, \qquad d(0)=d_0 \qquad \text{a.e. in } \Omega. \tag{4.11}$$

The above definition uses several tricky points, which seems in general quite inevitable for this sort of complicated problems, cf. also [40] for even more tricky definition. Here, let us note that we made the by-part integration in time in (4.10a,c,e) to avoid abstract duality pairing due to only weak estimates on $\varrho\ddot{\boldsymbol{u}}$, $\dot{c}$, and $\dot{w}$ we will have at disposal, cf. (5.34a-c) below. The other three initial conditions $\dot{\boldsymbol{u}}(0)=\boldsymbol{v}_0$, $c(0)=c_0$, and $w(0)=w_0$ are thus involved already in (4.10a,c,e). The by-part integration used in (4.10b) is to avoid the term $\int_Q\nabla\chi\cdot\nabla\dot{\chi}\,\mathrm{d}x\,\mathrm{d}t$ where $\nabla\dot{\chi}$ would not have a good sense. Also note that we used the by-part integration in time for the heat term induced by damage, i.e.

$$\int_{\bar{Q}}\alpha(\chi)z\dot{d}(\mathrm{d}x\mathrm{d}t)=\int_\Omega\alpha(\chi(T))z(T)d(T)\,\mathrm{d}x-\int_Q(\alpha'(\chi)\dot{\chi}z+\alpha(\chi)\dot{z})d\,\mathrm{d}x\mathrm{d}t-\int_\Omega\alpha(\chi(0))z(0)d(0)\,\mathrm{d}x \tag{4.12}$$

for z smooth with $z(T)=0$ in (4.10e) or with $z=1$ in (4.10f) to avoid usage of the measure $\dot{d}$ in Definition 4.1 although here it would be well possible because $\alpha(\chi)$ is a continuous function on $\bar{Q}$. More importantly, we balanced only the mechano-chemical energy $\mathscr{E}_{\rm MC}$ to avoid usage of $\theta(T)$ or of $w(T)$ which would not have a specified meaning as the temperature as well as the thermal part of the internal energy may be discontinuous in time instances where $\dot{d}$ concentrates.

Theorem 4.2. Let the assumptions (4.1)–(4.3) be valid. Then there exists a weak solution to the initial-boundary-value problem (3.7)–(3.9) in the sense of Definition 4.1 such that also $\varrho\ddot{\boldsymbol{u}}\in L^2(I;H^1(\Omega;\mathbb{R}^3)^*)$, $\dot{c}\in L^2(I;H^1(\Omega)^*)$, $\dot{w}\in\mathrm{Meas}(I;W^{1,r/(r-1)}(\Omega)^*)$, $\theta\ge0$ a.e. in Q. Moreover, the total-energy balance is satisfied "generically" in the sense that, for a.a. $t\in I$, it holds that

$$\mathscr{E}_{\rm TOT}(t)-\mathscr{E}_{\rm TOT}(0)=\int_0^t\Big(\int_\Omega\boldsymbol{f}\cdot\dot{\boldsymbol{u}}\,\mathrm{d}x+\int_\Gamma\boldsymbol{f}_{\rm s}\cdot\dot{\boldsymbol{u}}+q_{\rm s}+\mu h_{\rm s}\,\mathrm{d}S\Big)\mathrm{d}t, \tag{4.13}$$

where, referring to $\varphi_{\rm ME/CH}$ and $e_{\rm TH}$ from (3.5)–(3.6), the total energy is:

$$\mathscr{E}_{\rm TOT}(t)=\int_\Omega\Big(\varphi_{\rm ME/CH}\big(\boldsymbol{E}(t),\chi(t),d(t),c(t)\big)+e_{\rm TH}\big(\chi(t),\theta(t)\big)+\frac{\varrho}{2}\big|\dot{u}(t)\big|^2+\frac{1}{2}\kappa_1\big|\nabla\chi(t)\big|^2+\frac{1}{2}\kappa_2\big|\nabla d(t)\big|^2\Big)\,\mathrm{d}x.$$

We will prove this theorem in the next section by a constructive way which also suggest a conceptual numerical strategy which, after another discretisation in space, would allow for an efficient computer implementation.

Remark 4.3 (Poro-elastic model revisited). The poro-elastic example (3.12) does not comply with the second condition in (4.1d) unless λ, G, and M is independent of d. Also, (3.12) is incompatible with (4.1i) in general, although one could weaken this condition and then make finer splitting in the time-discretisation in Section 5 by considering (p,γ) separately from $(\boldsymbol{E},\pi_{\rm pl})$ in (5.1); here it however depends on the dissipation which should allow this separation. Anyhow, due to (4.1d), the example (3.12) has to be slightly modified. One option is to pose:

$$\begin{aligned}\varphi_{\rm TOT}(\boldsymbol{E},p,\gamma,c,d,\theta)=\frac{1}{2}\frac{\lambda(p,d)(\mathrm{tr}\,\boldsymbol{E})^2}{\sqrt{1+\epsilon(\mathrm{tr}\,\boldsymbol{E})^2}}+G(p,d)\frac{|\boldsymbol{E}|^2}{\sqrt{1+\epsilon|\boldsymbol{E}|^2}}+\frac{1}{2}M(p,d)\frac{|\beta\mathrm{tr}\,\boldsymbol{E}-\gamma+p|^2}{\sqrt{1+\epsilon(\mathrm{tr}\,\boldsymbol{E})^2}}\\+\frac{1}{2}\lambda_0(\mathrm{tr}\,\boldsymbol{E})^2+G_0|\boldsymbol{E}|^2+\frac{1}{2}k|\gamma-c|^2+c_{\rm v}\theta(\ln\theta-1)\end{aligned} \tag{4.14}$$

with $\epsilon>0$ presumably small regularing parameter and with $\lambda_0\ge0$ and $G_0>0$. Then (4.1d) is satisfied.

5. Time discretisation and the proof of existence of weak solutions

Our proof of Theorem 4.2 is based on the following strategy:

- A semi-implicit discretisation of the system (3.7) of a fractional-step type which decouples this system at each time level and is numerically stable under quite weak convexity requirements on $\varphi_{_{\rm TOT}}$, cf. also [44, Remark 8.25] for a general discussion. Namely, we use four steps in such a way that one solves separately (3.7a-b), then (3.7c), then (3.7d), and eventually (3.7e).
- The above specified splitting allows for only the relatively weak (partial) semi-convexity assumption (4.1i). In particular, we thus do not require any (semi)-convexity of $\varphi_{_{\rm ME/CH}}$ or even of $\varphi_{_{\rm ME}}$ itself which would exclude interesting applications like the examples in Section 3.
- Further key ingredient is an L^2-estimate of the driving force for (4.10b) together with the qualification of the dissipation potential ζ for χ to have a bounded subdifferential so that one can obtain the additional estimate $\Delta\chi\in L^2(Q;\mathbb{R}^N)$. This facilitates the by-part integration formula (5.74) and, if Ω is smooth, also the H^2-regularity of χ is needed to give a good sense to the dissipative-heat term $\alpha(\chi)\dot{d}$.

We use an equidistant partition of the time interval $I=I$ with a time step $\tau>0$, assuming $T/\tau\in\mathbb{N}$, and denote by $\{\boldsymbol{u}_\tau^k\}_{k=0}^{T/\tau}$ an approximation of the desired values $\boldsymbol{u}(k\tau)$, and similarly d_τ^k is to approximate $d(k\tau)$, etc. Further, let us abbreviate by $\mathfrak{d}_\tau^k$ the backward difference operator, i.e. e.g. $\mathfrak{d}_\tau^k\boldsymbol{u}:=\frac{\boldsymbol{u}_\tau^k-\boldsymbol{u}_\tau^{k-1}}{\tau}$, and similarly also $[\mathfrak{d}_\tau^k]^2\boldsymbol{u}=\mathfrak{d}_\tau^k[\mathfrak{d}_\tau^k\boldsymbol{u}]=\frac{\boldsymbol{u}_\tau^k-2\boldsymbol{u}_\tau^{k-1}+\boldsymbol{u}_\tau^{k-2}}{\tau^2}$, or $\mathfrak{d}_\tau^k d:=\frac{d_\tau^k-d_\tau^{k-1}}{\tau}$, $\mathfrak{d}_\tau^k c:=\frac{c_\tau^k-c_\tau^{k-1}}{\tau}$, etc. When evaluating $[\mathfrak{d}_\tau^k]^2\boldsymbol{u}$ for $k=1$, we let $\boldsymbol{u}_\tau^{-1}=\boldsymbol{u}_\tau^0-\tau\boldsymbol{v}_0$.

From a conceptual "algorithmic" viewpoint that may serve for a possible numerical implementation and for making the free-energy qualification as weak as possible, it is advantageous to make as fine splitting as possible. The finest splitting is essentially dictated by the considered de-coupled form of the dissipation energy, cf. also Rem. 5.8 below.

Step 1: We seek weak solution $\boldsymbol{u}_\tau^k$, and χ_τ^k to the following boundary-value problem (written in the classical formulation)

$$\varrho[\mathfrak{d}_\tau^k]^2\boldsymbol{u}-{\rm div}\big(\partial_{\boldsymbol{E}}\varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau\big)=\boldsymbol{f}_\tau^k \tag{5.1a}$$

$$\partial_{\dot\chi}\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1},\mathfrak{d}_\tau^k\chi)-\kappa_1\Delta\chi_\tau^k+\partial_\chi\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1})$$
$$+\partial_\chi\varphi_{_{\rm TH}}(\chi_\tau^{k-1},\theta_\tau^{k-1})-\mathbb{E}^\top{:}\big(\partial_{\boldsymbol{E}}\varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau\big)+\sigma_{{\rm r},\tau}^k\ni 0, \tag{5.1b}$$

$$\text{with}\ \ \boldsymbol{E}_\tau^k=\boldsymbol{\varepsilon}(\boldsymbol{u}_\tau^k)-\mathbb{E}\chi_\tau^k\ \ \text{and some}\ \ \sigma_{{\rm r},\tau}^k\in\partial\delta_K(\chi_\tau^k)\quad\text{on }\Omega, \tag{5.1c}$$

and with boundary conditions

$$\big(\partial_{\boldsymbol{E}}\varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau\big)\mathbf{n}=\boldsymbol{f}_{{\rm s},\tau}^k\qquad\text{and}\qquad\nabla\chi_\tau^k\cdot\mathbf{n}=0\quad\text{on }\Gamma. \tag{5.1d}$$

Step 2. We seek a weak solution c_τ^k and μ_τ^k to the boundary-value problem:

$$\mathfrak{d}_\tau^k c-{\rm div}\big(\mathbf{M}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^k\big)=0\quad\text{with}\ \ \mu_\tau^k=\partial_c\varphi_{_{\rm CH}}(\chi_\tau^k,c_\tau^k)\quad\text{on }\Omega, \tag{5.2a}$$

with boundary condition

$$\nabla\mu_\tau^k\cdot\mathbf{n}=0\quad\text{on }\Gamma. \tag{5.2b}$$

Step 3. We seek $d_\tau^k\in H^1(\Omega)$ as a (global) minimizer of the functional

$$d\mapsto\int_\Omega\varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d)-\alpha(\chi_\tau^k)d+\frac{\kappa_2}{2}|\nabla d|^2{\rm d}x \tag{5.3}$$

on the set $\{d{\in}H^1(\Omega);\ 0\le d\le d_\tau^{k-1}\}$.

Step 4. Eventually, we seek a weak solution θ_τ^k and w_τ^k to the boundary-value problem:

$$\frac{w_\tau^k-w_\tau^{k-1}}{\tau}-{\rm div}\big(\mathbf{K}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k,\theta_\tau^k)\nabla\theta_\tau^k\big)=\big(\partial_{\dot\chi}\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1},\mathfrak{d}_\tau^k\chi)+\partial_\chi\varphi_{_{\rm TH}}(\chi_\tau^k,\theta_\tau^k)\big){\cdot}\mathfrak{d}_\tau^k\chi$$
$$-\alpha(\chi_\tau^k)\mathfrak{d}_\tau^k d+\frac{\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}{:}\mathfrak{d}_\tau^k\boldsymbol{E}}{1+\tau|\mathfrak{d}_\tau^k\boldsymbol{E}|^2}+\frac{\mathbf{M}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^k\cdot\nabla\mu_\tau^k}{1+\tau|\nabla\mu_\tau^k|^2}\qquad\text{with}\quad w_\tau^k=e_{_{\rm TH}}(\chi_\tau^k,\theta_\tau^k) \tag{5.4a}$$

with the boundary condition

$$\mathbf{K}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k,\theta_\tau^k)\nabla\theta_\tau^k=q_{s,\tau}^k\quad\text{on }\Gamma. \tag{5.4b}$$

Of course, this recursive scheme is to be started for $k=1$ by putting

$$\boldsymbol{u}_\tau^0=\boldsymbol{u}_0,\qquad \boldsymbol{u}_\tau^{-1}=\boldsymbol{u}_0-\tau\boldsymbol{v}_0,\qquad \chi_\tau^0=\chi_0,\qquad c_\tau^0=c_0,\qquad d_\tau^0=d_0,\qquad w_\tau^0=w_0 \tag{5.5}$$

with w_0 from (3.9). An important feature of this scheme is that it decouples to four boundary-value problems, which (after a further spatial discretisation) can facilitate a numerical treatment and which is advantageously used even to show existence of approximate solutions. We also remark that the term $\partial_\chi\varphi_{\rm TH}$ is treated as lower-order terms. Note also that d_τ^k obtained in Step 3 is a weak solution to the boundary-value problem:

$$\partial_{\dot d}\xi(\chi_\tau^k,\mathfrak{d}_\tau^k d)+\partial_d\varphi_{\rm ME}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k)+s_{{\rm r},\tau}^k\ni\kappa_2\Delta d_\tau^k\quad\text{on }\Omega\quad\text{with}\quad\nabla d_\tau^k\cdot\mathbf{n}=0\quad\text{on }\Gamma, \tag{5.6}$$

with some $s_{{\rm d},\tau}^k\in$ and $s_{{\rm r},\tau}^k\in\partial\delta_{[0,\infty]}(d_\tau^k)$ on Ω. We however rely on the fact that d_τ^k is a special weak solution which is also the minimizer of the underlying potential (5.3). This need not be the same if $\varphi_{\rm ME}(\boldsymbol{E},\cdot)$ is not convex, i.e. if damage may undergo weakening effects.

Lemma 5.1 (Existence of the discrete solution). Let (4.1)–(4.3) hold. Then, for any $k=1,...,T/\tau$, (5.1)–(5.4) has a solution $\boldsymbol{u}_\tau^k\in H^1(\Omega;\mathbb{R}^3)$, $\chi_\tau^k\in H^1(\Omega;\mathbb{R}^N)$, $d_\tau^k\in H^1(\Omega)$, $\sigma_{{\rm r},\tau}^k\in L^2(\Omega;\mathbb{R}^N)$, $c_\tau^k\in H^1(\Omega)$, $\mu_\tau^k\in H^1(\Omega)$, $\theta_\tau^k\in H^1(\Omega)$ such that $\theta_\tau^k\ge0$.

Proof. Step 1: Let us consider the space $V=H^1(\Omega;\mathbb{R}^3)\times H^1(\Omega)$. The boundary-value problem (5.1) is of the form $A(\boldsymbol{u},\chi)\ni0$, with A a set-valued mapping from V to its dual V^* such that $A=\partial\Phi$, where

$$\begin{aligned}\Phi(\boldsymbol{u},\chi)=\int_\Omega\bigg(&\varphi_{\rm ME/CH}(\boldsymbol{\varepsilon}(\boldsymbol{u})-\mathbb{E}\chi,\chi,d_\tau^{k-1},c_\tau^{k-1})+\frac12\kappa_1|\nabla\chi|^2+\delta_K(\chi)\\&+\frac{\tau^2}{2}\varrho\Big|\frac{\boldsymbol{u}-2\boldsymbol{u}_\tau^{k-1}+\boldsymbol{u}_\tau^{k-2}}{\tau^2}\Big|^2+\frac{\tau}{2}\mathbb{D}\Big(\boldsymbol{\varepsilon}(\frac{\boldsymbol{u}-\boldsymbol{u}_\tau^{k-1}}{\tau})-\mathbb{E}\chi\Big):\Big(\boldsymbol{\varepsilon}(\frac{\boldsymbol{u}-\boldsymbol{u}_\tau^{k-1}}{\tau})-\mathbb{E}\chi\Big)\\&+\tau\zeta\Big(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1},\frac{\chi-\chi_\tau^{k-1}}{\tau}\Big)\\&+\partial_\chi\varphi_{\rm TH}(\chi_\tau^{k-1},\theta_\tau^{k-1})\cdot\chi+\boldsymbol{f}_\tau^k\cdot\boldsymbol{u}\bigg)\,{\rm d}x+\int_\Gamma\boldsymbol{f}_{{\rm s},\tau}^k\cdot\boldsymbol{u}\,{\rm d}S.\end{aligned} \tag{5.7}$$

Here it is understood that $\varrho=0$ in the quasistatic case. By (4.1i) and (4.1m), the potential Φ is weakly lower-semicontinuous although not necessarily convex here; in fact, later it will be convex if $\tau>0$ is small enough, cf. Lemma 5.3 below. Due to the terms δ_K and ζ, Φ is nonsmooth. Moreover, by (4.1g) it is also coercive. Hence, by using the direct method, cf. e.g. [44, Theorem 5.3], we can see that (5.1) has at least a solution. Next we observe that the solution satisfies an inclusion:

$$\partial_\chi(\Phi_1+\Phi_2)(\chi)+D\Phi_3(\chi)\ni0, \tag{5.8}$$

where the left-hand side is a subset of $H^1(\Omega;\mathbb{R}^N)^*$, with $\Phi_1(\chi)=\tau\int_\Omega\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},\theta_\tau^{k-1},\frac{\chi-\chi_\tau^{k-1}}{\tau})\,{\rm d}x$, $\Phi_2(\chi)=\int_\Omega\delta_K(\chi)\,{\rm d}x$ and with Φ_3 the remaining part of the potential Φ, which is Gateaux differentiable (we denote its Gateaux differential by $D\Phi_3$). Next, we observe that Φ_1 is convex, and by (4.1m) its domain is the whole space $H^1(\Omega;\mathbb{R}^N)$, and it is bounded from above in a bounded set of $H^1(\Omega;\mathbb{R}^N)$. Thus, by [56, Thm. 4.8], Φ_1 is locally Lipschiz continuous. Next, since ${\rm dom}(\Phi_2)\ne\emptyset$, there exists $\chi_0\in{\rm dom}\Phi_1\cap{\rm dom}\Phi_2$ such that Φ_1 is in particular continuous at χ_0. As both Φ_1 and Φ_2 are convex and lower semicontinuous, we conclude [56, Thm. 4.7] that:

$$\partial\Phi_1(\chi)+\partial\Phi_2(\chi)=\partial_\chi(\Phi_1+\Phi_2)(\chi). \tag{5.9}$$

Now, we can take a measurable selection $\sigma_{{\rm d},\tau}^k\in\tau\partial_\chi\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},\theta_\tau^{k-1},\frac{\chi-\chi_\tau^{k-1}}{\tau})$ and by (4.1m), $\sigma_{{\rm d},\tau}^k\in L^2(\Omega;\mathbb{R}^N)$. Then by comparison, we obtain $\sigma_{{\rm r},\tau}^k\in L^2(\Omega;\mathbb{R}^N)$, cf. also the arguments leading to (5.34e) below.

Step 2: We can treat (5.2) by a variational approach. We consider the function $\varphi_{\rm CH}^*(\chi_\tau^k,\cdot)$ defined as the Legendre transform of $\varphi_{\rm CH}(\chi_\tau^k,\cdot)$, and we notice that (5.2b) can be written as

$$c_\tau^k=\partial_\mu\varphi_{\rm CH}^*(\chi_\tau^k,\mu_\tau^k). \tag{5.10}$$

Then (5.2) is equivalent the following variational problem on $H^1(\Omega)$:

$$\text{minimize }\mu\mapsto\int_\Omega\frac{\varphi_{\rm CH}^*(\chi_\tau^k,\mu)-c_\tau^{k-1}\mu}{\tau}+\mathbf{M}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu\cdot\nabla\mu\,{\rm d}x, \tag{5.11}$$

which can be solved through the direct method. To this aim, we notice that, since the domain of $\varphi(\chi_\tau^k,d_\tau^{k-1},\cdot)$ is $\mathbb{R}$, its Legendre transform is coercive. Indeed, on writing for short $f(c)=\varphi_{\rm CH}(\chi_\tau^k,c)$, and on denoting by f^* the Legendre transform of f, we have $\lim_{|\mu|\to+\infty}f^*(\mu)/|\mu|=\lim_{|\mu|\to+\infty}\sup_c(({\rm sign}\mu)c-f(c)/|\mu|)\ge\lim_{|\mu|\to+\infty}({\rm sign}\mu)\overline{c}-f(\overline{c})/|\mu|)=({\rm sign}\mu)\overline{c}$ for every $\overline{c}\in\mathbb{R}$. Thus $\lim_{\mu\to+\infty}f^*(\mu)/\mu=+\infty$.

Step 3: The solution of (5.3) can be obtained simply by weak lower semicontinuity and coercivity arguments. Note that we do not require convexity of $\varphi_{\rm ME}(\boldsymbol{E},d,\cdot)$ so that the solution of (5.3) does not need to be unique.

Step 4: In this final step we solve the time-discrete heat equation (5.4a) with boundary conditions (5.4b). To this aim, we note that $\nabla\mu_\tau^k\in L^2(\Omega;\mathbb{R}^3)$. In particular, we have simply both $\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}{:}\mathfrak{d}_\tau^k\boldsymbol{E}/(1{+}\tau|\mathfrak{d}_\tau^k\boldsymbol{E}|^2)\in L^\infty(\Omega)$ and $\mathbf{M}(\mathsf{E}_{{\rm e},\tau}^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1})\nabla\mu_\tau^k{\cdot}\nabla\mu_\tau^k/(1{+}\tau|\nabla\mu_\tau^k|^2)\in L^\infty(\Omega)$, and thus the right-hand side of (5.4a) is in $L^2(\Omega)$. Therefore, eventually, we are to solve (5.4), which represents a semilinear heat-transfer equation with the right-hand side in $H^1(\Omega)^*$. The only nonlinearity with respect to θ_τ^k is in the terms $\mathbf{L}(\boldsymbol{\varepsilon}(\boldsymbol{u}_\tau^k),\chi_\tau^k,d_\tau^k,c_\tau^k,\theta_\tau^k)$ and $\partial_\chi\varphi_{\rm TH}(\chi_\tau^k,\theta_\tau^k)$. The later is needed to guarantee $\theta_\tau^k\ge0$. Anyhow, since this nonlinearity is of lower order, we can pass through it by compactness and strong convergence. Thus, it suffices for us to check coercivity of the underlying operator. To this aim, we test (5.4) by θ_τ^k. The terms on the right-hand side of (5.4a) containing θ_τ^k are estimated standardly by using Hölder's and Young's inequalities, and using the qualification (4.1q).

Having coercivity, we see that there exists at least one solution. Moreover, this solution satisfies $\theta_\tau^k\ge0$, which can be seen by testing (5.4) by the negative part of θ_τ^k and using that $\partial_\chi\varphi_{\rm TH}(\chi,\theta)=0$ for $\theta\le0$. $\square$

Remark 5.2. The delayed term s $\boldsymbol{E}_\tau^{k-1}$ and d_τ^{k-1} in (5.1b) and c_τ^{k-1} in (5.2a) allows us to treat (5.1) and (5.2) as variational problems. This does not create troubles in the limit passage, see also Step 5 in the proof of Proposition 5.5 below.

Let us define the piecewise affine interpolant $\boldsymbol{u}_\tau$ by

$$\boldsymbol{u}_\tau(t):=\frac{t-(k{-}1)\tau}{\tau}\boldsymbol{u}_\tau^k+\frac{k\tau-t}{\tau}\boldsymbol{u}_\tau^{k-1}\qquad\text{for }t\in[(k{-}1)\tau,k\tau]\tag{5.12a}$$

with $k=0,...,T/\tau$. Besides, we define also the backward piecewise constant interpolant $\bar{\boldsymbol{u}}_\tau$ and $\underline{\boldsymbol{u}}_\tau$ by

$$\bar{\boldsymbol{u}}_\tau(t):=\boldsymbol{u}_\tau^k,\qquad\text{for }t\in((k{-}1)\tau,k\tau]\ ,\ \ k=1,...,T/\tau,\tag{5.12b}$$

$$\underline{\boldsymbol{u}}_\tau(t):=\boldsymbol{u}_\tau^{k-1},\qquad\text{for }t\in[(k{-}1)\tau,k\tau)\ ,\ \ k=1,...,T/\tau.\tag{5.12c}$$

Similarly, we define also d_τ, $\overline{d}_\tau$, $\underline{d}_\tau$, $\overline{w}_\tau$, w_τ, $\overline{g}_\tau$, $\overline{\boldsymbol{f}}_{{\rm b},\tau}$, etc. We will also need the piecewise affine interpolant of the (piecewise constant) velocity $\dot{\boldsymbol{u}}_\tau$, which we denote by $\big[\dot{\boldsymbol{u}}_\tau\big]^{\rm i}$, i.e.

$$\big[\dot{\boldsymbol{u}}_\tau\big]^{\rm i}(t):=\frac{t{-}(k{-}1)\tau}{\tau}\,\frac{\boldsymbol{u}_\tau^k{-}\boldsymbol{u}_\tau^{k-1}}{\tau}+\frac{k\tau{-}t}{\tau}\,\frac{\boldsymbol{u}_\tau^{k-1}{-}\boldsymbol{u}_\tau^{k-2}}{\tau}\quad\text{for }t\in((k{-}1)\tau,k\tau].\tag{5.12d}$$

Note that $\ddot{\boldsymbol{u}}_\tau^{\rm i}:=\frac{\partial}{\partial t}\big[\dot{\boldsymbol{u}}_\tau\big]^{\rm i}$ is piecewise constant with the values $(\boldsymbol{u}_\tau^k{-}2\boldsymbol{u}_\tau^{k-1}{+}\boldsymbol{u}_\tau^{k-2})/\tau^2$ on the particular subintervals $((k{-}1)\tau,k\tau)$.

In terms of interpolants, we can write the approximate system (5.1)–(5.4) and the semi-stability information we can get from (5.3) in a more "condensed" form closer to the desired continuous system (3.7), namely:

$$\varrho\ddot{\boldsymbol{u}}_\tau^{\rm i}-{\rm div}\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau\big)=\overline{\boldsymbol{f}}_\tau\qquad\text{with }\ \overline{\boldsymbol{E}}_\tau=\boldsymbol{\varepsilon}(\bar{\boldsymbol{u}}_\tau){-}\mathbb{E}\bar\chi_\tau,\tag{5.13a}$$

$$\begin{aligned}&\partial_{\dot\chi}\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot\chi_\tau)-\kappa_1\Delta\bar\chi_\tau+\partial_\chi\varphi_{\rm ME/CH}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau)\\&\qquad+\partial_\chi\varphi_{\rm TH}(\underline{\chi}_\tau,\underline{\theta}_\tau)-\mathbb{E}^\top{:}\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau){+}\mathbb{D}\dot{\boldsymbol{E}}_\tau\big){+}\bar\sigma_{{\rm r},\tau}\ni0\quad\text{ with }\bar\sigma_{{\rm r},\tau}\in\partial\delta_K(\bar\chi_\tau),\end{aligned}\tag{5.13b}$$

$$\dot c_\tau-{\rm div}\big(\mathbf{M}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau\big)=0\qquad\text{with}\quad\bar\mu_\tau=\partial_c\varphi_{\rm CH}(\bar\chi_\tau,\bar c_\tau),\tag{5.13c}$$

$$\begin{aligned}&\int_\Omega\varphi_{\rm ME/CH}(\overline{\boldsymbol{E}}_\tau(t),\bar\chi_\tau(t),\overline{d}_\tau(t),\bar c_\tau(t))+\frac{\kappa_2}{2}|\nabla\overline{d}_\tau(t)|^2\,{\rm d}x\le\int_\Omega\Big(\varphi_{\rm ME/CH}(\overline{\boldsymbol{E}}_\tau(t),\bar\chi_\tau(t),\widetilde d,\bar c_\tau(t))\\&\quad+\frac{\kappa_2}{2}|\nabla\widetilde d|^2+\alpha(\bar\chi_\tau(t))(\widetilde d{-}\overline{d}_\tau(t))\Big)\,{\rm d}x\qquad\forall\widetilde d{\in}H^1(\Omega),\ 0\le\widetilde d\le\overline{d}_\tau(t)\text{ on }\Omega,\ \text{for a.a. }t{\in}I,\end{aligned}\tag{5.13d}$$

$$\begin{aligned}&\dot w_\tau-{\rm div}\big(\mathbf{K}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\overline{d}_\tau,\bar c_\tau,\bar\theta_\tau)\nabla\bar\theta_\tau\big)=\bar r_\tau\qquad\text{with}\quad\overline{w}_\tau=e_{\rm TH}(\bar\chi_\tau,\bar\theta_\tau)\quad\text{ and}\\&\quad\text{with}\ \ \bar r_\tau=\big(\bar s_{{\rm d},\tau}{+}\partial_\chi\varphi_{\rm TH}(\bar\chi_\tau,\bar\theta_\tau)\big){\cdot}\dot\chi_\tau-\alpha(\bar\chi_\tau)\dot d_\tau+\frac{\mathbb{D}\dot{\boldsymbol{E}}_\tau{:}\dot{\boldsymbol{E}}_\tau}{1{+}\tau|\dot{\boldsymbol{E}}_\tau|^2}+\frac{\mathbf{M}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau{\cdot}\nabla\bar\mu_\tau}{1+\tau|\nabla\bar\mu_\tau|^2},\end{aligned}\tag{5.13e}$$

$$\begin{aligned}&\int_\Omega\varphi_{\rm ME/CH}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k)+\frac{\varrho}{2}\big|\dot{\boldsymbol{u}}_\tau^k\big|^2+\frac{\kappa_1}{2}\big|\nabla\chi_\tau^k\big|^2+\frac{\kappa_2}{2}\big|\nabla d_\tau^k\big|^2\,{\rm d}x\\&\quad+\int_0^{k\tau}\!\!\int_\Omega\Big(\mathbb{D}\dot{\boldsymbol{E}}_\tau{:}\dot{\boldsymbol{E}}_\tau+\big((\partial_{\dot\chi}\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot\chi_\tau)-\sqrt{\tau}\dot\chi_\tau){+}\partial_\chi\varphi_{\rm TH}(\underline{\chi}_\tau,\underline{\theta}_\tau)\big){\cdot}\dot\chi_\tau-\alpha(\bar\chi_\tau)\dot d_\tau\\&\quad+\mathbf{M}(\overline{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau{\cdot}\nabla\bar\mu_\tau\Big)\,{\rm d}x{\rm d}t\le\int_0^{k\tau}\!\!\int_\Gamma\overline{\boldsymbol{f}}_{{\rm s},\tau}{\cdot}\dot{\boldsymbol{u}}_\tau{+}q_{{\rm s},\tau}{+}\bar\mu_\tau\bar h_{{\rm s},\tau}\,{\rm d}S+\mathscr{E}_{\rm MC}(0)\end{aligned}\tag{5.13f}$$

holding for any $k=0,...,T/\tau$, together with the corresponding boundary conditions

$$\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau\big)\mathbf{n}=\bar{\boldsymbol{f}}_{{\rm s},\tau}, \tag{5.14a}$$

$$\nabla\chi_\tau\cdot\mathbf{n}=0, \tag{5.14b}$$

$$\mathbf{M}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau\cdot\mathbf{n}=\bar h_{{\rm s},\tau}, \tag{5.14c}$$

$$\big(\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\bar d_\tau,\bar c_\tau,\bar\theta_\tau)\nabla\bar\theta_\tau\big)\cdot\mathbf{n}=\bar q_{{\rm s},\tau}. \tag{5.14d}$$

The discrete semi-stability (5.13d) has been obtained from minimizing (5.3) by comparing a solution d_τ^k against $\widetilde d$ and using the triangle inequality for $\xi(\chi_\tau^k,\cdot)$; here the positive degree-1 homogeneity of $\xi(\chi,\cdot)$ is used. Note that we just choose one global minimizer d_τ^k of (5.3) from possibly many, if $\varphi_{\rm ME}(\boldsymbol{E},\chi,\cdot)$ is not convex. The energy inequality (5.13f) which we will prove in Lemma 5.3 below is an analog of the mechanical/chemical energy (4.10f) over the time interval $[0,k\tau]$ and without making the by-part integration like (4.12). Note also the term $\sqrt{\tau}|\dot\chi_\tau|^2$ in (5.13f) which facilitates handling of non-convex energies $\varphi_{\rm ME}$ as admitted by the semi-convexity assumption (4.1i) but which disappers in the limit for $\tau\to0$, cf. [44, Rem. 8.24] for this trick.

Lemma 5.3 (First estimates). *Let again the assumptions of Lemma 5.1 hold. Then the mecano-chemical energy inequality* (5.13f) *holds and the following estimates hold uniformly with respect to the time-step provided* $\tau\le\min(1/M^2,T,4\epsilon^2)$ *with* M *from* (4.1i) *(or simply* $\tau\le T$ *if* $M=0$*):*

$$\big\|\boldsymbol{u}_\tau\big\|_{W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^3))\,\cap\,H^1(I;H^1(\Omega;\mathbb{R}^3))}\le C, \tag{5.15a}$$

$$\big\|\boldsymbol{E}_\tau\big\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \tag{5.15b}$$

$$\big\|\chi_\tau\big\|_{L^\infty(I;H^1(\Omega;\mathbb{R}^N))\,\cap\,H^1(I;L^2(\Omega;\mathbb{R}^N))\,\cap\,L^\infty(Q;\mathbb{R}^N)}\le C, \tag{5.15c}$$

$$\big\|c_\tau\big\|_{L^2(I;H^1(\Omega))}\le C, \tag{5.15d}$$

$$\big\|\mu_\tau\big\|_{L^2(I;H^1(\Omega))}\le C, \tag{5.15e}$$

$$\big\|d_\tau\big\|_{L^\infty(I;H^1(\Omega))\,\cap\,{\rm BV}(I;L^1(\Omega))\,\cap\,L^\infty(Q)}\le C, \tag{5.15f}$$

$$\big\|w_\tau\big\|_{L^\infty(I;L^1(\Omega))}\le C. \tag{5.15g}$$

Moreover, for every $1\le r<\frac54$ *there exists* $C_r>0$*, independent of* τ*, such that*

$$\big\|\nabla w_\tau\big\|_{L^r(Q;\mathbb{R}^3)}\le C_r, \tag{5.15h}$$

$$\big\|\nabla\theta_\tau\big\|_{L^r(Q;\mathbb{R}^3)}\le C_r, \tag{5.15i}$$

$$\|w_\tau\|_{L^{r/(2-r)}(Q)}\le C_r, \tag{5.15j}$$

$$\|\theta_\tau\|_{L^{r/(2-r)}(Q)}\le C_r. \tag{5.15k}$$

Proof. The strategy is to test the particular equations in (5.1)–(5.4) respectively by $\mathfrak{d}_\tau^k\boldsymbol{u}$, $\mathfrak{d}_\tau^k\chi$, μ_τ^k, $\mathfrak{d}_\tau^k d$, and $\frac12$. For (5.1a,b), we note that a standard argument using convexity of $(\boldsymbol{E},\chi)\mapsto\varphi_{\rm ME/CH}(\boldsymbol{E},\chi,c,d)+\delta_K(\chi)$ composed with the linear mapping $(\boldsymbol{u},\chi)\mapsto\boldsymbol{E}$, and of $\dot\chi\mapsto\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)$ yields:

$$\begin{aligned}\int_\Omega&\varrho[\mathfrak{d}_\tau^k]^2\boldsymbol{u}\cdot\mathfrak{d}_\tau^k\boldsymbol{u}+\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau^k\big):\boldsymbol{\varepsilon}(\mathfrak{d}_\tau^k\boldsymbol{u})\\&+\big(\partial_{\dot d}\zeta(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k,\theta_\tau^k,\mathfrak{d}_\tau^k\chi)+\partial_\chi\varphi_{\rm ME}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1})\\&-\mathbb{E}^\top:\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau^k\big)+\sigma_{{\rm r},\tau}^k\big)\cdot\mathfrak{d}_\tau^k\chi+\kappa_1\nabla\chi_\tau^k:\nabla\mathfrak{d}_\tau^k\chi\,{\rm d}x\\\ge\int_\Omega&\mathbb{D}\mathfrak{d}_\tau^k\boldsymbol{E}_\tau:\big(\boldsymbol{\varepsilon}(\mathfrak{d}_\tau^k\boldsymbol{u})-\mathbb{E}\mathfrak{d}_\tau^k\chi\big)+s_{{\rm d},\tau}^k+\partial_\chi\varphi_{\rm TH}(\chi_\tau^{k-1},\theta_\tau^{k-1}))\mathfrak{d}_\tau^k\chi\\&+\frac{\varrho}{2}|\mathfrak{d}_\tau^k\boldsymbol{u}|^2+\varphi_{\rm ME}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1})+\frac{\kappa_1}{2}|\nabla\chi_\tau^k|^2+\delta_K(\chi_\tau^k)\\&-\frac{\varrho}{2}|\mathfrak{d}_\tau^{k-1}\boldsymbol{u}|^2-\varphi_{\rm ME}(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1})-\frac{\kappa_1}{2}|\nabla\chi_\tau^{k-1}|^2-\delta_K(\chi_\tau^{k-1})\,{\rm d}x.\end{aligned} \tag{5.16}$$

Further, we execute the test of (5.2) relying on the convexity of $c\mapsto\varphi_{\rm CH}(\chi,c)$

$$\begin{aligned}\int_\Gamma h_{{\rm s},\tau}^k\mu_\tau^k\,{\rm d}S&=\int_\Omega\mu_\tau^k\mathfrak{d}_\tau^k c+\mathbf{M}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^k,\theta_\tau^{k-1})\nabla\mu_\tau^k\cdot\nabla\mu_\tau^k\,{\rm d}x\\&\ge\int_\Omega\varphi_{\rm CH}(\chi_\tau^k,c_\tau^k)-\varphi_{\rm CH}(\chi_\tau^k,c_\tau^{k-1})+\mathbf{M}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^k,\theta_\tau^{k-1})\nabla\mu_\tau^k\cdot\nabla\mu_\tau^k\,{\rm d}x.\end{aligned} \tag{5.17}$$

Moreover, we test (5.3) with d_τ^{k-1} to obtain

$$\int_\Omega \varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k)+\frac{\kappa_2}{2}|\nabla d_\tau^k|^2\,\mathrm{d}x \le \int_\Omega \varphi_{_{\rm ME}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1})+\frac{\kappa_2}{2}|\nabla d_\tau^{k-1}|^2-\alpha(\chi_\tau^k)(d_\tau^k-d_\tau^{k-1})\,\mathrm{d}x. \tag{5.18}$$

Relying on the semiconvexity (4.1i) of the mechano-chemical part $\varphi_{_{\rm ME}}$ of the free energy (see the argument in [44, Rem. 8.24]) and adding (5.16), (5.17), and (5.18), and recalling that $\varphi_{_{\rm ME/CH}}=\varphi_{_{\rm ME}}+\varphi_{_{\rm CH}}$, we benefit with the telescopic cancellation of the terms $\pm\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^k)$ and $\pm\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^{k-1},c_\tau^{k-1})$, and we obtain the following mechano-chemical energy balance:

$$\begin{aligned}
&\int_\Omega \frac{\varrho}{2}\big|\mathfrak{d}_\tau^k\boldsymbol{u}\big|^2+\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k)+\frac{\kappa_2}{2}|\nabla d_\tau^k|^2+\frac{\kappa_1}{2}|\nabla\chi_\tau^k|^2+\delta_K(\chi_\tau^k)+\delta_{[0,1]}(d_\tau^k)\,\mathrm{d}x\\
&\quad+\tau\sum_{j=1}^k\int_\Omega \mathbb{D}\mathfrak{d}_\tau^j\boldsymbol{E}:\mathfrak{d}_\tau^j\boldsymbol{E}+\big(\partial_{\dot\chi}\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1},\mathfrak{d}_\tau^j\chi)-\sqrt{\tau}\mathfrak{d}_\tau^j\chi\big)\cdot\mathfrak{d}_\tau^j\chi-\alpha(\chi_\tau^j)\cdot\mathfrak{d}_\tau^j d\\
&\qquad\qquad+\mathbf{M}(\boldsymbol{E}_\tau^{j-1},\chi_\tau^{j-1},d_\tau^{j-1},c_\tau^{j-1},\theta_\tau^{j-1})\nabla\mu_\tau^j\cdot\nabla\mu_\tau^j\mathrm{d}x\mathrm{d}t\\
&\le\int_\Omega\Big(\frac{\varrho}{2}|\boldsymbol{v}_0|^2+\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_0,\chi_0,d_0,c_0)+\frac{\kappa_2}{2}|\nabla d_0|^2+\frac{\kappa_1}{2}|\nabla\chi_0|^2\Big)\,\mathrm{d}x\\
&\qquad\qquad+\tau\sum_{j=1}^k\Big(\int_\Omega \boldsymbol{f}_\tau^j\cdot\mathfrak{d}_\tau^j\boldsymbol{u}\mathfrak{d}_\tau^j\chi+\int_\Gamma \boldsymbol{f}_{{\rm s},\tau}^j\cdot\mathfrak{d}_\tau^j\boldsymbol{u}+h_{{\rm s},\tau}^j\cdot\mu_\tau^j\mathrm{d}S\Big).
\end{aligned}$$

We also used that $\delta_K(\chi_0)+\delta_{[0,1]}(d_0)=0$. This proves (5.13f).

Finally, we test the heat equation (5.4) by 1/2, and we add the resulting equation to (5.16)–(5.18). This is not a physical test (which would be by 1 instead of 1/2) and thus, in this summation, the adiabatic terms do not cancel out. This scenario simplifies the implicit discretisation to let is decoupled by using θ_τ^{k-1} in $\varphi_{_{\rm TH}}$ in (5.1b) instead of θ_τ^k and also it allows to estimate w with the other variables simultaneously but it forces more restrictive assumption on the growth of heat capacity than physically necessary, cf. [44, Exercise 12.9]. Upon summing over k, we arrive at the following estimate:

$$\begin{aligned}
&\int_\Omega \frac12 w_\tau^k+\frac{\varrho}{2}\big|\mathfrak{d}_\tau^k\boldsymbol{u}\big|^2+\varphi_{_{\rm ME/CH}}(\boldsymbol{E}_\tau^k,\chi_\tau^k,d_\tau^k,c_\tau^k)+\frac{\kappa_2}{2}|\nabla d_\tau^k|^2+\frac{\kappa_1}{2}|\nabla\chi_\tau^k|^2+\delta_K(\chi_\tau^k)+\delta_{[0,1]}(d_\tau^k)\,\mathrm{d}x\\
&\quad+\tau\sum_{j=1}^k\int_\Omega \mathbb{D}\mathfrak{d}_\tau^j\boldsymbol{E}:\mathfrak{d}_\tau^j\boldsymbol{E}+\partial_{\dot\chi}\zeta(\boldsymbol{E}_\tau^{k-1},\chi_\tau^{k-1},d_\tau^{k-1},c_\tau^{k-1},\theta_\tau^{k-1},\mathfrak{d}_\tau^j\chi)\cdot\mathfrak{d}_\tau^j\chi-\alpha(\chi_\tau^j)\cdot\mathfrak{d}_\tau^j d\\
&\qquad\qquad+\frac12\mathbf{M}(\boldsymbol{E}_\tau^{j},\chi_\tau^{j},d_\tau^{j-1},c_\tau^{j-1},\theta_\tau^{j-1})\nabla\mu_\tau^j\cdot\nabla\mu_\tau^j\mathrm{d}x\mathrm{d}t\\
&\le\int_\Omega\Big(\frac12 e_{_{\rm TH}}(\chi_0,\theta_0)+\frac{\varrho}{2}|\boldsymbol{v}_0|^2+\varphi_{_{\rm CH}}(\chi_0,c_0)+\varphi_{_{\rm ME}}(\boldsymbol{E}_0,d_0,c_0)+\frac{\kappa_2}{2}|\nabla d_0|^2+\frac{\kappa_1}{2}|\nabla\chi_0|^2\Big)\,\mathrm{d}x\\
&\quad+\tau\sum_{j=1}^k\Big(\int_\Omega \boldsymbol{f}_\tau^j\cdot\mathfrak{d}_\tau^j\boldsymbol{u}\;+\Big(\frac12\partial_\chi\varphi_{_{\rm TH}}(\chi_\tau^j,\theta_\tau^j)-\partial_\chi\varphi_{_{\rm TH}}(\chi_\tau^{j-1},\theta_\tau^{j-1})\Big)\mathfrak{d}_\tau^j\chi+\int_\Gamma \boldsymbol{f}_{{\rm s},\tau}^j\cdot\mathfrak{d}_\tau^j\boldsymbol{u}+h_{{\rm s},\tau}^j\cdot\mu_\tau^j+\frac12 q_{{\rm s},\tau}^j\mathrm{d}S\Big).
\end{aligned}$$

Using (4.1q) and Holder's and Young's inequalities, followed by the discrete Gronwall lemma, we see that the left-hand side in the above inequality is bounded uniformly with respect to t for all $k=1,\ldots,T/\tau$. We therefore obtain the following bounds:

$$\|\dot{\boldsymbol{u}}_\tau\|_{L^\infty(L^2(\Omega;\mathbb{R}^3))}\le C, \tag{5.19a}$$

$$\|\varphi_{_{\rm ME}}(\overline{\boldsymbol{E}}_\tau,\overline{\chi}_\tau,\overline{d}_\tau)\|_{L^\infty(I;L^1(\Omega))}\le C, \tag{5.19b}$$

$$\|\varphi_{_{\rm CH}}(\overline{\chi}_\tau,\overline{c}_\tau)\|_{L^\infty(I;L^1(\Omega))}\le C, \tag{5.19c}$$

$$\|\nabla\chi_\tau\|_{L^\infty(L^2(\Omega;\mathbb{R}^{N\times3}))}\le C, \tag{5.19d}$$

$$\|\nabla d_\tau\|_{L^\infty(L^2(\Omega;\mathbb{R}^3))}\le C, \tag{5.19e}$$

$$\chi_\tau\in K\ \text{a.e. in } Q, \tag{5.19f}$$

$$\|\dot{\boldsymbol{E}}_\tau\|_{L^2(Q;\mathbb{R}^{3\times3})}\le C, \tag{5.19g}$$

$$\|\dot\chi_\tau\|_{L^2(Q;\mathbb{R}^N)}\le C, \tag{5.19h}$$

$$\|\dot d_\tau\|_{L^1(Q)}\le C, \tag{5.19i}$$

$$\|\nabla\mu_\tau\|_{L^2(Q;\mathbb{R}^3)}\le C, \tag{5.19j}$$

along with (5.15g). From (5.19b) and (4.1d) we immediately obtain the a-priori estimate (5.15b). Furthermore, from (5.19d,h) we get (5.15c). From (5.19e,i), combined with the initial condition for d contained in (4.2b), and from the monotonicity of d (see Step 3 of the discretization scheme at the beginning of this section) we obtain the bound (5.15f) on the damage variable. Moreover, since $\boldsymbol{\varepsilon}(\dot{\boldsymbol{u}}_\tau) = \dot{\boldsymbol{E}}_\tau + \mathbb{E}\dot{\chi}_\tau \in L^2(Q;\mathbb{R}^{3\times3})$, the estimates (5.19g,h) and Korn's inequality entail

$$\|\nabla\dot{\boldsymbol{u}}_\tau\|_{L^2(Q;\mathbb{R}^{3\times3})} \le C. \tag{5.20}$$

The estimate (5.15a) is now recovered from (5.16) and (5.20). Next, from (5.2b) taking a gradient of $\bar{\mu}_\tau = \partial_c\varphi_{\rm CH}(\bar{\chi}_\tau,\bar{c}_\tau)$, cf. (5.13c), and using the strong convexity assumption (4.1j), we obtain the following estimate on concentration gradient:

$$\nabla\bar{c}_\tau = [\partial^2_{cc}\varphi_{\rm CH}(\bar{\chi}_\tau,\bar{c}_\tau)]^{-1}\big(\nabla\bar{\mu}_\tau - \partial^2_{c\chi}\varphi_{\rm CH}(\bar{\chi}_\tau,\bar{c}_\tau)\nabla\bar{\chi}_\tau\big), \tag{5.21}$$

and hence, by (4.1pb), (5.19d, j), and (5.15e), we obtain

$$\|\nabla c_\tau\|_{L^2(Q;\mathbb{R}^3)} \le C. \tag{5.22}$$

Because of the coercivity assumption in (4.1g), the bounds (5.19c) and (5.22) imply (5.15d). Using (5.19j) and assumption (4.1l) we obtain (5.15e).

It remains for us to prove (5.15h)–(5.15k). Let us fix $r \in [1,5/4)$ and let us set

$$\phi(\omega) = \frac{1+\omega-(1+\omega)^{1-\eta}}{\eta(1-\eta)} \qquad \text{with} \quad \eta = \frac{5-4r}{3}. \tag{5.23}$$

We are going to exploit the following properties of ϕ:

$$\forall\omega\ge0: \quad \phi(\omega)\ge0, \quad \phi'(w)\le C, \quad 0<\epsilon\le\phi''(\omega)<\frac{1}{1+\omega}, \tag{5.24a}$$

$$\limsup_{\omega\to+\infty}\frac{1}{\phi''(\omega)\omega^{1+\eta}} \le C. \tag{5.24b}$$

By the second inequality in (5.24a), the function $\phi'(\bar{w}_\tau)$ is in $L^\infty(Q)$ and hence it is a legal test for (5.13e), whose right-hand side $\bar{r}_\tau$ is in $L^1(Q)$. By performing this test, and by exploiting the convexity of ϕ we arrive at:

$$\int_\Omega \phi(\bar{w}_\tau(T))\,\mathrm{d}x + \int_Q \phi''(\bar{w}_\tau)\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{c}_\tau,\bar{\theta}_\tau)\nabla\bar{\theta}_\tau\cdot\nabla\bar{w}_\tau\,\mathrm{d}x\,\mathrm{d}t \le C. \tag{5.25}$$

From the equation in the third line of (5.13e), recalling from (4.6) that $w\mapsto\vartheta(\chi,w)$ is the inverse of $\theta\mapsto e_{\rm TH}(\chi,\theta)$, we obtain

$$\bar{\theta}_\tau = \vartheta(\bar{\chi}_\tau,\bar{w}_\tau) \tag{5.26}$$

a.e. in Q. Furthermore, since $\bar{\theta}_\tau(t)\in H^1(\Omega)$, $\bar{\chi}_\tau(t)\in H^1(\Omega;\mathbb{R}^N)$, and $\bar{d}_\tau(t)\in H^1(\Omega;\mathbb{R})$ for all $t\in(0,T)$. By the chain rule for Sobolev functions, the equation (5.26) together with assumptions (4.7) and (4.8) implies that $\bar{\theta}_\tau(\cdot,t)\in H^1(\Omega)$ for all $t\in(0,T)$ with

$$\nabla\bar{\theta}_\tau = \partial_\chi\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{\chi}_\tau + \partial_w\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{w}_\tau \tag{5.27}$$

holding a.e. in Q.

Now, by (4.1k) and (4.7), we have

$$\phi''(\bar{w}_\tau)\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{\chi}_\tau,\bar{\theta}_\tau)\partial_w\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{w}_\tau\cdot\nabla\bar{w}_\tau \ge \epsilon_1\phi''(\bar{w}_\tau)|\nabla\bar{w}_\tau|^2, \tag{5.28}$$

with some $\epsilon_1>0$. Moreover, using, in the order, Holder's and Young's inequalities, the last inequality in (5.24a), the last line of (5.13e), and (4.6), we obtain, for δ sufficiently small,

$$\begin{aligned}
&\phi''(\bar{w}_\tau)\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{\chi}_\tau,\bar{\theta}_\tau)\partial_\chi\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{\chi}_\tau\cdot\nabla\bar{w}_\tau\\
&\qquad\ge -\frac{1}{2\delta}\phi''(\bar{w}_\tau)|\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{c}_\tau,\bar{\theta}_\tau)\partial_\chi\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{\chi}_\tau|^2 - \frac{\delta}{2}\phi''(\bar{w}_\tau)|\nabla\bar{w}_\tau|^2\\
&\qquad\ge -\frac{1}{2\delta}\Big|\frac{\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{c}_\tau,\bar{\theta}_\tau)\partial_\chi\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{\chi}_\tau}{\sqrt{1+\bar{w}_\tau}}\Big|^2 - \frac{\delta}{2}\phi''(\bar{w}_\tau)|\nabla\bar{w}_\tau|^2\\
&\qquad= -\frac{1}{2\delta}\Big|\frac{\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{c}_\tau,\bar{\theta}_\tau)\partial_\chi e_\vartheta(\bar{\chi}_\tau,\bar{\theta}_\tau)\nabla\bar{\chi}_\tau}{\partial_\theta e_{\rm TH}(\bar{\chi}_\tau,\bar{\theta}_\tau)\sqrt{1+e_{\rm TH}(\bar{\chi}_\tau,\bar{\theta}_\tau)}}\Big|^2 - \frac{\delta}{2}\phi''(\bar{w}_\tau)|\nabla\bar{w}_\tau|^2.
\end{aligned}\tag{5.29}$$

The above chain of inequalities, combined with Assumption (4.1r) and with the lower bound in (4.5) yields:

$$\phi''(\bar{w}_\tau)\mathbf{K}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\bar{d}_\tau,\bar{c}_\tau,\bar{\theta}_\tau)\partial_\chi\vartheta(\bar{\chi}_\tau,\bar{w}_\tau)\nabla\bar{\chi}_\tau\cdot\nabla\bar{w}_\tau \ge -\frac{C}{\delta}|\nabla\bar{\chi}_\tau|^2 - \frac{\delta}{2}\phi''(\bar{w}_\tau)|\nabla\bar{w}_\tau|^2. \tag{5.30}$$

By combining (5.27) with (5.29), and (5.28), we arrive at

$$\phi''(\overline{w}_\tau)\mathbf{K}(\overline{\boldsymbol{E}}_\tau,\overline{\chi}_\tau,\overline{d}_\tau,\overline{c}_\tau,\overline{\theta}_\tau)\nabla\overline{\theta}_\tau\cdot\nabla\overline{w}_\tau \ge (1-\delta)\phi''(\overline{w}_\tau)|\nabla\overline{w}_\tau|^2 - \frac{C}{\delta}|\nabla\overline{\chi}_\tau|^2. \tag{5.31}$$

Since ϕ is bounded from below, see (5.24a), and since $\nabla\overline{d}_\tau$ and $\nabla\overline{\chi}_\tau$ are bounded in $L^2(Q)$, see (5.19d,e), it follows from (5.25) and (5.31) that

$$\int_Q \phi''(\overline{w}_\tau)|\nabla\overline{w}_\tau|^2\,\mathrm{d}x\,\mathrm{d}t \le C. \tag{5.32}$$

Now, by Holder's inequality and by (5.24*b*) we have the bound

$$\begin{aligned}\int_Q \big|\nabla\overline{w}_\tau\big|^r\,\mathrm{d}x\,\mathrm{d}t &\le \Big(\int_Q \phi''(\overline{w}_\tau)\big|\nabla\overline{w}_\tau\big|^2\,\mathrm{d}x\,\mathrm{d}t\Big)^{r/2}\Big(\int_Q\Big(\frac{1}{\phi''(\overline{w}_\tau)^{r/2}}\Big)^{2/(2-r)}\mathrm{d}x\,\mathrm{d}t\Big)^{1-r/2}\\ &\le C\Big(1+\int_Q \big|\overline{w}_\tau\big|^{(2-r)r/(1+\eta)}\,\mathrm{d}t\Big)^{1-r/2}.\end{aligned} \tag{5.33}$$

Now, let us set $\lambda=\frac{2-r}{1+\eta}$. The choice (5.23) for η entails that $\frac{\lambda}{r}=1-\lambda+\frac{\lambda}{r^*}$, with $r^*=\frac{3r}{3-r}$ the exponent of the Sobolev embedding $L^{r^*}(\Omega)\subset W^{1,r}(\Omega)$. Thus, a standard interpolation argument based on Holder's inequality entails $\|\overline{w}_\tau\|_{L^{r(1+\eta)/(2-r)}(\Omega)}=\|\overline{w}_\tau\|_{L^{r/\lambda}(\Omega)}\le\|\overline{w}_\tau\|^{1-\lambda}_{L^1(\Omega)}\|\overline{w}_\tau\|^{\lambda}_{L^{r^*}(\Omega)}=\|\overline{w}_\tau\|^{r(1+\eta)/(2-r)}_{L^1(\Omega)}\|\overline{w}_\tau\|^{(2-r)/(1+\eta)}_{L^{r^*}(\Omega)}$. Hence, the Sobolev embedding and Poincaré's inequality yield

$$\big\|\overline{w}_\tau\big\|_{L^{r(1+\eta)/(2-r)}(\Omega)}\le C\big\|\overline{w}_\tau\big\|^{(r-1+\eta)/(1+\eta)}_{L^1(\Omega)}\Big(\big\|\overline{w}_\tau\big\|_{L^1(\Omega)}+\big\|\nabla\overline{w}_\tau\big\|_{L^r(\Omega)}\Big)^{(2-r)/(1+\eta)}.$$

Thus, on taking into account the bound $\|\overline{w}_\tau\|_{L^\infty(I;L^1(\Omega))}\le C$, which has already been established, we obtain $\int_Q|\nabla\overline{w}_\tau|^r\,\mathrm{d}x\,\mathrm{d}t\le C(1+\int_Q|\nabla\overline{w}_\tau|^r\,\mathrm{d}x\,\mathrm{d}t)^{1-r/2}$, whence (5.15h) and thence (5.15j). Finally, thanks to the boundedness of $\partial_\chi\vartheta$, *cf.* (4.8), by combining (5.27) with (5.19d-e), we obtain (5.15i). In view of (4.7), from (5.15j) we obtain (5.15k). □

Lemma 5.4 (Further estimates). *Under the assumption of Lemma 5.1, for some constant C and C_r independent of τ, it also holds:*

$$\big\|\varrho\ddot{\boldsymbol{u}}^{\mathrm{i}}_\tau\big\|_{L^2(I;H^1(\Omega;\mathbb{R}^3)^*)}\le C, \tag{5.34a}$$

$$\big\|\dot{w}_\tau\big\|_{L^1(I;W^{1,r/(r-1)}(\Omega)^*)}\le C_r \quad \text{with } r \text{ from (4.9e)}, \tag{5.34b}$$

$$\big\|\dot{c}_\tau\big\|_{L^2(I;H^1(\Omega)^*)}\le C, \tag{5.34c}$$

$$\big\|\Delta\chi_\tau\big\|_{L^2(Q;\mathbb{R}^N)}\le C, \tag{5.34d}$$

$$\big\|\sigma_{\mathrm{r},\tau}\big\|_{L^2(Q;\mathbb{R}^N)}\le C. \tag{5.34e}$$

Proof. The "dual" estimates (5.34a-c) follow by comparison from the time-discrete equations (5.13a,c,e) with the corresponding boundary conditions (5.14a,c,e).

In order to prove the remaining estimate (5.34d,e), we consider a measurable selection $\overline{\sigma}_{\mathrm{d},\tau}\in\partial_{\dot{d}}\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot{d}_\tau)$. We notice that, thanks to the growth assumption in (4.1m) and the estimate (5.15c), we have $\overline{\sigma}_{\mathrm{d},\tau}\in L^2(Q;\mathbb{R}^N)$. Thus, the equation in (5.13b) can be written as

$$\kappa_1\Delta\overline{\chi}_\tau+\overline{f}_\tau\in\partial\delta_K(\overline{\chi}_\tau), \tag{5.35}$$

where $\overline{f}_\tau=-\overline{\sigma}_{\mathrm{d},\tau}-\partial_\chi\varphi_{\mathrm{CH}}(\overline{\chi}_\tau,\underline{c}_\tau)-\partial_\chi\varphi_{\mathrm{ME}}(\overline{\boldsymbol{E}}_\tau,\overline{\chi}_\tau,\underline{d}_\tau)-\partial_\chi\varphi_\theta(\underline{\chi}_\tau,\underline{d}_\tau,\underline{\theta}_\tau)\in L^2(Q;\mathbb{R}^N)$. At this stage, (5.13b) is understood in the weak sense, so that $\Delta\overline{\chi}_\tau$ (and hence also $\overline{\sigma}_{\mathrm{r},\tau}$) are elements of $H^1(\Omega;\mathbb{R}^N)^*$. Let us introduce the Yosida regularization of δ_K, defined by $\delta_{K,\varepsilon}(\chi)=\inf_{\widetilde{\chi}\in\mathbb{R}^N}\big(\delta_K(\widetilde{\chi})+\frac12|\chi-\widetilde{\chi}|^2\big)$. Consider the *strictly convex* functional $\widetilde{\chi}\mapsto\int_\Omega\big(\frac12|\nabla\widetilde{\chi}|^2+\frac12|\widetilde{\chi}-\overline{\chi}_\tau|^2+\delta_\varepsilon(\widetilde{\chi})-\overline{f}_\tau\cdot\widetilde{\chi}\big)\,\mathrm{d}x$ over $H^1(\Omega;\mathbb{R}^N)$. The functional has a unique minimizer $\overline{\chi}_{\tau,\varepsilon}$, and this minimizer is the *unique solution* of the regularized elliptic equation

$$-\kappa_1\Delta\overline{\chi}_{\tau,\varepsilon}+\delta'_{K,\varepsilon}(\overline{\chi}_{\tau,\varepsilon})+\overline{\chi}_{\tau,\varepsilon}=\overline{f}_\tau+\overline{\chi}_\tau, \tag{5.36}$$

with boundary condition $\partial_n\overline{\chi}_{\tau,\varepsilon}=0$.

Testing (5.36) by $\overline{\chi}_{\tau,\varepsilon}$ and using $\delta'_{K,\varepsilon}(\overline{\chi}_{\tau,\varepsilon})\cdot\overline{\chi}_{\tau,\varepsilon}\ge C(|\overline{\chi}_{\tau,\varepsilon}|^2-1)$, together with Holder's and Young's inequalities we get $\int_\Omega\kappa_1|\nabla\overline{\chi}_{\tau,\varepsilon}|^2+C|\overline{\chi}_{\tau,\varepsilon}|^2\,\mathrm{d}x\le C|\Omega|+\frac1\delta\int_\Omega|\overline{f}_\tau|^2\,\mathrm{d}x+\delta\int_\Omega|\overline{\chi}_{\tau,\varepsilon}|^2\,\mathrm{d}x$ for any $\delta>0$. By the arbitrariness of δ, we obtain the bound $\|\overline{\chi}_{\tau,\varepsilon}\|_{H^1(\Omega;\mathbb{R}^N)}\le C$. Moreover, since δ'_ε is Lipschitz continuous although not uniformly in ε, we have $\delta'_\varepsilon(\bar\chi_{\tau,\varepsilon}) \le C(1+|\bar\chi_{\tau,\varepsilon}|)/\varepsilon$, and hence $\|\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\|_{L^2(\Omega;\mathbb{R}^N)} \le C/\varepsilon$. By comparison in (5.36), we obtain $\Delta\bar\chi_{\tau,\varepsilon} \in L^2(\Omega;\mathbb{R}^N)$. Thus we can test (5.36) by $-\Delta\bar\chi_{\tau,\varepsilon}$ and use

$$\int_\Omega -\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\cdot\Delta\bar\chi_{\tau,\varepsilon}\,\mathrm{d}x = \int_\Omega \nabla\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon}):\nabla\bar\chi_{\tau,\varepsilon}\,\mathrm{d}x = \int_\Omega \delta''_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})|\nabla\bar\chi_{\tau,\varepsilon}|^2\,\mathrm{d}x \ge 0$$

to obtain the inequality $\int_\Omega \kappa_1|\Delta\bar\chi_{\tau,\varepsilon}|^2 - \Delta\bar\chi_{\tau,\varepsilon}\cdot\bar\chi_{\tau,\varepsilon}\,\mathrm{d}x \le \int_\Omega(\bar f_\tau + \bar\chi_\tau)\bar\chi_{\tau,\varepsilon}\,\mathrm{d}x$. Again, the application of Hölder's and Young's inequalities, yields the estimate $\|\Delta\bar\chi_{\varepsilon,\tau}\|_{L^2(\Omega;\mathbb{R}^N)} \le C$. By comparison in (5.36), we still have the estimate $\|\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\|_{L^2(\Omega;\mathbb{R}^N)} = \|\kappa_1\Delta\bar\chi_{\tau,\varepsilon} - \bar\chi_{\tau,\varepsilon} + \bar f_\tau + \bar\chi_\tau\|_{L^2(\Omega;\mathbb{R}^N)} \le C$ now independent of ε. By the a priori bound derived above, there exists $\widetilde\chi_\tau \in H^1(\Omega;\mathbb{R}^N)$ and a subsequence of $\{\chi_{\tau,\varepsilon}\}_{\tau>0}$ such that $\bar\chi_{\tau,\varepsilon} \to \widetilde\chi_\tau$ weakly in $H^1(\Omega;\mathbb{R}^N)$ and strongly in $L^2(\Omega;\mathbb{R}^N)$, $\Delta\bar\chi_{\tau,\varepsilon} \to \Delta\widetilde\chi_\tau$ weakly in $L^2(\Omega;\mathbb{R}^N)$, and $\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon}) \to \widetilde\sigma_\mathrm{r}$ weakly in $L^2(\Omega;\mathbb{R}^N)$, with $\widetilde\sigma_\mathrm{r} = \kappa_1\Delta\widetilde\chi_\tau - \widetilde\chi_\tau + \bar f_\tau + \bar\chi_\tau$. In order to identify the limit $\widetilde\chi_\tau$, we consider an arbitrary $z \in L^2(\Omega;\mathbb{R}^N)$, and we write

$$\int_\Omega \delta_{K,\varepsilon}(z) - \delta_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\,\mathrm{d}x \ge \int_\Omega \delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\cdot(z-\bar\chi_{\tau,\varepsilon})\,\mathrm{d}x = \int_\Omega (\bar f_\tau + \bar\chi_\tau + \kappa_1\Delta\bar\chi_{\tau,\varepsilon} - \bar\chi_{\tau,\varepsilon})\cdot(z-\bar\chi_{\tau,\varepsilon})\,\mathrm{d}x. \quad (5.37)$$

Using standard properties of the Yosida regularization (see e.g. [44, Lemma 5.17]), we can pass to the limit in (5.37) to obtain $\int_\Omega \delta_K(z) - \delta_K(\widetilde\chi_\tau)\,\mathrm{d}x \ge \int_\Omega(\bar f_\tau + \bar\chi_\tau + \kappa_1\Delta\widetilde\chi_\tau - \widetilde\chi_\tau)\cdot(z-\widetilde\chi_\tau)\,\mathrm{d}x$. Thus, $\widetilde\chi_\tau$ solves the differential inclusion

$$\kappa_1\Delta\widetilde\chi - \widetilde\chi_\tau + \bar f_\tau + \bar\chi_\tau \in \partial\delta_K(\widetilde\chi_\tau) \quad (5.38)$$

with homogeneous Neumann condition on $\partial\Omega$. By comparing (5.35) with (5.38) and the corresponding boundary conditions, we see that $\bar\chi_\tau$ is a solution of (5.38) as well. On the other hand solving (5.38) is equivalent to minimizing a strictly convex functional, thus the solution of (5.38) is unique. We therefore conclude that $\widetilde\chi_\tau = \bar\chi_\tau$ and $\widetilde\sigma_\mathrm{r} = \kappa_1\Delta\bar\chi_\tau + \bar f_\tau = \bar\sigma_\mathrm{r}$. Consequently, on using the strong convergence of $\bar\chi_{\tau,\varepsilon}$ and the weak convergence of $\delta'_{K,\varepsilon}(\widetilde\chi_\tau)$ we arrive at:

$$\begin{aligned} 0 &\le \limsup_{\varepsilon\to0}\int_\Omega \kappa_1\delta''_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\nabla\bar\chi_{\tau,\varepsilon}:\nabla\bar\chi_{\tau,\varepsilon}\,\mathrm{d}x = \limsup_{\varepsilon\to0}\int_\Omega \big(-\kappa_1\Delta\bar\chi_{\tau,\varepsilon}\big)\cdot\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\,\mathrm{d}x \\ &= \limsup_{\varepsilon\to0}\int_\Omega \big(\bar f_\tau + \bar\chi_\tau - \delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon}) - \bar\chi_{\tau,\varepsilon}\big)\cdot\delta'_{K,\varepsilon}(\bar\chi_{\tau,\varepsilon})\,\mathrm{d}x \\ &\le \int_\Omega \big(\bar f_\tau + \bar\chi_\tau - \bar\sigma_{\mathrm{r},\tau} - \bar\chi_\tau\big)\cdot\bar\sigma_{\mathrm{r},\tau}\,\mathrm{d}x = \kappa_1\int_\Omega \Delta\bar\chi_\tau\cdot\bar\sigma_\tau\,\mathrm{d}x. \end{aligned}$$

Since $\big\|\bar f_\tau\big\|_{L^2(Q;\mathbb{R}^N)} \le C$, the test of (4.1j) with $\Delta\bar\chi_\tau$, with Holder's and Young's inequalities yields (5.34d). The bound (5.34e) follows by comparison. □

Proposition 5.5 (Convergence for $\tau \to 0$). *Let again the assumption of Lemma 5.1 hold and let Ω be smooth. Then there is a subsequence such that*

$$\boldsymbol{u}_\tau \to \boldsymbol{u} \qquad \textit{strongly in } H^1(I;H^1(\Omega;\mathbb{R}^3)), \quad (5.39a)$$
$$\chi_\tau \to \chi \qquad \textit{strongly in } H^1(I;L^2(\Omega;\mathbb{R}^N)) \cap C(\bar Q;\mathbb{R}^N), \quad (5.39b)$$
$$\bar c_\tau \to c \ \ \&\ \ \underline{c}_\tau \to c \qquad \textit{strongly in } L^2(Q), \quad (5.39c)$$
$$d_\tau(t) \to d(t) \qquad \textit{weakly in } H^1(\Omega)\ \ \forall t\in I, \quad (5.39d)$$
$$\dot d_\tau \to \dot d \qquad \textit{weakly* in } \mathrm{Meas}(\bar Q) \cong C(\bar Q)^*, \quad (5.39e)$$
$$\bar\theta_\tau \to \theta, \quad \underline{\theta}_\tau \to \theta \qquad \textit{strongly in } L^s(Q)\ \textit{ with any }\ 1 \le s < 5/3, \quad (5.39f)$$
$$\bar\mu_\tau \to \mu \qquad \textit{strongly in } L^2(I;H^1(\Omega)), \quad (5.39g)$$
$$\bar w_\tau \to w \ \ \&\ \ \underline{w}_\tau \to w \qquad \textit{strongly in } L^s(Q)\ \textit{ with any }\ 1 \le s < 5/3, \quad (5.39h)$$

and any $(\boldsymbol{u},\chi,c,d,\theta,\mu,w)$ obtained in this way is a weak solution to the initial-boundary-value problem (3.7)–(3.9) *according Definition 4.1 which also preserves the total energy in the sense* (4.13).

Proof. For clarity of exposition, we divide the proof to eleven particular steps.

Step 1: Selection of a converging subsequence. By Banach's selection principle, we select a weakly* converging subsequence with respect to the norms from the estimates (5.15) and (5.34), namely,

$$\boldsymbol{u}_\tau \to \boldsymbol{u} \qquad \text{weakly* in } W^{1,\infty}(I;L^2(\Omega;\mathbb{R}^3)) \cap H^1(I;H^1(\Omega;\mathbb{R}^3)) \quad (5.40a)$$

$$\begin{aligned}
&\boldsymbol{E}_\tau \to \boldsymbol{E} && \text{weakly in } H^1(I;L^2(\Omega;\mathbb{R}^{3\times3})) && (5.40b)\\
&\chi_\tau \to \chi && \text{weakly* in } L^\infty(I;H^1(\Omega;\mathbb{R}^N)) \cap H^1(I;L^2(\Omega;\mathbb{R}^N)) \cap L^\infty(Q;\mathbb{R}^N), && (5.40c)\\
&c_\tau \to c && \text{weakly in } L^2(I;H^1(\Omega)), && (5.40d)\\
&\dot c_\tau \to \dot c && \text{weakly in } L^2(I;H^1(\Omega)^*), && (5.40e)\\
&\mu_\tau \to \mu && \text{weakly in } L^2(I;H^1(\Omega)), && (5.40f)\\
&d_\tau \to d && \text{weakly* in } L^2(I;H^1(\Omega)) \cap L^\infty(Q), && (5.40g)\\
&\bar\sigma_{\mathrm{r},\tau} \to \sigma_{\mathrm{r}} && \text{weakly in } L^2(Q;\mathbb{R}^N), && (5.40h)\\
& && && (5.40i)
\end{aligned}$$

and also (5.39e). Moreover, by the BV-estimate (5.15f) and by Helly's selection principle, we can rely also on (5.39d) for a subsequence. We introduce the shorthand notation

$$\boldsymbol{v}_\tau = [\dot{\boldsymbol{u}}_\tau]^{\mathrm{i}} \qquad \text{and} \qquad \bar{\boldsymbol{v}}_\tau = \dot{\boldsymbol{u}}_\tau. \tag{5.41}$$

We also define $t_\tau := t - \tau[t/\tau]$. Then, we have $\bar{\boldsymbol{v}}_\tau - \boldsymbol{v}_\tau = (\tau - t_\tau)\dot{\boldsymbol{v}}_\tau$. Moreover,

$$\begin{aligned}\int_0^T\!\!\int_\Omega |\bar{\boldsymbol{v}}_\tau - \boldsymbol{v}_\tau|^2 \,\mathrm{d}x\,\mathrm{d}t &= \int_0^T\!\!\int_\Omega (\tau - t_\tau)(\boldsymbol{v}_\tau - \bar{\boldsymbol{v}}_\tau)\cdot\dot{\boldsymbol{v}}_\tau \,\mathrm{d}x\,\mathrm{d}t\\
&\le \tau\big\|\boldsymbol{v}_\tau - \bar{\boldsymbol{v}}_\tau\big\|_{L^2(I;H^1(\Omega;\mathbb{R}^3))}\big\|\dot{\boldsymbol{v}}_\tau\big\|_{L^2(I;H^1(\Omega;\mathbb{R}^3)^*)} \to 0.\end{aligned} \tag{5.42}$$

By (5.40a), $\bar{\boldsymbol{v}}_\tau \to \dot{\boldsymbol{u}}$ weakly in $L^2(I;H^1(\Omega;\mathbb{R}^3)$. Thus, (5.42) implies that also $\boldsymbol{v}_\tau \to \dot{\boldsymbol{u}}$ weakly* in $L^2(I;H^1(\Omega;\mathbb{R}^3))$. On taking into account that $\ddot{\boldsymbol{u}}_\tau^{\mathrm{i}} = \dot{\boldsymbol{v}}_\tau$ and using a standard argument to identify time derivatives (see for instance [44, Theorem 8.9]), we arrive at

$$\ddot{\boldsymbol{u}}_\tau^{\mathrm{i}} \to \ddot{\boldsymbol{u}} \text{ weakly in } L^2(I;H^1(\Omega;R^3)^*). \tag{5.43}$$

By Rellich's theorem we have the continuous and the compact embeddings $H^1(I;L^2(\Omega))\cap L^\infty(I;H^1(\Omega)) \subset H^1(Q) \Subset L^2(Q)$ so that (5.40c,f) imply

$$\chi_\tau \to \chi \text{ strongly in } L^2(Q;\mathbb{R}^N). \tag{5.44a}$$

Again, arguing as (5.42), we have that $\|\bar\chi_\tau - \chi_\tau\|_{L^2(Q;\mathbb{R}^N)} \to 0$ and similarly also for $\underline{\chi}_\tau$, cf. [44, Rem. 8.10], hence

$$\bar\chi_\tau \to \chi \ \text{ and } \ \underline{\chi}_\tau \to \chi \ \text{ strongly in } \ L^2(Q;\mathbb{R}^N). \tag{5.44b}$$

Using the Aubin-Lions theorem with the estimates (5.15d) and (5.34c), we obtain, for a subsequence,

$$c_\tau \to c \quad \text{strongly in} \quad L^2(I;L^q(\Omega)) \quad \forall 1 \le q < 6. \tag{5.45}$$

Moreover, we have $\int_0^T\!\int_\Omega |c_\tau - \underline{c}_\tau|^2 \,\mathrm{d}x\mathrm{d}t \le \tau\|\dot c_\tau\|_{L^2(I;H^1(\Omega)^*)}\|c_\tau - \underline{c}_\tau\|_{L^2(I;H^1(\Omega))} \to 0$ and similarly also for $\bar c_\tau$. Hence,

$$\bar c_\tau \to c \ \text{ and } \ \underline{c}_\tau \to c \ \text{ strongly in } \ L^2(Q). \tag{5.46}$$

Similarly, by using the generalized Aubin-Lions theorem relying on the boundedness of $\{\dot{\underline{d}}_\tau\}_{\tau>0}$ in $\mathrm{Meas}(I;L^1(\Omega))$, see [44, Corollary 7.9], we also have at disposal

$$\underline{d}_\tau \to d \ \text{ strongly in } \ L^2(Q). \tag{5.47}$$

Now, let $1 \le r < 5/4$ and $1 \le q < r^* = \frac{3r}{3-r}$. Then $L^q(\Omega)$ is compactly embedded in $W^{1,r}(\Omega)$. By (5.15h) and (5.15j), we have that $\|w_\tau\|_{L^r(I;W^{1,r}(\Omega))} \le C$. Thus, by (5.34b), thanks to the Aubin-Lions Lemma, there exists a subsequence such that $\|w_\tau - w\|_{L^r(I;L^q(\Omega))} \to 0$. Now, for any such q and r, let $\lambda(r,q) = (1 + \frac1r - \frac1q)^{-1}$. Then, we have $\frac{\lambda(r,q)}{r} = 1 - \lambda(r,q) + \frac{\lambda(r,q)}{q}$. Therefore, by interpolating between $L^\infty(I;L^1(\Omega))$ and $L^r(I;L^q(\Omega))$ (see [44, Proposition 1.41]), we have the inequality $\|w_\tau - w\|_{L^{r/\lambda(r,q)}(Q)} \le C\|w_\tau - w\|^{1-\lambda(r,q)}_{L^\infty(I;L^1(\Omega))}\|w_\tau - w\|^{\lambda(r,q)}_{L^r(I;L^q(\Omega))}$. Now, for $1 \le r < 5/4$ fixed, we have $\inf_{1\le q<r^*}\lambda(r,q) = (1 + \frac1r - \frac1{r^*})^{-1} = (1 + \frac1r - \frac{3-r}{3r})^{-1} = \frac34$. Thus, $\sup_{\substack{1\le r<5/4\\1\le q<r^*}} \frac{r}{\lambda(r,q)} = 5/3$. This gives

$$w_\tau \to w \text{ strongly in } L^s(Q) \quad \text{with any } 1 \le s < 5/3. \tag{5.48}$$

Next, we observe that $\dot{\bar w}_\tau$ is bounded in the space of $W^{1,r/(r-1)}(\Omega)^*$-valued Radon measures on I, since:

$$\big\|\dot{\bar w}_\tau\big\|_{\mathrm{Meas}(I;W^{1,r/(r-1)}(\Omega)^*)} = \sup_{\|\varphi\|_{C(I;W^{1,r/(r-1)}(\Omega)^*)}=1} \int_Q \bar w_\tau \dot\varphi \,\mathrm{d}x\,\mathrm{d}t$$

$$
\begin{aligned}
&= \sup_{\|\varphi\|_{C(I;W^{1,r/(r-1)}(\Omega)^*)}=1} \sum_{k=1}^{T/\tau} \int_\Omega w_\tau^k(\varphi(k\tau)-\varphi((k-1)\tau))\,\mathrm{d}x \\
&= \sup_{\|\varphi\|_{C(I;W^{1,r/(r-1)}(\Omega)^*)}=1} \int_\Omega w_\tau^{T/\tau}\varphi(T) - \sum_{k=1}^{T/\tau-1}\int_\Omega \big(w_\tau^{k+1}-w_\tau^k\big)\varphi(k\tau)\,\mathrm{d}x - w_\tau^1\varphi(0)\,\mathrm{d}x \\
&\le \big\|\dot{w}_\tau\big\|_{L^1(I;W^{1,r/(r-1)}(\Omega)^*)} \le C,
\end{aligned} \tag{5.49}
$$

where the last inequality follows from (5.34b). We can now use the generalized version of the Aubin-Lions Lemma in [44, Corollary 7.9] and interpolate with the estimate to conclude that there exists $\bar{w} \in L^s(Q)$ such that

$$
\bar{w}_\tau \to \bar{w} \quad \text{strongly in} \quad L^s(Q) \quad \text{with any} \quad 1 \le s < 5/3. \tag{5.50}
$$

Thanks to (5.48) and (5.50), in order to prove the first convergence statement in (5.39h) it suffices for us to show that $\bar{w} = w$. To this aim, we argue as in [44, Remark 8.10]:

$$
\begin{aligned}
&\big\|w_\tau - \bar{w}_\tau\big\|_{L^1(I;W^{1,r/(r-1)}(\Omega)^*)} = \sum_{k=1}^{T/\tau}\int_{(k-1)\tau}^{k}\Big\|\frac{t-k\tau}{\tau}(w_\tau^k - w_\tau^{k-1})\Big\|_{W^{1,r/(r-1)}(\Omega)^*}\,\mathrm{d}t \\
&\quad = \frac{\tau}{2}\sum_{k=1}^{T/\tau}\big\|w_\tau^k - w_\tau^{k-1}\big\|_{W^{1,r/(r-1)}(\Omega)^*} = \frac{\tau}{2}\sum_{k=1}^{T/\tau}\int_{(k-1)\tau}^{k}\big\|\dot{w}_\tau\big\|_{W^{1,r/(r-1)}(\Omega)^*}\,\mathrm{d}t = \frac{\tau}{2}\int_0^T\big\|\dot{w}_\tau\big\|_{W^{1,r/(r-1)}(\Omega)^*}\,\mathrm{d}t \to 0,
\end{aligned}
$$

where we have used the bound (5.34b). The second convergence statement in (5.39h) is arrived at using a similar argument.

In order to obtain the convergences in (5.39f), we invert (5.13e) with respect to $\bar{\theta}_\tau$ to obtain (*cf.* (4.6)):

$$
\bar{\theta}_\tau = \vartheta(\bar{\chi}_\tau, \bar{w}_\tau), \qquad \text{and} \qquad \underline{\theta}_\tau = \vartheta(\underline{\chi}_\tau, \underline{w}_\tau). \tag{5.51}
$$

Then, (5.39f) follows from the already-established convergences (5.39h) and (5.44b) by the contiuity of the Nemytskiĭ mapping associated to ϑ.

Step 2: Strong convergence of $\bar{\boldsymbol{E}}_\tau$. In this step we prove:

$$
\bar{\boldsymbol{E}}_\tau \to \boldsymbol{E} \quad \text{strongly in } L^2(Q;\mathbb{R}^{3\times 3}). \tag{5.52}
$$

Note that we already have the weak convergence. Thus, by (4.4),

$$
\begin{aligned}
\epsilon\|\bar{\boldsymbol{E}}_\tau - \boldsymbol{E}\|^2_{L^2(Q;\mathbb{R}^3)} &\le \int_Q \big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau) - \partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\bar{\chi}_\tau,\underline{d}_\tau)\big) : (\bar{\boldsymbol{E}}_\tau - \boldsymbol{E})\,\mathrm{d}x\,\mathrm{d}t \\
&= \int_Q \partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau) : (\boldsymbol{\varepsilon}(\bar{\boldsymbol{u}}_\tau) - \boldsymbol{\varepsilon}(\boldsymbol{u})) - \partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau) : \mathbb{E}(\bar{\chi}_\tau - \chi)\,\mathrm{d}x\,\mathrm{d}t \\
&\quad - \int_Q \partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\bar{\chi}_\tau,\underline{d}_\tau) : (\bar{\boldsymbol{E}}_\tau - \boldsymbol{E})\,\mathrm{d}x\,\mathrm{d}t.
\end{aligned} \tag{5.53}
$$

We are going to show that the right-hand side of (5.53) converges to 0 as $\tau \to 0$.

By (5.44b) and (5.47) and the continuity of the Nemytskiĭ mapping induced by $\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\cdot,\cdot)$ and by (5.40b), we have $\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\bar{\chi}_\tau,\underline{d}_\tau){:}(\boldsymbol{E}_\tau - \boldsymbol{E}) \to 0$ weakly in $L^1(Q)$. Also, by the boundedness of $\{\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau)\}_{\tau>0}$ in $L^2(Q;\mathbb{R}^{3\times3})$ and again by (5.44b), we have $\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau){:}\mathbb{E}(\bar{\chi}_\tau - \chi) \to 0$ strongly in $L^1(Q)$. Hence, relying on the discrete equation (5.13a), we can continue in estimation (5.53) as follows:

$$
\begin{aligned}
&\epsilon \limsup_{\tau\to 0}\|\bar{\boldsymbol{E}}_\tau - \boldsymbol{E}\|^2_{L^2(Q;\mathbb{R}^3)} \le \limsup_{\tau\to0}\int_Q \partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar{\chi}_\tau,\underline{d}_\tau){:}(\boldsymbol{\varepsilon}(\bar{\boldsymbol{u}}_\tau) - \boldsymbol{\varepsilon}(\boldsymbol{u}))\,\mathrm{d}x\,\mathrm{d}t. \\
&\quad = \limsup_{\tau\to0}\int_Q (\bar{\boldsymbol{f}}_\tau - \varrho\ddot{\boldsymbol{u}}_\tau^{\rm i})\cdot(\bar{\boldsymbol{u}}_\tau - \boldsymbol{u})\,\mathrm{d}x\,\mathrm{d}t - \int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau : (\bar{\boldsymbol{E}}_\tau - \boldsymbol{E})\,\mathrm{d}x\,\mathrm{d}t \\
&\quad \le \lim_{\tau\to0}\Big(\int_\Omega \varrho\dot{\boldsymbol{u}}_\tau(0)\cdot\bar{\boldsymbol{u}}_\tau(\tau) - \varrho\dot{\boldsymbol{u}}_\tau(T)\cdot\bar{\boldsymbol{u}}_\tau(T)\,\mathrm{d}x + \int_\tau^T\!\!\int_\Omega \varrho\dot{\boldsymbol{u}}_\tau(\cdot-\tau){\cdot}\dot{\boldsymbol{u}}_\tau\,\mathrm{d}x\mathrm{d}t + \int_Q \varrho\ddot{\boldsymbol{u}}_\tau^{\rm i}{\cdot}\boldsymbol{u}\,\mathrm{d}x\mathrm{d}t\Big) \\
&\qquad + \lim_{\tau\to0}\int_\Omega \bar{\boldsymbol{f}}_\tau\cdot(\bar{\boldsymbol{u}}_\tau - \boldsymbol{u})\,\mathrm{d}x\mathrm{d}t - \liminf_{\tau\to0}\int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau : (\boldsymbol{E}_\tau - \boldsymbol{E})\,\mathrm{d}x\,\mathrm{d}t \\
&\quad = \int_\Omega \varrho\dot{\boldsymbol{u}}(0){\cdot}\boldsymbol{u}(0) - \varrho\dot{\boldsymbol{u}}(T){\cdot}\boldsymbol{u}(T)\,\mathrm{d}x + \int_Q \varrho|\dot{\boldsymbol{u}}|^2 + \varrho\ddot{\boldsymbol{u}}{\cdot}\boldsymbol{u}\,\mathrm{d}x\mathrm{d}t
\end{aligned}
$$

$$
\begin{aligned}
&-\liminf_{\tau\to 0}\int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau:\boldsymbol{E}_\tau\,\mathrm{d}x\,\mathrm{d}t+\lim_{\tau\to 0}\int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau:\boldsymbol{E}\,\mathrm{d}x\,\mathrm{d}t\\
&=\liminf_{\tau\to 0}\frac12\int_\Omega\big(\mathbb{D}\boldsymbol{E}_\tau(T):\boldsymbol{E}_\tau(T)-\mathbb{D}\boldsymbol{E}_0:\boldsymbol{E}_0\big)\,\mathrm{d}x-\frac12\int_\Omega\big(\mathbb{D}\boldsymbol{E}(T):\boldsymbol{E}(T)-\mathbb{D}\boldsymbol{E}_0:\boldsymbol{E}_0\big)\,\mathrm{d}x\le 0. \qquad (5.54)
\end{aligned}
$$

Here we also used the discrete by-part summation, cf. e.g. [44, Remark 11.38] and that, since $\bar{\boldsymbol{E}}_\tau-\boldsymbol{E}_\tau=(\tau k-t)\dot{\boldsymbol{E}}_\tau$ for $t\in((k-1)\tau,k\tau)$ and since $\mathbb{D}$ is positive, we have $\int_Q\mathbb{D}\dot{\boldsymbol{E}}_\tau:(\bar{\boldsymbol{E}}_\tau-\boldsymbol{E}_\tau)\,\mathrm{d}x\,\mathrm{d}t\ge 0$. Also we used the weak convergence $\boldsymbol{E}_\tau(T)\rightharpoonup\boldsymbol{E}(T)$ in $L^2(\Omega;\mathbb{R}^{3\times3})$, which is readily verified through $\int_\Omega\boldsymbol{E}_\tau(T):\widetilde{\boldsymbol{E}}\,\mathrm{d}x=\int_0^T\!\int_\Omega\dot{\boldsymbol{E}}_\tau:\widetilde{\boldsymbol{E}}\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\boldsymbol{E}_\tau(0):\widetilde{\boldsymbol{E}}\,\mathrm{d}x\ \to\ \int_0^T\!\int_\Omega\dot{\boldsymbol{E}}:\widetilde{\boldsymbol{E}}\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\boldsymbol{E}(0):\widetilde{\boldsymbol{E}}\,\mathrm{d}x=\int_\Omega\boldsymbol{E}(T):\widetilde{\boldsymbol{E}}\,\mathrm{d}x$ holding for $\widetilde{\boldsymbol{E}}\in L^2(\Omega;\mathbb{R}^{3\times3})$ arbitrary. Moreover, we also used that $\{\varrho\ddot{\boldsymbol{u}}_\tau^{\mathrm{i}}\}_{\tau>0}$ converges weakly* in a space which is in duality to the space where $\dot{\boldsymbol{u}}$ lives, and in particular also the $\varrho\ddot{\boldsymbol{u}}$ is in duality with $\dot{\boldsymbol{u}}$:

$$
\dot{\boldsymbol{u}}\in L^2(I;H^1(\Omega;\mathbb{R}^3))\quad\text{and}\quad\varrho\ddot{\boldsymbol{u}}\in L^2(I;H^1(\Omega;\mathbb{R}^3)^*). \qquad (5.55)
$$

Step 3: Convergence in the semilinear mechanical part. Because of the smoothness of $\varphi_{\rm ME}$ and of the strong convergence of $\bar{\boldsymbol{E}}_\tau$, $\bar\chi_\tau$, and $\underline{d}_\tau$ already established and stated, respectively, in (5.52), (5.44b), and (5.47), we have

$$
\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)\to\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\quad\text{in}\quad L^2(Q;\mathbb{R}^{3\times3}). \qquad (5.56)
$$

by continuity of the Nemytskiĭ mapping induced by $\varphi_{\rm ME}$. The limit passage in (5.13a) is then done.

Step 4: Limit passage in the phase-field equation. We rewrite (5.13d) as two variational inequalities:

$$
\begin{aligned}
&\int_Q\big(\bar\sigma_{\mathrm{r},\tau}+\partial_\chi\varphi_{\rm ME/CH}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau)+\partial_\chi\varphi_{\rm TH}(\underline{\chi}_\tau,\underline{\theta}_\tau)-\mathbb{E}^\top:(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau)\big)\cdot(v-\dot\chi_\tau)\\
&\qquad+\kappa_1\nabla\bar\chi_\tau:(\nabla v-\nabla\dot\chi_\tau)+\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,v)\,\mathrm{d}x\mathrm{d}t\\
&\qquad\qquad\ge\int_Q-\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot\chi_\tau)\,\mathrm{d}x\mathrm{d}t\qquad\forall v\in L^2(I;H^1(\Omega;\mathbb{R}^N)), \qquad (5.57a)\\
&\int_Q\bar\sigma_{\mathrm{r},\tau}\cdot(v-\bar\chi_\tau)\,\mathrm{d}x\mathrm{d}t\ge 0\qquad\qquad\forall v\in L^2(Q;\mathbb{R}^N),\ \ v\in K\text{ a.e. in }Q. \qquad (5.57b)
\end{aligned}
$$

The limit passage in (5.57b) is easy because $\bar\sigma_{\mathrm{r},\tau}\to\sigma_{\mathrm{r}}$ weakly in $L^2(Q;\mathbb{R}^N)$ and $\bar\chi_\tau\to\chi$ strongly in $L^2(Q;\mathbb{R}^N)$ has already been proved in Step 2; thus $\sigma_{\mathrm{r}}\in N_K(\chi)$ is shown. Now we can make a limit passage in (5.57a). Here on the left-hand side we have collected all terms that need to be handled through a continuity or a weak upper semicontinuity, while the right-hand side is to be treated by weak lower semicontinuity. We benefit from the already proven strong convergence of $\underline{d}_\tau$, $\underline{c}_\tau$, and $\bar{\boldsymbol{E}}_\tau$. The limit passage in $\partial_\chi\varphi_{\rm ME/CH}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau)\cdot\dot\chi_\tau$ and $\partial_\chi\varphi_{\rm TH}(\underline{\chi}_\tau,\underline{\theta}_\tau)\cdot\dot\chi_\tau$ is simply by continuity. Furthermore, we have

$$
\begin{aligned}
\limsup_{\tau\to0}\int_Q-\kappa_1\nabla\bar\chi_\tau\cdot\nabla\dot\chi_\tau\,\mathrm{d}x\mathrm{d}t&\le\int_\Omega\frac{\kappa_1}{2}\big|\nabla\chi_0\big|^2\,\mathrm{d}x-\liminf_{\tau\to0}\int_\Omega\frac{\kappa_1}{2}\big|\nabla\chi(T)\big|^2\,\mathrm{d}x\\
&\le\int_\Omega\frac{\kappa_1}{2}\big|\nabla\chi_0\big|^2-\frac{\kappa_1}{2}\big|\nabla\chi(T)\big|^2\,\mathrm{d}x. \qquad (5.58)
\end{aligned}
$$

The only difficult term is $\mathbb{E}^\top:\mathbb{D}\dot{\boldsymbol{E}}_\tau\dot\chi_\tau$ because so far we know only a weak convergence of both $\dot{\boldsymbol{E}}_\tau$ and $\dot\chi_\tau$. This requires quite tricky chain of arguments:

$$
\begin{aligned}
&\limsup_{\tau\to0}\int_Q\mathbb{E}^\top:\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau\big)\dot\chi_\tau\,\mathrm{d}x\,\mathrm{d}t\\
&=\limsup_{\tau\to0}\int_Q\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau\big):\big(\boldsymbol{\varepsilon}(\dot{\boldsymbol{u}}_\tau)-\dot{\boldsymbol{E}}_\tau\big)\,\mathrm{d}x\,\mathrm{d}t\\
&=-\liminf_{\tau\to0}\int_Q\big(\varrho\ddot{\boldsymbol{u}}_\tau^{\mathrm{i}}-\bar{\boldsymbol{f}}_\tau\big)\cdot\dot{\boldsymbol{u}}_\tau+\big(\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau)+\mathbb{D}\dot{\boldsymbol{E}}_\tau\big):\dot{\boldsymbol{E}}_\tau\,\mathrm{d}x\,\mathrm{d}t+\lim_{\tau\to0}\int_\Sigma\bar{\boldsymbol{f}}_{\mathrm{s},\tau}\cdot\dot{\boldsymbol{u}}_\tau\,\mathrm{d}S\,\mathrm{d}t\\
&\le-\liminf_{\tau\to0}\Big(\frac12\int_\Omega\varrho|\dot{\boldsymbol{u}}_\tau(T)|^2\,\mathrm{d}x+\int_Q\mathbb{D}\dot{\boldsymbol{E}}_\tau:\dot{\boldsymbol{E}}_\tau\,\mathrm{d}x\,\mathrm{d}t\Big)\\
&\quad+\frac12\int_\Omega\varrho|\dot{\boldsymbol{u}}(0)|^2\,\mathrm{d}x+\lim_{\tau\to0}\Big(\int_Q\bar{\boldsymbol{f}}_\tau\cdot\dot{\boldsymbol{u}}_\tau-\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau):\dot{\boldsymbol{E}}_\tau\,\mathrm{d}x\,\mathrm{d}t+\int_\Sigma\bar{\boldsymbol{f}}_{\mathrm{s},\tau}\cdot\dot{\boldsymbol{u}}_\tau\,\mathrm{d}S\,\mathrm{d}t\Big)
\end{aligned}
$$

$$
\begin{aligned}
&\le -\frac{1}{2}\int_\Omega \varrho|\dot{\boldsymbol u}(T)|^2\,\mathrm{d}x - \int_Q \mathbb{D}\dot{\boldsymbol E}:\dot{\boldsymbol E}\,\mathrm{d}x\,\mathrm{d}t\\
&\quad+\frac{1}{2}\int_\Omega \varrho|\dot{\boldsymbol u}(0)|^2\,\mathrm{d}x + \int_Q \boldsymbol f\cdot\dot{\boldsymbol u} - \partial_{\boldsymbol E}\varphi_{\rm ME}(\boldsymbol E,\chi,d):\dot{\boldsymbol E}\,\mathrm{d}x\,\mathrm{d}t + \int_\Sigma \boldsymbol f_{\rm s}\cdot\dot{\boldsymbol u}\,\mathrm{d}S\,\mathrm{d}t\\
&= -\int_0^T \langle\varrho\ddot{\boldsymbol u},\dot{\boldsymbol u}\rangle\,\mathrm{d}t + \int_Q \boldsymbol f\cdot\dot{\boldsymbol u} - \big(\partial_{\boldsymbol E}\varphi_{\rm ME}(\boldsymbol E,\chi,d)+\mathbb{D}\dot{\boldsymbol E}\big):\dot{\boldsymbol E}\,\mathrm{d}x\,\mathrm{d}t + \int_\Sigma \boldsymbol f_{\rm s}\cdot\dot{\boldsymbol u}\,\mathrm{d}S\,\mathrm{d}t\\
&= \int_Q \mathbb{E}^\top : \big(\partial_{\boldsymbol E}\varphi_{\rm ME}(\boldsymbol E,\chi,d)+\mathbb{D}\dot{\boldsymbol E}\big)\dot\chi\,\mathrm{d}x\,\mathrm{d}t.
\end{aligned}
\tag{5.59}
$$

Here, the first equality used just $\dot\chi_\tau = \boldsymbol\varepsilon(\dot{\boldsymbol u}_\tau) - \dot{\boldsymbol E}_\tau$, the second one used the force balance (5.13a) with the boundary conditions (5.14a) tested by $\dot u_\tau$, then we used the discrete by-part integration (or, in fact, summation) $\frac{1}{2}|\dot{\boldsymbol u}_\tau(T)|^2 - \frac{1}{2}|\dot{\boldsymbol u}(0)|^2 \le \int_0^T \ddot{\boldsymbol u}_\tau^{\rm i}\cdot\dot{\boldsymbol u}_\tau\mathrm{d}t$ on Ω, then semicontinuity arguments, then the by-part integration formula

$$
\int_0^T \langle\varrho\ddot{\boldsymbol u},\dot{\boldsymbol u}\rangle\,\mathrm{d}t = \int_\Omega \frac{\varrho}{2}\big|\dot{\boldsymbol u}(T)\big|^2 - \frac{\varrho}{2}\big|\dot{\boldsymbol u}(0)\big|^2\,\mathrm{d}x. \tag{5.60}
$$

relying on the fact that, by (5.55), $\varrho\ddot{\boldsymbol u}$ and $\dot{\boldsymbol u}$ are in duality, then the limit force equilibrium we proved already in Step 3, and at the end still $\mathbb{E}\dot\chi = \boldsymbol\varepsilon(\dot{\boldsymbol u}) - \dot{\boldsymbol E}$. The limit in $\int_Q \bar\sigma_{{\rm r},\tau}\cdot\dot\chi_\tau\,\mathrm{d}x\mathrm{d}t$ is simple because, for any $\bar\sigma_{{\rm r},\tau}\in N_K(\dot\chi_\tau)$, this integral equals to $\int_\Omega \delta_K(\chi_\tau(T)) - \delta_K(\chi_0)\,\mathrm{d}x = 0$. Eventually, the limit passage in the right-hand side of (5.57a) is by convexity of $\zeta(\boldsymbol E,\chi,d,c,\theta,\cdot)$ and the weak lower semi-continuity

$$
\liminf_{\tau\to0}\int_Q \zeta(\underline{\boldsymbol E}_\tau,\underline\chi_\tau,\underline d_\tau,\underline c_\tau,\underline\theta_\tau,\dot\chi_\tau)\,\mathrm{d}x\mathrm{d}t \ge \int_Q \zeta(\boldsymbol E,\chi,d,c,\theta,\dot\chi)\,\mathrm{d}x\mathrm{d}t. \tag{5.61}
$$

Here we also used that $\underline{\boldsymbol E}_\tau \to \boldsymbol E$, which follows from (5.52) and from

$$
\|\bar{\boldsymbol E}_\tau - \underline{\boldsymbol E}_\tau\|_{L^2(Q;\mathbb{R}^{3\times3})} \le \tau\|\dot{\boldsymbol E}_\tau\|_{L^2(Q;\mathbb{R}^{3\times3})} \to 0. \tag{5.62}
$$

Step 5: Limit passage in the diffusion equation. By the strong convergence of $\bar{\boldsymbol E}_\tau$, $\bar\chi_\tau$, $\underline d_\tau$, and $\underline c_\tau$ established in (5.52), (5.44b), (5.46), and (5.39f), and by assumption of boundedness (4.1k) of $\mathbf M$ and by the Nemytskii-mapping continuity argument, we have that

$$
\mathbf M(\bar{\boldsymbol E}_\tau,\bar\chi_\tau,\underline d_\tau,\underline c_\tau) \to \mathbf M(\boldsymbol E,\chi,c,d) \quad \text{strongly in} \quad L^p(Q) \quad \forall 1\le p<+\infty. \tag{5.63}
$$

Now, owing to (5.40e), (5.40f), and (5.63), we can pass to the limit in the first of (5.13c). In order to pass to the limit in the second of (5.13c), we observe that by the aforementioned a.e. convergence of $\bar\chi_\tau$, $\underline d_\tau$, and $\underline c_\tau$ in Q and by the continuity of $\partial_c\varphi_{\rm CH}$, we have

$$
\bar\mu_\tau = \partial_c\varphi_{\rm CH}(\bar\chi_\tau,\bar c_\tau) \to \partial_c\varphi_{\rm CH}(\chi,c) \text{ a.e. in } Q, \tag{5.64}
$$

for some subsequence. By comparing (5.64) with (5.40f) we conclude that

$$
\mu = \partial_c\varphi_{\rm CH}(\chi,c). \tag{5.65}
$$

Step 6: Limit passage in the semi-stability (5.13d) *towards* (4.10d). The mutual recovery sequence in the sense of [33] for (5.13d) uses the sophisticated construction of M. Thomas [52, 53]. For all $t\in I$, we have

$$
\bar d_\tau(t) \to d(t) \quad \text{weakly in} \quad H^1(\Omega). \tag{5.66}
$$

Consider a competitor $\widetilde d$ of $d(t)$ in (4.10d). It suffices to consider the case

$$
\widetilde d(x) \le d(x,t) \quad \text{for a.e. } x\in\Omega, \tag{5.67}
$$

since otherwise the right-hand side the inequality (4.10d) is $+\infty$.

We define the sequence

$$
\widetilde d_\tau(x,t) = \min\big\{(\widetilde d(x)-\varepsilon_\tau)^+,\bar d_\tau(x,t)\big\} \qquad \text{with} \qquad \varepsilon_\tau = \big\|\bar d_\tau(t) - d(t)\big\|_{L^q(\Omega)}^{1/2}. \tag{5.68}
$$

with $1\le q<6$. It is immediate that $\widetilde d_\tau\in H^1(\Omega)$ and $\widetilde d_\tau(t) < \bar d_\tau(t)$. Moreover, for $A_\tau(t) = \{x\in\Omega : \widetilde d(x) - \varepsilon_\tau \le \bar d_\tau(x,t)\}$, we have:

$$
\nabla\widetilde d_\tau(x,t) = \begin{cases} \nabla\widetilde d(x) & \forall x\in A_\tau(t),\\ \nabla\bar d_\tau(x,t) & \forall x\in\Omega\setminus A_\tau(t), \end{cases} \tag{5.69}
$$

Consequently

$$\liminf_{\tau\to 0}\int_\Omega \big|\nabla\overline{d}_\tau(x,t)\big|^2-\big|\nabla\widetilde{d}_\tau(x,t)\big|^2\,\mathrm{d}x=\liminf_{\tau\to 0}\int_{A_\tau}\big|\nabla\overline{d}_\tau(x,t)\big|^2-\big|\nabla\widetilde{d}(x)\big|^2\,\mathrm{d}x. \tag{5.70}$$

Because of (5.67), we have $|\overline{d}_\tau(x,t)-d(x)|\le\varepsilon_\tau\Rightarrow x\in A_\tau(t)$. Thus, $\Omega\setminus A_\tau(t)\subset\{x\in\Omega:|\overline{d}_\tau(x,t)-\widetilde{d}(x)|\ge\varepsilon_\tau\}$. Using Markov's inequality and the weak convergence of $\overline{d}_\tau(t)$ to $d(t)$ in $H^1(\Omega)$, we obtain

$$\big|\Omega\backslash A_\tau(t)\big|\le\frac{1}{\varepsilon_\tau^q}\int_\Omega\big|\overline{d}_\tau(x,t)-d(x,t)\big|^q\mathrm{d}x=\big\|\overline{d}_\tau(t)-d(t)\big\|_{L^q(\Omega)}^{q/2}\to 0 \tag{5.71}$$

where $|\Omega\backslash A_\tau(t)|$ denoted the Lebesgue measure of the set $\Omega\backslash A_\tau(t)$. Given a set C, let δ_C be its indicator function. It is shown in [53] that

$$\delta_{A_\tau(t)}\nabla\overline{d}_\tau(t)\to\nabla d(t)\qquad\text{weakly in }\ L^2(\Omega;\mathbb{R}^3). \tag{5.72}$$

On the other hand we have, trivially, that $\delta_{A_\tau(t)}\nabla\widetilde{d}$ converges strongly to $\nabla\widetilde{d}$. Thus, from (5.70) we find, by lower semicontinuity,

$$\begin{aligned}\liminf_{\tau\to 0}\int_\Omega|\nabla\overline{d}_\tau(x,t)|^2-|\nabla\widetilde{d}_\tau(x,t)|^2\,\mathrm{d}x&=\liminf_{\tau\to 0}\int_\Omega\delta_{A_\tau(t)}(x)|\nabla\overline{d}_\tau(x,t)|^2\,\mathrm{d}x-\lim_{\tau\to 0}\int_{A_\tau(t)}|\nabla\widetilde{d}(x)|^2\,\mathrm{d}x\\&\ge\int_\Omega|\nabla d_\tau(x,t)|^2\,\mathrm{d}x-\int_A|\nabla\widetilde{d}(x)|^2\,\mathrm{d}x.\end{aligned} \tag{5.73}$$

With this result, the limit passage in the semi-stability condition is easily achieved for a.e. $t\in I$, on taking into account that $\overline{\boldsymbol{E}}(t)\to\boldsymbol{E}(t)$ strongly in $L^2(\Omega;\mathbb{R}^{3\times3})$; furthermore, $\overline{\chi}_\tau(t)\to\chi(t)$ strongly in $L^q(\Omega;\mathbb{R}^N)$, and $\overline{c}_\tau(t)\to c(t)$ strongly in $L^q(\Omega;\mathbb{R})$.

Step 7: Mechanical/chemical energy conservation (4.10f). This is standardly achieved by testing the mechano-chemical equations (3.7a–d) respectively by $\dot{\boldsymbol{u}}$, $\dot\chi$, μ, and $\dot d$, and by using the chain rule to integrate with respect to t. Here, however, (3.7d) has to be specially treated because $\dot d$ can be a measure.

Making the first test legal, we again need $\varrho\ddot{\boldsymbol{u}}$ to be in duality with $\dot{\boldsymbol{u}}$, cf. (5.55), and make use of (5.60). For the second mentioned test, we need $\Delta\chi\in L^2(Q)$ to have the integration-by-part formula at our disposal. The regularity of $\Delta\chi$ follows from the estimate (5.34d) and weak convergence. The proof of the by-part integration formula is rather technical because $\chi:I\to H^1(\Omega;\mathbb{R}^N)$ is actually only a weakly continuous function but not necessarily strongly continuous. The desired formula is

$$\int_Q\Delta\chi\cdot\dot\chi\,\mathrm{d}x\mathrm{d}t=\frac12\int_\Omega|\nabla\chi_0|^2-|\nabla\chi(T)|^2\,\mathrm{d}x. \tag{5.74}$$

Its proof is a bit tricky and can be done either by a mollification in space [36, Formula (3.69)] and or in time by a time-difference technique [18, Formula (2.15)]. Also we use that $\sigma_{\rm r}\in L^2(Q;\mathbb{R}^N)$ is in duality with $\dot\chi\in L^2(Q;\mathbb{R}^N)$, so that the integral $\int_Q\sigma_{\rm r}\cdot\dot\chi\,\mathrm{d}x\mathrm{d}t$ has a sense and simply equals to 0 because $\sigma_{\rm r}\in\partial\delta_K(\chi)$ has been proved in Step 4 and because $\delta_K(\chi_0)=0$ has been assumed, cf. (4.2b).

Also, $\dot c\in L^2(I;H^1(\Omega)^*)$ is in duality with $\mu\in L^2(I;H^1(\Omega))$ as well as $\dot\chi\in L^2(Q;\mathbb{R}^N)$ is in duality with $\partial_\chi\varphi_{\rm CH}(\chi,c)\in L^2(Q;\mathbb{R}^N)$, cf. (5.34c) with (5.39g) and (4.1e) so that we obtain

$$\int_0^T\Big(\langle\dot c,\mu\rangle+\int_\Omega\partial_\chi\varphi_{\rm CH}(\chi,c)\cdot\dot\chi\,\mathrm{d}x\Big)\mathrm{d}t=\int_\Omega\varphi_{\rm CH}(\chi(T),c(T))-\varphi_{\rm CH}(\chi_0,c_0)\,\mathrm{d}x. \tag{5.75}$$

Eventually, we use the Riemann-sum approximation of Lebesgue integrals and semi-stability as devised in [9, 32], cf. also [43, Formulas (4.68)–(4.74)] for a combination with rate-dependent mechanical part. In fact, the Riemann sums can range only a.a. points from I and thus the semi-stability need not hold at every time but only at almost each times. By this way we obtain

$$\begin{aligned}&\int_\Omega\varphi_{\rm ME}(\boldsymbol{E}(T),\chi(T),d(T))+\frac{\kappa_2}{2}|\nabla d(T)|^2+\alpha(\chi(T))d(T)\,\mathrm{d}x+\int_Q\alpha'(\chi)\dot\chi d\,\mathrm{d}x\mathrm{d}t\\&\quad=\int_\Omega\varphi_{\rm ME}(\boldsymbol{E}_0,\chi_0,d_0)+\frac{\kappa_2}{2}|\nabla d_0|^2+\alpha(\chi_0)d_0\,\mathrm{d}x-\int_Q\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\dot{\boldsymbol{E}}+\partial_\chi\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\dot\chi\,\mathrm{d}x\mathrm{d}t.\end{aligned} \tag{5.76}$$

Again we used that $\dot{\boldsymbol{E}}\in L^2(Q;\mathbb{R}^{3\times3})$ and $\dot\chi\in L^2(Q;\mathbb{R}^N)$ are in duality with $\partial_{\boldsymbol{E}}\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\in L^2(Q;\mathbb{R}^{3\times3})$ and $\partial_\chi\varphi_{\rm ME}(\boldsymbol{E},\chi,d)\dot\chi$, respectively. Here we also used the semi-stability of the initial condition d_0 assumed in (4.2c).

Eventually, by summing up all four obtained partial balances, we obtain (4.10f).

Step 8: Strong convergence of $\dot{\boldsymbol{E}}_\tau$, $\dot\chi_\tau$, and $\nabla\bar\mu_\tau$. Using the discrete mechano-chemical energy imbalance (5.13f) and eventually the energy equality (4.10f), we can write

$$
\begin{aligned}
&\int_Q \mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}} + \partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\cdot\dot\chi + \mathbf{M}(\boldsymbol{E},d,c,\theta)\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t\\
&\quad\le \liminf_{\tau\to0}\int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau{:}\dot{\boldsymbol{E}}_\tau + \partial_{\dot\chi}\zeta(\underline{\boldsymbol{E}}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot\chi_\tau)\cdot\dot\chi_\tau + \mathbf{M}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau{\cdot}\nabla\bar\mu_\tau\\
&\quad\le \limsup_{\tau\to0}\int_Q \mathbb{D}\dot{\boldsymbol{E}}_\tau{:}\dot{\boldsymbol{E}}_\tau + \partial_{\dot\chi}\zeta(\boldsymbol{E}_\tau,\underline{\chi}_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau,\dot\chi_\tau)\cdot\dot\chi + \mathbf{M}(\bar{\boldsymbol{E}}_\tau,\bar\chi_\tau,\underline{d}_\tau,\underline{c}_\tau,\underline{\theta}_\tau)\nabla\bar\mu_\tau{\cdot}\nabla\bar\mu_\tau\,\mathrm{d}x\mathrm{d}t\\
&\quad\le \limsup_{\tau\to0}\bigg(\mathscr{E}_{\rm MC}(0)-\int_\Omega\frac{\varrho}{2}\big|\dot{\boldsymbol{u}}_\tau(T)\big|^2+\varphi_{\rm ME/CH}(\boldsymbol{E}_\tau(T),\chi_\tau(T),d_\tau(T),c_\tau(T))\\
&\qquad\qquad+\frac{\kappa_1}{2}\big|\nabla\chi_\tau(T)\big|^2+\frac{\kappa_2}{2}\big|\nabla d_\tau(T)\big|^2\mathrm{d}x-\int_\Sigma\bar{\boldsymbol{f}}_{{\rm s},\tau}{\cdot}\dot{\boldsymbol{u}}_\tau\,\mathrm{d}S\mathrm{d}t-\int_Q\bar{\boldsymbol{f}}_\tau{\cdot}\dot{\boldsymbol{u}}_\tau+\alpha(\bar\chi_\tau)\dot d_\tau\,\mathrm{d}x\mathrm{d}t\bigg)\\
&\quad\le \mathscr{E}_{\rm MC}(0)-\mathscr{E}_{\rm MC}(T)-\int_\Sigma\boldsymbol{f}_{\rm s}{\cdot}\dot{\boldsymbol{u}}\,\mathrm{d}S\mathrm{d}t-\int_Q\boldsymbol{f}{\cdot}\dot{\boldsymbol{u}}\,\mathrm{d}x\mathrm{d}t-\int_Q\alpha'(\chi)\dot\chi d\,\mathrm{d}x\,\mathrm{d}t-\int_\Omega\alpha(\chi(T))d(T)-\alpha(\chi_0)d_0\,\mathrm{d}x\\
&\quad=\int_Q \mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}} + \partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)\cdot\dot\chi + \mathbf{M}(\boldsymbol{E},d,c,\theta)\nabla\mu{\cdot}\nabla\mu\,\mathrm{d}x\mathrm{d}t.
\end{aligned}\tag{5.77}
$$

Note that in the last inequality we have made use of the discrete by-part integration (= summation) formula for the following calculations, being a discrete analogue of (4.12) with $z=1$:

$$
\begin{aligned}
\lim_{\tau\to0}\int_Q\alpha(\bar\chi_\tau)\dot d_\tau\,\mathrm{d}x\,\mathrm{d}t &= \lim_{\tau\to0}\sum_{k=1}^{T/\tau}\int_\Omega\alpha(\chi_\tau^k)(d_\tau^k-d_\tau^{k-1})\,\mathrm{d}x\\
&=\lim_{\tau\to0}\bigg(\int_\Omega\alpha(\chi_\tau^{T/\tau})d_\tau^{T/\tau}\,\mathrm{d}x-\sum_{k=1}^{T/\tau}\int_\Omega\big(\alpha(\chi_\tau^k)-\alpha(\chi_\tau^{k-1})\big)d_\tau^{k-1}\,\mathrm{d}x\bigg)-\int_\Omega\alpha(\chi_\tau^0)d_\tau^0\,\mathrm{d}x\\
&=\lim_{\tau\to0}\bigg(\int_\Omega\alpha(\chi_\tau(T))d_\tau(T)\,\mathrm{d}x-\int_Q\big(\alpha'(\chi_\tau)\dot\chi_\tau\underline{d}_\tau+r_\tau\underline{d}_\tau\big)\,\mathrm{d}x\,\mathrm{d}t\bigg)-\int_\Omega\alpha(\chi_0)d_0\,\mathrm{d}x\\
&=\int_\Omega\alpha(\chi(T))d(T)\,\mathrm{d}x-\int_Q\big(\alpha'(\chi)\dot\chi d+0\big)\,\mathrm{d}x\,\mathrm{d}t-\int_\Omega\alpha(\chi_0)d_0\,\mathrm{d}x,
\end{aligned}
$$

where we have set $d_\tau^{-1}=d_\tau^0=d_0$ and where r_τ denotes the difference between $[\alpha(\chi_\tau)]^{^\centerdot}$ and the piece-wise constant-in-time function with values $(\alpha(\chi_\tau^k)-\alpha(\chi_\tau^k))/\tau$ on the interval $((k-1)\tau,k\tau)$; here we used differentiability assumption on α stated in (4.1o) and the estimate $|r_\tau|\le\tau^2(\sup_{\mathbb{R}^N}\alpha'')|\dot\chi_\tau|^2$ so that

$$
\Big|\int_Q r_\tau\underline{d}_\tau\,\mathrm{d}x\,\mathrm{d}t\Big|\le\tau^2\big(\sup_{\mathbb{R}^N}\alpha''\big)\int_Q\big|\dot\chi_\tau\big|^2d_\tau\,\mathrm{d}x\,\mathrm{d}t\le\tau^2\big(\sup_{\mathbb{R}^N}\alpha''\big)\big\|\dot\chi_\tau\big\|^2_{L^2(Q;\mathbb{R}^N)}\big\|d_\tau\big\|_{L^\infty(Q)}=\mathscr{O}(\tau^2)\to0
$$

for $\tau\to0$. To converge $\alpha'(\chi_\tau)\dot\chi_\tau\underline{d}_\tau$ to $\alpha'(\chi)\dot\chi d$ weakly in $L^1(Q)$, we used (5.44b) together with (5.40c), and (5.47). The last equality in (5.77) has been proved in Step 7. Altogether, we can write "lim" and "=" everywhere in (5.77) and, together with the already proved weak convergence, we obtain the desired strong convergence of $\dot{\boldsymbol{E}}_\tau$ and $\dot\chi_\tau$ and $\nabla\bar\mu_\tau$ in $L^2(Q)$-spaces. Here we rely on the well-known concept of compactness via convexity ([55, 56]) with some modifications. In particular, for technical details about the term $\mathbf{M}\nabla\mu{\cdot}\nabla\mu$ with the nonconstant coefficient $\mathbf{M}=\mathbf{M}(\boldsymbol{E},d,c,\theta)$, we refer to [49, Formula (4.25)].

Step 9: Limit passage in the heat equation (5.13e). Having proved the strong convergence in Steps 3 and 9, the right-hand side of (5.13e) converges strongly in $L^1(Q)$ except the term $\alpha(\chi)\dot d$ but even this term converges weakly∗ in Meas$(\bar Q)$, cf. Step 7, which is sufficient to the limit passage towards (3.7e), which is then easy.

Step 10: Total-energy conservation (4.13) *at almost each time.* Considering $t_*\in[0,T)$ fixed, we use the test function

$$
z_\epsilon(t)=\begin{cases}1 & \text{if } t\le t_*,\\ 1+(t_*-t)/\epsilon & \text{if } t_*\le t\le t_*+\epsilon,\\ 0 & \text{if } t\ge t_*+\epsilon\end{cases}\tag{5.78}
$$

for (4.10e). Using that $\dot z=0$ for $t\in[0,t_*]\cup[t_*+\epsilon,T]$ and that $\nabla z=0$, this test leads to

$$
\begin{aligned}
\frac{1}{\epsilon}\int_{t_*}^{t_*+\epsilon}\!\!\int_\Omega w\,\mathrm{d}x\,\mathrm{d}t&=\int_0^{t_*}\!\!\int_\Omega\Big(\big(\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)+\partial_\chi\varphi_{\rm TH}(\chi,\theta)+\alpha'(\chi)d\big){\cdot}\dot\chi+\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu{\cdot}\nabla\mu\\
&\qquad+\mathbb{D}\dot{\boldsymbol{E}}{:}\dot{\boldsymbol{E}}\Big)\,\mathrm{d}x\,\mathrm{d}t+\frac{1}{\epsilon}\int_{t*}^{t_*+\epsilon}\!\!\int_\Omega\alpha(\chi)d\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\big(w_0+\alpha(\chi_0)d_0\big)\,\mathrm{d}x+\int_\Sigma q_{\rm s}\,\mathrm{d}S\,\mathrm{d}t+o_t(\epsilon)
\end{aligned}\tag{5.79}
$$

with $o_{t_*}(\epsilon)$ abbreviating the corresponding integrals over $[t_*,t_*+\epsilon]$. We have $\lim_{\epsilon\to0}o_{t_*}(\epsilon)=0$ for any t_* due to absolute continuity of the Lebesgue integral. Considering however t_* as a right Lebesgue point of the functions $t\mapsto\int_\Omega w(x,t)\,\mathrm{d}x$ and $t\mapsto\int_\Omega\alpha(\chi(x,t))d(x,t)\,\mathrm{d}x$, in the limit for $\epsilon\to0+$ we obtain

$$\int_\Omega w(t_*)\,\mathrm{d}x\,\mathrm{d}t=\int_0^{t_*}\!\!\int_\Omega\Big(\big(\partial_{\dot\chi}\zeta(\boldsymbol{E},\chi,c,d,\theta,\dot\chi)+\partial_\chi\varphi_{\rm TH}(\chi,\theta)+\alpha'(\chi)d\big)\cdot\dot\chi+\mathbf{M}(\boldsymbol{E},\chi,c,d,\theta)\nabla\mu\cdot\nabla\mu$$
$$+\mathbb{D}\dot{\boldsymbol{E}}:\dot{\boldsymbol{E}}\Big)\,\mathrm{d}x\,\mathrm{d}t+\int_\Omega\alpha(\chi(t_*))d(t_*)\,\mathrm{d}x+\int_\Omega\big(w_0+\alpha(\chi_0)d_0\big)\,\mathrm{d}x+\int_0^{t_*}\!\!\int_\Gamma q_{\rm s}\,\mathrm{d}S\,\mathrm{d}t. \tag{5.80}$$

Such points t_*'s has a full Lebesgue measure on I. Eventually, we get (4.13) by summing (5.80) with mechanical/chemical energy balance (4.10f) written for t_* instead of T obtained already in Step 8 by obvious modification of the arguments there. □

Remark 5.6 (*Damageable viscosity*). One may want to include damageable viscosity in the model through a constitutive equation of the form $\boldsymbol{S}_{\rm d}=\mathbb{D}(d)\dot{\boldsymbol{E}}$ for the viscous part of the stress. With this modification, when performing integration by parts in (5.54), the additional term $-\int_Q\frac{\partial}{\partial t}\mathbb{D}(d_\tau)\boldsymbol{E}_\tau:\boldsymbol{E}_\tau\,dxdt$ would appear. Passage to the limit through lower semicontinuity would still be possible if the tensor $\frac{\partial}{\partial t}\mathbb{D}(d_\tau)$ is non-positive. This could rely on the unidirectional evolution of d adopted in this paper and monotone dependence of $\mathbb{D}$ on damage, in the sense of the so-called Löwner ordering, namely $(\mathbb{D}(d_1)-\mathbb{D}(d_2))\boldsymbol{E}:\boldsymbol{E}\le0$ if $d_1<d_2$.

Remark 5.7 (*Decoupling between concentration and strain).* Our assumption (3.4) rules out any direct coupling between strain and concentration. We need a decoupling between concentration and strain to avoid an explicit dependence of chemical potential on strain, which would lead to the appearance of the gradient of strain in the formulation. Indeed, in order to pass to the limit in the nonlinear equation:

$$\mu=\partial_c\varphi_{\rm CH}(\chi,c) \tag{5.81}$$

which defines chemical potential, we exploit the strong convergence of c in a suitable L^p space, cf. (5.39d) above. In order to obtain such convergence, we rely on the standard Aubin-Lions compactness theorem, whose application requires estimates on $\dot c$ and ∇c. The natural energetic estimate provides us with a control on $\nabla\mu$ (*cf.* (5.15e)), but not on ∇c. To control of the latter (cf. the estimate (5.15d) above) we take the gradient of (5.81) at the approximation level, see (5.21) in the proof of Lemma 5.3. If we were allowed $\partial^2_{c\boldsymbol{E}}\varphi\neq0$, then $\nabla\boldsymbol{E}$ would have appeared in that estimate. To give a concrete example, let us consider a toy model with no phase field χ, no damage variable d, and no temperature θ. Let us assume that the following strain decomposition:

$$\boldsymbol{\varepsilon}(\boldsymbol{u})=\boldsymbol{E}+c\mathbb{E} \tag{5.82}$$

holds, where $\mathbb{E}$ is a constant second-order symmetric tensor. In this case, the dissipation inequality takes the form

$$\dot\psi-\mu\dot c\le\boldsymbol{S}:\dot{\boldsymbol{E}}+\boldsymbol{S}:\mathbb{E}\dot c-\mathbf{h}\cdot\nabla\mu. \tag{5.83}$$

Then, the application of the Coleman-Noll argument yields, for chemical potential, a constitutive equation of the form

$$\mu=\partial_c\psi(\boldsymbol{E},c)+\boldsymbol{S}:\mathbb{E}. \tag{5.84}$$

Suppose that we take $\psi=\frac12\mathbb{C}\boldsymbol{E}:\boldsymbol{E}$. Then, if we rule out viscoelastic dissipation the constitutive equation for the stress is $\boldsymbol{S}=\mathbb{C}\boldsymbol{E}$. From (5.84) we have

$$\partial^2_{cc}\psi(\boldsymbol{E},c)\nabla c=\nabla\mu-\mathbb{E}^\top:\mathbb{C}\nabla\boldsymbol{E} \tag{5.85}$$

Clearly, there is no hope to control the second term on the right-hand side of (5.85), unless we have some control on $\nabla\boldsymbol{E}$, which however cannot be expected. This issue may be circumvented by allowing a dependence of free energy on ∇c, for instance by adding a term proportional to $|\nabla c|^2$. As discussed, for instance, in [14], this term describes capillarity effects, and would lead to a system of Cahn–Hilliard type [7], similar to those studied in [16]. Alternatively, one might think of reformulating the model in the framework of non-simple materials, by allowing for instance the free energy to depend on $\nabla\boldsymbol{E}$ and by introducing hyperstress. In this case, however, issues would arise from the choice of traction boundary conditions in non-smooth domain [39].

Remark 5.8 (*Quasistatic inviscid model).* Some models in literature neglect inertia and viscosity by putting $\varrho=0$ and $\mathbb{D}=0$, see e.g. [5, 23]. The semi-implicit scheme can then be spit naturally to five fractional step, each of them for each variable $\mathbf{u}$, χ, d, c, and θ separately by replacing χ^k_τ in (5.1a) by χ^{k-1}_τ. Instead of (4.1i), it would suffice to require $\varphi_{\rm ME}(\cdot,\chi,d)$ and $\varphi_{\rm ME}(\boldsymbol{E},\cdot,d)+\frac12M|\cdot|^2$ convex. In this case, however, we would have to remove the dependence of ζ on $\boldsymbol{E}$ because we would lose the estimate (5.62), which relies on viscosity. Also e.g. thermal expansion leading usually to adiabatic terms containing $\dot{\boldsymbol{E}}$ would have to be excluded, although some particular studies resulting to spatially constant temperature does exist, cf. [30].

Remark 5.9 (*Viscous damage and higher regularity of displacements).* We already pointed out that in the case of rate-dependent evolution of damage (i.e. if the dissipation pseudopotential ξ would be quadratic), the variable d may be incorporated into the vectorial variable χ, which would still obey an evolution equation having the structure of (3.7b). This variant has recently been investigated in [41] in the case of thermal coupling. It is worth pointing out that its mathematical analysis would however require $L^2(Q)$ regularity of the term $\partial_d\varphi_{\rm ME}(\boldsymbol{E},\chi,d)$. Such regularity would in general not be compatible with the quadratic growth of $\varphi_{\rm ME}$ with respect to $\boldsymbol{E}$. In order to better elucidate this point, let us take $\varphi_{\rm ME} = \frac{1}{2}\mathbb{C}(d)\boldsymbol{E}{:}\boldsymbol{E}$. In order to guarantee the above-mentioned regularity, we would need $L^4(Q)$ regularity of $\boldsymbol{E}$, which in general cannot be expected without additional assumptions. Yet, higher regularity of displacements may be proved through a sophisticated technique based on testing the standard-force balance by $-{\rm div}(\boldsymbol{\varepsilon}(\dot{\mathbf{u}}))$, as in [6], and also in [41]. This estimate would however require the assumption that acceleration vanishes on the whole boundary, which in turn would restrict the applicability of the model to affine-in-time Dirichlet boundary conditions for $\mathbf{u}$.

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