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A model of gravitational differentiation of compressible self-gravitating planets

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A model of gravitational differentiation of compressible self-gravitating planets

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Abstract

We present a dynamic model for inhomogeneous viscoelastic media at finite strains. The model features a Kelvin–Voigt rheology, and includes a self-generated gravitational field in the actual evolving configuration. In particular, a fully Eulerian approach is adopted. We specialize the model to viscoelastic (barotropic) fluids and prove existence and a certain regularity of global weak solutions by a Faedo–Galerkin semi-discretization technique. Then, an extension to multi-component chemically reacting viscoelastic fluids based on a phenomenological approach by Eckart and Prigogine, is advanced and studied. The model is inspired by planetary geophysics. In particular, it describes gravitational differentiation of inhomogeneous planets and moons, possibly undergoing volumetric phase transitions.

1 Introduction

Self-gravitating inhomogeneous media provide a rich class of interesting problems in continuum mechanics, a prominent application being planetary geophysics. A detailed understanding of the processes of planetary formation and early evolution is currently available. In addition, the dynamics of the interiors of planets and their moons is relatively well understood, in particular in relation with the Solar planetary system and the planet Earth, cf. [BaW15, Con16, Ger19, GeY07, STO04].

After a relatively short time (tens or hundreds of millions of years) of accretion from a rather homogeneous stellar disc of dust, meteoroids, and asteroids, on a much longer period (billions of years) planets *differentiate*. Self-gravitation drives the dynamics inside the mantle, eventually leading to the formation of a *core-mantle* structure. This occurs as effect of the different densities of the mantle constituents, i.e., the heavier media (metals), which are strongly attracted towards the planet core, and the lighter ones (silicates and volatile elements forming liquid oceans or gaseous atmospheres), which are subjected to buoyancy. The onset of so-called Rayleigh-Taylor instability of interfaces between media with different densities can be observed. A similar evolution happens also in the development of big moons of planets.

Self-gravitation also governs the subsequent evolution of planets and moons interiors. In particular, gravity is responsible for the formation of plumes and slabs in the mantle, which are accompanied by various volumetric *phase transitions* and related buoyancy effects. Silicates in the Earth mantle undergo several quite sharp volumetric transitions. This happens at pressures of about 14 GPa (olivine transforms to wadsleyite) and 23 GPa (spinel transforms to perovskite and magnesiowüstite), which in Earth's mantle occur at a depth of 410 km and 660 km, respectively, cf., e.g., [Chr95, Con16, Ger19, HeW01, TS*94]. These volumetric transformations are related with the loss of strict convexity (or, accounting for hysteresis, non-convexity of the stored energy $\phi_{\rm ref}$ as a function of the determinant $J = \det \boldsymbol{F}$ of the deformation gradient (i.e., *loss of polyconvexity* in terms of $\boldsymbol{F}$ itself).

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The aim of this paper is to present and analyze a dynamic model able to capture the basic features of planets and moons differentiation under self-gravitation. In particular, we model an inhomogeneous viscoelastic medium at finite strains by assuming the so-called Kelvin-Voigt rheology and including the effects of the self-generated gravitational field. A crucial aspect of our approach is that it is formulated in the actual evolving configuration, making it fully Eulerian. Mainly for analytical reasons (but see Remarks 3.3 and 4.1 for a discussion), we restrict ourselves to the discussion of the isothermal case. Note nonetheless that thermal effects and temperature dependence of material parameters play a vital role in the evolution of planets' and moons' interiors. We refrain however to discuss thermal effects here, as these would require a much longer tractate. We specifically study the case of barotropic fluids, as well as the multicomponent case. Both in the single component and in the multicomponent case, we are able to prove the existence of weak solutions by means of a Galerkin approximation technique.

Before starting our discussion of the evolutionary model, let us mention some available contributions on the equilibrium of self-gravitating systems. By assuming spherical symmetry, a collection of results, together with an historical account, are provided in the monograph [MüW16]. Existence of equilibria of a hyperelastic solid under self-gravitation has been investigated in [CaL15]. Some alternative Eulerian analysis in case of spheres and multiple and stratified spherical shells is in [AlC19, AlC20]. Again in the spherical setting, the phenomenon of gravitational collapse and the possible existence of multiple equilibria are discussed in [JK*19], together with the ensuing bifurcation dynamics.

The case of nonlinear elastic models for polytropic fluids are considered in [Cal22] both in the Lagrangian and the Eulerian setting. In the case of the stationary Navier-Stokes under barotropic pressure with $p(\rho) \approx a\rho^\gamma$ for $\gamma > 4/3$, existence of equilibria has been established in [Sec94], and the stability of radially symmetric solutions and their free boundary have been studied in [StZ99]. In addition, a number of contributions explore the relativistic setting, again in the spherical case, see [AlC17, AnC14] among many others.

In the dynamic case, the reference setting is that of Navier-Stokes-Poisson systems. Note that these are parted into two distinct classes, depending on the repulsive versus attractive nature of the Poisson subsystem. These indeed correspond to the modeling of electrically charged versus self-gravitating fluids. The literature in the repulsive case is extensive, see, for instance [CD*21, Don03, DoM08, HeT20, LMZ10a, TaZ10, LMZ10b, Zhe12]. Concerning the attractive case, which is the case of our interest, we start by mentioning the local existence result in [StZ99], as well as the global existence result for weak solutions on bounded domains with pressure law $p(\rho) = a\rho^\gamma$, $\gamma > 3/2$, in [KoS08]. Existence in an external domain is tackled in [DuF04, DF*01, JiT09a] for $p(\rho) = a\rho^\gamma$, $\gamma > 3/2$, and in [DF*04] for $p(\cdot)$ non-monotone. Global existence in $\mathbb{R}^n$ for $4/3 < \gamma \leq 3/2$ and for radially symmetric initial data has been proved in [JiT10]. The stability and stabilization of spherical solutions in an external domain is treated in [DuZ05]. Eventually, a result on strong-weak uniqueness is in [Bas22], and the existence of an absorbing set for large times has been obtained in [JiT09b] for $\gamma > 5/3$ and later in [GJY12] for $\gamma > 3/2$. Local existence for self-gravitating inviscid liquid bodies with varying shape was shown in [StZ99] and, in the degenerate (inviscid) case of the Euler-Poisson system, in [GLL20].

The novelty of our paper relies on the treatment of general *inhomogeneous*, as well *multicomponent* materials. Note that the discussion of inhomogeneous or multicomponent materials is instrumental to the description of differentiation dynamics in planets' mantle. Our way of modeling the inhomogeneity of the material relies on the use of the *reference mapping* $\boldsymbol{\xi}(t,\cdot)$ mapping the Eulerian or spatial point $\boldsymbol{x} \in \boldsymbol{y}(t,\Omega)$ back into the reference domain configuration Ω. By studying the transport of $\boldsymbol{\xi}$ along with the velocity field $\boldsymbol{v}(t,\boldsymbol{x})$ we can trace the inhomogeneities that are imprinted into the material at the reference point $\boldsymbol{\xi}(t,\boldsymbol{x})$. Using a suitable hyperviscosity (cf., 3.4), we are able to derive the necessary regularity properties for $\boldsymbol{\xi}$ to treat quite general material laws, see (5.2). In particular, our analysis covers the case of a general non-monotone barotropic pressure with growth $\sim \rho^\gamma$ with $\gamma > 6/5$; cf., assumption (5.2b) with Remark 4.2 below.

The plan of the paper is as follows. Section 2 recalls basic notations and standard concepts from kinematic of finite-strain continuum mechanics. In Section 3, we introduce the model for self-gravitating inhomogeneous viscoelastic bodies, and its energetics is discussed. Section 4 then specifies the model to visco-elastic Navier-Stokes fluids with Kelvin-Voigt rheology in the volumetric part. In Section 5, we present a result on existence and regularity of weak solutions to an initial-boundary-value problem for the inhomogeneous self-gravitating system. In order to achieve this goal, we perform an approximation and Galerkin discretization of (most of) the equations. Eventually, in Section 6, we present and analyze a *multi-component* version of the previous model, employing the Eckart-Prigogine approach.

2 Kinematics at finite strains

Let us start by recalling some basic notion from the general theory of large (or finite) deformations in continuum mechanics, cf., e.g., [GFA10, Mar19].

The basic quantity describing the time-dependent evolution of a deformable body is the (referential) *deformation* or *motion* $\boldsymbol{y} : I\times\Omega \to \mathbb{R}^3$, where $I = [0, T]$ and $T > 0$ is some given final time. For all time instants $t \in I$, the deformation $\boldsymbol{y}(t, \cdot)$ maps the *reference configuration* $\Omega \subset \mathbb{R}^3$ of the deformable body to its *actual* configuration $\boldsymbol{y}(t, \Omega)$, a subset of the *physical space* $\mathbb{R}^3$. In what follows, we indicate *referential coordinates* by $\boldsymbol{X} \in \Omega$ and *actual coordinates* by $\boldsymbol{x} \in \mathbb{R}^3$. By assuming $\boldsymbol{y}(t, \cdot)$ to be globally invertible, we indicate its inverse by $\boldsymbol{\xi}(t, \cdot) = \boldsymbol{y}^{-1}(t, \cdot) : \boldsymbol{y}(t, \Omega) \to \Omega$. Such $\boldsymbol{\xi}$ is usually referred to as *return* or *reference mapping*, or sometimes *inverse motion*. Two basic kinematic quantities are the Lagrangian velocity $\boldsymbol{v}_{\rm R} = \frac{\partial}{\partial t}\boldsymbol{y}$ and the Lagrangian deformation gradient $\boldsymbol{F}_{\rm R} = \nabla_{\boldsymbol{X}}\boldsymbol{y}$. Starting from these, one defines the Eulerian velocity $\boldsymbol{v}(t, \boldsymbol{x}) = \boldsymbol{v}_{\rm R}(t, \boldsymbol{\xi}(t, \boldsymbol{x}))$ and the Eulerian deformation gradient $\boldsymbol{F}(t, \boldsymbol{x}) = \boldsymbol{F}_{\rm R}(t, \boldsymbol{\xi}(t, \boldsymbol{x}))$. Here and throughout the article, having the Eulerian velocity at disposal, we use the dot-notation $(\cdot)^{\boldsymbol{\cdot}} = \frac{\partial}{\partial t} + \boldsymbol{v}\cdot\nabla_{\boldsymbol{x}}$ to indicate the *convective time derivative* applied to scalars or, componentwise, to vectors or tensors. The velocity gradient $\nabla\boldsymbol{v}$ fulfills $\nabla\boldsymbol{v} = \nabla_{\boldsymbol{X}}\boldsymbol{v}\nabla_{\boldsymbol{x}}\boldsymbol{X} = \dot{\boldsymbol{F}}\boldsymbol{F}^{-1}$, where we used the chain-rule and the fact that $\boldsymbol{F}^{-1} = (\nabla_{\boldsymbol{X}}\boldsymbol{x})^{-1} = \nabla_{\boldsymbol{x}}\boldsymbol{X}$. This gives the *evolution-and-transport* equation for the deformation gradient

$$\dot{\boldsymbol{F}} = (\nabla\boldsymbol{v})\boldsymbol{F}\,. \tag{2.1}$$

From this, we also obtain the evolution-and-transport equation for Jacobian $\det\boldsymbol{F}$ and its reciprocal $1/\det\boldsymbol{F}$, namely,

$$\overline{\det\boldsymbol{F}}^{\boldsymbol{\cdot}} = (\det\boldsymbol{F}){\rm div}\,\boldsymbol{v} \quad \text{and} \quad \overline{\Big(\frac{1}{\det\boldsymbol{F}}\Big)}^{\boldsymbol{\cdot}} = -\frac{{\rm div}\,\boldsymbol{v}}{\det\boldsymbol{F}}\,. \tag{2.2}$$

The return mapping $\boldsymbol{\xi}$ satisfies the transport equation

$$\dot{\boldsymbol{\xi}} = \boldsymbol{0} \tag{2.3}$$

which simply expresses the fact that the material properties encoded in the material point $\boldsymbol{X} = \boldsymbol{\xi}(t, \boldsymbol{x})$ move along with the particles in the flow. Moreover, one has that $\boldsymbol{F} = (\nabla\boldsymbol{\xi})^{-1}$.

As $\boldsymbol{F}$ depends on $\boldsymbol{x}$, equalities (2.1)–(2.3) will be assumed to hold for almost all $\boldsymbol{x} \in \boldsymbol{y}(t, \Omega)$. Here, we take advantage of the boundary condition $\boldsymbol{v}\cdot\boldsymbol{n} = 0$ imposed below, with $\boldsymbol{n}$ being the outward unit normal to the boundary of the actual domain. This boundary condition implies that the actual domain $\mathit{\Omega} = \boldsymbol{y}(t, \Omega)$ does not evolve in time, i.e., $\mathit{\Omega} = \Omega$. The stress $\boldsymbol{T}$ and the pressure p defined in (3.5a) and (4.3a) are also functions of $\boldsymbol{x}$. In particular, all models under consideration in the following will be fully Eulerian.

3 Self-gravitating inhomogeneous viscoelastic media

We consider a simple model for a self-gravitating bounded body with a fixed shape. Planets and moons are typically composed by many components. By referring to the Earth, as well as to other planets and moons of the solar system, one should minimally consider three components, namely, metals, silicates, and a gaseous atmosphere. The latter is often adopted for the so-called *sticky-air approach* (cf. [Cra12]) to allow for a fixed and smooth domain $\mathit{\Omega}$. We are thus led to consider here a spatially inhomogeneous material with a given referential mass density $\rho_{\rm ref} = \rho_{\rm ref}(\boldsymbol{X}) > 0$ at some initial time $t = 0$ and stored energy $\varphi_{\rm ref}(\boldsymbol{X}, \cdot) : \mathbb{R}^{3\times3} \to \mathbb{R}$ acting on $\boldsymbol{F}$. We preliminarily assume that the body follows the *Kelvin-Voigt rheology*, which is the simplest viscoelastic solid-type rheology. In the following, two inhomogeneous viscosity coefficients ν_1 and ν_2 will be introduced.

We will use the shorthand notation $(\cdot)^{\boldsymbol{\xi}}$ in order to indicate the composition with $\boldsymbol{\xi}$ within a referential quantify when substituting $\boldsymbol{X}$ by $\boldsymbol{\xi}(t, \boldsymbol{x})$. In particular, $\boldsymbol{F} = \boldsymbol{F}_{\rm R}^{\boldsymbol{\xi}}$ and $\boldsymbol{v} = \boldsymbol{v}_{\rm R}^{\boldsymbol{\xi}}$. This notation is meant to emphasize the spatial inhomogeneity of the material.

The referential density $\varrho_{\rm R} = \varrho_{\rm R}(\boldsymbol{X})$ in the deformed configuration is $\varrho_{\rm R} = \rho_{\rm ref}/\det \boldsymbol{F}_{\rm R}$ while the actual Eulerian mass density $\varrho = \varrho(t, \boldsymbol{x})$ is $\varrho_{\rm R}^{\boldsymbol{\xi}} = \rho_{\rm ref}^{\boldsymbol{\xi}}/\det \boldsymbol{F}_{\rm R}^{\boldsymbol{\xi}}$, i.e.,

$$\varrho = \frac{\rho_{\rm ref}^{\boldsymbol{\xi}}}{\det \boldsymbol{F}} = \det(\nabla\boldsymbol{\xi})\rho_{\rm ref}^{\boldsymbol{\xi}} \,. \tag{3.1}$$

Likewise, the referential stored energy reads $\varphi_{\rm R} = \varphi_{\rm R}(\boldsymbol{X}, \boldsymbol{F}_{\rm R}) = \varphi_{\rm ref}(\boldsymbol{X}, \boldsymbol{F}_{\rm R})/\det \boldsymbol{F}_{\rm R}$ and the actual Eulerian stored energy is $\varphi = \varphi(t, \boldsymbol{x}, \boldsymbol{F}) = \varphi_{\rm ref}^{\boldsymbol{\xi}}(t, \boldsymbol{x}, \boldsymbol{F})/\det \boldsymbol{F}$. Note that now φ is dependent on time t. In what follows, we will often simply write $\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})$ instead of $\varphi_{\rm ref}^{\boldsymbol{\xi}}(t, \boldsymbol{x}, \boldsymbol{F})$.

Given equation (2.1), relation (3.1) is equivalent to the evolution-and-transport equation for the actual mass density

$$\dot{\varrho} = -\varrho \,{\rm div}\, \boldsymbol{v} \quad \text{with the initial condition} \quad \varrho|_{t=0} = \frac{\rho_{\rm ref}^{\boldsymbol{\xi}}|_{t=0}}{\det \boldsymbol{F}|_{t=0}} \,. \tag{3.2}$$

A distinct advantage of working in a fully Eulerian setting is the simplicity with which one can incorporate in the model interactions with actual fields. Relevant to our endeavor is in particular the gravitational acceleration field $\boldsymbol{g} = -\nabla V$ ensuing from the *gravitational potential* V. We introduce a simplification of the model by posing the system in a bounded and smooth albeit possibly large domain $U \subset \mathbb{R}^3$, which plays the role of *universe*. In addition, we assume that the gravitational potential V takes the constant value $V_{\rm B}$ outside U. The rationale of this choice is that, by possibly taking U large enough, the effect of assuming the universe U to be bounded on the dynamic of the planet is expected to be negligible. Note that our system will be completely independent of the constant $V_{\rm B}$. This is particularly relevant in connection with the choice of U. Note that well-known that the actual value of the gravitational potential on the Earth surface depends on whether one considers only a single planet, the whole Solar System, or the whole galaxy Milky Way, and is given roughly by 60 MJ/kg, 900 MJ/kg, or more than 130 GJ/kg, respectively. Fixing a specific value $V_{\rm B}$ in (3.6) will in fact be shown to be immaterial in our framework, see (3.10) below.

The gravitational potential V is governed by the Poisson equation

$$\Delta V = \begin{cases} G\varrho \ \text{ with } \ \varrho = \det(\nabla\boldsymbol{\xi})\rho_{\rm ref}^{\boldsymbol{\xi}} & \text{on } \varOmega\,, \\ G\varrho_{\rm ext} & \text{on } U\setminus\varOmega, \end{cases} \tag{3.3}$$

where G is the gravitational constant and $\varrho_{\rm ext} = \varrho_{\rm ext}(t,\boldsymbol{x})$ is a given external, possibly time-dependent mass density distributed around $\varOmega$, which may model tidal effects. In fact, we will introduce a further simplification by assuming that the mass $\varrho_{\rm ext}$ does not feel the presence of the mass ϱ. In what follows, we will consider both ϱ and $\varrho_{\rm ext}$ to be defined on the whole U by extending them to 0 outside $\varOmega$ and $U\setminus\varOmega$, respectively.

The geometric setting of the model is illustrated in Figure 1.

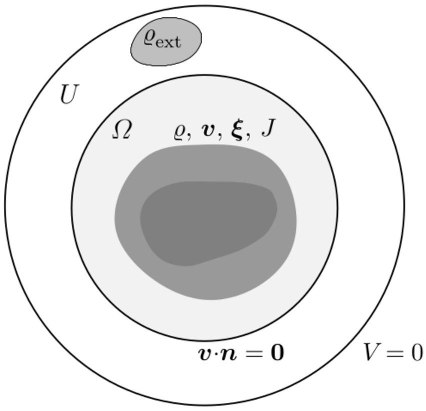

Fig. 1: The schematic geometry of the fixed bounded domain $\varOmega\subset U$ where the self-gravitating medium is evolving with velocity $\boldsymbol{v}$. The universe U, where the external mass density $\varrho_{\rm ext} = \varrho_{\rm ext}(t,\boldsymbol{x})$ outside $\varOmega$ is prescribed, is considered to be very large, so that the gravitational potential V can be assumed to be constant out of it. The boundary conditions on $\partial\varOmega$ and ∂U are depicted too, with $\boldsymbol{n}$ denoting the unit normal to the boundary $\partial\varOmega$.

The conservative and the dissipative parts of the Cauchy stress acting on the body are defined standardly (cf. Remark 3.2) as

$$\boldsymbol{T} = \frac{[\varphi_{\rm ref}^{\boldsymbol{\xi}}]'_{\boldsymbol{F}}(\boldsymbol{F})\boldsymbol{F}^\top}{\det\boldsymbol{F}} = [\varphi_{\rm ref}^{\boldsymbol{\xi}}]'_{\boldsymbol{F}}((\nabla\boldsymbol{\xi})^{-1}){\rm Cof}(\nabla\boldsymbol{\xi}) \quad \text{and} \tag{3.4a}$$

$$\boldsymbol{D} = \nu_1^{\boldsymbol{\xi}}\boldsymbol{e}(\boldsymbol{v}) - {\rm div}\big(\nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\big)\,. \tag{3.4b}$$

The Kelvin-Voigt rheology corresponds to considering the total stress as $\boldsymbol{T}+\boldsymbol{D}$. Note that $\boldsymbol{D}$ contains a standard Newtonian term $\nu_1^{\boldsymbol{\xi}}\boldsymbol{e}(\boldsymbol{v})$ and the hyperviscous stress $-{\rm div}\big(\nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\big)$, see Remark 3.2 for a discussion.

The full model system is formulated in the unknowns $(\boldsymbol{v}, \boldsymbol{\xi}, V)$ and results from the momentum equilibrium, (2.1), namely,

$$\varrho\dot{\boldsymbol{v}} = \mathrm{div}\big(\boldsymbol{T}{+}\boldsymbol{D}\big) - \varrho\nabla V \quad \text{on } \Omega \quad \text{with } \boldsymbol{T} \text{ and } \boldsymbol{D} \text{ from (3.4) and } \varrho \text{ from (3.1)}, \tag{3.5a}$$

$$\dot{\boldsymbol{\xi}} = \boldsymbol{0} \quad \text{on } \Omega\,, \tag{3.5b}$$

$$\Delta V = G\big(\varrho{+}\varrho_{\rm ext}\big) \quad \text{on } U\,. \tag{3.5c}$$

We complement this system by the boundary conditions

$$\boldsymbol{v}{\cdot}\boldsymbol{n} = 0\,, \quad \big((\boldsymbol{T}{+}\boldsymbol{D})\boldsymbol{n} - \mathrm{div}_{\rm s}(\nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\boldsymbol{n})\big)_{\rm T} = \boldsymbol{0}\,, \quad \nabla\boldsymbol{e}(\boldsymbol{v}){:}(\boldsymbol{n}{\otimes}\boldsymbol{n}) = \boldsymbol{0} \ \text{ on } \partial\Omega, \tag{3.6a}$$

$$V = V_{\rm B} \ \text{ on } \partial U\,. \tag{3.6b}$$

Here, $(\cdot)_{\rm T}$ indicates the tangential component of a vector at $\partial\Omega$ and $V_{\rm B}$ is the above mentioned arbitrary constant for the value of the gravitational field outside U. The $(d{-}1)$-dimensional surface divergence is defined as

$$\mathrm{div}_{\rm s} = \mathrm{tr}(\nabla_{\rm s}) \quad \text{with} \quad \nabla_{\rm s}\bullet = \nabla\bullet - \frac{\partial\bullet}{\partial\boldsymbol{n}}\boldsymbol{n}\,, \tag{3.7}$$

where $\mathrm{tr}(\cdot)$ is the trace of a $(d{-}1){\times}(d{-}1)$-matrix and $\nabla_{\rm s}$ denotes the surface gradient. Let us again remark the crucial role of the impenetrability boundary condition $\boldsymbol{v}{\cdot}\boldsymbol{n} = 0$, indeed allowing system (3.5a,b) to be formulated in the fixed domain Ω.

The energetics of system (3.5) can be revealed by testing (3.5a) by $\boldsymbol{v}$ and (3.5c) by $\frac{\partial}{\partial t}V$. The former test quite standardly employs the Green formula over Ω (for the ν_2 term one uses the formula twice, combined with a surface Green formula on $\partial\Omega$) in view of the first and the second boundary conditions in (3.6a). In fact, following [Rou22a, Sec. 3] we start from position (3.4a) and compute

$$\begin{aligned}\boldsymbol{T} &= \frac{\big[\varphi_{\rm ref}^{\boldsymbol{\xi}}\big]'_{\boldsymbol{F}}(\boldsymbol{F})\boldsymbol{F}^\top}{\det\boldsymbol{F}} = \frac{\big[\varphi_{\rm ref}^{\boldsymbol{\xi}}\big]'_{\boldsymbol{F}}(\boldsymbol{F}) - \varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})\boldsymbol{F}^{-\top}}{\det\boldsymbol{F}}\boldsymbol{F}^\top + \frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\boldsymbol{I}\\ &= \bigg(\frac{\big[\varphi_{\rm ref}^{\boldsymbol{\xi}}\big]'_{\boldsymbol{F}}(\boldsymbol{F})}{\det\boldsymbol{F}} - \frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})\mathrm{Cof}\boldsymbol{F}}{(\det\boldsymbol{F})^2}\bigg)\boldsymbol{F}^\top + \frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\boldsymbol{I} = \bigg[\frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg]'_{\boldsymbol{F}}\boldsymbol{F}^\top + \frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\boldsymbol{I}.\end{aligned} \tag{3.8}$$

where $\boldsymbol{I}$ denotes the identity matrix. Moreover, we have that

$$\frac{\partial}{\partial t}\bigg(\frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg) = \frac{\big[[\varphi_{\rm ref}]'_{\boldsymbol{X}}\big]^{\boldsymbol{\xi}}}{\det\boldsymbol{F}}\cdot\frac{\partial\boldsymbol{\xi}}{\partial t} + \bigg[\frac{\varphi_{\rm ref}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg]'_{\boldsymbol{F}}{:}\frac{\partial\boldsymbol{F}}{\partial t} \quad \text{and} \tag{3.9a}$$

$$\nabla\bigg(\frac{\varphi_{\rm ref}^{\boldsymbol{\xi}}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg) = \frac{\big[[\varphi_{\rm ref}]'_{\boldsymbol{X}}\big]^{\boldsymbol{\xi}}}{\det\boldsymbol{F}}\cdot(\boldsymbol{v}{\cdot}\nabla)\boldsymbol{\xi} + \bigg[\frac{\varphi_{\rm ref}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg]'_{\boldsymbol{F}}{:}(\boldsymbol{v}{\cdot}\nabla)\boldsymbol{F}. \tag{3.9b}$$

By testing the force $-\mathrm{div}(\boldsymbol{T}+\boldsymbol{D})$ by the velocity $\boldsymbol{v}$ and using the boundary conditions (3.6a) we hence get

$$\begin{aligned}-\int_\Omega \mathrm{div}(\boldsymbol{T}{+}\boldsymbol{D}){\cdot}\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} &\overset{(3.6a)}{=} \int_\Omega(\boldsymbol{T}{+}\boldsymbol{D}){:}\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\\ &\underset{(3.8)}{=} \int_\Omega\bigg[\frac{\varphi_{\rm ref}(\boldsymbol{F})}{\det\boldsymbol{F}}\bigg]'_{\boldsymbol{F}}\boldsymbol{F}^\top{:}\nabla\boldsymbol{v} + \frac{\varphi_{\rm ref}(\boldsymbol{F})\boldsymbol{I}}{\det\boldsymbol{F}}{:}\nabla\boldsymbol{v} + \boldsymbol{D}{:}\nabla\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\end{aligned}$$

$$
\begin{aligned}
&= \int_\Omega \Big[\frac{\varphi_{\rm ref}(\boldsymbol F)}{\det \boldsymbol F}\Big]'_{\boldsymbol F}{:}\nabla\boldsymbol v\boldsymbol F + \frac{\varphi_{\rm ref}(\boldsymbol F)}{\det \boldsymbol F}{\rm div}\,\boldsymbol v + \boldsymbol D{:}\nabla\boldsymbol v\,{\rm d}\boldsymbol x\\
&\overset{(2.1)}{=} \int_\Omega \Big[\frac{\varphi_{\rm ref}(\boldsymbol F)}{\det \boldsymbol F}\Big]'_{\boldsymbol F}{:}\dot{\boldsymbol F} + \frac{\varphi_{\rm ref}(\boldsymbol F)}{\det \boldsymbol F}{\rm div}\,\boldsymbol v + \boldsymbol D{:}\nabla\boldsymbol v\,{\rm d}\boldsymbol x\\
&\overset{(3.9)}{=} \int_\Omega \frac{\partial}{\partial t}\Big(\frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\Big) + \nabla\Big(\frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\Big){\cdot}\boldsymbol v + \frac{\varphi_{\rm ref}(\boldsymbol F)}{\det \boldsymbol F}{\rm div}\,\boldsymbol v\,{\rm d}\boldsymbol x\\
&\qquad\qquad - \int_\Omega \frac{\big[[\varphi_{\rm ref}]'_{\boldsymbol X}\big]^{\boldsymbol\xi}}{\det \boldsymbol F}{:}\Big(\frac{\partial\boldsymbol\xi}{\partial t} + \boldsymbol v{\cdot}\nabla\boldsymbol\xi\Big) + \boldsymbol D{:}\nabla\boldsymbol v\,{\rm d}\boldsymbol x\\
&\overset{(2.3)}{=} \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\,{\rm d}\boldsymbol x + \int_\Omega {\rm div}\Big(\frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\boldsymbol v\Big)\,{\rm d}\boldsymbol x + \int_\Omega \boldsymbol D{:}\nabla\boldsymbol v\,{\rm d}\boldsymbol x\\
&\overset{(2.3)}{=} \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\,{\rm d}\boldsymbol x + \int_{\partial\Omega} \frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\,(\boldsymbol v{\cdot}\boldsymbol n)\,{\rm d}S + \int_\Omega \boldsymbol D{:}\nabla\boldsymbol v\,{\rm d}\boldsymbol x\\
&= \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\varphi_{\rm ref}^{\boldsymbol\xi}(\boldsymbol F)}{\det \boldsymbol F}\,{\rm d}\boldsymbol x + \int_\Omega \nu_1^{\boldsymbol\xi}|\boldsymbol e(\boldsymbol v)|^2 + \nu_2^{\boldsymbol\xi}|\nabla\boldsymbol e(\boldsymbol v)|^q{\rm d}\boldsymbol x.
\end{aligned}
$$

By testing the inertial force $\varrho\dot{\boldsymbol v}$ by $\boldsymbol v$, it is paramount to use (3.5b) together with (3.1) and $\boldsymbol F = (\nabla\boldsymbol\xi)^{-1}$, inducing the continuity equation (3.2). In particular, one has

$$
\frac{\partial}{\partial t}\Big(\frac{\varrho|\boldsymbol v|^2}{2}\Big) = \varrho\boldsymbol v{\cdot}\frac{\partial}{\partial t}\boldsymbol v - \frac12{\rm div}(\varrho\boldsymbol v)|\boldsymbol v|^2.
$$

Hence, by using again the Green formula and $\boldsymbol v{\cdot}\boldsymbol n = 0$, we obtain

$$
\frac{\rm d}{{\rm d}t}\int_\Omega \frac{\varrho|\boldsymbol v|^2}{2}\,{\rm d}\boldsymbol x = \int_\Omega \varrho\dot{\boldsymbol v}{\cdot}\boldsymbol v\,{\rm d}\boldsymbol x.
$$

On the other hand, testing (3.5c) on $\partial V/\partial t$ we obtain

$$
\begin{aligned}
\frac{\rm d}{{\rm d}t}\int_U \frac{|\nabla V|^2}{2G}\,{\rm d}\boldsymbol x &= \frac{\rm d}{{\rm d}t}\int_U \frac{|\nabla(V{-}V_{\rm B})|^2}{2G}\,{\rm d}\boldsymbol x \overset{(3.6b)}{=} -\int_U \frac{\Delta(V{-}V_{\rm B})}{G}\frac{\partial(V{-}V_{\rm B})}{\partial t}\,{\rm d}\boldsymbol x\\
&\overset{(3.5c)}{=} -\int_U(\varrho{+}\varrho_{\rm ext})\frac{\partial(V{-}V_{\rm B})}{\partial t}\,{\rm d}\boldsymbol x = \int_U\Big(\frac{\partial\varrho}{\partial t}{+}\frac{\partial\varrho_{\rm ext}}{\partial t}\Big)(V{-}V_{\rm B})\,{\rm d}\boldsymbol x - \frac{\rm d}{{\rm d}t}\int_U(\varrho{+}\varrho_{\rm ext})(V{-}V_{\rm B})\,{\rm d}\boldsymbol x\\
&\overset{(3.2)}{=} -\int_\Omega {\rm div}(\varrho\boldsymbol v)\,(V{-}V_{\rm B})\,{\rm d}\boldsymbol x + \int_{U\setminus\Omega}\frac{\partial\varrho_{\rm ext}}{\partial t}(V{-}V_{\rm B})\,{\rm d}\boldsymbol x - \frac{\rm d}{{\rm d}t}\int_U(\varrho{+}\varrho_{\rm ext})(V{-}V_{\rm B})\,{\rm d}\boldsymbol x\\
&= \int_\Omega \varrho\boldsymbol v{\cdot}\nabla(V{-}V_{\rm B})\,{\rm d}\boldsymbol x + \int_{U\setminus\Omega}\frac{\partial\varrho_{\rm ext}}{\partial t}(V{-}V_{\rm B})\,{\rm d}\boldsymbol x - \frac{\rm d}{{\rm d}t}\int_U(\varrho{+}\varrho_{\rm ext})(V{-}V_{\rm B})\,{\rm d}\boldsymbol x\\
&= \int_\Omega \varrho\boldsymbol v{\cdot}\nabla V\,{\rm d}\boldsymbol x + \int_{U\setminus\Omega}\frac{\partial\varrho_{\rm ext}}{\partial t}V\,{\rm d}\boldsymbol x - \frac{\rm d}{{\rm d}t}\int_\Omega \varrho V\,{\rm d}\boldsymbol x - \frac{\rm d}{{\rm d}t}\int_{U\setminus\Omega}\varrho_{\rm ext}V\,{\rm d}\boldsymbol x
\end{aligned}
\tag{3.10}
$$

with ϱ from (3.1), where we also used the fact that $\int_\Omega \varrho\,{\rm d}\boldsymbol x$ is constant. Note that the Green formula on U used in (3.10) hinges on the boundary condition $V = V_{\rm B}$ on ∂U while the Green formula on Ω used again the boundary condition $\boldsymbol v{\cdot}\boldsymbol n = 0$. The equality in (3.10) is nonetheless independent of the value $V_{\rm B}$. By noticing that the term $\varrho\boldsymbol{v}\cdot\nabla V = \varrho\nabla V\cdot\boldsymbol{v}$ arises also when testing (3.5a) by $\boldsymbol{v}$ where it is to be substituted from (3.10), we obtain the mechanical energy-dissipation balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\bigg(\int_\Omega \underbrace{\frac{\varrho}{2}|\boldsymbol{v}|^2}_{\substack{\text{kinetic}\\\text{energy}}} + \underbrace{\frac{\varphi^{\boldsymbol{\xi}}_{\text{ref}}(\boldsymbol{F})}{\det \boldsymbol{F}}}_{\substack{\text{stored}\\\text{energy}}} + \underbrace{\varrho V}_{\substack{\text{energy of } \varrho \text{ in}\\\text{gravitational}\\\text{field } V}}\,\mathrm{d}\boldsymbol{x} + \int_U \underbrace{\frac{|\nabla V|^2}{2G}}_{\substack{\text{energy of}\\\text{gravitational}\\\text{field}}}\mathrm{d}\boldsymbol{x} + \int_{U\setminus\Omega} \underbrace{\varrho_{\text{ext}}V\mathrm{d}\boldsymbol{x}}_{\substack{\text{energy of } \varrho_{\text{ext}}\\\text{in gravitational}\\\text{field } V}}\bigg)$$
$$+\int_\Omega \underbrace{\nu_1^{\boldsymbol{\xi}}|\boldsymbol{e}(\boldsymbol{v})|^2 + \nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^q}_{\substack{=:\,\xi \text{ dissipation rate due}\\\text{to viscosity}}}\,\mathrm{d}\boldsymbol{x} = \int_{U\setminus\Omega} \underbrace{\frac{\partial\varrho_{\text{ext}}}{\partial t}V}_{\substack{\text{power of}\\\text{external mass in}\\\text{gravitational field}}}\mathrm{d}\boldsymbol{x}\,. \tag{3.11}$$

Remark 3.1 (*Variational structure of* (3.5)**).** To elucidate the variational structure of the system (3.5) requires some care, because the potential equation (3.3) for V provides a concave contribution to the free energy

$$(\boldsymbol{y},V)\mapsto \int_\Omega \varphi_{\text{ref}}(\boldsymbol{X},\nabla\boldsymbol{y}) + \varrho_{\text{ref}}\big(\boldsymbol{X},V\circ\boldsymbol{y}\big)\,\mathrm{d}\boldsymbol{X} + \int_{U\setminus\Omega}\varrho_{\text{ext}}(\boldsymbol{x})V(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x} - \int_U \frac{|\nabla V(\boldsymbol{x})|^2}{2G}\,\mathrm{d}\boldsymbol{x}\,.$$

Note that the latter features a mixture of referential and actual terms. By taking the variation of the free energy with respect to the gravitational potential V and using $V\circ\boldsymbol{y}(\boldsymbol{X}) = V(\boldsymbol{x})$ we obtain (3.3). On the other hand, the variation with respect to $\boldsymbol{y}$ produces the first Piola-Kirchhoff stress tensor and the gravitational force $\varrho_{\text{R}}(\nabla V\circ\boldsymbol{y})$, which correspond to $\boldsymbol{T}$ and $\varrho_{\text{R}}\nabla V = \varrho\nabla V$ when written in the Eulerian setting of (3.5a).

Remark 3.2 (*Gradient theories in rates)***.** Higher-order theories in solid mechanics are well established and used for various reasons. By introducing a further length scale into the problem, additional hyperstresses occur, which in turn usually contribute crucial compactness for the mathematical analysis. Such high-order models are generally referred to as *nonsimple materials*. Both the conservative and the dissipative stress can feature higher gradients. In (3.5) we consider an hyperstress on the dissipative part, an option which is particularly well tailored to rate formulations, having the advantage to provide additional regularity for the velocity field $\boldsymbol{v}$. Our approach follows the theory by E. Fried and M. Gurtin [FrG06], as already considered in the general nonlinear context of *multipolar fluids* by J. Nečas at al. [Neč94, NNŠ91, NeR92, NeŠ91] and as originally inspired by R. A. Toupin [Tou62] and R. D. Mindlin [Min64].

Remark 3.3 (*Anisothermal extension)***.** Heat exchange and transfer plays an important role with respect to the differentiation phenomenon in self-gravitating planets and moons. Although presently neglected in our model, thermal effects could also be considered. On the one hand, one may let material parameters be dependent on temperature, here denoted by θ. On the other hand, by assuming the (referential) free energy $\psi_{\text{ref}} = \psi_{\text{ref}}(\boldsymbol{X},\boldsymbol{F},\theta)$ to be additively decomposed as $\psi_{\text{ref}}(\boldsymbol{X},\boldsymbol{F},\theta) = \varphi_{\text{ref}}(\boldsymbol{X},\boldsymbol{F}) + \gamma_{\text{ref}}(\boldsymbol{X},\boldsymbol{F},\theta)$ with $\gamma_{\text{ref}}(\boldsymbol{X},\boldsymbol{F},0) = 0$, the heat equation reads

$$\frac{\partial w}{\partial t} + \mathrm{div}\big(\boldsymbol{v}w{+}\boldsymbol{j}\big) = \xi + \frac{[\gamma^\xi_{\text{ref}}]'_{\boldsymbol{F}}(\boldsymbol{F},\theta)}{\det\boldsymbol{F}}{:}\dot{\boldsymbol{F}} \quad \text{with} \quad w = \frac{\gamma^\xi_{\text{ref}}(\boldsymbol{F},\theta){-}\theta[\gamma^\xi_{\text{ref}}]'_\theta(\boldsymbol{F},\theta)}{\det\boldsymbol{F}}\,, \tag{3.12}$$

where the heat production rate ξ is specified in (3.11) and the heat flux $\boldsymbol{j}$ is governed by the Fourier law $\boldsymbol{j} = -k^{\boldsymbol{\xi}}\nabla\theta$ with a heat-conduction coefficient $k = k(\boldsymbol{X},\det\boldsymbol{F},\theta)$. Then, the viscosity coefficients ν_1 and ν_2 can be assumed to depend on temperature, as well. The physical meaning of the quantity w is of that of the thermal part of the (actual) internal energy. By complementing relation (3.12) to the system (3.5), the ensuing anisothermal coupled model then reproduces the expected energetics. In addition, it complies with the Clausius-Duhem entropy inequality, cf. [Rou22b] and it is hence thermodynamically consistent.

4 Kelvin-Voigt/Navier-Stokes viscoelastic fluid

Differentiation by self-gravitation in planets and moons occurs on very long time scales. Within such a time scale, solid-type rheologies (as the Kelvin-Voigt one from Section 3) have limited relevance and one should resort to fluid rheologies in the deviatoric components instead. Different options are available. Classical choices in geophysics are the Andrade and the Jeffreys rheologies, both allowing for the propagation of elastic shear waves. Such waves are however of relatively low importance on the time scale of planetary evolution. As such, we resort here to a simpler variant, which goes under the name of Newton or Stokes or, in the current convective setting, of Navier-Stokes rheology and does not allow for propagation of shear waves. The Navier-Stokes rheology can be obtained in the frame of the above introduced Kelvin-Voigt model by assuming that the elastic shear response vanishes, i.e., that $\varphi_{\rm ref}$ depends only on the volumetric part $(\det \boldsymbol{F})^{1/3}\boldsymbol{I}$ of $\boldsymbol{F}$. Thus, we let

$$\varphi_{\rm ref}(\boldsymbol{X},\boldsymbol{F}) = \phi_{\rm ref}(\boldsymbol{X},J) \quad \text{with} \quad J=\det\boldsymbol{F} \tag{4.1}$$

for some $\phi_{\rm ref}: \varOmega\times(0,\infty)\to\mathbb{R}$, cf., e.g., [MaH83, p. 10] or also [Rou22a]. By recalling that $\det'(\cdot)={\rm Cof}(\cdot)$ and $F^{-1}={\rm Cof}F^\top/\det F$, the conservative part of the Cauchy stress reduces to

$$\begin{aligned}\boldsymbol{T} &= \frac{[\varphi_{\rm ref}]'_{\boldsymbol{F}}(\boldsymbol{X},\boldsymbol{F})\boldsymbol{F}^\top}{\det\boldsymbol{F}} = [\phi_{\rm ref}]'_J(\boldsymbol{X},\det\boldsymbol{F})\frac{\det'(\boldsymbol{F})\boldsymbol{F}^\top}{\det\boldsymbol{F}}\\ &= [\phi_{\rm ref}]'_J(\boldsymbol{X},\det\boldsymbol{F})\frac{({\rm Cof}\,\boldsymbol{F})\boldsymbol{F}^\top}{\det\boldsymbol{F}} = [\phi_{\rm ref}]'_J(\boldsymbol{X},J)\boldsymbol{I}\,,\end{aligned} \tag{4.2}$$

(compare with (3.8)), where $[\phi_{\rm ref}]'_J$ has a physical interpretation of a (negative) pressure.

Under the fluidic ansatz (4.1), by taking (4.2) and (3.1) into account, system (3.5) reads

$$\varrho\dot{\boldsymbol{v}} = {\rm div}\big(\nu_1^{\boldsymbol{\xi}}\boldsymbol{e}(\boldsymbol{v}) - {\rm div}\big(\nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\big)\big) - \nabla p - \varrho\nabla V$$
$$\text{with}\ \ p=-[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J\Big(\frac{1}{\det(\nabla\boldsymbol{\xi})}\Big) \ \ \text{and}\ \ \varrho=\det(\nabla\boldsymbol{\xi})\rho_{\rm ref}^{\boldsymbol{\xi}}\,, \tag{4.3a}$$

$$\dot{\boldsymbol{\xi}} = \boldsymbol{0}, \qquad \text{on } \varOmega\,, \tag{4.3b}$$

$$\Delta V = G\big(\varrho{+}\varrho_{\rm ext}\big) \quad \text{on } U\,. \tag{4.3c}$$

System (4.3) is usually referred to as the compressible Navier-Stokes-Poisson system. We complement it with the boundary conditions (3.6).

The energetics for system (4.3) follows along the same lines of that of system (3.5). Let us explicitly show how to handle the conservative part of the stress, i.e., the term ${\rm div}\,\boldsymbol{T}{\cdot}\boldsymbol{v}$, which now reads as $\nabla p{\cdot}\boldsymbol{v}$ with $p=-[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J(J)$. The analogous of computations (3.9) in the fluidic setting (4.1) are

$$\frac{\partial}{\partial t}\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J)}{J}\Big) = \frac{\big[[\phi_{\rm ref}]'_{\boldsymbol{X}}\big]^{\boldsymbol{\xi}}(J)}{J}{\cdot}\frac{\partial\boldsymbol{\xi}}{\partial t} + \Big[\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J)}{J}\Big]'_J\frac{\partial J}{\partial t} \tag{4.4a}$$

$$\nabla\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J)}{J}\Big){\cdot}\boldsymbol{v} = \frac{\big[[\phi_{\rm ref}]'_{\boldsymbol{X}}\big]^{\boldsymbol{\xi}}(J)}{J}{\cdot}(\boldsymbol{v}{\cdot}\nabla)\boldsymbol{\xi} + \Big[\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J)}{J}\Big]'_J\boldsymbol{v}{\cdot}\nabla J\,. \tag{4.4b}$$

Making use of (2.2) we find

$$\int_\varOmega \nabla p{\cdot}\boldsymbol{v}\,{\rm d}\boldsymbol{x} = -\int_\varOmega \nabla[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J(J){\cdot}\boldsymbol{v}\,{\rm d}\boldsymbol{x} = \int_\varOmega [\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J(J){\rm div}\,\boldsymbol{v}\,{\rm d}\boldsymbol{x} - \int_{\partial\varOmega}[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J(J)\underbrace{\boldsymbol{v}{\cdot}\boldsymbol{n}}_{=\,0}\,{\rm d}S$$

$$
\begin{aligned}
&\overset{(2.2)}{=} \int_\Omega \frac{[\phi_{\rm ref}^{\boldsymbol\xi}]'_J(J)}{J}\dot J\,{\rm d}\boldsymbol x = \int_\Omega \bigg(\Big[\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\Big]'_J + \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J^2}\bigg)\dot J\,{\rm d}\boldsymbol x\\
&\overset{(2.2)}{=} \int_\Omega \Big[\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\Big]'_J\frac{\partial J}{\partial t} + \Big[\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\Big]'_J\boldsymbol v{\cdot}\nabla J + \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}{\rm div}\,\boldsymbol v\,{\rm d}\boldsymbol x\\
&\overset{(4.4)}{=} \int_\Omega \frac{\partial}{\partial t}\Big(\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\Big) + \nabla\Big(\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\Big){\cdot}\boldsymbol v - \frac{\big[[\phi_{\rm ref}]'_{\boldsymbol X}\big]^{\boldsymbol\xi}(J)}{J}{\cdot}\underbrace{\Big(\frac{\partial\boldsymbol\xi}{\partial t}{+}(\boldsymbol v{\cdot}\nabla)\boldsymbol\xi\Big)}_{=\,0\text{ due to (4.3b)}} + \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}{\rm div}\,\boldsymbol v\,{\rm d}\boldsymbol x\\
&= \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\,{\rm d}\boldsymbol x + \int_\Omega {\rm div}\Big(\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\boldsymbol v\Big)\,{\rm d}\boldsymbol x\\
&= \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\,{\rm d}\boldsymbol x + \int_{\partial\Omega} \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\underbrace{\boldsymbol v{\cdot}\boldsymbol n}_{=\,0}\,{\rm d}S = \frac{\rm d}{{\rm d}t}\int_\Omega \frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}\,{\rm d}\boldsymbol x\,. \qquad (4.5)
\end{aligned}
$$

Note that these computations require sufficient smoothness of $\phi_{\rm ref}$ with respect to $\boldsymbol X$, so that $[\phi_{\rm ref}]'_{\boldsymbol X}$ is integrable. On the other hand, from the application point of view, it is desirable to consider sharp interfaces between different materials, which leads to jumps in $\phi_{\rm ref}(\cdot,J):\Omega\to\mathbb R$. Such material laws could also be rigorously accounted for, at the expense of more refined arguments, cf. [Rou22a] and Remark 5.5.

Altogether, under assumptions (4.1) the energy balance now reads

$$
\begin{aligned}
&\frac{\rm d}{{\rm d}t}\bigg(\int_\Omega \underbrace{\frac{\rho_{\rm ref}^{\boldsymbol\xi}}{2J}|\boldsymbol v|^2}_{\substack{\text{kinetic}\\ \text{energy}}} + \underbrace{\frac{\phi_{\rm ref}^{\boldsymbol\xi}(J)}{J}}_{\substack{\text{actual}\\ \text{stored}\\ \text{energy}}} + \underbrace{\frac{\rho_{\rm ref}^{\boldsymbol\xi}}{J}V}_{\substack{\text{energy of }\varrho\text{ in}\\ \text{gravitational}\\ \text{field }V}}\,{\rm d}\boldsymbol x + \int_U \underbrace{\frac{|\nabla V|^2}{2G}}_{\substack{\text{energy of}\\ \text{gravitational}\\ \text{field}}}\,{\rm d}\boldsymbol x + \int_{U\setminus\Omega}\underbrace{\varrho_{\rm ext}V}_{\substack{\text{energy of }\varrho_{\rm ext}\\ \text{in gravitational}\\ \text{field }V}}\,{\rm d}\boldsymbol x\bigg)\\
&\qquad + \int_\Omega \underbrace{\nu_1^{\boldsymbol\xi}|\boldsymbol e(\boldsymbol v)|^2 + \nu_2^{\boldsymbol\xi}|\nabla\boldsymbol e(\boldsymbol v)|^q}_{\substack{=:\,\eta\text{ dissipation rate}\\ \text{due to viscosity}}}\,{\rm d}\boldsymbol x = \int_{U\setminus\Omega}\underbrace{\frac{\partial\varrho_{\rm ext}}{\partial t}V}_{\substack{\text{power of}\\ \text{external forces}}}\,{\rm d}\boldsymbol x\,. \qquad (4.6)
\end{aligned}
$$

Remark 4.1 (*Anisothermal extension)***.** In the spirit of Remark 3.3, also in case of assumption (4.1) the model can be extended to the anisothermal case by letting the material parameters depend on the temperature θ, e.g., the (referential) free energy can be taken as $\psi_{\rm ref}=\psi_{\rm ref}(\boldsymbol X,J,\theta)$. Considering the split $\psi_{\rm ref}(\boldsymbol X,J,\theta)=\phi_{\rm ref}(\boldsymbol X,J)+\gamma_{\rm ref}(\boldsymbol X,J,\theta)$ with $\gamma_{\rm ref}(\boldsymbol X,J,0)=0$, the (actual) pressure p in (3.5a) reads $p=-[\phi_{\rm ref}^{\boldsymbol\xi}]'_J(\boldsymbol x,J)$ $-[\gamma_{\rm ref}^{\boldsymbol\xi}]'_J(\boldsymbol x,J,\theta)$. Hence, the ensuing heat equation is

$$
\frac{\partial w}{\partial t} + {\rm div}\big(\boldsymbol v w{+}\boldsymbol j\big) = \eta + [\gamma_{\rm ref}^{\boldsymbol\xi}]'_J(J,\theta){\rm div}\,\boldsymbol v \quad\text{with}\quad w = \frac{\gamma_{\rm ref}^{\boldsymbol\xi}(J,\theta){-}\theta[\gamma_{\rm ref}^{\boldsymbol\xi}]'_\theta(J,\theta)}{J}\,, \qquad (4.7)
$$

where the heat production rate η is defined in (4.6). This anisothermal version of the model again reproduces the expected energetics and complies with the Clausius-Duhem inequality. In particular, it can be checked to be thermodynamically consistent.

Remark 4.2 (*State equation)***.** In fluid thermomechanics, the state equation relates density, pressure, and temperature. Here, in view of Remark 4.1 and the fact that $\varrho=\rho_{\rm ref}/J$, this relation at a current material point reads as $p=-\phi'_{\rm ref}(\rho_{\rm ref}/\varrho)-[\gamma_{\rm ref}]'_J(\rho_{\rm ref}/\varrho,\theta)$. In the isothermal situation, where $\gamma_{\rm ref}\equiv0$, the relation $p=-\phi'_{\rm ref}(\rho_{\rm ref}/\varrho)$ represents a so-called *isentropic state equation* while the fluid is said to be *barotropic*, i.e., its density depends only on pressure.

5 Analysis of the viscoelastic fluid problem

We present here an existence result for weak solutions to system (4.3). Moreover, we prove that such weak solutions fulfill the energy balance (4.6). Note that in order to obtain (4.6), as well as the corresponding a-priori estimates, one needs a Poincaré inequality to control the terms $\int_\Omega \varrho V\,\mathrm{d}\boldsymbol{x}$, $\int_U \varrho_{\rm ext} V\,\mathrm{d}\boldsymbol{x}$, and $\int_U \frac{\partial}{\partial t}\varrho_{\rm ext} V\,\mathrm{d}\boldsymbol{x}$, which have no sign, through $\int_{\mathbb{R}^3}|\nabla V|^2\,\mathrm{d}\boldsymbol{x}$. This once again asks U to be budded.

We are interested in an initial-value problem for system (4.3). The initial conditions are prescribed as

$$\boldsymbol{v}|_{t=0}=\boldsymbol{v}_0 \quad\text{and}\quad \boldsymbol{\xi}|_{t=0}=\boldsymbol{\xi}_0\,. \tag{5.1}$$

We will use the standard notation for Lebesgue and Sobolev spaces, namely $L^p(\Omega;\mathbb{R}^n)$ for Lebesgue measurable functions $\Omega\to\mathbb{R}^n$ whose Euclidean norm has integrable p-power, $W^{k,p}(\Omega;\mathbb{R}^m)$ for functions from $L^p(\Omega;\mathbb{R}^m)$ whose distributional derivatives up to the order k have their Euclidean norm integrable with p-power, and $W^{k,p}_0(\Omega;\mathbb{R}^m)$ for the subspace of $W^{k,p}(\Omega;\mathbb{R}^m)$ of functions with zero trace on $\partial\Omega$. We also use $H^k=W^{k,2}$ and $H^k_0=W^{k,2}_0$. The notation p^* will denote the optimal exponent for the embedding $W^{1,p}(\Omega)\subset L^{p^*}(\Omega)$, i.e., $p^*=dp/(d-p)$ for $p<d$ while $p^*\ge 1$ arbitrary for $p=d$ or $p^*=+\infty$ for $p>d$. Moreover, for a Banach space X and for $I=[0,T]$, we will use the notation $L^p(I;X)$ for the Bochner space of Bochner measurable functions $I\to X$ whose norm is in $L^p(I)$ while $W^{1,p}(I;X)$ indicates the functions $I\to X$ whose distributional derivative is in $L^p(I;X)$. Moreover, $C(\cdot)$ and $C^k(\cdot)$ will denote spaces of continuous and k-times continuously differentiable functions, respectively. Eventually, $C_{\rm w}(I;X)$ and ${\rm BV}(I;X)$ will denote the Banach space of weakly continuous functions $I\to X$ and functions with bounded variations, respectively, and $C_{\rm b}(\cdot)$ will stand for continuous bounded functions.

In the following, we use the symbol C to indicate a generic positive constant depending on data and possibly changing from line to line. We impose the following assumptions on the data:

$$\Omega\subset\subset U\subset\mathbb{R}^3 \text{ are open, bounded, and } C^{1,1}\text{-regular}, \tag{5.2a}$$

$$\phi_{\rm ref}\in C^1(\overline\Omega\times(0,+\infty)),\ \ \exists\,\epsilon>0,\ \alpha>1/5\ \ \forall \boldsymbol{X}\in\Omega,\ J>0:\ \ \phi_{\rm ref}(\boldsymbol{X},J)\ge\frac{\epsilon}{J^\alpha}\,, \tag{5.2b}$$

$$\nu_1,\nu_2\in C(\overline\Omega)\,,\quad \min(\nu_1,\nu_2)>0\,,\quad q>3\ \ \text{(for q occurring in (3.4))}\,, \tag{5.2c}$$

$$\rho_{\rm ref}\in C(\overline\Omega)\,,\quad \rho_{\rm ref}>0\,,\quad G>0\,,\quad \varrho_{\rm ext}\in W^{1,1}(I;L^{6/5}(U\backslash\Omega))\,, \tag{5.2d}$$

$$\boldsymbol{v}_0\in L^2(\Omega;\mathbb{R}^3)\,,\quad \boldsymbol{\xi}_0\in W^{2,r}(\Omega;\mathbb{R}^3)\ \text{ with }\ r>3\,,\quad 1/\det(\nabla\boldsymbol{\xi}_0)>0\ \text{ on }\overline\Omega\,. \tag{5.2e}$$

Note that $\phi_{\rm ref}(\boldsymbol{X},\cdot)$ need not be convex, hence $\boldsymbol{F}\mapsto\phi_{\rm ref}(\boldsymbol{X},\det\boldsymbol{F})$ need not be polyconvex. In view of the problem being independent of the actual value of the constant $V_{\rm B}$, with no loss of generality we choose $V_{\rm B}=0$ in (3.6b) for simplicity.

Definition 5.1 (Weak solutions of system (4.3))**.** *A triplet $(\boldsymbol{v},\boldsymbol{\xi},V)$ with $\boldsymbol{v}\in C_{\rm w}(I;L^2(\Omega;\mathbb{R}^3))\cap L^2(I;W^{2,q}(\Omega;\mathbb{R}^3))$, $\boldsymbol{\xi}\in C_{\rm w}(I;W^{2,r}(\Omega;\mathbb{R}^3))\cap W^{1,1}(I\times\Omega;\mathbb{R}^3)$, and $V\in C_{\rm w}(I;H^2_0(U))$ is a* weak solution *of the boundary-value problem* (4.3) *with the boundary conditions* (3.6) *and with the initial condition* (5.1) *if*

$$\int_0^T\!\!\int_\Omega\bigg(\Big(\nu_1^{\boldsymbol{\xi}}\boldsymbol{e}(\boldsymbol{v})-\det(\nabla\boldsymbol{\xi})\varrho_{\rm ref}^{\boldsymbol{\xi}}\boldsymbol{v}\otimes\boldsymbol{v}\Big){:}\boldsymbol{e}(\widetilde{\boldsymbol{v}})+\nu_2^{\boldsymbol{\xi}}|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v}){\vdots}\nabla\boldsymbol{e}(\widetilde{\boldsymbol{v}})-\det(\nabla\boldsymbol{\xi})\varrho_{\rm ref}^{\boldsymbol{\xi}}\boldsymbol{v}{\cdot}\frac{\partial\widetilde{\boldsymbol{v}}}{\partial t}$$
$$+\,[\phi_{\rm ref}^{\boldsymbol{\xi}}]_J'\Big(\frac{1}{\det(\nabla\boldsymbol{\xi})}\Big){\rm div}\,\widetilde{\boldsymbol{v}}+\det(\nabla\boldsymbol{\xi})\varrho_{\rm ref}^{\boldsymbol{\xi}}\nabla V{\cdot}\widetilde{\boldsymbol{v}}\bigg)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t=\int_\Omega\frac{\varrho_{\rm ref}^{\boldsymbol{\xi}_0}\boldsymbol{v}_0}{J_0}{\cdot}\widetilde{\boldsymbol{v}}(0)\,\mathrm{d}\boldsymbol{x} \tag{5.3}$$

holds for all $\widetilde{\boldsymbol{v}} \in C^\infty(I\times\overline{\Omega};\mathbb{R}^3)$ *with* $\widetilde{\boldsymbol{v}}\cdot\boldsymbol{n} = 0$ *and* $\widetilde{\boldsymbol{v}}(T) = \boldsymbol{0}$*,* (4.3b) *hold a.e. on* $I\times\Omega$ *with* $\boldsymbol{\xi}(0) = \boldsymbol{\xi}_0$ *on* Ω*, and* (4.3c) *holds a.e. on* $I\times U$*.*

Theorem 5.2 (Existence of solutions of (4.3))**.** *Let assumptions* (5.2) *hold. Then:*

(i) *there exists a weak solution* $(\boldsymbol{v}, \boldsymbol{\xi}, V)$ *of system* (4.3)*.*

(ii) *Weak solutions of system* (4.3) *satisfy the energy-dissipation balance* (4.6) *when integrated over the time interval* $[0, t]$ *for all* $t \in I$*.*

Proof. The proof relies on a *semi-Galerkin* approximation and is divided into four steps.

Step 1: semi-Galerkin approximation. We perform a Galerkin approximation of the momentum equation (4.3a) for $\boldsymbol{v}$ but leave the Poisson equation (4.3c) for V not discretized, relying on the invertibility of the the Laplacian operator $-\Delta : H^2_0(U) \to L^2(U)$. Similarly, we do not discretize the transport equation (4.3b) for $\boldsymbol{\xi}$ and rely on [RoS22, Lemma 3.2] for its weak solvability.

In order to approximate the momentum equation (4.3a), we introduce a family of nested finite-dimensional subspaces $\{\mathscr{V}_k\}_{k=0}^\infty$ whose union is dense in $W^{2,q}(\Omega;\mathbb{R}^3)$. Without loss of generality, we may assume $\boldsymbol{v}_0 \in \mathscr{V}_0$.

The global existence on the whole time interval $[0, T]$ of a solution of such regularized and semi-discretized system, which will be denoted by $(\boldsymbol{v}_k, \boldsymbol{\xi}_k, V_k)$, can be proved to exist by the standard successive-prolongation argument, on the basis of the uniform-in-time estimates proved below.

Setting $J_k := \det(\nabla\boldsymbol{\xi}_k)$ and $\varrho_k := \rho_{\rm ref}^{\boldsymbol{\xi}_k}/J_k$, we can rely on the evolution-and-transport equations

$$\frac{\partial J_k}{\partial t} = (\operatorname{div}\boldsymbol{v}_k)\, J_k - \boldsymbol{v}_k\cdot\nabla J_k \quad \text{and} \quad \frac{\partial \varrho_k}{\partial t} = -\operatorname{div}(\varrho_k\boldsymbol{v}_k) \tag{5.4}$$

with the initial conditions $J_k(0) = 1/\det(\nabla\boldsymbol{\xi}_0)$ and $\varrho_k(0) := \rho_{\rm ref}^{\boldsymbol{\xi}_0}/J_0$, respectively, cf. (2.2) and (3.2). Here, we crucially used the fact that the transport equation (4.3b) is not discretized.

Step 2: first a-priori estimates. We test the Galerkin approximate versions of (4.3a) and (4.3c) by $\boldsymbol{v}_k$ and V_k, respectively, and use (5.4). The discretized velocity field $\boldsymbol{v}_k$ is in $L^2(I;W^{1,\infty}(\Omega;\mathbb{R}^3))$, so that J_k, which fulfills the non-discretized transport-and-evolution equation (5.4), stays positive on $I\times\Omega$; here assumption (5.2e) is used, cf. [RoS22, Lemma 3.2]. By abbreviating $\overline{\nu}_i = \min \nu_i(\boldsymbol{X})$ for $i = 1, 2$, we find

$$\begin{aligned}
&\int_\Omega \frac{\varrho_k}{2}|\boldsymbol{v}_k|^2 + \frac{\epsilon}{J_k^{\alpha+1}(t)}\mathrm{d}\boldsymbol{x} + \int_U \frac{|\nabla V_k(t)|^2}{2G}\mathrm{d}\boldsymbol{x} + \int_0^t\!\!\int_\Omega \overline{\nu}_1|\boldsymbol{e}(\boldsymbol{v}_k)|^2 + \overline{\nu}_2|\nabla\boldsymbol{e}(\boldsymbol{v}_k)|^q\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t\\
&\overset{(5.2)}{\leq} \int_\Omega \frac{\rho_{\rm ref}^{\boldsymbol{\xi}_k(t)}}{2J_k(t)}|\boldsymbol{v}_k(t)|^2 + \frac{\phi_{\rm ref}^{\boldsymbol{\xi}_k(t)}(J_k(t))}{J_k(t)}\mathrm{d}\boldsymbol{x}\\
&\qquad\qquad + \int_U \frac{|\nabla V_k(t)|^2}{2G}\,\mathrm{d}\boldsymbol{x} + \int_0^t\!\!\int_\Omega \nu_1^{\boldsymbol{\xi}_k}|\boldsymbol{e}(\boldsymbol{v}_k)|^2 + \nu_2^{\boldsymbol{\xi}_k}|\nabla\boldsymbol{e}(\boldsymbol{v}_k)|^q\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t\\
&\overset{(4.6)}{=} \int_0^t\!\!\int_\Omega \frac{\partial\varrho_{\rm ext}}{\partial t}V_k\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t - \int_\Omega \frac{\rho_{\rm ref}^{\boldsymbol{\xi}_k(t)}}{J_k(t)}V_k(t)\,\mathrm{d}\boldsymbol{x} - \int_{U\setminus\Omega}\varrho_{\rm ext}(t)V_k(t)\,\mathrm{d}\boldsymbol{x}\\
&\quad + \int_\Omega \frac{\rho_{\rm ref}^{\boldsymbol{\xi}_0}}{J_0}V_k(0) + \frac{\rho_{\rm ref}^{\boldsymbol{\xi}_0}}{J_0}|\boldsymbol{v}_0|^2 + \frac{\phi_{\rm ref}^{\boldsymbol{\xi}_0}(J_0)}{J_0}\,\mathrm{d}\boldsymbol{x} + \int_{U\setminus\Omega}\varrho_{\rm ext}(0)V_k(0)\,\mathrm{d}\boldsymbol{x} + \int_U \frac{|\nabla V_k(0)|^2}{2G}\,\mathrm{d}\boldsymbol{x}
\end{aligned}$$

$$\le C_\delta + \|\varrho_{\rm ext}(t)\|^{6/5}_{L^{6/5}(U\setminus\Omega)} + \delta\Big\|\frac{1}{J^{\alpha+1}(t)}\Big\|_{L^1(\Omega)} + \delta\|\nabla V_k(t)\|^2_{L^2(U;\mathbb{R}^3)}$$
$$+\int_0^t \Big\|\frac{\partial\varrho_{\rm ext}}{\partial t}\Big\|^{6/5}_{L^{6/5}(U\setminus\Omega)}\big(1{+}\|\nabla V_k\|^2_{L^2(U;\mathbb{R}^3)}\big)\,{\rm d}t \tag{5.5}$$

with α from (5.2b), and with C_δ depending on $\delta > 0$ and $\|\varrho_{\rm ref}\|_{L^\infty(\Omega)}$, where $\delta > 0$ will later be taken to be small. Here above, we used the Hölder and Young inequalities and the embedding $H^1(U) \subset L^6(U)$ to obtain the estimate

$$-\int_\Omega \frac{\rho^{\boldsymbol{\xi}_k(t)}_{\rm ref}}{J_k(t)} V_k(t)\,{\rm d}\boldsymbol{x} \le C\|\rho_{\rm ref}\|_{L^\infty(\Omega)}\Big\|\frac{1}{J_k(t)}\Big\|_{L^{\alpha+1}(\Omega)}\|V_k(t)\|_{L^6(U)}$$
$$\le C\|\rho_{\rm ref}\|_{L^\infty(\Omega)}\Big\|\frac{1}{J_k(t)}\Big\|_{L^{\alpha+1}(\Omega)}\|\nabla V_k(t)\|_{L^2(U;\mathbb{R}^3)}$$
$$\le C_\delta + \delta\Big\|\frac{1}{J_k(t)}\Big\|^{\alpha+1}_{L^{\alpha+1}(\Omega)} + \delta\|\nabla V_k(t)\|^2_{L^2(U;\mathbb{R}^3)} \tag{5.6}$$

where we have used $\alpha > 1/5$ from (5.2b) and taken $\delta > 0$ arbitrarily small (not necessarily the same as in (5.5)).

From this, taking $\delta > 0$ in (5.5) sufficiently small and using the Gronwall inequality, we obtain the a-priori bounds

$$\big\|\sqrt{\varrho_k}\boldsymbol{v}_k\big\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \le C\,, \tag{5.7a}$$
$$\|\boldsymbol{e}(\boldsymbol{v}_k)\|_{L^2(I;W^{1,q}(\Omega;\mathbb{R}^{3\times3}))} \le C\,, \tag{5.7b}$$
$$\|V_k\|_{L^\infty(I;H^1(U))} \le C\,. \tag{5.7c}$$

By using [RoS22, Lemma 3.2], from (5.4) for J_k and assumption (5.2e) we further obtain

$$\|J_k\|_{L^\infty(I;W^{1,r}(\Omega))} \le C \ \text{ and } \ \min J_k > 1/C\,. \tag{5.7d}$$

From (4.3b), i.e., $\frac{\partial}{\partial t}\boldsymbol{\xi}_k = -(\boldsymbol{v}_k{\cdot}\nabla)\boldsymbol{\xi}_k$ and thus also $\frac{\partial}{\partial t}\nabla\boldsymbol{\xi}_k = -(\boldsymbol{v}_k{\cdot}\nabla)\nabla\boldsymbol{\xi}_k - (\nabla\boldsymbol{\xi}_k)\nabla\boldsymbol{v}_k$ and taking advantage of the regularity of the initial value $\nabla\boldsymbol{\xi}_0 \in W^{1,r}(\Omega;\mathbb{R}^{d\times d})$, again by [RoS22, Lemma 3.2] we also obtain

$$\|\boldsymbol{\xi}_k\|_{L^\infty(I;W^{2,r}(\Omega;\mathbb{R}^3))} \le C\,. \tag{5.7e}$$

Since $\boldsymbol{v}_k = (\sqrt{\varrho_k}\boldsymbol{v}_k)\,(1/\sqrt{\varrho_k}) = (\sqrt{\varrho_k}\boldsymbol{v}_k)\sqrt{J_k}/\sqrt{\varrho^{\boldsymbol{\xi}_k}_{\rm ref}}$, from (5.7a) and (5.7d) we eventually obtain

$$\|\boldsymbol{v}_k\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \le \frac{\|J_k\|^{1/2}_{L^\infty(I\times\Omega)}}{\min\varrho_{\rm ref}(\overline{\Omega})^{1/2}}\big\|\sqrt{\varrho_k}\boldsymbol{v}_k\big\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))} \le C\,. \tag{5.7f}$$

From (5.4) for J_k we obtain a bound for $\frac{\partial}{\partial t}J_k$ in $L^q(I;L^r(\Omega))$ and, similarly, from $\frac{\partial}{\partial t}\boldsymbol{\xi}_k = -(\boldsymbol{v}_k{\cdot}\nabla)\boldsymbol{\xi}_k$, we obtain a bound for $\frac{\partial}{\partial t}\boldsymbol{\xi}_k$ in $L^q(I;L^r(\Omega;\mathbb{R}^3))$. This additionally provides a bound on $\frac{\partial}{\partial t}\nabla\boldsymbol{\xi}_k$, which we will not use, however. From $\frac{\partial}{\partial t}V_k = \Delta^{-1}(\frac{\partial}{\partial t}\varrho_k + \frac{\partial}{\partial t}\varrho_{\rm ext})$ with $\frac{\partial}{\partial t}\varrho_k \in L^q(I;L^r(\Omega))$ and $\frac{\partial}{\partial t}\varrho_{\rm ext} \in L^1(L^{6/5}(U\setminus\Omega))$, we obtain a bound for $\frac{\partial}{\partial t}V_k$ in $L^1(I;W^{2,6/5}(U))$.

Step 3: limit passage with $k \to \infty$. By the Banach selection principle, we select a weakly* convergent subsequence and $(\varrho, \boldsymbol{v}, \boldsymbol{\xi}, J, V)$ such that

$$\varrho_k \to \varrho \qquad \text{weakly* in } L^\infty(I; W^{1,r}(\Omega)) \cap W^{1,q}(I; L^r(\Omega)), \tag{5.8a}$$
$$\boldsymbol{v}_k \to \boldsymbol{v} \qquad \text{weakly* in } L^\infty(I; L^2(\Omega;\mathbb{R}^3)) \cap L^2(I; W^{2,q}(\Omega;\mathbb{R}^3)) \tag{5.8b}$$
$$\boldsymbol{\xi}_k \to \boldsymbol{\xi} \qquad \text{weakly* in } L^\infty(I; W^{2,r}(\Omega;\mathbb{R}^3)) \cap W^{1,q}(I; L^2(\Omega;\mathbb{R}^3)), \tag{5.8c}$$
$$J_k \to J \qquad \text{weakly* in } L^\infty(I; W^{1,r}(\Omega)) \cap W^{1,q}(I; L^r(\Omega)), \tag{5.8d}$$
$$V_k \to V \qquad \text{weakly* in } L^\infty(I; H^2(U)) \cap \mathrm{BV}(I; W^{2,6/5}(U)). \tag{5.8e}$$

Recalling that $r > d$, by the Aubin-Lions Lemma, the convergences (5.8a,c,d) are also strong

$$J_k \to J \qquad \text{strongly in } C(I{\times}\overline{\Omega}), \tag{5.8f}$$
$$\varrho_k \to \varrho = \rho_{\rm ref}^{\boldsymbol{\xi}}/J \qquad \text{strongly in } C(I{\times}\overline{\Omega}), \text{ and} \tag{5.8g}$$
$$\boldsymbol{\xi}_k \to \boldsymbol{\xi} \qquad \text{strongly in } C(I{\times}\overline{\Omega};\mathbb{R}^3). \tag{5.8h}$$

Moreover, $\varrho_k\boldsymbol{v}_k \to \varrho\boldsymbol{v}$ and $\boldsymbol{v}_k \to \boldsymbol{v}$ strongly in $L^c(I{\times}\Omega;\mathbb{R}^3)$ for all $1 \le c < 4$, cf. [RoS22] for details. From the mentioned strong convergence of ϱ_k and the Poisson equation (4.3c), we further obtain

$$\nabla V_k \to \nabla V \qquad \text{strongly in } L^\infty(I; L^2(U;\mathbb{R}^3)). \tag{5.8i}$$

We now use the Galerkin approximation of the momentum equation (4.3a) tested by $\widetilde{\boldsymbol{v}} = \boldsymbol{v}_k - \widetilde{\boldsymbol{v}}_k$ where $\widetilde{\boldsymbol{v}}_k : I \to \mathscr{V}_k$ is an approximation of $\boldsymbol{v}$ such that $\widetilde{\boldsymbol{v}}_k \to \boldsymbol{v}$ strongly in $L^\infty(I; L^2(\Omega;\mathbb{R}^d))$ and $\nabla\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k) \to \nabla\boldsymbol{e}(\boldsymbol{v})$ strongly in $L^q(I{\times}\Omega;\mathbb{R}^{d\times d\times d})$ for $k \to \infty$. Using also inequality (5.7d) and the calculus

$$\int_\Omega \frac{\varrho_k(T)}{2}\big|\boldsymbol{v}_k(T){-}\boldsymbol{v}(T)\big|^2 \mathrm{d}\boldsymbol{x} = \int_0^T\!\!\int_\Omega \Big(\frac{\partial}{\partial t}(\varrho_k\boldsymbol{v}_k) + \mathrm{div}(\varrho_k\boldsymbol{v}_k{\otimes}\boldsymbol{v}_k)\Big){\cdot}\boldsymbol{v}_k\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$
$$+\int_\Omega \frac{\varrho_0}{2}|\boldsymbol{v}_0|^2 - \varrho_k(T)\boldsymbol{v}_k(T){\cdot}\boldsymbol{v}(T) + \frac{\varrho_k(T)}{2}|\boldsymbol{v}(T)|^2 \mathrm{d}\boldsymbol{x}, \tag{5.9}$$

we can estimate

$$\frac{\min\rho_{\rm ref}(\overline{\Omega})}{2\|J_k(T)\|_{L^\infty(\Omega)}}\big\|\boldsymbol{v}_k(T){-}\boldsymbol{v}(T)\big\|^2_{L^2(\Omega;\mathbb{R}^3)} + \bar\nu_2\,c_q\,\|\nabla\boldsymbol{e}(\boldsymbol{v}_k{-}\boldsymbol{v})\|^q_{L^q(I\times\Omega;\mathbb{R}^{3\times3\times3})}$$
$$\le \int_\Omega \frac{\varrho_k(T)}{2}\big|\boldsymbol{v}_k(T){-}\boldsymbol{v}(T)\big|^2\,\mathrm{d}\boldsymbol{x} + \int_0^T\!\!\int_\Omega \bigg(\nu_1^{\boldsymbol{\xi}_k}\boldsymbol{e}(\boldsymbol{v}_k{-}\boldsymbol{v}_\varepsilon){:}\boldsymbol{e}(\boldsymbol{v}_k{-}\boldsymbol{v}_\varepsilon)$$
$$+ \nu_2^{\boldsymbol{\xi}_k}\big(|\nabla\boldsymbol{e}(\boldsymbol{v}_k)|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v}_k) - |\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\big)\vdots\nabla\boldsymbol{e}(\boldsymbol{v}_k{-}\boldsymbol{v})\bigg)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$
$$= \int_0^T\!\!\int_\Omega \bigg(p_k\mathrm{div}(\boldsymbol{v}_k{-}\widetilde{\boldsymbol{v}}_k) - \varrho_k\nabla V_k{\cdot}(\boldsymbol{v}_k{-}\widetilde{\boldsymbol{v}}_k) - \nu_1^{\boldsymbol{\xi}_k}\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k){:}\boldsymbol{e}(\boldsymbol{v}_k{-}\widetilde{\boldsymbol{v}}_k)$$
$$- \nu_2^{\boldsymbol{\xi}_k}|\nabla\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k)|^{q-2}\nabla\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k)\vdots\nabla\boldsymbol{e}(\boldsymbol{v}_k{-}\widetilde{\boldsymbol{v}}_k) + \Big(\frac{\partial}{\partial t}(\varrho_k\boldsymbol{v}_k) + \mathrm{div}(\varrho_k\boldsymbol{v}_k{\otimes}\boldsymbol{v}_k)\Big){\cdot}\widetilde{\boldsymbol{v}}_k\bigg)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$
$$+ \int_\Omega\bigg(\frac{\varrho_0}{2}|\boldsymbol{v}_0|^2 - \varrho_k(T)\boldsymbol{v}_k(T){\cdot}\widetilde{\boldsymbol{v}}_k(T) + \frac{\varrho_k(T)}{2}|\widetilde{\boldsymbol{v}}_k(T)|^2\bigg)\,\mathrm{d}\boldsymbol{x} + \mathscr{O}_k \stackrel{k\to\infty}{\longrightarrow} 0 \tag{5.10}$$

with $p_k = -[\phi_{\rm ref}^{\boldsymbol{\xi}_k}]'_J(J_k)$ converging strongly in $C(I\times\overline{\Omega})$ and with $c_q > 0$ so that the inequality $c_q|G-\widetilde{G}|^q \le (|G|^{q-2}G - |\widetilde{G}|^{q-2}\widetilde{G})\vdots(G-\widetilde{G})$ holds. The remainder term $\mathscr{O}_k$ in (5.10) is

$$\mathscr{O}_k = \int_\Omega \frac{\varrho_k(T)}{2}\boldsymbol{v}_k(T)\cdot\big(\widetilde{\boldsymbol{v}}_k(T)-\boldsymbol{v}(T)\big)\,\mathrm{d}\boldsymbol{x} \\ + \int_0^T\!\!\int_\Omega \nu_1^{\boldsymbol{\xi}_k}\boldsymbol{e}(\boldsymbol{v}_k):\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k-\boldsymbol{v}) + \nu_2^{\boldsymbol{\xi}_k}|\nabla\boldsymbol{e}(\boldsymbol{v}_k)|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v}_k)\vdots\nabla\boldsymbol{e}(\widetilde{\boldsymbol{v}}_k-\boldsymbol{v})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

and it converges to zero due to the strong approximation properties of the approximation $\widetilde{\boldsymbol{v}}_k$ of $\boldsymbol{v}$. Here, we also used the convergences above. Thus, we obtain the strong convergence

$$\boldsymbol{v}_k \to \boldsymbol{v}_\varepsilon \qquad \text{strongly in } L^q(I;W^{2,q}(\Omega;\mathbb{R}^3)) \tag{5.11a}$$

together with $\boldsymbol{v}_k(T) \to \boldsymbol{v}_\varepsilon(T)$ in $L^2(\Omega;\mathbb{R}^d)$. In fact, by performing this computation at a generic time $t \in (0,T)$ instead of T, we obtain

$$\boldsymbol{v}_k(t) \to \boldsymbol{v}(t) \qquad \text{strongly in } L^2(\Omega;\mathbb{R}^3) \text{ for any } t\in I. \tag{5.11b}$$

Owing to these convergences, the passage to the limit in the semi-discrete system is straightforward. In particular, the limit is a weak solution of the system in the sense of Definition 5.1. By differentiating (4.3c) in time and taking into account that $\frac{\partial}{\partial t}\varrho \in L^p(I;L^r(\Omega))$, from the assumption $\frac{\partial}{\partial t}\varrho_{\rm ext} \in L^1(I;L^{6/5}(\Omega))$ we have that $V \in W^{1,1}(I;W_0^{2,6/5}(U))$ and, in particular, $V \in C_{\rm w}(I;W_0^{2,6/5}(U))$. Here, we used the classical elliptic $W^{2,p}$-regularity theory [ADN64, Gri85] as well as the fact that the right-hand side $\varrho_{\rm ext} \in W^{1,1}(I;L^{6/5}(U))$ is fixed, so that the limit time derivative is integrable.

Step 4: energy-dissipation balance. To conclude the proof, we now check that the calculations leading to (3.11) in the variant (4.6), in particular (4.5), are indeed legitimate. Here, we simply refer to [Rou22a, Sec. 3] or [RoS22, Sec. 3] where this check has been already performed. With respect to these references, additional care has to be given here in order to obtain (3.10), since the mechanical load $\nabla p + \varrho\nabla V$ in the momentum equation (4.3a) has to be shown to be in duality with $\boldsymbol{v} \in L^\infty(I;L^2(\Omega;\mathbb{R}^3)) \cap L^q(I;W^{2,q}(\Omega;\mathbb{R}^3))$. This follows however as p is in $L^\infty(I;W^{1,r}(\Omega))$ so that ∇p is in $L^1(I;L^2(\Omega;\mathbb{R}^3))$, and the restriction of ∇V to Ω is in $L^\infty(I;L^2(\Omega;\mathbb{R}^3))$. Note in addition that $\frac{\partial}{\partial t}V$ needs to be in $L^1(I;L^6(U))$ in order to be in duality with the equation (4.3c). This however follows from $\frac{\partial}{\partial t}V \in L^1(I;W_0^{2,6/5}(U))$ which has been proved in Step 3. □

Remark 5.3 (*Long time scales*)**.** Having in mind the self-gravitational differentiation of planets during long time scales, when the initial configuration is successively forgotten, discussing the validity of the above estimates for $T\to\infty$ is relevant. The constants in the bounds in (5.7d-f) depend on the regularity of the initial conditions and are possibly (exponentially) increasing in time. On the other hand, estimates (5.7a,c) are controlled by the material properties and can pass to the limit $T\to\infty$ (at least after neglecting the effect of a moving external mass $\varrho_{\rm ext}$). Moreover, from (5.5) we have an estimate of $1/J$ in $L^\infty(0,+\infty;L^{1+\alpha}(\Omega))$. For $\alpha \ge 3/2$, also the linear momentum $\varrho\boldsymbol{v} = \sqrt{\varrho}\boldsymbol{v}(\rho_{\rm ref}^{\boldsymbol{\xi}}/J)^{1/2}$ is bounded, specifically

$$\|\varrho\boldsymbol{v}\|_{L^\infty(0,+\infty;L^{(4\alpha+2)/(2\alpha+5)}(\Omega;\mathbb{R}^3))} \\ \le \sqrt{\max\rho_{\rm ref}(\overline{\Omega})}\big\|\sqrt{\varrho}\boldsymbol{v}\big\|_{L^\infty(0,+\infty;L^2(\Omega;\mathbb{R}^3))}\Big\|\frac{1}{\sqrt{J}}\Big\|_{L^\infty(0,+\infty;L^{\alpha+1/2}(\Omega))}$$

$$= \sqrt{\max \rho_{\rm ref}(\overline{\Omega})} \big\| \sqrt{\varrho} \boldsymbol{v} \big\|_{L^\infty(0,+\infty;L^2(\Omega;\mathbb{R}^3))} \bigg\| \frac{1}{J^{\alpha+1}} \bigg\|^{(2\alpha+2)/(2\alpha+1)}_{L^\infty(0,+\infty;L^{\alpha+1}(\Omega))}$$

and the right-hand side of (5.7a) is bounded.

Remark 5.4 (*Pressure dependent viscosities)***.** Often, viscosity coefficients depend (beside temperature, not considered here) also on the pressure [RSV09] and may vary, in particular during phase transitions in some materials [SS*77, SN*12]. This can be taken into account by letting $\nu_1 = \nu_1(\boldsymbol{X}, J)$ and $\nu_2 = \nu_2(\boldsymbol{X}, J)$ depend on J.

Remark 5.5 (*Sharp interfaces)***.** In many applications (and in particular in planetary geophysics), the solid is composed by very different materials. Correspondingly the reference data $\phi_{\rm ref}(\cdot, J)$ and $\rho_{\rm ref}$ as well as the viscosities $\nu_1(\cdot, J)$ and $\nu_2(\cdot, J)$ are ideally discontinuous with respect to $\boldsymbol{X}$, as opposed to (5.2). This makes the substitutions with $\boldsymbol{\xi}$ analytically more complicated, as one cannot use the continuity of the implied Nemytskiĭ mapping (composition), as actually used in the above proof. Instead, one has to modify the free-slip boundary condition (3.6) and assume a stick condition $\boldsymbol{v} = \boldsymbol{0}$ on $\partial\Omega$. This, together with the local invertibility $\det(\nabla\boldsymbol{\xi}(t)) > 0$, would ensure the global invertibility of $\boldsymbol{\xi}$, eventually allowing to apply a change of variable. The reader is referred to [Rou22a, Sec. 4] for additional details in a similar setting. Let us just record that this approach hinges on a bound for the distorsion, which in turn ensures that referential interfaces between the regions occupied by different materials remain of null measure in the actual deformed configuration.

6 Multicomponent materials

The different regions of planets and moons are actually composed by many distinct materials (cf., e.g., [Con16, STO04]). These materials, may undergo pressure-dependent chemical reactions, combined with diffusion. In this section, we extend the model by including the description of the different constituent of the solid by means of a concentration vector $\boldsymbol{c} = (c_1, ..., c_n)$. We assume that the viscoelastic response of the solid depends on the composition, namely, we let $\nu_1 = \nu_1(\boldsymbol{X}, J, \boldsymbol{c})$, $\nu_2 = \nu_2(\boldsymbol{X}, J, \boldsymbol{c})$, as well as $\phi_{\rm ref} = \phi_{\rm ref}(\boldsymbol{X}, J, \boldsymbol{c})$. On the other hand, we assume the mass density to be independent of $\boldsymbol{c}$, so that ϱ is still determined by (3.1), cf. Remark 6.3 below. Without loss of generality, we take the number n of constituents to be the same in all regions (hence n is independent of $\boldsymbol{X}$). Of course, the components of $\boldsymbol{c}$ are to be non-negative and to satisfy $\sum_{i=1}^n c_i = 1$ a.e. in $I{\times}\Omega$. In other words, $\boldsymbol{c}$ takes values in the so-called Gibbs' simplex

$$\triangle_1^+ := \{(c_1, ..., c_n) \in \mathbb{R}^n;\ \sum_{i=1}^n c_i = 1 \ \text{ and } \ \forall i:\ c_i \geq 0\}.$$

The single-component system (4.3) is then expanded to its multi-component variant as

$$\varrho\dot{\boldsymbol{v}} = {\rm div}\big(\nu_1^{\boldsymbol{\xi}}(\boldsymbol{c})\boldsymbol{e}(\boldsymbol{v}) - {\rm div}\big(\nu_2^{\boldsymbol{\xi}}(\boldsymbol{c})|\nabla\boldsymbol{e}(\boldsymbol{v})|^{q-2}\nabla\boldsymbol{e}(\boldsymbol{v})\big)\big) - \nabla p - \varrho\nabla V$$

$$\text{where} \quad p = -\frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_J(J,\boldsymbol{c})}{J} \quad \text{and} \quad \varrho = \frac{\rho_{\rm ref}^{\boldsymbol{\xi}}}{J} \ \text{ with } \ J = \frac{1}{\det(\nabla\boldsymbol{\xi})}\,, \tag{6.1a}$$

$$\dot{\boldsymbol{c}} = {\rm div}\big(\mathbb{M}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\nabla\boldsymbol{\mu}\big) - \boldsymbol{r}^{\boldsymbol{\xi}}(J,\boldsymbol{c}) \tag{6.1b}$$

$$\text{with} \quad \boldsymbol{\mu} \in \frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J} + \boldsymbol{N}(\boldsymbol{c})\,, \tag{6.1c}$$

$$\dot{\boldsymbol{\xi}} = \mathbf{0}, \qquad\qquad \text{on } \Omega\,, \tag{6.1d}$$

$$\Delta V = G\big(\varrho{+}\varrho_{\rm ext}\big) \qquad \text{on } U\,, \tag{6.1e}$$

where $\boldsymbol{N}(\boldsymbol{c})$ in (6.1c) denotes the normal cone to the convex set $\triangle_1^+$ at $\boldsymbol{c}$. In particular, $\boldsymbol{N}(\cdot) : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ is a maximal monotone set-valued mapping. In fact, the term $\boldsymbol{N}(\boldsymbol{c})$ in (6.1c) contributes a Lagrange multiplier (= a “pressure”) corresponding to the constraints $\sum_{i=1}^n c_i = 1$ and $c_i \geq 0$. Such multiplier ensures the validity of the constraints throughout the evolution. In this context, the use of such a multiplier dates at least back to E and Palffy-Muhoray [EP97], who nonetheless generalized an (essentially) 1D-model by De Gennes [dGe80]. We also refer to [OtE97] for a discussion of local versus a nonlocal mixture models, where our approach corresponds to the nonlocal model with multiplier $\lambda(t,\boldsymbol{x})\mathbf{1} \in \boldsymbol{N}(\boldsymbol{c})$ with $\mathbf{1} = (1,\ldots,1) \in \mathbb{R}^n$ associated with the constraint $\boldsymbol{c}(t,\boldsymbol{x}) \in \triangle_1^+$, see also Remark 6.4.

Relation (6.1b) features the $n{\times}n$ mobility matrix $\mathbb{M} = \mathbb{M}(\boldsymbol{X},J,\boldsymbol{c})$ and the chemical-reaction rate $\boldsymbol{r} = \boldsymbol{r}(\boldsymbol{X},J,\boldsymbol{c})$. The mobility matrix $\mathbb{M}(\boldsymbol{X},J,\boldsymbol{c})$ is assumed to be symmetric in order to comply with the Onsager principle. In addition, it is assumed to be positive semi-definite to comply with the Clausius-Duhem inequality and thus the 2nd-law of thermodynamics. For analytical reasons, we assume $\mathbb{M}$ to be uniformly positive definite, as this allows to control the chemical-potential gradient and, indirectly, also the concentration gradients. The mass conservation within chemical reactions imposes that the reaction rates $\boldsymbol{r} = (r_1,\ldots,r_n)$ satisfy the condition

$$\forall(\boldsymbol{X},J,\boldsymbol{c}) \in \Omega{\times}\mathbb{R}^+{\times}\triangle_1^+ :\ \sum_{i=1}^n r_i(\boldsymbol{X},J,\boldsymbol{c}) = 0\,. \tag{6.2}$$

Note that we are following here the phenomenological approach by Eckart and Prigogine [Eck40, Pri47] by assuming that all component have the same velocity $\boldsymbol{v}$. A less phenomenological, truly rational-thermodynamical alternative would be to assume that each constituent has its own velocity, as in the Truesdell [Tru68] approach.

The boundary conditions (3.6) are complemented by the boundary condition $\boldsymbol{n}{\cdot}\mathbb{M}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\nabla\boldsymbol{\mu} = \mathbf{0}$ on $\partial\Omega$ for (6.1b), expressing that there is no flux of the constituents across $\partial\Omega$. The energetics of the model can be deduced as in Section 4, now combined with (6.1b) tested by $\boldsymbol{\mu}$, which leads to

$$\int_\Omega \dot{\boldsymbol{c}}{\cdot}\boldsymbol{\mu}\,\mathrm{d}\boldsymbol{x} = -\int_\Omega \boldsymbol{r}^{\boldsymbol{\xi}}(J,\boldsymbol{c}){\cdot}\boldsymbol{\mu} + \nabla\boldsymbol{\mu}{:}\mathbb{M}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\nabla\boldsymbol{\mu}\,\mathrm{d}\boldsymbol{x}\,, \tag{6.3}$$

and further using (6.1c) tested by $\dot{\boldsymbol{c}}$. We modify (4.5) to be merged with a part of (6.1c) tested by $\dot{\boldsymbol{c}}$. Specifically, also using (2.3) similarly as in (4.5), we have

$$\begin{aligned}
\int_\Omega \boldsymbol{\mu}{\cdot}\dot{\boldsymbol{c}} + \nabla p{\cdot}\boldsymbol{v}\,\mathrm{d}\boldsymbol{x} &= \int_\Omega \boldsymbol{\mu}{\cdot}\dot{\boldsymbol{c}} - p{\cdot}\mathrm{div}\boldsymbol{v} = \int_\Omega \frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]_{\boldsymbol{c}}'(J,\boldsymbol{c})}{J}{\cdot}\dot{\boldsymbol{c}} + \frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]_J'(J,\boldsymbol{c})}{J}\dot{J}\,\mathrm{d}\boldsymbol{x}\\
&= \int_\Omega \bigg(\Big[\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big]_J' + \frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J^2}\bigg)\dot{J} + \frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]_{\boldsymbol{c}}'(J,\boldsymbol{c})}{J}{\cdot}\dot{\boldsymbol{c}}\,\mathrm{d}\boldsymbol{x}\\
&= \int_\Omega \frac{\partial}{\partial t}\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big) + \Big[\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big]_J'\boldsymbol{v}{\cdot}\nabla J + \Big[\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big]_{\boldsymbol{c}}'{\cdot}(\boldsymbol{v}{\cdot}\nabla)\boldsymbol{c} + \frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\mathrm{div}\,\boldsymbol{v}\\
&= \int_\Omega \frac{\partial}{\partial t}\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big) + \nabla\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\Big){\cdot}\boldsymbol{v} + \frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\mathrm{div}\,\boldsymbol{v}\,\mathrm{d}\boldsymbol{x}\\
&= \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\,\mathrm{d}\boldsymbol{x} + \int_\Omega \mathrm{div}\Big(\frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\,\boldsymbol{v}\Big)\,\mathrm{d}\boldsymbol{x} = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{\phi_{\rm ref}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\,\mathrm{d}\boldsymbol{x}\,.
\end{aligned} \tag{6.4}$$

The remaining term arising from $\boldsymbol{N}(\boldsymbol{c})$ in (6.1c) tested by $\dot{\boldsymbol{c}}$ can be proved to vanish, provided that $\boldsymbol{c}(0,\boldsymbol{x}) \in \triangle_1^+$. Indeed, let $\delta_{\triangle_1^+}$ be the indicator function of $\triangle_1^+$ and $\boldsymbol{\eta} \in \boldsymbol{N}(\boldsymbol{c})$ a.e. in $I{\times}\Omega$. By comparison from (6.1c) one will find that $\boldsymbol{\eta} \in L^2(I{\times}\Omega;\mathbb{R}^n)$ (under the assumption (6.9a) below). Hence, the classical chain rule for convex functions (see, for instance [Vis96, Prop. XI.4.11]) ensures that

$$\boldsymbol{\eta}{\cdot}\dot{\boldsymbol{c}} = \boldsymbol{\eta}{\cdot}\frac{\partial \boldsymbol{c}}{\partial t} + \boldsymbol{\eta}{\cdot}(\boldsymbol{v}{\cdot}\nabla)\boldsymbol{c} = \dot{\overline{\delta_{\triangle_1^+}(\boldsymbol{c})}} = 0 \tag{6.5}$$

a.e. in $I{\times}\Omega$, the last equality following from the fact that $\boldsymbol{c} \in \triangle_1^+$ a.e. in $I{\times}\Omega$. In fact, by comparison from (6.1c) one can see that $\boldsymbol{\eta} \in L^2(I{\times}\Omega;\mathbb{R}^n)$ under the assumption (6.9a) below, as needed in [Vis96] for a rigorous proof of (6.5).

We hence deduce the energy-dissipation balance

$$\frac{\mathrm{d}}{\mathrm{d}t}\Bigg(\int_\Omega \underbrace{\frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}}}{2J}|\boldsymbol{v}|^2}_{\substack{\text{kinetic}\\ \text{energy}}} + \underbrace{\frac{\phi_{\mathrm{ref}}^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}}_{\substack{\text{actual}\\ \text{stored}\\ \text{energy}}} + \underbrace{\frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}}}{J}V}_{\substack{\text{energy of } \varrho \text{ in}\\ \text{gravitational}\\ \text{field } V}}\,\mathrm{d}\boldsymbol{x} + \int_U \underbrace{\frac{|\nabla V|^2}{2G}}_{\substack{\text{energy of}\\ \text{gravitational}\\ \text{field}}}\mathrm{d}\boldsymbol{x} + \int_{U\setminus\Omega} \underbrace{\varrho_{\mathrm{ext}} V}_{\substack{\text{energy of } \varrho_{\mathrm{ext}}\\ \text{in gravitational}\\ \text{field } V}}\mathrm{d}\boldsymbol{x}\Bigg)$$
$$+ \int_\Omega \underbrace{\nu_1^{\boldsymbol{\xi}}(\boldsymbol{c})|\boldsymbol{e}(\boldsymbol{v})|^2 + \nu_2^{\boldsymbol{\xi}}(\boldsymbol{c})|\nabla\boldsymbol{e}(\boldsymbol{v})|^q}_{\substack{\text{dissipation rate}\\ \text{due to viscosity}}} + \underbrace{\mathbb{M}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\nabla\boldsymbol{\mu}{:}\nabla\boldsymbol{\mu}}_{\substack{\text{dissipation rate}\\ \text{due to diffusion}}} + \underbrace{\boldsymbol{r}^{\boldsymbol{\xi}}(J,\boldsymbol{c}){\cdot}\boldsymbol{\mu}}_{\substack{\text{dissipation rate}\\ \text{due to reactions}}}\,\mathrm{d}\boldsymbol{x}$$
$$= \int_{U\setminus\Omega} \underbrace{\frac{\partial \varrho_{\mathrm{ext}}}{\partial t}V}_{\substack{\text{gravitational power}\\ \text{of external mass}}}\,\mathrm{d}\boldsymbol{x}\,. \tag{6.6}$$

The initial conditions (5.1) now include a prescription for $\boldsymbol{c}$ and read

$$\boldsymbol{v}|_{t=0} = \boldsymbol{v}_0\,, \quad \boldsymbol{\xi}|_{t=0} = \boldsymbol{\xi}_0\,, \quad \text{and} \quad \boldsymbol{c}|_{t=0} = \boldsymbol{c}_0 \in \triangle_1^+\,. \tag{6.7}$$

Definition 6.1 (Weak solutions of the system (6.1))**.** *The quintuple $(\boldsymbol{v},\boldsymbol{c},\boldsymbol{\mu},\boldsymbol{\xi},V)$ is a* weak solution *of the boundary-value problem for the system* (6.1) *with the boundary conditions* (3.6) *together with $(\boldsymbol{n}{\cdot}\nabla)\boldsymbol{\mu} = \boldsymbol{0}$ on $\partial\Omega$ and with the initial conditions* (6.7) *if $(\boldsymbol{v},\boldsymbol{\xi},V)$ is as in Definition 5.1 with* (5.3) *holding with $\nu_1^{\boldsymbol{\xi}} = \nu_1^{\boldsymbol{\xi}}(\boldsymbol{c})$ and $\nu_2^{\boldsymbol{\xi}} = \nu_2^{\boldsymbol{\xi}}(\boldsymbol{c})$ and if $\boldsymbol{c} \in L^2(I;H^1(\Omega;\mathbb{R}^n))$ and $\boldsymbol{\mu} \in L^2(I;H^1(\Omega;\mathbb{R}^n))$ satisfy $0 \le c_i \le 1$ and $\sum_{i=1}^n c_i = 1$ a.e. on $I{\times}\Omega$, the integral identity*

$$\int_0^T\!\!\int_\Omega \mathbb{M}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\nabla\boldsymbol{\mu}{:}\nabla\widetilde{\boldsymbol{\mu}} + \big((\boldsymbol{v}{\cdot}\nabla)\boldsymbol{c} + \boldsymbol{r}^{\boldsymbol{\xi}}(J,\boldsymbol{c})\big){\cdot}\widetilde{\boldsymbol{\mu}} - \boldsymbol{c}{\cdot}\frac{\partial\widetilde{\boldsymbol{\mu}}}{\partial t}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t = \int_\Omega \boldsymbol{c}_0{\cdot}\widetilde{\boldsymbol{\mu}}(0)\,\mathrm{d}\boldsymbol{x} \tag{6.8}$$

holds for any $\widetilde{\boldsymbol{\mu}} \in H^1(I{\times}\Omega;\mathbb{R}^n)$ with $\widetilde{\boldsymbol{\mu}}(T) = \boldsymbol{0}$, and the inclusion (6.1c) *holds a.e. on $I{\times}\Omega$.*

In order to treat the multi-component case, the assumptions on data have to be specified as follows, where we use the short-hand $\mathfrak{D} := \overline{\Omega}{\times}(0,+\infty){\times}\mathbb{R}^n$:

$$\phi_{\mathrm{ref}}(\boldsymbol{X},J,\boldsymbol{c}) = \phi_{\mathrm{r},0}(\boldsymbol{X},J) + \phi_{\mathrm{r},1}(\boldsymbol{X},J,\boldsymbol{c}),\ \ \phi_{\mathrm{r},0} \in C^1(\overline{\Omega}{\times}(0,+\infty))\,,$$
$$\phi_{\mathrm{r},1} \in C^1(\mathfrak{D}) \ \ \text{with} \ \ [\phi_{\mathrm{r},1}]'_{\boldsymbol{c}} \in C^1(\mathfrak{D}) \ \ \text{and} \ \ [\phi_{\mathrm{r},1}]''_{\boldsymbol{cc}} \in C_{\mathrm{b}}(\mathfrak{D};\mathbb{R}^{n\times n}),$$

$$\exists\,\epsilon>0,\ \alpha>1/5\,,\ \ \forall \boldsymbol{X}\in\Omega,\ J>0,\ \boldsymbol{c}\in\mathbb{R}^n:\ \ \phi_{\mathrm{r},0}(\boldsymbol{X},J)\geq\frac{\epsilon}{J^\alpha}\,,$$

$$\phi_{\mathrm{r},1}(\boldsymbol{X},J,\boldsymbol{c})\geq 0\,,\quad \big|[\phi_{\mathrm{r},1}]'_J(\boldsymbol{X},J,\boldsymbol{c})\big|\leq\frac{1}{\epsilon J^{(\alpha+1)/2}}\,,\ \text{ and }\ [\phi_{\mathrm{r},1}]''_{\boldsymbol{cc}}(\boldsymbol{X},J,\boldsymbol{c})\geq\epsilon\,, \tag{6.9a}$$

$$\mathbb{M}\in C_{\mathrm{b}}(\mathfrak{D};\mathbb{R}^{(n\times3)^2}_{\mathrm{sym}})\,,\qquad \forall G\in\mathbb{R}^{n\times 3}:\inf\nolimits_{(\boldsymbol{X},J,\boldsymbol{c})\in\mathfrak{D}} G^\top{:}\mathbb{M}(\boldsymbol{X},J,\boldsymbol{c}){:}G\geq\epsilon|G|^2\,, \tag{6.9b}$$

$$\boldsymbol{r}(\boldsymbol{X},J,c)=\mathbb{K}(\boldsymbol{X},J,\boldsymbol{c})[\phi_{\mathrm{r},1}]'_{\boldsymbol{c}}(\boldsymbol{X},J,\boldsymbol{c})\ \text{ with some }\ \mathbb{K}\in C_{\mathrm{b}}(\mathfrak{D};\mathbb{R}^{n\times n}_{\mathrm{sym}}),\ \ \mathbb{K}\boldsymbol{1}=\boldsymbol{0},\ \text{and}$$

$$\forall\,\boldsymbol{\mu}\in\mathbb{R}^n,\ \sum_{i=1}^n\mu_i=0:\ \ \inf\nolimits_{(\boldsymbol{X},J,\boldsymbol{c})\in\mathfrak{D}}\boldsymbol{\mu}{\cdot}\mathbb{K}(\boldsymbol{X},J,\boldsymbol{c})\boldsymbol{\mu}\geq\epsilon|\boldsymbol{\mu}|^2, \tag{6.9c}$$

$$\nu_1,\nu_2\in C(\overline{\Omega}{\times}\mathbb{R}^n)\,,\quad \inf\nolimits_{\overline{\Omega}\times\mathbb{R}^n}\min(\nu_1,\nu_2)>0\,,\quad q>3\,. \tag{6.9d}$$

Note that (6.9a) in particular implies that $\phi_{\mathrm{ref}}(\boldsymbol{X},J,\cdot)$ is uniformly convex with respect to $\boldsymbol{c}$. For the purposes of the mathematical study, this implies that the diffusion equation defined via (6.1b)-(6.1c) is parabolic. The fact that the reaction terms $\boldsymbol{r}$ can be written in the form $\mathbb{K}\,[\phi_{\mathrm{r},1}]'_{\boldsymbol{c}}$ (under the condition of detailed balance) was observed in [Mie11], see also [MaM20] and Remark 6.5 below. The condition $\mathbb{K}\boldsymbol{1}=\boldsymbol{0}$ in (6.9c) guarantees (6.2). Note also that assumptions are formulated also for $\boldsymbol{c}\in\mathbb{R}^n\setminus\triangle_1^+$, which is required as we will use an exterior-penalty technique below.

Theorem 6.2 (Existence of weak solutions of system (6.1))**.** *Let assumptions* (5.2a)*,* (5.2d)*,* (5.2e)*, and* (6.9) *hold. Then:*

(i) *there exists a weak solution of system* (6.1)*.*

(ii) *Weak solutions of system* (6.1) *satisfy the energy-dissipation balance* (6.6) *when integrated over the time interval* $[0,t]$ *with any* $t\in I$*.*

Proof. We argue by approximation and subdivide the proof into seven subsequent steps. In addition to a semi-Galerkin approximation in the spirit of Section 5, now used also for (6.1b), we perform a regularization of the indicator function $\delta_{\triangle_1^+}(\cdot)$ by an exterior penalization.

Step 1: regularized problem. The multivalued mapping $\boldsymbol{N}(\cdot)$ in (6.1c) is regularized by introducing a penalization $\mathcal{P}_\varepsilon$ of the indicator function of the Gibbs' simplex $\triangle_1^+$ defined here, for any $\varepsilon>0$, by

$$\mathcal{P}_\varepsilon(\boldsymbol{c})=\frac{1}{2\varepsilon}\sum_{i=1}^n\min(0,c_i)^2+\frac{1}{2\varepsilon}\Big(\sum_{i=1}^n c_i-1\Big)^2.$$

Note that $\mathcal{P}_\varepsilon$ is convex and continuously differentiable. As $\varepsilon\to 0$ one has that $\mathcal{P}_\varepsilon\to\delta_{\triangle_1^+}$ pointwise and increasing.

The regularized problem is obtained by replacing $\boldsymbol{N}$ in (6.1c) by the derivative $\mathcal{P}'_\varepsilon$. The inclusion (6.1c) turns into the equation

$$\boldsymbol{\mu}=\frac{[\phi^{\boldsymbol{\xi}}_{\mathrm{ref}}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J}+\mathcal{P}'_\varepsilon(\boldsymbol{c})\,. \tag{6.10}$$

This choice also regularizes the reaction terms $\boldsymbol{r}$ as

$$\boldsymbol{r}^{\boldsymbol{\xi}}_\varepsilon=\mathbb{K}^{\boldsymbol{\xi}}\boldsymbol{\mu}=\mathbb{K}^{\boldsymbol{\xi}}\Big(\frac{1}{J}[\phi^{\boldsymbol{\xi}}_{\mathrm{ref}}]'_{\boldsymbol{c}}(J,\boldsymbol{c})+\mathcal{P}'_\varepsilon(\boldsymbol{c})\Big). \tag{6.11}$$

The weak solution of the boundary-value problem for the system (6.1a,b,d,e) and (6.10) with the boundary conditions (3.6) together with $(\boldsymbol{n}\cdot\nabla)\boldsymbol{\mu} = \mathbf{0}$ on $\partial\Omega$ and the initial condition (6.7) will be denoted by $(\boldsymbol{v}_\varepsilon, \boldsymbol{c}_\varepsilon, \boldsymbol{\mu}_\varepsilon, \boldsymbol{\xi}_\varepsilon, V_\varepsilon)$. Its existence is proved in Step 4 below.

Step 2: semi-Galerkin approximation. We perform a Galerkin approximation of the momentum equation (6.1) for $\boldsymbol{v}$ as in Section 5 and of the diffusion equation (6.1b) for $\boldsymbol{c}$. On the other hand, we do not approximate in space the transport equation (6.1d) for $\boldsymbol{\xi}$ but rather rely on [RoS22, Lemma 3.2] for its weak solvability. Moreover, we do not approximate neither the Poisson equation (6.1e) nor the regularized nonlinear equation (6.10).

Specifically, we again use a nested finite-dimensional subspaces $\{\mathscr{V}_k\}_{k=0}^\infty$ for the momentum equation (6.1a). For the Galerkin approximation of the diffusion equation (6.1b) we use a second collection of nested finite-dimensional subspaces $\{\mathscr{Z}_k\}_{k=0}^\infty$ whose union is dense in $H^1(\Omega;\mathbb{R}^n)$. Without loss of generality, we may assume $\boldsymbol{v}_0 \in \mathscr{V}_0$ and $\boldsymbol{c}_0 \in \mathscr{Z}_0$.

We directly substitute $\boldsymbol{\mu}$ from (6.10) into (6.1b) to obtain a parabolic equation for $\boldsymbol{c}_\varepsilon$. It should be emphasized that the physically motivated tests leading to the discrete energy-dissipation balance (6.6) cannot be performed at the Galerkin-discretization level because $\dot{\boldsymbol{c}}_{\varepsilon k} = \frac{\partial}{\partial t}\boldsymbol{c}_{\varepsilon k} + (\boldsymbol{v}_{\varepsilon k}\cdot\nabla)\boldsymbol{c}_{\varepsilon k}$ is not a legitimate test for the discretized equation for $\boldsymbol{\mu}_{\varepsilon k}$. This calls for implementing another estimation strategy. Moving from (6.10) we have that

$$\begin{aligned}\nabla\boldsymbol{\mu} = {}&\Big(\frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]''_{\boldsymbol{cc}}(J,\boldsymbol{c})}{J} + \mathcal{P}''_\varepsilon(\boldsymbol{c})\Big)\nabla\boldsymbol{c}\\ &+ \Big(\frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]''_{J\boldsymbol{c}}(J,\boldsymbol{c})}{J} - \frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J^2}\Big)\nabla J + \frac{[[\phi_{\rm ref}]''_{\boldsymbol{X}\boldsymbol{c}}]^{\boldsymbol{\xi}}(J,\boldsymbol{c})}{J}\nabla\boldsymbol{\xi}\end{aligned} \tag{6.12}$$

so that, by substituting (6.10) into (6.1b) we obtain the semilinear parabolic equation for $\boldsymbol{c}_{\varepsilon k}$:

$$\begin{aligned}\frac{\partial\boldsymbol{c}_{\varepsilon k}}{\partial t} - {\rm div}\big(M_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla\boldsymbol{c}_{\varepsilon k}\big) = {}&{\rm div}\Big(R_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla J_{\varepsilon k}\\ &+S_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla\boldsymbol{\xi}_{\varepsilon k}\Big) - (\boldsymbol{v}_{\varepsilon k}\cdot\nabla)\boldsymbol{c}_{\varepsilon k} - \boldsymbol{r}^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\\ \text{with }\ R_\varepsilon(\boldsymbol{X},J,\boldsymbol{c}) := {}& M_\varepsilon(\boldsymbol{X},J,\boldsymbol{c})\Big(\frac{[\phi_{\rm ref}]''_{J\boldsymbol{c}}(\boldsymbol{X},J,\boldsymbol{c})}{J} - \frac{[\phi_{\rm ref}]'_{\boldsymbol{c}}(\boldsymbol{X},J,\boldsymbol{c})}{J^2}\Big),\\ S_\varepsilon(\boldsymbol{X},J,\boldsymbol{c}) := {}& M_\varepsilon(\boldsymbol{X},J,\boldsymbol{c})\frac{[\phi_{\rm ref}]''_{\boldsymbol{X}\boldsymbol{c}}(\boldsymbol{X},J,\boldsymbol{c})}{J}\,,\quad\text{and}\\ M_\varepsilon(\boldsymbol{X},J,\boldsymbol{c}) := {}& \mathbb{M}(\boldsymbol{X},J,\boldsymbol{c})\Big(\frac{[\phi_{\rm ref}]''_{\boldsymbol{cc}}(\boldsymbol{X},J,\boldsymbol{c})}{J} + \mathcal{P}''_\varepsilon(\boldsymbol{c})\Big)^{-1}.\end{aligned} \tag{6.13}$$

The global existence on the whole time interval $I = [0,T]$ of a solution of such regularized and semi-discretized system, which we denote by

$$(\boldsymbol{v}_{\varepsilon k}, \boldsymbol{c}_{\varepsilon k}, \boldsymbol{\xi}_{\varepsilon k}, V_{\varepsilon k}) : I \to \mathscr{V}_k \times \mathscr{Z}_k \times W^{2,r}(\Omega;\mathbb{R}^d) \times H^1(U),$$

results from a standard successive-prolongation argument, on the basis of the uniform-in-time estimates proved below.

Step 3: first a-priori estimates. We first test (6.1a,e) separately. Specifically, we test the Galerkin discretization of (6.1a) by $\boldsymbol{v}_{\varepsilon k}$ and test (6.1e) by $V_{\varepsilon k}$, also using (6.1d). The discretized velocity field $\boldsymbol{v}_{\varepsilon k}$ is in $L^2(I;W^{1,\infty}(\Omega;\mathbb{R}^d))$ so that $J_{\varepsilon k} = 1/\det(\nabla\boldsymbol{\xi}_{\varepsilon k})$, which fulfills the non-discretized transport-and-evolution equation (5.4), stays positive on $I\times\Omega$. Here, assumption (5.2e) has been used [RoS22, Lemma 3.2].

By arguing as in (5.5), abbreviating $\overline{\nu}_i = \inf \nu_i(\boldsymbol{X}, \boldsymbol{c})$ with $i = 1, 2$, and using also (4.5) for $\phi_{\mathrm{r},0}$ in place of ϕ_{ref} and assumption (6.9a), we obtain

$$
\begin{aligned}
&\int_\Omega \frac{\varrho_{\varepsilon k}}{2}|\boldsymbol{v}_{\varepsilon k}|^2 + \frac{\epsilon}{J_{\varepsilon k}^{\alpha+1}(t)}\mathrm{d}\boldsymbol{x} + \int_U \frac{|\nabla V_{\varepsilon k}(t)|^2}{2G}\mathrm{d}\boldsymbol{x} + \int_0^t\!\!\int_\Omega \overline{\nu}_1|\boldsymbol{e}(\boldsymbol{v}_{\varepsilon k})|^2 + \overline{\nu}_2|\nabla\boldsymbol{e}(\boldsymbol{v}_{\varepsilon k})|^q \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \\
&\overset{(5.2)}{\le} \int_\Omega \frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}_{\varepsilon k}(t)}}{2J_{\varepsilon k}(t)}|\boldsymbol{v}_{\varepsilon k}(t)|^2 + \frac{\phi_{\mathrm{r},0}^{\boldsymbol{\xi}_{\varepsilon k}(t)}(J_{\varepsilon k}(t))}{J_{\varepsilon k}(t)}\mathrm{d}\boldsymbol{x} \\
&\qquad\qquad + \int_U \frac{|\nabla V_{\varepsilon k}(t)|^2}{2G}\,\mathrm{d}\boldsymbol{x} + \int_0^t\!\!\int_\Omega \nu_1^{\boldsymbol{\xi}_{\varepsilon k}}(\boldsymbol{c}_{\varepsilon k})|\boldsymbol{e}(\boldsymbol{v}_{\varepsilon k})|^2 + \nu_2^{\boldsymbol{\xi}_{\varepsilon k}}(\boldsymbol{c}_{\varepsilon k})|\nabla\boldsymbol{e}(\boldsymbol{v}_{\varepsilon k})|^q \,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \\
&\overset{(5.5)}{=} \int_0^t\!\!\int_{U\setminus\Omega} \frac{\partial\varrho_{\mathrm{ext}}}{\partial t}V_{\varepsilon k} + \big[\phi_{\mathrm{r},1}^{\boldsymbol{\xi}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\big]_J'\mathrm{div}\,\boldsymbol{v}_{\varepsilon k}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t - \int_\Omega \frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}_{\varepsilon k}(t)}}{J_{\varepsilon k}(t)}V_{\varepsilon k}(t)\,\mathrm{d}\boldsymbol{x} - \int_{U\setminus\Omega}\varrho_{\mathrm{ext}}(t)V_{\varepsilon k}(t)\,\mathrm{d}\boldsymbol{x} \\
&\quad + \int_\Omega \frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}_0}}{J_0}V_{\varepsilon k}(0) + \frac{\rho_{\mathrm{ref}}^{\boldsymbol{\xi}_0}}{J_0}|\boldsymbol{v}_0|^2 + \frac{\phi_{\mathrm{r},0}^{\boldsymbol{\xi}_0}(J_0)}{J_0}\,\mathrm{d}\boldsymbol{x} + \int_{U\setminus\Omega}\varrho_{\mathrm{ext}}(0)V_{\varepsilon k}(0)\,\mathrm{d}\boldsymbol{x} + \int_U \frac{|\nabla V_{\varepsilon k}(0)|^2}{2G}\,\mathrm{d}\boldsymbol{x} \\
&\le C_\delta + \|\varrho_{\mathrm{ext}}(t)\|_{L^{6/5}(U\setminus\Omega)}^{6/5} + \delta\Big\|\frac{1}{J_{\varepsilon k}^{\alpha+1}(t)}\Big\|_{L^1(\Omega)} + \delta\|\nabla V_{\varepsilon k}(t)\|_{L^2(U;\mathbb{R}^3)}^2 \\
&\quad + \int_0^t \bigg(\Big\|\frac{\partial\varrho_{\mathrm{ext}}}{\partial t}\Big\|_{L^{6/5}(U\setminus\Omega)}^{6/5}\big(1+\|\nabla V_{\varepsilon k}\|_{L^2(U;\mathbb{R}^3)}^2\big) + \frac{1}{\epsilon}\Big\|\frac{1}{\epsilon J_{\varepsilon k}^{\alpha+1}}\Big\|_{L^1(\Omega)} + \big\|\mathrm{div}\,\boldsymbol{v}_{\varepsilon k}\big\|_{L^2(\Omega)}^2\bigg)\,\mathrm{d}t\,.
\end{aligned}
$$

From this, taking $\delta > 0$ sufficiently small and using the Gronwall inequality, we obtain the a-priori bounds

$$
\|\boldsymbol{v}_{\varepsilon k}\|_{L^q(I;W^{2,q}(\Omega;\mathbb{R}^3))} \le C_\varepsilon, \tag{6.14a}
$$

$$
\|V_{\varepsilon k}\|_{L^\infty(I;H^1(U))} \le C_\varepsilon\,. \tag{6.14b}
$$

From the equations for $\boldsymbol{\xi}$ and J and assumption (5.2e), by using [RoS22, Lemma 3.2] we also obtain

$$
\|\boldsymbol{\xi}_{\varepsilon k}\|_{L^\infty(I;W^{2,r}(\Omega;\mathbb{R}^3))} \le C_\varepsilon\,, \quad \|J_{\varepsilon k}\|_{L^\infty(I;W^{1,r}(\Omega))} \le C_\varepsilon\,, \ \text{ and } \ \min J_{\varepsilon k} > 1/C_\varepsilon\,. \tag{6.14c}
$$

It should be noted that C_ε here depends possibly on ε but is independent of k. From (6.14c), we also obtain a bound for $\varrho_{\varepsilon k} = \rho_{\mathrm{ref}}^{\boldsymbol{\xi}_{\varepsilon k}}/J_{\varepsilon k}$ in $L^\infty(I;W^{1,r}(\Omega))$.

Next, we test the parabolic equation (6.13) by $\boldsymbol{c}_{\varepsilon k}$. From (6.14), we have that $R^{\boldsymbol{\xi}_{\varepsilon k}}$ is bounded in $L^\infty(I\times\Omega;\mathbb{R}^{n\times 3}))$. Using the Green formula for

$$
\int_\Omega ((\boldsymbol{v}\cdot\nabla)\boldsymbol{c})\cdot\boldsymbol{c}\,\mathrm{d}\boldsymbol{x} = -\frac{1}{2}\int_\Omega (\mathrm{div}\,\boldsymbol{v})|\boldsymbol{c}|^2\mathrm{d}\boldsymbol{x}
$$

and the assumption (6.9c), this test gives

$$
\begin{aligned}
&\int_\Omega \frac{|\boldsymbol{c}_{\varepsilon k}(t)|^2}{2}\,\mathrm{d}\boldsymbol{x} + \int_0^t\!\!\int_\Omega M_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla\boldsymbol{c}_{\varepsilon k}{:}\nabla\boldsymbol{c}_{\varepsilon k}\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \\
&= \int_0^t\!\!\int_\Omega R_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla J_{\varepsilon k}{:}\nabla\boldsymbol{c}_{\varepsilon k} - \boldsymbol{r}_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\cdot\boldsymbol{c}_{\varepsilon k} - \frac{1}{2}(\mathrm{div}\,\boldsymbol{v}_{\varepsilon k})|\boldsymbol{c}_{\varepsilon k}|^2\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \\
&\le \int_0^t \bigg(\delta\|\nabla\boldsymbol{c}_{\varepsilon k}\|_{L^2(\Omega;\mathbb{R}^{n\times 3})}^2 + \frac{1}{4\delta}\|R_\varepsilon^{\boldsymbol{\xi}_{\varepsilon k}}(J_{\varepsilon k},\boldsymbol{c}_{\varepsilon k})\nabla J_{\varepsilon k}\|_{L^2(\Omega;\mathbb{R}^{n\times 3})}^2
\end{aligned}
$$

$$+ C_\varepsilon\big(|\Omega| + \|\boldsymbol{c}_{\varepsilon k}\|^2_{L^2(\Omega;\mathbb{R}^n)}\big) + \|\mathrm{div}\, \boldsymbol{v}_{\varepsilon k}\|_{L^\infty(\Omega)}\|\boldsymbol{c}_{\varepsilon k}\|^2_{L^2(\Omega;\mathbb{R}^n)}\bigg)\,\mathrm{d}t\,. \tag{6.15}$$

Here we estimated $|\boldsymbol{r}^{\boldsymbol{\xi}}_\varepsilon| = \big|\mathbb{K}^{\boldsymbol{\xi}}\,\big(\frac{1}{J_\varepsilon}[\phi_{\mathrm{r},1}]'_{\boldsymbol{c}} + \mathcal{P}'_\varepsilon(\boldsymbol{c})\big)\big| \le C_\varepsilon(1+|\boldsymbol{c}|)$ by using that $|\mathbb{K}| \le C$ from (6.9c), $|[\phi_{\mathrm{r},1}]'_{\boldsymbol{c}}| \le C(1+|\boldsymbol{c}|)$ from (6.9a), and $|\mathcal{P}'_\varepsilon(\boldsymbol{c})| \le C(1+|\boldsymbol{c}|)/\varepsilon$ and by exploiting estimate (6.14c).

By the uniform positive definiteness of $M_\varepsilon(\cdot,\cdot)$, choosing $\delta > 0$ sufficiently small and exploiting the Gronwall inequality, we also obtain

$$\|\boldsymbol{c}_{\varepsilon k}\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^n))\,\cap\, L^2(I;H^1(\Omega;\mathbb{R}^n))} \le C\,. \tag{6.16}$$

From (6.10) and (6.12), we obtain the bound for $\boldsymbol{\mu}_{\varepsilon k}$ in $L^\infty(I;L^2(\Omega;\mathbb{R}^n)) \,\cap\, L^2(I;H^1(\Omega;\mathbb{R}^n))$ uniformly in k, depending possibly on $\varepsilon > 0$.

Step 4: limit passage for $k \to \infty$. By the Banach selection principle, we select a weakly* convergent subsequence and $(\varrho_\varepsilon, \boldsymbol{v}_\varepsilon, \boldsymbol{\xi}_\varepsilon, J_\varepsilon, V_\varepsilon, \boldsymbol{c}_\varepsilon, \boldsymbol{\mu}_\varepsilon)$ such that the convergences (5.8) (still for fixed value

$\varepsilon > 0$) hold, together with

$$\boldsymbol{c}_{\varepsilon k} \to \boldsymbol{c}_\varepsilon \qquad \text{weakly* in } L^\infty(I;L^2(\Omega;\mathbb{R}^n)) \,\cap\, L^2(I;H^1(\Omega;\mathbb{R}^n))\,, \tag{6.17a}$$

$$\boldsymbol{\mu}_{\varepsilon k} \to \boldsymbol{\mu}_\varepsilon \qquad \text{weakly* in } L^\infty(I;L^2(\Omega;\mathbb{R}^n)) \,\cap\, L^2(I;H^1(\Omega;\mathbb{R}^n))\,. \tag{6.17b}$$

From (6.13), we deduce a bound on $\frac{\partial}{\partial t}\boldsymbol{c}_{\varepsilon k}$ in the respective semi-norms induced by the Faedo-Galerkin discretization by the finite-dimensional subspaces $\mathscr{Z}_k$. By the (generalized) Aubin-Lions theorem, we obtain the strong convergence $\boldsymbol{c}_{\varepsilon k} \to \boldsymbol{c}_\varepsilon$ in $L^s(I{\times}\Omega;\mathbb{R}^n)$ for any $1 \le s < 10/3$. From (6.10), such strong convergence also holds for $\boldsymbol{\mu}_{\varepsilon k} \to \boldsymbol{\mu}_\varepsilon$.

Adapting the argument leading to (5.8)–(5.11) towards the weak formulation of (6.1b) with (6.10) is then easy.

Step 5: "physically motivated" a-priori estimates. As $\boldsymbol{c}_\varepsilon$ is not discretized, we can test (6.10) by $\dot{\boldsymbol{c}}_\varepsilon = \frac{\partial}{\partial t}\boldsymbol{c}_\varepsilon + (\boldsymbol{v}_\varepsilon{\cdot}\nabla)\boldsymbol{c}_\varepsilon$. Together with the other tests, we thus obtain the analogous energy-dissipation balance to (6.6), now for the ε-solution and with the additional left-hand-side term $\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \mathcal{P}_\varepsilon(\boldsymbol{c}_\varepsilon)\,\mathrm{d}\boldsymbol{x}$. This delivers a-priori estimates, similarly as those obtained in (5.5), with the additional energy estimate

$$\int_\Omega \mathcal{P}_\varepsilon\big(\boldsymbol{c}_\varepsilon(t,\boldsymbol{x})\big)\,\mathrm{d}\boldsymbol{x} \le C \quad \text{for all } t \in I. \tag{6.18}$$

Let us introduce now the orthogonal projection $\mathbb{P} : \mathbb{R}^n \to \mathbb{R}^n$ to the subspace $\{\boldsymbol{\mu} \in \mathbb{R}^n \,|\, \sum_1^n \mu_i = 0\}$, namely,

$$(\mathbb{P}\boldsymbol{\mu})_i = \mu_i - \frac{1}{n}\sum_{j=1}^n \mu_j = \frac{1}{n}\sum_{j=1}^n (\mu_i - \mu_j) \quad \text{for } i = 1,\dots,j,$$

so that

$$\mathbb{P}\boldsymbol{\mu} = \boldsymbol{\mu} - \Big(\frac{1}{n}\sum_{j=1}^n \mu_j\Big)\mathbf{1} = \boldsymbol{\mu} - \frac{1}{n}(\boldsymbol{\mu}{\cdot}\mathbf{1})\mathbf{1}.$$

Taking into account (6.9c) so that specifically $\mathbb{K}\mathbf{1} = \mathbf{0}$, the reaction term in the estimate gives

$$\int_0^T\!\!\int_\Omega \boldsymbol{r}^{\boldsymbol{\xi}_\varepsilon}_\varepsilon(J_\varepsilon,\boldsymbol{c}_\varepsilon){\cdot}\boldsymbol{\mu}_\varepsilon\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t = \int_0^T\!\!\int_\Omega \boldsymbol{\mu}_\varepsilon{\cdot}\mathbb{K}\boldsymbol{\mu}_\varepsilon\,\mathrm{d}\boldsymbol{x}\mathrm{d}t = \int_0^T\!\!\int_\Omega \mathbb{P}\boldsymbol{\mu}_\varepsilon{\cdot}\mathbb{K}\,\mathbb{P}\boldsymbol{\mu}_\varepsilon\,\mathrm{d}\boldsymbol{x}\mathrm{d}t \ge \epsilon\int_0^T\!\!\int_\Omega |\mathbb{P}\boldsymbol{\mu}_\varepsilon|^2\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t.$$

We thus obtain estimates as in (6.14), but for ε-solution, together with additional estimates

$$\|\mathbb{P}\boldsymbol{\mu}_\varepsilon\|_{L^2(I\times\Omega;\mathbb{R}^n)} + \|\nabla\boldsymbol{\mu}_\varepsilon\|_{L^2(I\times\Omega;\mathbb{R}^{n\times3})} \le C\,, \quad \|\boldsymbol{c}_\varepsilon\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^n))} \le C\,, \tag{6.19a}$$

$$\Big\|\sum_{i=1}^n c_{i,\varepsilon} - 1\Big\|_{L^\infty(I;L^2(\Omega))} \le C\sqrt{\varepsilon}\,, \ \text{ and} \tag{6.19b}$$

$$\|\min(0,c_{i,\varepsilon})\|_{L^\infty(I;L^2(\Omega))} \le C\sqrt{\varepsilon} \quad \text{for any } \ i=1,...,n\,, \tag{6.19c}$$

where the constants C are independent of ε. Note in addition that the projection $\mathbb{P}$ commutes with differentiation, namely $\nabla\mathbb{P}\boldsymbol{\mu}_\varepsilon = \mathbb{P}\nabla\boldsymbol{\mu}_\varepsilon$, where the latter projection is intended column-wise. This fact and (6.19a) in particular ensure that

$$\|\mathbb{P}\boldsymbol{\mu}_\varepsilon\|_{L^2(I;H^1(\Omega;\mathbb{R}^n))} \le C\,, \tag{6.19d}$$

Moreover, using (6.12) written in the equivalent form

$$\nabla\boldsymbol{c}_\varepsilon = \Big(\frac{[\phi_{\rm ref}^{\boldsymbol{\xi}}]''_{\boldsymbol{c}\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J} + \mathcal{P}''_\varepsilon(\boldsymbol{c}_\varepsilon)\Big)^{-1}\bigg(\nabla\boldsymbol{\mu}_\varepsilon - \frac{J_\varepsilon[\phi_{\rm ref}^{\boldsymbol{\xi}}]''_{J\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon) - [\phi_{\rm ref}^{\boldsymbol{\xi}}]'_{\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J^2}\nabla J_\varepsilon - \frac{[[\phi_{\rm ref}]''_{\boldsymbol{X}\boldsymbol{c}}]^{\boldsymbol{\xi}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J_\varepsilon}\nabla\boldsymbol{\xi}\bigg)\,,$$

we obtain the estimate

$$\|\nabla\boldsymbol{c}_\varepsilon\|_{L^2(I\times\Omega;\mathbb{R}^{n\times3})} \le C \tag{6.19e}$$

independently of $\varepsilon>0$. In addition, (6.19a) allow for using (6.1b) written for ε-solution to obtain the estimate

$$\Big\|\frac{\partial\boldsymbol{c}_\varepsilon}{\partial t}\Big\|_{L^2(I;H^1(\Omega;\mathbb{R}^n)^*)} \le C\,. \tag{6.19f}$$

Here, the bound on $\nabla\boldsymbol{\mu}_\varepsilon$ from (6.19a) is used.

Step 6: convergence for $\varepsilon\to0$. As in Step 4, we select a weakly* convergent subsequence and find $(\varrho,\boldsymbol{v},\boldsymbol{\xi}, V,\boldsymbol{c},\boldsymbol{\mu})$ such that

$$\varrho_\varepsilon \to \varrho \qquad \text{weakly* in } \ L^\infty(I;W^{1,r}(\Omega)) \,\cap\, W^{1,p}(I;L^r(\Omega))\,, \tag{6.20a}$$

$$\boldsymbol{v}_\varepsilon \to \boldsymbol{v} \qquad \text{weakly* in } \ L^\infty(I;W^{2,r}(\Omega;\mathbb{R}^3)) \,\cap\, W^{1,p}(I;L^2(\Omega;\mathbb{R}^3))\,, \tag{6.20b}$$

$$\boldsymbol{\xi}_\varepsilon \to \boldsymbol{\xi} \qquad \text{weakly* in } \ L^\infty(I;W^{2,r}(\Omega;\mathbb{R}^3)) \,\cap\, W^{1,p}(I;L^2(\Omega;\mathbb{R}^3))\,, \tag{6.20c}$$

$$V_\varepsilon \to V \qquad \text{weakly* in } \ L^\infty(I;H^2(U)) \,\cap\, BV(I;W^{2,6/5}(U))\,, \tag{6.20d}$$

$$\boldsymbol{c}_\varepsilon \to \boldsymbol{c} \qquad \text{weakly in } \ L^2(I;H^1(\Omega;\mathbb{R}^n)) \,\cap\, H^1(I;H^1(\Omega;\mathbb{R}^n)^*)\,, \tag{6.20e}$$

$$\mathbb{Q}\boldsymbol{\mu}_\varepsilon \to \boldsymbol{\mu} \qquad \text{weakly in } \ L^2(I;H^1(\Omega;\mathbb{R}^n))\,, \tag{6.20f}$$

where $\boldsymbol{\mu}(t,\cdot)=\mathbb{Q}\boldsymbol{\mu}(t,\cdot)$ and the projection $\mathbb{Q}: L^2(\Omega;\mathbb{R}^n)\to L^2(\Omega;\mathbb{R}^n)$ is defined via

$$(\mathbb{Q}\boldsymbol{\mu})(x) = \boldsymbol{\mu}(x) - \bigg(\frac{1}{n|\Omega|}\int_\Omega \boldsymbol{\mu}(y)\cdot\mathbf{1}\,{\rm d}y\bigg)\mathbf{1}.$$

To justify convergence (6.20f) we observe that $\int_\Omega \big(|\nabla\boldsymbol{\mu}|^2{+}|\mathbb{P}\boldsymbol{\mu}|^2\big)\mathrm{d}\boldsymbol{x} = 0$ implies first, by using $\nabla\boldsymbol{\mu} = 0$ that $\boldsymbol{\mu}(x) = \boldsymbol{\eta}$ for a constant vector $\boldsymbol{\eta} \in \mathbb{R}^n$. Second, using $\mathbb{P}\boldsymbol{\eta} = 0$ we have $\boldsymbol{\eta} = \alpha\mathbf{1}$ for a constant $\alpha \in \mathbb{R}$. Hence, we have $\mathbb{Q}\boldsymbol{\mu} = 0$. Thus, by repeating the classical compactness argument for showing Poincaré's inequality, we find a constant $c_\mathbb{Q} > 0$ such that

$$\forall\,\boldsymbol{\mu} \in H^1(\Omega;\mathbb{R}^n) \text{ with } \mathbb{Q}\boldsymbol{\mu} = 0: \quad \int_\Omega \big(|\nabla\boldsymbol{\mu}|^2 + |\mathbb{P}\boldsymbol{\mu}|^2\big)\,\mathrm{d}\boldsymbol{x} \geq c_\mathbb{Q}\|\boldsymbol{\mu}\|^2_{H^1(\Omega;\mathbb{R}^n)}.$$

Thus, with (6.19a) we obtain the a priori estimate

$$\|\mathbb{Q}\boldsymbol{\mu}_\varepsilon\|_{L^2(I;H^1(\Omega;R^n))} \leq C$$

and (6.20f) follows. The Aubin-Lions lemma and (6.20c) and (6.20e) yield the strong convergences

$$\boldsymbol{\xi}_\varepsilon \to \boldsymbol{\xi} \quad \text{strongly in } C(I{\times}\overline{\Omega};\mathbb{R}^3)\,, \tag{6.21a}$$

$$J_\varepsilon \to J \quad \text{strongly in } C(I{\times}\overline{\Omega})\,, \tag{6.21b}$$

$$\boldsymbol{c}_\varepsilon \to \boldsymbol{c} \quad \text{strongly in } L^s(I{\times}\Omega;\mathbb{R}^n)\ \ \forall 1 \leq s < 6\,. \tag{6.21c}$$

In addition to the argument used for proving Theorem 6.2, we need to pass to the limit in the semi-linear transport-and-diffusion equation (6.1b) formulated weakly. This is however straightforward, so that we omit details.

The only remaining issue is to pass to the limit in (6.10) written at level ε in the form of the variational inequality

$$\int_0^T\!\!\int_\Omega \mathcal{P}_\varepsilon(\boldsymbol{c}_\varepsilon) + \Big(\boldsymbol{\mu}_\varepsilon - \frac{[\phi_{\mathrm{ref}}^{\boldsymbol{\xi}_\varepsilon}]'_{\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J_\varepsilon}\Big)\cdot(\widetilde{\boldsymbol{c}}_\varepsilon - \boldsymbol{c}_\varepsilon)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \leq \int_0^T\!\!\int_\Omega \mathcal{P}_\varepsilon(\widetilde{\boldsymbol{c}}_\varepsilon)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \tag{6.22}$$

for $i = 1,...,n$, for all $\widetilde{\boldsymbol{c}}_\varepsilon \in L^2(I{\times}\Omega;\mathbb{R}^n)$. The bounds (6.19b,c) entail that the limit $\boldsymbol{c}$ is valued in $\triangle_1^+$ almost everywhere in $I \times \Omega$. We aim at proving that $\boldsymbol{c}$ satisfies

$$\int_0^T\!\!\int_\Omega \Big(\boldsymbol{\mu} - \frac{[\phi_{\mathrm{ref}}^{\boldsymbol{\xi}}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J}\Big)\cdot(\widehat{\boldsymbol{c}} - \boldsymbol{c})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t \leq 0 \tag{6.23}$$

for all $\widehat{\boldsymbol{c}} \in L^2(I{\times}\Omega;\mathbb{R}^n)$ valued in $\triangle_1^+$ a.e. on $I{\times}\Omega$. We first observe that (6.19b) allows to write

$$\boldsymbol{c}_\varepsilon(t,x) = \frac{1+\alpha_\varepsilon(t)}{n}\mathbf{1} + \big(\mathbb{Q}\boldsymbol{c}_\varepsilon\big)(t,x), \quad \text{where } \|\alpha_\varepsilon\|_{L^\infty(I)} \leq C\sqrt{\varepsilon}.$$

To construct good test function $\widetilde{\boldsymbol{c}}_\varepsilon$ for (6.22) we fix a small $\delta > 0$ and choose $\widehat{\boldsymbol{c}}$ with

$$\widehat{\boldsymbol{c}}(t,x) \in \triangle_1^+ \text{ and } \min \widehat{c}_i(t,x) \geq \delta \quad \text{and set } \widetilde{\boldsymbol{c}}_\varepsilon = \frac{\alpha_\varepsilon(t)}{n}\mathbf{1} + \widehat{\boldsymbol{c}}.$$

In particular, we have $\widetilde{\boldsymbol{c}}_\varepsilon - \boldsymbol{c}_\varepsilon = \mathbb{Q}\big(\widehat{\boldsymbol{c}} - \boldsymbol{c}_\varepsilon\big)$. By using the weak convergences (6.20e,f) and the strong convergences (6.21), we obtain

$$\int_0^T\!\!\int_\Omega \Big(\boldsymbol{\mu}_\varepsilon - \frac{[\phi_{\mathrm{ref}}^{\boldsymbol{\xi}_\varepsilon}]'_{\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J_\varepsilon}\Big)\cdot(\widetilde{\boldsymbol{c}}_\varepsilon - \boldsymbol{c}_\varepsilon)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t = \int_0^T\!\!\int_\Omega \Big(\mathbb{Q}\boldsymbol{\mu}_\varepsilon - \mathbb{Q}\frac{[\phi_{\mathrm{ref}}^{\boldsymbol{\xi}_\varepsilon}]'_{\boldsymbol{c}}(J_\varepsilon,\boldsymbol{c}_\varepsilon)}{J_\varepsilon}\Big)\cdot(\widehat{\boldsymbol{c}} - \boldsymbol{c}_\varepsilon)\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$

$$\longrightarrow \int_0^T\!\!\int_\Omega \Big(\boldsymbol{\mu} - \mathbb{Q}\frac{[\phi^{\boldsymbol{\xi}}_{\rm ref}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J}\Big)\cdot(\widehat{\boldsymbol{c}}-\boldsymbol{c})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t = \int_0^T\!\!\int_\Omega \Big(\boldsymbol{\mu} - \frac{[\phi^{\boldsymbol{\xi}}_{\rm ref}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J}\Big)\cdot\mathbb{Q}(\widehat{\boldsymbol{c}}-\boldsymbol{c})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t$$
$$= \int_0^T\!\!\int_\Omega \Big(\boldsymbol{\mu} - \frac{[\phi^{\boldsymbol{\xi}}_{\rm ref}]'_{\boldsymbol{c}}(J,\boldsymbol{c})}{J}\Big)\cdot(\widehat{\boldsymbol{c}}-\boldsymbol{c})\,\mathrm{d}\boldsymbol{x}\,\mathrm{d}t\,,$$

where we have also used $\mathbb{Q}(\widehat{\boldsymbol{c}}-\boldsymbol{c}) = \widehat{\boldsymbol{c}}-\boldsymbol{c}$, coming from the fact that $\boldsymbol{c}$, $\widehat{\boldsymbol{c}} \in \triangle_1^+$.

Moreover, our construction guarantees $\widetilde{c}_{\varepsilon,i}(t,x) = \alpha_\varepsilon(t)/n + \widehat{c}_i(t,x) \geq -C\sqrt{\varepsilon}+\delta \geq 0$ for sufficiently small $\varepsilon > 0$. Hence, we have $\mathcal{P}_\varepsilon(\widetilde{\boldsymbol{c}}_\varepsilon) = \big(\alpha_\varepsilon + \widehat{\boldsymbol{c}}\cdot\mathbf{1} - 1\big)^2/(2\varepsilon) = \alpha_\varepsilon^2/(2\varepsilon)$ since $\widehat{\boldsymbol{c}} \in \triangle_1^+$. With this, $\mathcal{P}_\varepsilon(\boldsymbol{c}_\varepsilon) \geq (\boldsymbol{c}_\varepsilon\cdot\mathbf{1}-1)^2/(2\varepsilon)$, and $\alpha_\varepsilon(t) = \frac{1}{|\Omega|}\int_\Omega \big(\boldsymbol{c}_\varepsilon(t,y)\cdot\mathbf{1}-1\big)\,\mathrm{d}y$ we find

$$\int_0^T\!\!\int_\Omega \big(\mathcal{P}_\varepsilon(\boldsymbol{c}_\varepsilon) - \mathcal{P}_\varepsilon(\widetilde{\boldsymbol{c}}_\varepsilon)\big)\,\mathrm{d}x\,\mathrm{d}t \geq \frac{1}{2\varepsilon}\int_0^T\!\!\int_\Omega \Big(\big(\boldsymbol{c}_\varepsilon\cdot\mathbf{1}-1\big)^2 - \big(\alpha_\varepsilon\big)^2\Big)\,\mathrm{d}x\,\mathrm{d}t \;\geq\; \frac{1}{2\varepsilon}\int_0^T 0\,\mathrm{d}t = 0.$$

Hence, by collecting all terms on the left-hand side, we can pass to the $\liminf \varepsilon \to 0$ in (6.22) and obtain (6.23) for all $\widehat{\boldsymbol{c}}$ satisfying $\min \widehat{c}_i(t,x) \geq \delta$. Since $\delta > 0$ was arbitrary, the desired variational inequality (6.23) holds for all test functions.

Step 7: energy-dissipation balance. In addition to the argumentation used in the proof of Theorem 5.2(ii), we now use that $\frac{\partial}{\partial t}\boldsymbol{c} + (\boldsymbol{v}\cdot\nabla)\boldsymbol{c} \in L^2(I;H^1(\Omega;\mathbb{R}^n)^*)$. Note also that $(\boldsymbol{v}\cdot\nabla)\boldsymbol{c}$ lies in $L^2(I;L^2(\Omega;\mathbb{R}^n))$ and can be tested by $\boldsymbol{\mu}$ and integrated by parts. Here the indeterminacy of $\boldsymbol{\mu}$ with respect to spatially constant multiples of $\mathbf{1}$ does not matter, because from $\boldsymbol{c}(t,x) \in \triangle_1^+$ we have $\boldsymbol{c}(t,\boldsymbol{x})\cdot\mathbf{1} = 0$ in $I\times\Omega$. Thus, the energy balance follows as for Theorem 5.2(ii). □

Remark 6.3 (*Composition-dependent mass density*). It would be desirable to make the mass density depends also on composition, cf. e.g. [Ger19, Ch.2]. In our present modeling level, this would mean $\rho_{\rm ref} = \rho_{\rm ref}(\boldsymbol{X},\boldsymbol{c})$ and hence, by (3.1) we would have $\varrho = \rho^{\boldsymbol{\xi}}_{\rm ref}(\boldsymbol{c})/J$. Repeating the calculation in (2.2) and (2.3) continuity equation (3.2) would be extended to

$$\dot{\varrho} + (\operatorname{div}\boldsymbol{v})\varrho = \frac{[\varrho^{\boldsymbol{\xi}}_{\rm ref}]'_{\boldsymbol{c}}(\boldsymbol{c})}{J}\cdot\dot{\boldsymbol{c}}\,. \tag{6.24}$$

Thus, the principle of mass conservation would be violated, and further mathematical difficulties would arise in the kinetic energy and the gravitational energy (3.10). Hence, a proper modeling of a concentration-dependent mass density would need a truly multiphase modeling that exceeds beyond the Eckart-Prigogine approximation and is left to future research.

Remark 6.4 (*An alternative approach*). Keeping the sum of diffusion fluxes to 0 can also be achieved without directly constraining $\sum_{j=1}^n c_j = 1$ by tuning the mobility matrix to satisfy $\sum_{j=1}^n \mathbb{M}_{ij}(\boldsymbol{X},J,\boldsymbol{c}) = 0$, which is the "local model" in the sense of [OtE97]. In this case, condition $\sum_{i=1}^n c_i = 1$ is kept during the evolution if it holds at the initial time. This can be seen by summing up (6.1b) for $i = 1,...,n$, which gives $\frac{\partial}{\partial t}(\sum_{i=1}^n c_i) = \operatorname{div}\big(\sum_{i,j=1}^n \mathbb{M}^{\boldsymbol{\xi}}_{ij}(J,\boldsymbol{c})\nabla\mu_j\big) + \sum_1^n r^{\boldsymbol{\xi}}_i(J,\boldsymbol{c})) = \operatorname{div}\mathbf{0} + 0 = 0$. This allows to us avoid the constraint $\sum_{i=1}^n c_i = 1$ from $\boldsymbol{N}(\cdot)$ in (6.1c). For equal mobilities of each chemical components, possibly dependent on pressure and local composition, denoted by $m = m(\boldsymbol{X},J,\boldsymbol{c})$, one usually considers the so-called Maxwell-Stefan mobility matrix

$$\mathbb{M}(\boldsymbol{X},J,\boldsymbol{c}) = m(\boldsymbol{X},J,\boldsymbol{c})\big(\operatorname{diag}(\boldsymbol{c}) - \boldsymbol{c}\otimes\boldsymbol{c}\big)\,, \tag{6.25}$$

cf. e.g. [Gio99, BoD23]. This matrix has the kernel $\mathbf{1}$ and hence is only positive semidefinite; moreover it degenerates further for $c_i \approx 0$. This makes its usage analytically more difficult than our simplified model with a general symmetric positive matrix as imposed in (6.1).

Remark 6.5 (*General reaction stoichiometry*)**.** For general reaction systems the assumption that $\mathbb{K}$ in (6.9c) is positive definite on the orthogonal complement of $\mathbf{1}$ may be too restrictive. In general, one has a stoichiometric subspace $\boldsymbol{S} \subset \mathbb{R}^n$ such that $\boldsymbol{r} \in \boldsymbol{S}$. Defining $\mathbb{P}_S : \mathbb{R}^n \to \boldsymbol{S} \subset \mathbb{R}^n$ to be the orthogonal projection and $\mathbb{Q}_S = I - \mathbb{P}_S$ the complementing projection, one can then assume that there is a symmetric reaction matrix $\mathbb{K}$ such that $\mu \cdot \mathbb{K}(\boldsymbol{X}, J, \boldsymbol{c})\mu \geq \epsilon|\mathbb{P}_S\mu|^2$. The above analysis can easily be generalized to this case, if we use that $\mathbb{Q}_S \int_\Omega \boldsymbol{c}(t, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$ is conserved along solutions, that $\mathbb{P}_S\boldsymbol{\mu}$ is controlled by the dissipation, and that we can assume $\mathbb{Q}_S \int_\Omega \boldsymbol{\mu}(t, \boldsymbol{x})\,\mathrm{d}\boldsymbol{x} = 0$ without loss of generality.

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