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Analysis of improved Nernst–Planck–Poisson models of compressible isothermal electrolytes

Wolfgang Dreyer, Pierre-Étienne Druet, Paul Gajewski and Clemens Guhlke

Abstract. We consider an improved Nernst–Planck–Poisson model first proposed by Dreyer et al. in 2013 for compressible isothermal electrolytes in non-equilibrium. The elastic deformation of the medium, that induces an inherent coupling of mass and momentum transport, is taken into account. The model consists of convection–diffusion–reaction equations for the constituents of the mixture, of the Navier–Stokes equation for the barycentric velocity and of the Poisson equation for the electrical potential. Due to the principle of mass conservation, cross-diffusion phenomena must occur, and the mobility matrix (Onsager matrix) has a non-trivial kernel. In this paper, we establish the existence of a global-in-time weak solution, allowing for a general structure of the mobility tensor and for chemical reactions with fast nonlinear rates in the bulk and on the active boundary. We characterise the singular states of the system, showing that the chemical species can vanish only globally in space, and that this phenomenon must be concentrated in a compact set of measure zero in time.

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1. Introduction

Increasing the efficiency of actual high-performance energy storage systems requires an exact understanding of their fundamental physical principles. Of particular interest is ion transport in electrolytes, for instance in lithium-ion batteries. In the neighbourhood of interfaces, the classical description using the Nernst–Planck theory is failing for various reasons (see [11,12]): first of all, the Nernst–Planck model neglects the high pressures induced by the Lorentz force that affect the charge transport. Secondly, it does not take into account the interaction between the solvent and the charged constituents. A third drawback of the Nernst–Planck theory is the widely used assumption of local charge neutrality. This assumption completely fails in the vicinity of the boundaries where electric charges accumulate. An improved model able to remedy these deficiencies was proposed in the paper [12]. In [11,13], this model was further extended to include (i) finite volume effects of the constituents, (ii) the viscosity of the mixture and (iii) chemical reactions in the bulk and on electrochemical interfaces. The improved model rests on three supporting pillars:

- The universal conservation principles for mass, electrical charge, momentum and energy;
- The entropy principle for bulk and surfaces, which allows to choose thermodynamically consistent material models;
- A special construction of the free energy-functional, designed in the papers [13,26] for electrolytes.

Throughout the paper, we shall focus on the isothermal case and need to formulate *universal balance equations* only for mass, momentum and charge. If the considered electrolyte is a fluid mixture of N

chemical substances, these equations assume the form

$$\begin{aligned} \partial_t\rho_i + \operatorname{div}(\rho_i\, v + J^i) &= r_i \qquad\qquad \text{for } i = 1,\ldots,N,\\ \partial_t(\varrho\, v) + \operatorname{div}(\varrho\, v\otimes v - \mathbb{S}) + \nabla p &= -\, n^F\, \nabla\phi,\\ -\epsilon_0\, \operatorname{div}((1+\chi)\,\nabla\phi) &= n^F, \end{aligned}$$

where the main variables are the mass densities $\rho_1,\ldots,\rho_N$ of the substances in the mixture, the components v_1, v_2, v_3 of the velocity field and the electric potential ϕ. Notice that we overall denote by ϱ the total mass density $\sum_{i=1}^N \rho_i$ of the electrolyte. In the right-hand side of the Navier–Stokes equations, the contribution $-n^F\,\nabla\phi$ is the Lorentz or Coulomb force. The density of free charges is $n^F := \sum_{i=1}^N \bar{Z}_i\,\rho_i$ with constants $\bar{Z}_1,\ldots,\bar{Z}_N$. Assuming a linear description of dielectric displacement in the electrolyte, the evolution of ϕ is driven by the Poisson equation with the universal Gauss constant ϵ_0 and the susceptibility χ of the electrolyte, here likewise assumed constant.

The diffusion fluxes $J^1,\ldots,J^N$, the reaction densities $r_1,\ldots,r_N$ and the components $\mathbb{S}$ (viscous stress) and p (thermodynamic pressure) of the stress tensor, represent physical phenomena that dissipate energy. In order to provide constitutive equations for these quantities, relating them to the main variables, our model uses the entropy principle as a guideline—after the universal conservation laws, this is the second pillar.

The chemical potentials, denoted by $\mu_1,\ldots,\mu_N$, are the essential pivot making the link between the densities and the thermodynamic consistent description of transport mechanisms. They are defined as derivatives of a free energy density $\varrho\psi$ via $\mu_i := \partial_{\rho_i}\varrho\psi$ for $i = 1,\ldots,N$. In the paper, we restrict to free energy densities of the form $\varrho\psi = h(\theta,\,\rho_1,\ldots,\rho_N)$, where the function h encodes the energetic behaviour (volume extension and mixing entropy) of the electrolyte without the electromagnetic contribution. Recall that the absolute temperature θ, which is assumed fixed, is only a parameter (isothermal case).

For the diffusion fluxes, the gradients $\nabla(\mu_j/\theta)+(\bar{Z}_j/\theta)\,\nabla\phi$ for $j = 1,\ldots,N$ are identified as the driving forces for the diffusion process, and the thermodynamic consistent model postulates the proportionality

$$J^i = -\sum_{j=1}^N M_{i,j}(\rho_1,\ldots,\rho_N)\left(\nabla\frac{\mu_j}{\theta} + \frac{\bar{Z}_j}{\theta}\,\nabla\phi\right) \text{for } i = 1,\ldots,N,$$

where the factor $\{M_{i,j}(\rho)\}_{i,j=1,\ldots,N}$ shall be called the mobility tensor. If $M(\rho)$ is positive semi-definite for all states, this definition of the diffusion fluxes guarantees that the contribution of diffusion to the production of entropy is non-negative.

In order to model the reactions $r_1,\ldots,r_N$ in a similar spirit, we shall make use of constitutive equations proposed first in [13] to obtain a closure equation of the form

$$r_i = -\sum_{k=1}^s \gamma_i^k\,\partial_k\Psi(\gamma^{\mathsf{T}}\mu)),$$

where s is the number of active reactions, $\{\gamma_i^k\}\in\mathbb{R}^{s\times N}$ is a matrix of stoichiometric coefficients, and $\Psi:\mathbb{R}^s\to\mathbb{R}$ a convex potential. Here, we denoted by μ the vector $(\mu_1,\ldots,\mu_N)$ of chemical potential.

The pressure shall obey the Gibbs–Duhem equation

$$p = -\varrho\psi + \sum_{i=1}^N \rho_i\,\mu_i = -h(\theta,\,\rho_1,\ldots,\rho_N) + \sum_{i=1}^N \rho_i\, h_{\rho_i}(\theta,\,\rho_1,\ldots,\rho_N).$$

Finally, the analysis of the entropy production shows that the viscous stress $\mathbb{S}$ can be consistently chosen of standard Newtonian form with constant coefficients. We will restrict for convenience to this simplifying assumption. Together with the Poisson equation to determine the electric potential, the final PDE model assumes the form

$$\partial_t \rho_i + \operatorname{div}\left(\rho_i\, v - \sum_{j=1}^N M_{i,j}(\rho)\,(\nabla h_{\rho_j}(\rho) + \bar{Z}_j\,\nabla\phi)\right) = -\sum_{k=1}^s \gamma_i^k\,\partial_k\Psi(\gamma^{\mathsf{T}} h_\rho(\rho)) \quad \text{for } i = 1,\dots,N, \tag{1}$$

$$\partial_t(\varrho\, v) + \operatorname{div}(\varrho\, v\otimes v - \mathbb{S}(\nabla v)) + \nabla\left(-h(\rho) + \sum_{i=1}^N \rho_i\, h_{\rho_i}(\rho)\right) = -\sum_{i=1}^N \rho_i\,\bar{Z}_i\,\nabla\phi, \tag{2}$$

where we omit for convenience every dependence on temperature, and write for simplicity $\rho = (\rho_1,\dots,\rho_N)$ in the arguments of M and h. We see that, for a known free energy potential h, these equations form a closed system for the variables ρ and v. To close the PDE system, we choose the free energy

$$h(\rho) = \sum_{i=1}^N \rho_i\, c_i + F\left(\sum_{i=1}^N \bar{V}_i\,\rho_i\right) + k_B\theta \sum_{i=1}^N \frac{\rho_i}{m_i}\left(\ln(\rho_i/m_i) - \ln\left(\sum_{j=1}^N (\rho_j/m_j)\right)\right), \tag{3}$$

where c_i, $m_i > 0$, $\bar{V}_i > 0$ are certain constants, k_B is the Boltzmann constant, and F a nonlinear function describing the volume extension of the mixture. We refer to Sects. 2.1, 2.2, and 2.3 for in-depth discussions of the three steps of the model derivation after the papers [11–13] and the book [20]. We explain (3) in Sect. 2.3 in more details.

From the viewpoint of analysis we first remark that, up to the complex looking definition of the thermodynamic pressure imposed by the multicomponent character, Eqs. (2) are very similar to the single-component compressible Navier–Stokes equations. They shall indeed allow the same type of natural bounds.

However, in the new model, the diffusion fluxes in (1) cannot be brought into the standard diagonal form assumed by the Nernst–Planck theory, and this for at least two reasons. At first, the matrix M is subject to the zero column-sum constraint $\sum_{i=1}^N M_{i,j} = 0$ due to the fact that we model diffusion fluxes. At second, the choice (3) of the free energy potential h leads, unlike the case of the standard Boltzmann entropy $\rho\log\rho$, to a nondiagonal Hessian. Hence, the diffusion tensor is in general both nondiagonal and singular. As to this last point, the equations in (1) cannot constitute a parabolic system for the variables $\rho_1,\dots,\rho_N$. Indeed, summing up over $i = 1,\dots,N$ and using the zero column-sup side-condition for M, we derive the continuity equation $\partial_t\varrho + \operatorname{div}(\varrho\, v) = 0$. This shows that one component of the solution vector is driven by an hyperbolic equation. Thus, whereas classical models of electrochemistry yield diagonal drift–diffusion or diffusion–reaction systems, the new model for electrolytes exhibits a completely different structure and must be studied with techniques of mathematical fluid dynamics.

In the present paper, we establish the existence of a global-in-time weak solution. Our result is consistent with the physical definitions and restrictions concerning the objects h, M, $\hat{R}$ and p. In particular, we allow for

1. A general structure of the mobility tensor with a non-trivial kernel;
2. Chemical reactions of arbitrary growth rate in the bulk and on the active part of the boundary;
3. A pressure contribution to the diffusion flux, which is encoded in the choice of the free energy.

A feature worth to note separately is the original thermodynamic modelling for the reaction rates. The choice of Ψ discussed here does not lead to the structure of products of monomials in the concentrations. As a consequence, energy dissipation yields a control of the reaction terms in Orlicz classes associated with the dual potential Ψ^*, and global-in-time weak solutions can be defined without the help of the renormalisation techniques (see [17]) necessary to handle models traditionally called 'of mass action type' (see, a. o., [4,6,17,21–23,30]).

In addition to the existence statements, we are able to characterise the singularities of the system associated with the *vanishing of species*. We show that, except for the occurrence of a complete vacuum—which is entirely non-physical in the range of validity of the model—the mass density of a species can vanish *only globally in the spatial domain* and that this phenomenon is concentrated *in a compact set of measure zero in time*.

Our method relies at first on *a priori* estimates that result from the thermodynamically consistent modelling, and from the conservation of total mass. The estimates are partly a consequence of known results for the Poisson equation or the Navier–Stokes equations, but we can regard the estimates on the chemical potentials of the mixture constituents, in particular in the presence of chemical reactions, as original (Theorem 11.3). The control on diffusion gradients and the chemical reactions is used to reveal a relationship between the blow-up of *differences of chemical potentials* and the entire vanishing of certain groups of species. In order to exclude the latter phenomenon, a restriction on the *initial net masses* of the involved constituents turns out sufficient.

Compactness techniques constitute the second fundament of our method. Note that the Aubin–Lions compactness Lemma and its generalisations, which are typically invoked in similar investigations (see for instance [8]), attain their limit in the context of the PDE system (1), (2), (3) due to the complexity of the relationship between time derivatives (transport) and diffusion gradients. We exploit the original ideas of [24] based on structural PDE arguments as an adequate substitute. Moreover, we invoke the compactness properties of the Navier–Stokes operator established first in [28] and extended in [15] to show compactness for the total mass density.

Since large parts of the modelling work in [12] are original and not yet well known in the mathematical literature devoted to the analysis of models for the electrolyte, we are not able to quote a direct precursor for our analysis in the context of electrochemistry. Similar models are known only in the context of multicomponent gas dynamics. We refer to the book [18] for an overview about models in this area and for first insights into their strong solution analysis. It is to note that the global weak solution analysis of multicomponent flow models is, up to few exceptions, widely unexplored. Let us here mention the papers [31] and [34] where models of compressible mixtures with energy balance, but without electric field, were studied. These models are not derived from exactly the same thermodynamic principles that are used in our study: Particularly, the constitutive equations for the pressure, for the diffusion fluxes and for the reaction terms, are different in [31] and in [12]. The compactness question occurs there like in our analysis but is solved assuming a special structure of the viscosity tensor, called Bresch–Desjardins condition. The latter allows to obtain estimates on the density gradient, a device which is not at our disposal here. A further difference between the two mixture models concerns cross-diffusion, which is described in [31] and [34] by a special choice of the mobility matrix, whereas we allow for general symmetric positive semi-definite matrices. Note that the mobility matrix must be symmetric at least in a binary mixture.

Among recent less directly related investigations let us mention: In the context of general diffusion, [2], [25]; for models with simplified diffusion and pressure laws [4,16]; for the analysis of incompressible models of Nernst–Planck–Poisson type [5,7,22].

Due to the length of the investigation, let us point out at three main parts in the manuscript. The first part consists of Sects. 2–7. Here, we derive the model, we set up, for the functional analytic treatment, an equivalent formulation which exhibits more stability against extreme behaviour (species vanishing, vacuum), and we propose a survey of the main mathematical results. The second part (Sects. 8–11) is devoted to the construction of approximate solutions respecting the natural *a priori* estimates. The third part (Sects. 12, 13, 14) is concerned with the investigation of compactness properties, and with the proof of convergence of the approximation scheme.

2. Improved Nernst–Planck–Poisson model

The model will be introduced following [13]. It is formulated for the *normal regime of the system*, in particular it is assumed that the mass densities of the constituents do not vanish. Throughout the paper, the bounded domain $\Omega \subset \mathbb{R}^3$ is representing an electrolytic mixture. The boundary of Ω possesses a disjoint decomposition $\partial\Omega = \Gamma \cup \Sigma$: The surface Γ represents an active *interface* between an electrode and the electrolyte, where chemical reactions and adsorption may occur. The other surface Σ represents an inert outer wall with no reactions and no adsorption.

The mixture consists of $N \in \mathbb{N}$ species denoted by $A_1, \dots, A_N$. A molecule of A_i has the elementary mass $m_i > 0$ and, as ions are involved, it carries a multiple $z_i \in \mathbb{Z}$ of the elementary charge e_0.

We assume that the system is isothermal so that the absolute temperature, denoted by θ, is a positive constant. Under the isothermal assumption, the thermodynamic state of the mixture at time $t \in [0, T]$ is described by the mass densities $\rho_1, \dots, \rho_N$ of the species, the barycentric velocity v of the mixture and the electric field E. As usual in electrochemistry, a quasi-static approximation of the electric field is considered, i.e. the magnetic field is constant and the electric field satisfies $E = -\nabla\phi$. The scalar function ϕ is called electrical potential.

The active boundary Γ can be viewed as a mixture of $N^\Gamma = N + N^{\text{ext}}$ constituents denoted by $A_1, \dots, A_{N^\Gamma}$, where the additional N^{ext} constituents take into account the species of the adjacent exterior matter, i.e. electrode species. Thus, we only consider surface chemical reactions with participating species that also exist in the adjacent bulk domains. The surface constituents have the surface mass densities $\rho_1^\Gamma, \dots, \rho_{N^\Gamma}^\Gamma$.

We consider $s \in \mathbb{N}$ chemical reactions in the bulk and $s^\Gamma \in \mathbb{N}$ surface reactions on the boundary Γ, respectively. The k^{th} chemical reaction in the bulk ($k \in \{1, \dots, s\}$) and on the boundary ($k \in \{1, \dots, s^\Gamma\}$) possesses the general structure

$$a_1^k A_1 + \cdots + a_N^k A_N \underset{R_k^b}{\overset{R_k^f}{\rightleftharpoons}} b_1^k A_1 + \cdots + b_N^k A_N,$$

$$a_{\Gamma,1}^k A_1 + \cdots + a_{\Gamma,N^\Gamma}^k A_{N^\Gamma} \underset{R_k^{\Gamma,b}}{\overset{R_k^{\Gamma,f}}{\rightleftharpoons}} b_{\Gamma,1}^k A_1 + \cdots + b_{\Gamma,N^\Gamma}^k A_{N^\Gamma}.$$

The constants a_i^k, b_i^k and $a_{\Gamma,i}^k$, $b_{\Gamma,i}^k$ are positive integers called stoichiometric coefficients. For $k = 1, \dots, s$, we define a vectorial coefficient associated with the k^{th} bulk reaction via

$$\gamma^k \in \mathbb{R}^N, \quad \gamma_i^k := (a_i^k - b_i^k)\, m_i, \quad \text{for } i = 1, \dots, N.$$

Due to the inclusion of the masses, $\gamma^1, \dots, \gamma^s$ are not the usual stoichiometric vectors, but this will simplify the notation. The forward reaction rate of the k^{th} reaction is $R_k^f > 0$, and the backward reaction rate is $R_k^b > 0$. The net reaction rate of the k^{th} reaction is defined as

$$R_k = R_k^f - R_k^b \quad \text{for } k = 1, \dots, s\ .$$

The same definitions hold for the surface reactions on Γ. Here, the vectorial coefficients are defined via

$$\gamma_\Gamma^k \in \mathbb{R}^{N^\Gamma}, \quad \gamma_{\Gamma,i}^k := (a_{\Gamma,i}^k - b_{\Gamma,i}^k)\, m_i, \quad \text{for } i = 1, \dots, N^\Gamma,$$

and the surface reaction rates are $R_k^\Gamma = R_k^{\Gamma,f} - R_k^{\Gamma,b}$ for $k = 1, \dots, s^\Gamma$. Since charge and mass are conserved in every single reaction

$$\begin{aligned} &\sum_{i=1}^{N} \gamma_i^k = 0 \quad \text{and} \quad \sum_{i=1}^{N} \tfrac{z_i}{m_i}\, \gamma_i^k = 0, \quad \text{for } k = 1, \dots, s, \\ &\sum_{i=1}^{N^\Gamma} \gamma_{\Gamma,i}^k = 0 \quad \text{and} \quad \sum_{i=1}^{N^\Gamma} \tfrac{z_i}{m_i}\, \gamma_{\Gamma,i}^k = 0, \quad \text{for } k = 1, \dots, s^\Gamma. \end{aligned} \tag{4}$$

2.1. Balance equations in the bulk

In the isothermal case, the evolution of the thermodynamic state is described by the equations of partial mass balances, of momentum balance, and by the Poisson equation.

In $]0,T[\times\Omega$ the mixture obeys for $i=1,\ldots,N$ the partial mass balances

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}(\rho_i\, v + J^i) = \sum_{k=1}^{s} \gamma_i^k\, R_k.$$

Here, v denotes the *barycentric velocity* of the mixture, while $J^1,\ldots,J^N$ are called the diffusion fluxes. The total mass is defined as $\varrho = \sum_{i=1}^{N} \rho_i$. Together with v it has to satisfy the continuity equation

$$\frac{\partial \varrho}{\partial t} + \operatorname{div}(\varrho\, v) = 0. \tag{5}$$

Thus, the conservation of total mass yields additional constraints on the diffusion fluxes and the mass productions:

$$\sum_{i=1}^{N} J^i = 0 \quad \text{and} \quad \sum_{i=1}^{N} r_i = 0\ . \tag{6}$$

While the constraint $(6)_2$ is a consequence of the conservation of mass in every chemical reaction (cf. (4)), the side condition on the diffusion fluxes has to be guaranteed by an appropriate constitutive modelling.

The principle momentum balance possesses the expression

$$\frac{\partial \varrho\, v}{\partial t} + \operatorname{div}(\varrho\, v\otimes v - \sigma) = \varrho\, b + n^F E.$$

Herein σ denotes the Cauchy stress tensor, $\varrho\, b$ is the force density due to gravitation, and the symbol $n^F E$ stands for the Lorentz force due to the electric field. The quantity n^F represents the free charge density that is defined via

$$n^F = e_0 \sum_{i=1}^{N} \frac{z_i}{m_i}\, \rho_i\ . \tag{7}$$

Throughout the paper, we are going to neglect the gravitational force that plays no role in the analysis.

In the electrostatic setting the balance equation for the electric field reduces to the Poisson equation for the electrical potential,

$$-\epsilon_0\,(1+\chi)\,\triangle\phi = n^F. \tag{8}$$

Here, $\chi > 0$ is the constant susceptibility of the electrolyte.

2.2. Constitutive equations

The constitutive equations for the mass fluxes, the reaction rates and the stress tensor can be derived from one single free energy density $\varrho\psi$ of a general form

$$\varrho\psi = h(\theta,\, \rho_1,\ldots,\rho_N)\ . \tag{9}$$

The derivatives

$$\mu_i := \frac{\partial h}{\partial \rho_i}(\theta,\rho_1,\ldots,\rho_N) \tag{10}$$

are called *chemical potentials*, In the isothermal setting, the balance equations and the free energy density yield a local *entropy production* $\xi = \xi_D + \xi_R + \xi_V \geq 0$ with three contributions due to diffusion, ξ_D, reaction, ξ_R, and viscosity, ξ_V (see [3,13,29]). A constitutive model that relies on the free energy function of the form (9) implies explicit expressions for the three entropy productions as binary products. From these expressions, we may derive constitutive equations that yield three separate non-negative entropy productions. For more details regarding the derivation of the entropy production, we refer to [3,9,29]. In [3], it is shown how cross-effects revealing the Onsager symmetry can be introduced.

Diffusion fluxes The entropy production due to diffusion reads

$$\xi_D = -\sum_{i=1}^{N} J^i \cdot D^i, \text{ with } D^i := \nabla \frac{\mu_i}{\theta} - \frac{e_0}{\theta}\frac{z_i}{m_i} E, \quad \text{for } i = 1, \ldots, N.$$

Here, $D^1, \ldots, D^N$ are the thermodynamic driving forces for diffusion, The simplest constitutive ansatz for the diffusion fluxes $J^1, \ldots, J^N$ that implies $\xi_D \geq 0$ is given by

$$J^i = -\sum_{j=1}^{N} M_{i,j}\, D^j \quad \text{for } i = 1, \ldots, N.$$

The proportionality factor $M \in \mathbb{R}^{N\times N}_{\text{sym}}$ is called the *mobility matrix*. It is positive semi-definite and may depend on ρ. Moreover, the side condition $\sum_{i=1}^{N} J^i = 0$ is complied with if the mobility matrix satisfies

$$\sum_{i=1}^{N} M_{i,j} = 0 \quad \text{for } j = 1, \ldots, N. \tag{11}$$

For instance, following the paper [12], one can construct M from an empirical mobility matrix $M_{\text{emp}}(\rho)$ and a linear operator $\mathcal{P} : \mathbb{R}^N \to \mathbb{R}^{N-1} \times \{0\}$ via

$$M := \mathcal{P}^T M_{\text{emp}}\, \mathcal{P}, \qquad M_{\text{emp}} := \text{diag}(d_1\, \rho_1, \ldots, d_{N-1}\, \rho_{N-1}, 1), \tag{12}$$

where $d_1, \ldots, d_{N-1} > 0$ are diffusion constants, and the lines of the matrix $\mathcal{P}$ are given by the differences $e^i - e^N$ of standard basis vectors for $i = 1, \ldots, N$. In fact, any operator $\mathcal{P}$ that satisfies for $i = 1, \ldots, N$ the condition $\sum_{j=1}^{N} \mathcal{P}_{i,j} = 0$ can be chosen in (12) in order that (11) is valid. However our analytical results do not rely on the particular structure (12) of the matrix M.

Reaction rates The entropy production due to chemical reactions assumes the form

$$\xi_{\text{R}} = -\sum_{k=1}^{s} R_k\, D^{\text{R}}_k\ . \tag{13}$$

The driving forces $D^{\text{R}}_1, \ldots, D^{\text{R}}_s$ are defined, for $k = 1, \ldots, s$, via $D^{\text{R}}_k = \sum_{i=1}^{N} \gamma_i^k\, \mu_i$. To achieve $\xi_{\text{R}} \geq 0$, we assume that the vector of production rates are derived from a convex, non-negative potential

$$R = -\nabla_{D^{\text{R}}} \Psi(D^{\text{R}}), \quad \text{with } \Psi : \mathbb{R}^s \to \mathbb{R} \text{ convex and } \nabla_{D^{\text{R}}} \Psi(0) = 0\ . \tag{14}$$

This choice is in fact more general than in [13], where the following potential is employed,

$$\Psi = -\sum_{k=1}^{s} \tfrac{1}{\beta_k \alpha_k} e^{-\beta_k \alpha_k D^{\text{R}}_k} \Big(1 + \tfrac{\beta_k}{1-\beta_k} e^{\alpha_k D^{\text{R}}_k}\Big) + C\ ,$$

with positive constants $\alpha_1, \ldots, \alpha_s$ and constants $\beta_1, \ldots \beta_s \in]0,\, 1[$, $C \in \mathbb{R}$ arbitrary. The latter corresponds to an ansatz of Arrhenius type, which is widely used in chemistry,

$$R_k = e^{-\beta_k\, A_k\, D^{\text{R}}_k}\, (1 - e^{A_k\, D^{\text{R}}_k})\ . \tag{15}$$

Stress tensor The entropy production due to viscosity is $\xi_V = \frac{1}{2}(\sigma + p\ \text{Id}) : D(v)$, with the driving force $D(v) = (\partial_i v_j + \partial_j v_i)_{i,j=1,\ldots,3}$, and the identity matrix Id. We split the Cauchy stress tensor into a viscous part $\mathbb{S}^{\rm visc}$ and the pressure p via $\sigma = -p\,\mathrm{Id} + \mathbb{S}^{\rm visc}$. Then, the material pressure can be calculated from the free energy function (9). The resulting representation is called Gibbs–Duhem equation and reads

$$p := -h + \sum_{i=1}^{N} \rho_i\, \mu_i \ . \tag{16}$$

The simplest constitutive choice for the viscous stress tensor $\mathbb{S}^{\rm visc}$ satisfying $\xi_V \geq 0$ describes a Newtonian fluid. It reads

$$\mathbb{S}^{\rm visc} = \eta\ D(v) + \lambda\ \operatorname{div} v\ \mathrm{Id}, \tag{17}$$

where $\eta > 0$ is the shear viscosity, and the coefficient λ of bulk viscosity satisfies $\lambda + \frac{2}{3}\,\eta \geq 0$.

2.3. Choice of the free energy function

The constitutive model is derived from a free energy density of the general form (9). To describe an elastic mixture, the free energy density $\varrho\psi$ is additively split into three contributions,

$$h = \sum_{i=1}^{N} \rho_i\, \mu_i^{\rm ref} + h^{\rm mech} + h^{\rm mix}. \tag{18}$$

The constants $\mu_i^{\rm ref}$ $(i = 1,\ldots,N)$ are related to the reference states of the pure constituents. The contribution $h^{\rm mech}$ is the mechanical part of the free energy that is neglected in the classical Nernst–Planck theory. The function $h^{\rm mix}$ represents the mixing entropy.

In the presentation of [11,12], the contributions $h^{\rm mech}$ and $h^{\rm mix}$ are naturally given as functions of the *number densities* $n_1,\ldots,n_N$ of the constituents. These are defined via $n_i := \rho_i/m_i$ $(i = 1,\ldots,N)$. The number fractions are defined via $y_i := n_i/\sum_{j=1}^{N} n_j$ for $i = 1,\ldots,N$.

The mechanical free energy is associated with the isotropic elastic deformation of the mixture. It takes into account different *reference partial volumes* $V_1,\ldots,V_N \in \mathbb{R}_+$ of the constituents. Assuming a constant bulk compression modulus $K > 0$, the mechanical free energy according to [11] is a function of the mixture volume $\sum_{i=1}^{N} n_i\, V_i$:

$$h^{\rm mech} = (K - p_{\rm ref}) \left(1 - \sum_{i=1}^{N} n_i\, V_i\right) + K \left(\sum_{i=1}^{N} n_i\, V_i\right)\ \ln\left(\sum_{i=1}^{N} n_i\, V_i\right).$$

Here, $p_{\rm ref}$ is a constant reference value of the pressure. Another possible choice, corresponding to a polynomial state-equation (Tait equation), is

$$h^{\rm mech} = (K - p_{\rm ref}) \left(1 - \sum_{i=1}^{N} n_i\, V_i\right) + \frac{K}{\alpha} \left(\left(\sum_{i=1}^{N} n_i\, V_i\right)^{\alpha} - \sum_{i=1}^{N} n_i\, V_i\right),\ \alpha > 1.$$

For the sake of generality, we express $h^{\rm mech}$ in the form

$$h^{\rm mech} = F(\sum_{i=1}^{N} n_i\, V_i) + C \sum_{i=1}^{N} n_i\, V_i, \qquad F : \mathbb{R}_+ \to \mathbb{R} \text{ convex.} \tag{19}$$

Dreyer et al. use $F(x) := x\, \ln x + C_1$ for an ideal mixture, whereas the Tait equation corresponds to $F(x) = c_\alpha\, x^\alpha + C_2$. The contribution $h^{\rm mix}$ results from the entropy of mixing and is given by

$$h^{\rm mix} := \left(\sum_{i=1}^{N} n_i\right)\ k_B\ \theta\ \sum_{i=1}^{N} y_i\ \ln y_i, \tag{20}$$

where k_B is the Boltzmann constant.

2.4. The model for the boundary Γ

The active boundary Γ represents an interface between the electrolyte and an *external material*. In the most important application, the external material is an electrode which is likewise a mixture of $N^{\mathrm{ext}} \in \mathbb{N}$ constituents. Here, we have analogous quantities to those that occur in the electrolyte, namely the barycentric velocity, and diffusion fluxes and so on. To distinguish between the electrolyte and the external material, we make use of the suffix $^{\mathrm{ext}}$ in connection with external quantities.

In this paper, we assume for simplicity that the constituents occurring on Γ also exist in the bulk, either in the electrolyte or in the external material. Thus, the interface Γ is a mixture of $N^\Gamma = N + N^{\mathrm{ext}}$ constituents. The equations of an interface representing a surface mixture are derivable in the context of surface thermodynamics, and we refer the interested reader to [1,13,20]. As in the bulk, there are universal surface balance equations and material-depending surface constitutive equations. To simplify the surface equations, we assume on $]0,T[\times\Gamma$:

(a) Time variations of the surface mass densities and tangential transport are negligible in comparison to mass transfer across the surface and to chemical surface reactions.
(b) The interface is fixed in space, i.e. the interfacial normal speed is zero.
(c) There is no velocity slip and the normal barycentric velocity is equal to the interfacial normal speed, i.e. we have $v = 0$ on $]0,T[\times\Gamma$.

Surface mass balances and surface reaction rates In what follows the interfacial unit normal ν points into the external material. Under the assumptions (a), (b), (c), the surface mass balance equations on $]0,T[\times\Gamma$ reduce to

$$0 = \begin{cases} r_i^\Gamma + J^i \cdot \nu & \text{for } i = 1,\dots,N, \\ r_{N+i}^\Gamma - J^{\mathrm{ext},i} \cdot \nu & \text{for } i = 1,\dots,N^{\mathrm{ext}}. \end{cases} \tag{21}$$

Here, we make use of the convention that the N first species on Γ are the electrolyte constituents, while the constituents with indices $N+1,\dots,N+N^{\mathrm{ext}}$ are the external ones.

It remains to specify the surface mass production r^Γ due to surface reactions. As in the bulk, the production r^Γ is related to the surface reaction rates R^Γ by

$$r_i^\Gamma = \sum_{k=1}^{s^\Gamma} \gamma_{\Gamma,i}^k\, R_k^\Gamma \quad \text{for } i = 1,\dots,N^\Gamma\ .$$

The interfacial entropy production ξ_{R}^Γ due to chemical reaction is (see [13])

$$\xi_{\mathrm{R}}^\Gamma = -\sum_{k=1}^{s^\Gamma} R_k^\Gamma\, D_k^{\Gamma,\mathrm{R}} \geq 0, \qquad D_k^{\Gamma,\mathrm{R}} := \sum_{i=1}^{N^\Gamma} \gamma_{\Gamma,i}^k\, \mu_i^\Gamma \quad \text{for } k = 1,\dots,s^\Gamma\ .$$

The entropy production of the surface has the same structure as the corresponding entropy production in the bulk (13). Thus, in order to satisfy the entropy inequality, an ansatz similar to (14), (15) may be used. We assume the existence of a potential Ψ^Γ so that

$$R^\Gamma = -\nabla_{D^{\Gamma,\mathrm{R}}}\Psi^\Gamma(D^{\Gamma,\mathrm{R}}), \quad \Psi^\Gamma : \mathbb{R}^{s^\Gamma} \to \mathbb{R} \text{ convex s. t. } \nabla_{D^{\Gamma,\mathrm{R}}}\Psi^\Gamma(0) = 0\ . \tag{22}$$

Normal diffusion fluxes Under the assumptions (a), (b) and (c), the constitutive equations proposed in [13,20] for the normal diffusion fluxes at $]0,T[\times\Gamma$ simplify to

$$\begin{aligned} J^i\cdot\nu &= \sum_{j=1}^{N} M^{\Gamma}_{i,j}\,(\mu_j-\mu^{\Gamma}_j) \quad \text{for } i=1,\dots,N\ , \\ J^{\text{ext},i}\cdot\nu &= -\sum_{j=1}^{N^{\text{ext}}} M^{\Gamma,\text{ext}}_{i,j}\,(\mu^{\text{ext}}_j-\mu^{\Gamma}_{N+j}) \qquad \text{for } i=1,\dots,N^{\text{ext}}. \end{aligned} \tag{23}$$

Here, $\mu^{\Gamma}_1,\dots,\mu^{\Gamma}_N$ are the surface chemical potentials of the electrolytic species, whereas the quantities $\mu^{\Gamma}_{N+1},\dots,\mu^{\Gamma}_{N+N^{\text{ext}}}$ are associated with the external species. These equations describe the adsorption of a constituent from the bulk to the surface. The kinetics of this process is controlled by positive semi-definite matrices

$$M^{\Gamma}\in\mathbb{R}^{N\times N}_{\text{sym}} \qquad \text{and} \qquad M^{\Gamma,\text{ext}}\in\mathbb{R}^{N^{\text{ext}}\times N^{\text{ext}}}_{\text{sym}}.$$

Simpler form of the transmission conditions In the general thermodynamic setting, the surface chemical potentials are derivatives of a surface free energy. Due to the assumption of stationary surface equations, and that the boundary is fixed, we are able to formulate all surface equations in terms of the bulk chemical potentials. From a mathematical viewpoint the equation system (21), (23) only serves to eliminate the surface chemical potentials μ^{Γ} in order to calculate the external fluxes of the electrolytic species (see the appendix, section C).

Denoting by $\mathrm{R}(M^{\Gamma})$ the range of M^{Γ}, we define $\hat{s}^{\Gamma} := \dim\mathrm{R}(M^{\Gamma})$, and we choose basis vectors $\hat{\gamma}^1,\dots,\hat{\gamma}^{\hat{s}^{\Gamma}}$ for $\mathrm{R}(M^{\Gamma})$. The conditions (21), (23) allow to represent the flux of the electrolytic species via

$$J^i\cdot\nu = -\hat{r}_i - J^0_i \quad \text{for } i=1,\dots,N.$$

Here, the *external response* J^0 is a mapping from $[0,T]\times\Gamma$ into $\operatorname{span}\{\hat{\gamma}^1,\dots,\hat{\gamma}^{\hat{s}^{\Gamma}}\}$. The *modified reaction term* $\hat{r}$ is a map on $[0,T]\times\Gamma\times\mathbb{R}^{\hat{s}^{\Gamma}}$, which possesses the structure

$$\hat{r}_i = \sum_{k=1}^{\hat{s}^{\Gamma}} \hat{R}^{\Gamma}(t,\,x,\,\hat{\gamma}^1\cdot\mu,\dots,\hat{\gamma}^{\hat{s}^{\Gamma}}\cdot\mu)\,\hat{\gamma}^k_i \quad \text{for } i=1,\dots,N. \tag{24}$$

Moreover, there is a convex non-negative potential $\hat{\Psi}^{\Gamma}:[0,T]\times\Gamma\times\mathbb{R}^{\hat{s}^{\Gamma}}\to\mathbb{R}$ such that $\hat{R}^{\Gamma}(t,\,x,\,D) = -\nabla_D\hat{\Psi}^{\Gamma}(t,\,x,\,D)$ for all $(t,x,D)\in[0,T]\times\Gamma\times\mathbb{R}^{\hat{s}^{\Gamma}}$, and $\nabla_D\hat{\Psi}^{\Gamma}(t,\,x,\,0)=0$ for all $(t,x)\in[0,T]\times\Gamma$. The data μ^{ext}, M^{Γ} and $M^{\Gamma,\text{ext}}$ are included in the position dependence of J^0 and $\hat{\Psi}^{\Gamma}$. In the analysis we shall for simplicity assume that this J^0 and this $\hat{\Psi}^{\Gamma}$ are the boundary data. In applications the solution of a few additional nonlinear algebraic equations are necessary to compute them.

Electrical potential The boundary condition for the electrical potential can be derived from Maxwell's equations for surfaces, which are satisfied in the quasi-static stetting by a continuous electrical potential (see [13]). On $]0,T[\times\Gamma$ we impose the condition $\phi=\phi_0$, where ϕ_0 is the given electric potential at $]0,T[\times\Gamma$.

3. Summary of model equations

Domain Ω Summarising, the evolution of the state (ρ, v, φ) in $]0,T[\times\Omega$ is described by the PDE-system

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}\left(\rho_i\, v - \sum_{j=1}^{N} M_{i,j}(\rho)\,(\nabla(\mu_j/\theta) + \tfrac{e_0}{\theta}\,\tfrac{z_j}{m_j}\,\nabla\phi)\right) = -\sum_{k=1}^{s} \gamma_i^k\, \partial_{D_k^{\mathrm{R}}}\Psi(\gamma^1\cdot\mu,\dots,\gamma^s\cdot\mu), \quad (25)$$

$$\frac{\partial \varrho\, v}{\partial t} + \operatorname{div}(\varrho\, v\otimes v - \mathbb{S}^{\mathrm{visc}}(\nabla v)) + \nabla\left(-h(\theta,\,\rho) + \sum_{i=1}^{N}\rho_i\,\mu_i\right) = -e_0\left(\sum_{i=1}^{N}\tfrac{z_i}{m_i}\,\rho_i\right)\nabla\phi, \quad (26)$$

$$-\epsilon_0\,(1+\chi)\,\triangle\phi = e_0\sum_{i=1}^{N}\tfrac{z_i}{m_i}\,\rho_i. \quad (27)$$

Here, the chemical potentials μ_i are related to the densities via (10), the function h is chosen of the form (18) with (19) and (20), and $\mathbb{S}^{\mathrm{visc}}$ is subject to (17).

Boundary Γ We have on $]0,T[\times\Gamma$ the boundary conditions

$$0 = \sum_{k=1}^{s^\Gamma}\gamma_\Gamma^k\,R_k^\Gamma + \left(J - J^{\mathrm{ext}}\right)\cdot\nu\ , \quad (28)$$

$$J\cdot\nu = M^\Gamma\,(\mu-\mu^\Gamma) \quad \text{for electrolyte constituents,} \quad (29)$$

$$J^{\mathrm{ext}}\cdot\nu = -M^{\Gamma,\mathrm{ext}}\,(\mu^{\mathrm{ext}} - \mu^\Gamma_{N+\cdot}) \quad \text{for external constituents,} \quad (30)$$

$$v = 0\ , \quad (31)$$

$$\phi = \phi_0\ , \quad (32)$$

where the external chemical potentials μ^{ext}, the external potential ϕ_0 and the kinetic matrices M^Γ and $M^{\Gamma,\mathrm{ext}}$ are given. The reaction rates R^Γ are satisfying (22). Recall that the conditions (28) represent N^Γ equations and are a shorter form for (21). Alternatively to (28), (29) and (30),

$$J\cdot\nu = \sum_{k=1}^{\hat{s}^\Gamma}\partial_{\hat{D}_k^{\mathrm{R}}}\hat{\Psi}^\Gamma(t,\,x,\,\hat{\gamma}^1\cdot\mu,\dots,\hat{\gamma}^{\hat{s}^\Gamma}\cdot\mu)\,\hat{\gamma}^k - J^0 \qquad \text{for electrolyte constituents.} \quad (33)$$

Boundary $\boldsymbol{\Sigma}$ We choose as simple as possible a model on the surface $]0,T[\times\Sigma$ where basically all effects can be neglected: No mass flux $(\rho_i\,v + J^i)\cdot\nu = 0$ for $i = 1,\dots,N$; Complete adherence of the fluid $v = 0$; No surface charge $\nabla\phi\cdot\nu = 0$.

Initial conditions Initial conditions are prescribed for the variables $\rho_1,\dots,\rho_N$. We denote them ρ_i^0, $i = 1,\dots,N$. Moreover, an initial state v^0 is also given for the velocity vector.

4. Notation

To get rid of overstressed indexing, we simplify the notation by making use of vectors. For instance, we denote ρ the vector of mass densities, n the vector of number densities, i.e.

$$\rho := (\rho_1,\rho_2,\dots,\rho_N)\in\mathbb{R}^N, \quad n := (n_1,n_2,\dots,n_N)\in\mathbb{R}^N.$$

Moreover, we define the vector $\mathbb{1} := 1^N := (1,\,1,\dots,1)\in\mathbb{R}^N$, and we introduce the quotients of charge over mass $e^0\,z_i/m_i =: \bar{Z}_i$, and of volume over mass $V_i/m_i =: \bar{V}_i$ as vectors via

$$\bar{Z} := e^0\,(\tfrac{z_1}{m_1},\,\tfrac{z_2}{m_2},\dots,\tfrac{z_N}{m_N})\in\mathbb{R}^N, \quad \bar{V} := (\tfrac{V_1}{m_1},\,\tfrac{V_2}{m_2},\dots,\tfrac{V_N}{m_N})\in\mathbb{R}^N\ .$$

Using these conventions, we have a. o. the identities $\varrho = \mathbb{1}\cdot\rho$, $n^F = \bar{Z}\cdot\rho$, $n\cdot V = \rho\cdot\bar{V}$, etc.

With $\mathbb{R}_+ =]0, +\infty[$ and $\mathbb{R}_{0,+} := [0, +\infty[$, we define $\mathbb{R}^N_+ := (\mathbb{R}_+)^N$ and $\mathbb{R}^N_{0,+} = (\mathbb{R}_{0,+})^N$.

The diffusion fluxes $J^1, \ldots, J^N$ span a rectangular matrix $J = \{J^i_j\} \in \mathbb{R}^{N\times 3}$. The upper index corresponds to the lines of this matrix. Vectors of $\mathbb{R}^N$ are multiplicated from the left, as for instance in $\mathbb{1} \cdot J = \sum_{i=1}^N J^i$ which is an identity in $\mathbb{R}^3$.

The vectors $\gamma^1, \ldots, \gamma^s$ span a rectangular matrix $\gamma = \{\gamma^k_i\} \in \mathbb{R}^{s\times N}$. The upper index corresponds to the line of the matrix. Vectors of $\mathbb{R}^s$ are multiplicated from the left, as for instance in the identity $r = R \cdot \gamma = \sum_{k=1}^s R_k \, \gamma^k$ in $\mathbb{R}^N$. Analogously the vectors $\gamma^1_\Gamma, \ldots, \gamma^{s^\Gamma}_\Gamma$ span a rectangular matrix $\gamma_\Gamma = \{\gamma^k_{\Gamma,i}\} \in \mathbb{R}^{s^\Gamma \times N^\Gamma}$. In order to describe the reactions, we shall further make use of the abbreviations $\bar{R} : \mathbb{R}^s \to \mathbb{R}^s$, $\bar{R} := -\nabla_{D^{\mathrm{R}}} \Psi$ and $\hat{R}^\Gamma : \mathbb{R}^{\hat{s}^\Gamma} \to \mathbb{R}^{\hat{s}^\Gamma}$, $\hat{R}^\Gamma := -\nabla_{\hat{D}^{\mathrm{R}}} \hat{\Psi}^\Gamma$.

For notational simplicity, we introduce the positive constant

$$\bar{\chi} := \epsilon_0 \, (1 + \chi).$$

Moreover, since the constants K, k_B and θ play no role in the analysis we shall, for the sake of simplicity, normalise them to one.

We denote with λ_1 the Lebesgue measure on $]0, T[$, with λ_3 the Lebesgue measure on Ω, and with λ_4 the Lebesgue measure on Q. If the context is clear enough, we also employ the abbreviation $|\cdot|$ for the Lebesgue measure of a set indifferently of its dimension.

Functional classes We define $Q_t =]0, t[\times\Omega$ and $S_t :=]0, t[\times\Gamma$. We set $Q := Q_T$ and $S := S_T$. For $1 \leq p,\, q < +\infty$, we employ the notations $L^{p,q}(Q) \cong L^p(0, T;\, L^q(\Omega))$.

We make use of standard Sobolev spaces for spatial domains and space-time domains. In particular, recall that $W^{1,0}_p(Q) \cong L^p(0, T;\, W^{1,p}(\Omega))$. We define $W^{1,0}_{p,S}(Q) := \{u \in W^{1,0}_p(Q) \,:\, \mathrm{trace}(u) = 0 \text{ in } L^p(S)\}$.

For a convex, non-negative potential $\Psi \in C(\mathbb{R}^s)$, $s \geq 1$ (and for its conjugate Ψ^*), the vectorial Orlicz *classes* $L_\Psi(Q;\, \mathbb{R}^s)$ and $L_{\Psi^*}(Q;\, \mathbb{R}^s)$ are well known. We make use of the notation

$$[D^{\mathrm{R}}]_{L_\Psi(Q;\,\mathbb{R}^s)} := \int_{Q_T} \Psi(D^{\mathrm{R}}(t,\, x))\, \mathrm{d}x\, \mathrm{d}t.$$

For $\hat{\Psi}^\Gamma \in L^\infty(S;\, C^2(\mathbb{R}^{\hat{s}^\Gamma}))$, we define a vectorial Orlicz class $L_{\hat{\Psi}^\Gamma}(S;\, \mathbb{R}^{\hat{s}^\Gamma})$ as the set of all measurable $\hat{D}^{\Gamma,\mathrm{R}} : S \to \mathbb{R}^{\hat{s}^\Gamma}$ such that

$$[\hat{D}^{\Gamma,\mathrm{R}}]_{L_{\hat{\Psi}^\Gamma}(S;\,\mathbb{R}^{\hat{s}^\Gamma})} := \int_S \hat{\Psi}^\Gamma(t,\, x,\, \hat{D}^{\Gamma,\mathrm{R}}(t,\, x))\, \mathrm{d}S(x)\, \mathrm{d}t < +\infty.$$

5. Mathematical assumptions on the data

From the thermodynamic viewpoint, the free energy function h, the mobility matrix M and the potentials Ψ, Ψ^Γ are the essential objects determining the properties of the constitutive equations. Mathematical results can be obtained under suitable restrictions to these objects. In addition, restrictions are as usual necessary concerning the geometry and the quality of boundary and initial states. In this investigation, we are not concerned with pointing at optimal classes for the second type of data.

Assumptions on the free energy function Our estimates on the (relative) chemical potentials require the special form (18), where the mixing entropy obeys the precise representation (20). We allow for a certain generality only at the level of the function h^{mech} which we assume of the form (19).

Thereby, we assume that F belongs to $C^2(\mathbb{R}_+) \cap C(\mathbb{R}_{0,+})$ and is a strictly convex function. Moreover, we assume that there are $3/2 < \alpha < +\infty$ and constants $0 < c_0,\, c_1$ such that

$$F(s) \geq c_0\, s^\alpha - c_1, \quad \text{for all } s > 0, \tag{34}$$

and that there are positive constants $k_0 < k_1$, $k_2 < k_3$ and $s_1 > s_0 > 0$ such that

$$\frac{k_0}{s} \le F''(s) \le \frac{k_1}{s} \quad \text{for all } s \in]0, s_0], \quad k_2\, s^{\alpha-2} \le F''(s) \le k_3\, s^{\alpha-2} \quad \text{for all } s \in [s_1, +\infty[. \tag{35}$$

For the analysis, we further crucially need that $F' : \mathbb{R}_+ \to \mathbb{R}$ is surjective. This is not satisfied for instance by the pure polynomial ansatz according to Tait, but it always follows from (35) in connection with the strict convexity of F. The assumptions (34), (35) cover the typical choice $F(s) = s \ln s$—as for instance in [12]—in the range of finite densities, but require superlinear growth for large arguments. The restriction $\alpha > 3/2$ is imposed by the available methods for the weak solution analysis of (single-component) Navier–Stokes equations.

Assumptions on the mobility matrix M is symmetric and positive semi-definite. Throughout the paper, we assume that M is mass conservative, that is

$$M\mathbb{1} = 0. \tag{36}$$

Moreover, we assume that the entries of M are continuous functions of the vector ρ of the partial mass densities, with at most linear-growth in ρ.

Except for these few points, the exact structure of the mobility matrix is a delicate topic (in particular, there are connections to the Maxwell–Stefan theory, see [3,18]). In this paper we restrict ourselves to the assumption that M has rank $N-1$ independently on ρ. In other words, denoting $0 = \lambda_1(M) \le \lambda_2(M) \le \ldots \le \lambda_N(M)$ the eigenvalues of the matrix M, we assume that there are positive constants $0 < \underline{\lambda} \le \overline{\lambda}$ such that

$$\underline{\lambda} \le \lambda_i(M(\rho)) \le \overline{\lambda}\,(1 + |\rho|) \qquad \text{for all } i = 2, 3, \ldots, N,\ \rho \in \mathbb{R}^N_+. \tag{37}$$

Let us remark that due to this assumption, only regularisations of the original ansatz of the paper [12] are included in the analysis: In formula (12), we must, for example, apply a cut-off from below to the entries of the empirical matrix M_{emp}.

Assumptions on the reaction rates The reaction rates are derived from a strictly convex, non-negative potential[1] $\Psi \in C^2(\mathbb{R}^s)$. It is possible to consider general convex potentials with super linear growth but, for the sake of technical simplicity, we shall require at least linear growth of the rates via

$$\inf_{D^{\mathrm{R}} \in \mathbb{R}^s} \lambda_{\min}(D^2\Psi(D^{\mathrm{R}})) > 0, \qquad \inf_{D^{\Gamma,\mathrm{R}} \in \mathbb{R}^{s^\Gamma}} \lambda_{\min}(D^2\Psi^\Gamma(D^{\Gamma,\mathrm{R}})) > 0. \tag{38}$$

As to the adsorption coefficients M^Γ and $M^{\Gamma,\text{ext}}$ occurring in the boundary conditions (29), (30) they play in the analysis a role comparable to linear reactions. We assume them to be symmetric and positive semi-definite constant matrices. Moreover, in connection to the no slip condition (31), it is no restriction to require that $M^\Gamma\, 1^N = 0$ and $M^{\Gamma,\text{ext}}\, 1^{N^{\text{ext}}} = 0$. Under these conditions, the modified reaction potential $\hat{\Psi}^\Gamma$ on the boundary fulfils (see appendix, section C for a proof)

$$\inf_{\hat{D}^{\Gamma,\mathrm{R}} \in \mathbb{R}^{\hat{s}^\Gamma},\, (t,x) \in [0,T] \times \Gamma} \lambda_{\min}(D^2\hat{\Psi}^\Gamma(t, x,\, D^{\Gamma,\mathrm{R}})) > 0. \tag{39}$$

Assumptions on the domain Ω *and the boundary* Γ. $\Omega \subset \mathbb{R}^3$ is bounded and of class $\mathcal{C}^{0,1}$. In connection with the optimal regularity of the solution to the Poisson equation with mixed-boundary conditions, we introduce the exponent $r(\Omega, \Gamma)$ as the sup. of all numbers in the range $[2, +\infty[$ such that

$$-\triangle u = f \text{ in } [W^{1,\beta'}_\Gamma(\Omega)]^* \text{ implies } u \in W^{1,\beta}_\Gamma(\Omega)$$
$$\text{for all } f \in [W^{1,\beta'}_\Gamma(\Omega)]^* \text{ and all } \beta \in]r', r[\text{ with } r' := \frac{r}{r-1}. \tag{40}$$

[1]It is always possible to achieve the non-negativity, because the model only requires that Ψ has a global minimum in zero, but its value is not prescribed.

It is well known that $r(\Omega, \Gamma) > 2$ in general (see [19] a. o.), but there are numerous situations where, depending on the boundary of the domain and the structure of the surface Γ, the optimal exponent satisfies $r(\Omega, \Gamma) > 3$ (see [10] for results and discussions on this topic). We require that

$$\alpha' := \frac{\alpha}{\alpha - 1} < r, \tag{41}$$

with α from (34). This of course might be a restriction only if $\alpha < 2$.

Assumptions on the remaining boundary data We consider only non-degenerate initial and boundary data, whereby we mean that

$$\begin{aligned} \rho^0 &\in L^\infty(\Omega;\, (\mathbb{R}_+)^N), \\ v^0 &\in L^\infty(\Omega;\, \mathbb{R}^3), \\ \phi_0 &\in L^\infty(0,T;\, W^{1,r}(\Omega)) \cap L^\infty(]0,T[\times\Omega), \\ \partial_t\phi_0 &\in W^{1,0}_2(]0,T[\times\Omega) \cap L^{\alpha'}(]0,T[\times\Omega), \\ \mu^{\text{ext}} &\in L^\infty(]0,T[\times\Gamma;\, \mathbb{R}^{N^{\text{ext}}}). \end{aligned} \tag{42}$$

Note that the last assumption in (42) guarantees that $J^0 \in L^\infty(]0,T[\times\Gamma;\, \{\hat{\gamma}^1, \ldots \hat{\gamma}^{\hat{s}^\Gamma}\})$ (see the appendix, section C). Therefore, there are coefficients $\jmath_1, \ldots, \jmath_{\hat{s}^\Gamma} \in L^\infty([]0,T[\times\Gamma)$ such that

$$J^0_i := \sum_{k=1}^{\hat{s}^\Gamma} \jmath_k(t,\, x)\, \hat{\gamma}^k_i. \tag{43}$$

The reaction vectors: critical manifold For the analysis of our special model of chemical reactions, we need to introduce a technical notion. Denote $W \subseteq \mathbb{1}^\perp \subset \mathbb{R}^N$ the linear subspace given by

$$W := \text{span}\left\{\gamma^1, \ldots, \gamma^s,\, \hat{\gamma}^1, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}\right\}. \tag{44}$$

Recall that $\hat{\gamma}^1, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}$ are the reduced reaction vectors associated with the matrix M^Γ. They are elements from $\mathbb{1}^\perp$. Call *selection* S of cardinality $|S| \leq N$ a subset $\{i_1, \ldots, i_{|S|}\}$ of $\{1, \ldots, N\}$ such that $i_1 < \ldots < i_{|S|}$. For every selection, we introduce the corresponding projector $P_S : \mathbb{R}^N \to \mathbb{R}^N$ via $P_S(\xi)_i = \xi_i$ for $i \in S$, and $P_S(\xi)_i = 0$ otherwise. We define a linear subspace $W_S \subset \mathbb{R}^N$ via

$$W_S := \text{span}\left\{P_S(\gamma^1), \ldots, P_S(\gamma^s),\, P_S(\hat{\gamma}^1), \ldots, P_S(\hat{\gamma}^{\hat{s}^\Gamma})\right\}.$$

The selection S will be called *uncritical* if $\dim(W_S) = |S|$ and *critical* otherwise.

For every selection S, we denote S^{c} the complementary index set $\{1, \ldots, N\}\backslash S$. It can easily be shown that the manifold

$$\mathcal{M}_{\text{crit}} := \mathbb{R}^N_+ \cap \bigcup_{S \subset \{1,\ldots,N\},\, S \text{ critical}} W_S \times P_{S^\perp}(\mathbb{R}^N) \tag{45}$$

is the finite union of submanifolds of dimension at most $N-1$. We say that the *initial compatibility condition* is satisfied if the vector of initial net masses $\bar{\rho}_0 := \int_\Omega \rho^0 \, \mathrm{d}x \in \mathbb{R}^N_+$ satisfies $\bar{\rho}_0 \notin \mathcal{M}_{\text{crit}}$.

6. Identification of natural variables in the equations of mass transfer

The three following factors affect the solution concept and the analysis of Eq. (25):

- State-constraints ($\rho \geq 0$);
- The mobility matrix has a non-trivial kernel ($M\,\mathbb{1} = 0$). The PDE system is not parabolic;
- For weak solutions, the continuity equation $\partial_t \varrho + \text{div}(\varrho\, v) = 0$ might generate a local vacuum.

6.1. State-constraints

The pair of vector fields $(\rho, \mu) : [0,T]\times\Omega \to \mathbb{R}^N_+ \times \mathbb{R}^N$ is subject to the *algebraic relation* $\mu = \nabla_\rho h(\rho)$ (cf. (10)). Obviously: The vector of mass densities ρ must belong to the domain of the free energy function, while the vector of chemical potentials belongs to its image.

Meaningful choices of the function h must in general guarantee that the domain of $\nabla_\rho h$ is a subset of $\mathbb{R}^N_+$. Indeed, the algebraic constraint on ρ must be comply with the physical non-negativity restriction on the mass densities. The vector of chemical potentials μ must belong to the image of $\nabla_\rho h$. There are models, for instance the special constitutive assumption (18) with Tait equation for F, for which this image is a true subset of $\mathbb{R}^N$.

These algebraic state-constraints are a fundamental obstacle to the application of a functional analytic method to prove the solvability of the model. In order to overcome this difficulty, we exploit a particular observation: *For the special constitutive assumption* (18), we can show that $\nabla_\rho h : \mathbb{R}^N_+ \to \mathbb{R}^N$ is a bijection if the first derivative of the function F is surjective onto $\mathbb{R}$. At least for a relevant particular choice of h, the PDE system is *unconstrained* in μ, and the chemical potentials are a favourable set of variables to perform existence theory or numerical approximation. This was already noted in the context of multicomponent gas dynamics (see [18], [25], [7]).

6.2. A 'hyperbolic' component

Diffusion and chemical reactions are the dissipative structures that provide a control on the vector μ. But the fluxes $J^1,\ldots,J^N$ and the functions $r_1,\ldots,r_N$ occurring in the system (25) in fact only depend on the projection of the vector μ on the subspace $\mathbb{1}^\perp := \{\xi \in \mathbb{R}^N : \xi\cdot\mathbb{1} = 0\}$ (see the side condition (11) for the diffusion fluxes, and the restriction (4) on the vectors $\gamma^1,\ldots,\gamma^s$).

Thus, natural estimates can be obtained only for a $(N-1)$-dimensional projection of the vector μ. Due to this observation it was noted in [12] that a *change of variables* is advantageous in order to define the solution. It is to note that this tool is also known from precursor investigations under the concept of entropic variables: We refer to [18] for an overview. Following these ideas, we keep as main variables:

(a) On the one hand, one coordinate of the vector field ρ, namely the total mass density $\varrho = \rho\cdot\mathbb{1}$. This is the 'hyperbolic' component subject to the continuity equation (5);
(b) On the other hand, $N-1$ coordinates of the vector of chemical potentials μ defined via a projection onto the linear space $\mathbb{1}^\perp \subset \mathbb{R}^N$.

The possibility of these choices relies on an algebraic result that we want to afore mention here (See Sect. 8, Corollary 8.3 for the proof).

Proposition 6.1. *Assume that the free energy function h satisfies the ansatz* (18), (19), (20), *and that the function F occurring in* (19) *belongs to $C^2(\mathbb{R}_+)\cap C(\mathbb{R}_{0,+})$, is strictly convex, and possesses a surjective first derivative F'. Let $\xi^1,\ldots,\xi^N \in \mathbb{R}^N$ be a basis of $\mathbb{R}^N$ such that $\xi^N = \mathbb{1}$, and let $\eta^1,\ldots,\eta^N \in \mathbb{R}^N$ be the vectors such that $\xi^i\cdot\eta^j = \delta^j_i$ for $i,j = 1,\ldots,N$. We define a projector $\Pi : \mathbb{R}^N \to \mathbb{R}^{N-1}$ and an extension operator $\mathcal{E} : \mathbb{R}^{N-1} \to \mathbb{R}^N$ associated with the basis $\{\xi^i\}_{i=1\ldots,N}$ via*

$$\Pi X := (X\cdot\eta^1,\ldots,X\cdot\eta^{N-1}) \quad \text{for } X \in \mathbb{R}^N, \quad \mathcal{E}\, q := \sum_{k=1}^{N-1} q_k\,\xi^k \quad \text{for } q \in \mathbb{R}^{N-1}.$$

Then, there are mappings $\mathscr{R} \in C^1(\mathbb{R}_+\times\mathbb{R}^{N-1}; \mathbb{R}^N_+)$ and $\mathscr{M} \in C^1(\mathbb{R}_+\times\mathbb{R}^{N-1}; \mathbb{R})$ such that the nonlinear algebraic equations $\mu = \nabla_\rho h(\rho)$ are valid for $\mu \in \mathbb{R}^N$ and $\rho \in \mathbb{R}^N_+$ if and only if there are $\varrho \in \mathbb{R}_+$ and $q \in \mathbb{R}^{N-1}$ such that

$$\rho = \mathscr{R}(\varrho, q), \quad \rho\cdot\mathbb{1} = \varrho \qquad \text{and} \qquad \Pi\mu = q, \quad \mu\cdot\eta^N = \mathscr{M}(\varrho, q). \tag{46}$$

In view of Proposition 6.1, we equivalently define a solution to the system of Eq. (25) as a pair $(\varrho,\, q)$, with a function $\varrho :]0,T[\times\Omega \to \mathbb{R}_+$ and a vector field $q :]0,T[\times\Omega \to \mathbb{R}^{N-1}$ such that

$$\partial_t \mathscr{R}(\varrho,\, q) + \operatorname{div}(\mathscr{R}(\varrho,\, q)\, v - M(\mathscr{R}(\varrho,\, q))\, (\nabla \mathcal{E}\, q + \bar{Z}\, \nabla\phi)) = \bar{R}(\gamma^1 \cdot \mathcal{E}q, \ldots, \gamma^s \cdot \mathcal{E}q)\, \gamma. \tag{47}$$

For instance, one might choose $\xi^i = e^i$ $(i = 1, \ldots, N-1)$. In this case, $\eta^k = e^k - e^N$ for $k = 1, \ldots, N-1$ and $\eta^N = e^N$. Thus, $\Pi\mu$ is the vector $(\mu_1 - \mu_N, \ldots, \mu_{N-1} - \mu_N)$. For this reason, we propose to call *relative chemical potentials* the components of the new variable q.

In order to reexpress also in (26) and (27), the other occurrences of the original variables ρ, μ, we use the following equivalences relying on (46):

$$p = -h(\rho) + \sum_{i=1}^{N} \rho_i\, \mu_i = (-F + \mathrm{id}\, F')\, \big(\bar{V} \cdot \mathscr{R}(\varrho,\, q)\big) =: P(\varrho,\, q),$$
$$n^F = \bar{Z} \cdot \rho = \bar{Z} \cdot \mathscr{R}(\varrho,\, q).$$

Remark 6.2.
- It might be of importance to allow for a general Π, as its choice can be suited to the structure of the mobility matrix (e.g. (12)) in order to simplify the structure of the diffusion.
- In [14], we relaxed the lower bound in the condition (37) and used another strategy to introduce relative chemical potentials: define $\hat{q} \in \partial\mathbb{R}^N_-$ via $\hat{q} := \mu - \max_{i=1,\ldots,N} \mu_i\, \mathbb{1}$.

6.3. Vacuum oscillations

Although the pre-suppositions of the free energy model (18) in fact completely fail if the total mass density is below a lower critical value, the mathematical analysis cannot exclude the occurrence of a complete vacuum.

For our analytical treatment, a vacuum is characterised by the fact that the variables ϱ and q are 'decoupled' because the mapping $q \mapsto \mathscr{R}(\varrho = 0,\, q)$ is trivial on the entire $\mathbb{R}^{N-1}$. A concrete technical difficulty is raised concerning the compactness. Estimates on time-derivative are available only for the ρ-variables and do not transfer one to one to the q variables, since a sequence of mass densities $\rho^n = \mathscr{R}(\varrho_n,\, q^n)$ $(n \in \mathbb{N})$ such that $\varrho_n \to 0$ would converge strongly even if the corresponding q^n exhibit *oscillatory behaviour*.

Since the reaction densities are nonlinear expressions of $q_1, \ldots, q_{N-1}$, the vacuum-oscillations affect the concept of the solution at this level: The representation $R = -\partial_{D^{\mathrm{R}}} \Psi(\gamma^1 \cdot \mathcal{E}q, \ldots, \gamma^s \cdot \mathcal{E}q)$ for the production rates is restricted to the set where ϱ is strictly positive. An analogous situation occurs at the boundary $]0,T[\times\Gamma$ whenever it is in contact with a vacuum.

In order to include the possibility of this extreme behaviour, we relax the concept of a solution to (25), (28), (29), (30). It now contains four entries: the scalar $\varrho :]0,T[\times\Omega \to \mathbb{R}_+$ (total mass density) and the vector field $q :]0,T[\times\Omega \to \mathbb{R}^{N-1}$ (relative chemical potentials) like in the natural definition, but also the production factors in the bulk $R :]0,T[\times\Omega \to \mathbb{R}^s$ and on the interface $R^\Gamma :]0,T[\times\Gamma \to \mathbb{R}^{\hat{s}^\Gamma}$. We define the vacuum-free set via

$$Q^+(\varrho) := \{(t,x) \in]0,\, T[\times\Omega \,:\, \varrho(t,x) > 0\}.$$

For the representation of the bulk reactions, we require $r = \sum_{k=1}^{s} \gamma^k\, R_k$ with the following weaker condition:

$$R = \bar{R}(\gamma^1 \cdot \mathcal{E}q, \ldots, \gamma^s \cdot \mathcal{E}q) \text{ in } Q^+(\varrho). \tag{48}$$

We introduce a set $S^+(\varrho) \subseteq]0,T[\times\Gamma$ as the subset of all $(t,x) \in]0,T[\times\Gamma$ such that there is an open neighbourhood $U_{t,x}$ with the property

$$\lambda_4\Big(U_{t,x} \cap \{(s,y) \in]0,T[\times\Omega \,:\, \varrho(s,\,y)=0\}\Big) = 0.$$

For the concept of the solution, we ask for the representation $\hat{r} = \sum_{k=1}^{\hat{s}^\Gamma} \hat{\gamma}^k\, R^\Gamma_k$ together with

$$R^\Gamma = \hat{R}^\Gamma(t,\,x,\,\hat{\gamma}^1\cdot\mathcal{E}q,\ldots,\hat{\gamma}^{\hat{s}^\Gamma}\cdot\mathcal{E}q) \text{ in } S^+(\varrho). \tag{49}$$

7. The mathematical results

7.1. The solution class

For $t>0$, we recall that $Q_t =]0,t[\times\Omega$, $Q=Q_T$ and that $S_t =]0,t[\times\Gamma$, $S=S_T$. Exploiting the preliminary considerations of Sect. 6, a solution vector to the entire system (25), (26), (27) with boundary conditions (28), (29), (30), (31), (32) and initial conditions (=: Problem (P)) is composed of the scalars $\varrho : Q\to\mathbb{R}_+$ (total mass density) and $\phi : Q\to\mathbb{R}$ (electrical potential) and of the vector fields $q : Q\to\mathbb{R}^{N-1}$ (relative chemical potentials), and $v : Q\to\mathbb{R}^3$ (barycentric velocity field). If we want to account for the possibility of vacuum, the production factors are not everywhere functions of these components only. Thus, we also introduce $R : Q\to\mathbb{R}^s$, $R^\Gamma : S\to\mathbb{R}^{\hat{s}^\Gamma}$ as variables. For a given vector $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$, we introduce on the base of Proposition 6.1 the auxiliary variables

$$\rho = \mathscr{R}(\varrho,\,q), \tag{50a}$$

$$J = -M(\rho)\,D, \quad D := \nabla\mathcal{E}\,q + \bar{Z}\,\nabla\phi, \tag{50b}$$

$$r = \sum_{k=1}^{s}\gamma^k\,R_k, \quad D^{\mathrm{R}}_k := \gamma^k\cdot\mathcal{E}q \quad \text{for } k=1,\ldots,s, \tag{50c}$$

$$\hat{r} = \sum_{k=1}^{\hat{s}^\Gamma}\hat{\gamma}^k\,R^\Gamma_k, \quad \hat{D}^{\Gamma,\mathrm{R}}_k := \hat{\gamma}^k\cdot\mathcal{E}q \quad \text{for } k=1,\ldots,\hat{s}^\Gamma, \tag{50d}$$

$$p = P(\varrho,\,q), \tag{50e}$$

$$n^F = \rho\cdot\bar{Z}. \tag{50f}$$

An essential property of solutions is the mass and energy conservation.

Definition 7.1. We say that $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$ satisfies the *(global) energy (in)equality* with free energy function h and mobility matrix M if and only if the associated fields and variables (50) satisfy, for almost all $t\in]0,T[$,

$$\begin{aligned}
&\int_\Omega \left\{\frac{1}{2}\,\varrho\,v^2 + \frac{1}{2}\,\bar{\chi}\,|\nabla\phi|^2 + h(\rho)\right\}(t)\,\mathrm{d}x \\
&\quad + \int_{Q_t}\{\mathbb{S}(\nabla v)\,:\,\nabla v + M\,D\,:\,D + (\Psi(D^{\mathrm{R}}) + \Psi^*(-R))\} + \int_{S_t}\{\hat{\Psi}^\Gamma(\cdot,\,\hat{D}^{\Gamma,\mathrm{R}}) + (\hat{\Psi}^\Gamma)^*(\cdot,\,-R^\Gamma)\} \\
&\overset{(\leq)}{=} \int_\Omega\left\{\frac{1}{2}\,\varrho_0\,|v^0|^2 + \frac{1}{2}\,\bar{\chi}\,|\nabla\phi_0(0)|^2 + h(\rho^0)\right\}\mathrm{d}x - \int_\Omega \left\{n^F\,\phi_0 - \bar{\chi}\,\nabla\phi\cdot\nabla\phi_0\right\}\Big|_0^t\,\mathrm{d}x \\
&\quad + \int_{Q_t}\{n^F\,\phi_{0,t} - \bar{\chi}\,\nabla\phi\cdot\nabla\phi_{0,t}\} + \int_{S_t}\{(\hat{r}+J^0)\cdot\bar{Z}\,\phi_0 + J^0\cdot\mathcal{E}q\}.
\end{aligned} \tag{51}$$

We say that $(\varrho,\, q,\, v,\, \phi,\, R,\, R^{\Gamma})$ satisfies the *balance of net masses* if the vector field

$$\bar{\rho} := \int_{\Omega} \rho \,\mathrm{d}x = \int_{\Omega} \mathscr{R}(\varrho,\, q)\,\mathrm{d}x, \tag{52}$$

is subject to

$$\bar{\rho}(t) = \bar{\rho}^0 + \int_0^t \left\{ \int_{\Omega} r + \int_{\Gamma} (\hat{r} + J^0) \right\}(s)\,\mathrm{d}s \quad \text{for all } t \in [0, T]. \tag{53}$$

The conservation of energy provides the natural bounds that will allow to define the weak solution. We introduce what one could call a *natural class* $\mathcal{B}$, because this class naturally arises from the global energy and mass conservation identities associated with the model. The class $\mathcal{B}$ reflects the regularity of the weak solution and depends on several parameters

- The final time $T > 0$, the domain Ω and the partition $\Gamma \cup \Sigma$ of its boundary (see (40));
- The choice of the free energy function h and in particular the growth exponent of (34);
- The mobility matrix M, in particular its rank denoted by $\operatorname{rk} M$;
- The choice of the potentials Ψ and Ψ^{Γ} for the reaction densities.

The variables ϱ, ϕ and v will satisfy the conditions

$$\varrho \in L^{\infty,\alpha}(Q_T;\, \mathbb{R}_{0,+}), \tag{54}$$

$$v \in W^{1,0}_{2,S}(Q_T;\, \mathbb{R}^3), \tag{55}$$

$$\sqrt{\varrho}\, v \in L^{\infty,2}(Q_T;\, \mathbb{R}^3), \tag{56}$$

$$\phi \in L^{\infty}(Q_T), \quad \nabla\phi \in L^{\infty,\beta}(Q_T;\, \mathbb{R}^3), \tag{57}$$

with the exponents $\alpha > 3/2$ and $r(\Omega, \Gamma) > 2$ of the conditions (34) and (40), and with

$$\beta := \min\left\{ r(\Omega,\, \Gamma),\, \frac{3\alpha}{(3-\alpha)^+} \right\}. \tag{58}$$

For the variables R and R^{Γ}, we consider the conditions

$$-R \in L_{\Psi^*}(Q;\, \mathbb{R}^s), \quad -R^{\Gamma} \in L_{(\hat{\Psi}^{\Gamma})^*}(S;\, \mathbb{R}^{\hat{s}^{\Gamma}}). \tag{59}$$

For the variable q, a control is achieved on the spatial gradient thanks to the assumption (37). However, in the context of flux boundary conditions, the bound on the L^1-norm is a non-trivial problem. We shall nevertheless obtain, in Theorem 11.3, the integrability in time via complex estimates involving the diffusion gradient, the reactions and the conservation of total mass. Under the assumption (38) of at least quadratic potentials, a natural class for the variable q is then

$$q \in W^{1,0}_2(Q;\, \mathbb{R}^{N-1}). \tag{60}$$

Due to the dissipation of chemical reactions, the variable q also satisfies the additional conditions

$$(\gamma^1 \cdot \mathcal{E}q, \ldots, \gamma^s \cdot \mathcal{E}q) \in L_{\Psi}(Q_T;\, \mathbb{R}^s), \quad (\hat{\gamma}^1 \cdot \mathcal{E}q, \ldots, \hat{\gamma}^{\hat{s}^{\Gamma}} \cdot \mathcal{E}q) \in L_{\hat{\Psi}^{\Gamma}}(S_T;\, \mathbb{R}^{\hat{s}^{\Gamma}}). \tag{61}$$

The natural class $\mathcal{B}$ also encodes an information concerning the conservation of global mass (integration of (25) over Ω, (53)). We additionally introduce a non-negative function $\Phi^* \in C([0,T]^2)$, $\Phi^*(t,\, t) = 0$ constructed from the functions Ψ, Ψ^{Γ} (and thus from R and R^{Γ}) via

$$\Phi^*(t_1,\, t_2) := \sup_{[-R]_{L_{\Psi^*}(Q)} \le C_0} \left| \int_{t_1}^{t_2} \int_{\Omega} R \cdot \gamma \right| + \sup_{[-\hat{R}]_{L_{(\hat{\Psi}^{\Gamma})^*}(S)} \le C_0} \left| \int_{t_1}^{t_2} \int_{\Gamma} \hat{R} \cdot \hat{\gamma} \right| + (t_2 - t_1), \tag{62}$$

for all $0 \leq t_1 \leq t_2 \leq T$. Here, C_0 is an appropriate constant that we will choose later. For a function $u \in C^1([0,T])$, we define a weighted modulus of uniform continuity via

$$[u]_{C_{\Phi^*}([0,T])} := \sup_{t_1,\, t_2 \in [0,T]} \frac{|u(t_1) - u(t_2)|}{\Phi^*(t_1,\, t_2)}.$$

Definition 7.2. If $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)$ fulfils (54)–(57) and (59), (60), (61), we define

$$\begin{aligned}
&[(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,\mathrm{rk}\, M,\,\Psi,\,\Psi^\Gamma)}\\
:=\quad & \|\varrho\|_{L^{\infty,\alpha}(Q)} + \|v\|_{W^{1,0}_2(Q;\,\mathbb{R}^3)} + \|\sqrt{\varrho}\, v\|_{L^{\infty,2}(Q;\,\mathbb{R}^3)} + \|\phi\|_{L^\infty(Q)} + \|\nabla\phi\|_{L^{\infty,\beta}(Q;\,\mathbb{R}^3)}\\
&+ \|q\|_{W^{1,0}_2(Q;\,\mathbb{R}^{N-1})} + [D^{\mathrm{R}}]_{L_\Psi(Q;\,\mathbb{R}^s)} + [\hat{D}^{\Gamma,\mathrm{R}}]_{L_{\hat{\Psi}^\Gamma}(S;\,\mathbb{R}^{\hat{s}^\Gamma})} + \|J\|_{L^{2,\,\frac{2\alpha}{1+\alpha}}(Q;\,\mathbb{R}^{N\times 3})}\\
&+ [-R]_{L_{\Psi^*}(Q;\,\mathbb{R}^s)} + [-R^\Gamma]_{L_{(\hat{\Psi}^\Gamma)^*}(S;\,\mathbb{R}^{\hat{s}^\Gamma})} + \|p\|_{L^{\min\{1+\frac{1}{\alpha},\,\frac{5}{3}-\frac{1}{\alpha}\}}(Q)} + [\bar{\rho}]_{C_{\Phi^*}([0,T];\,\mathbb{R}^N)},
\end{aligned}$$

where D^{R}, J, p are defined in (50), and $\bar{\rho}$ in (52). We say that $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)$ belongs to the class $\mathcal{B}(T,\,\Omega,\,\alpha, \mathrm{rk}\, M,\,\Psi,\,\Psi^\Gamma)$ if and only if the number $[(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,\mathrm{rk}\, M,\,\Psi,\,\Psi^\Gamma)}$ is finite.

Definition 7.3. We call a vector $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma) \in \mathcal{B}(T,\,\Omega,\,\alpha,\, N-1,\,\Psi,\,\Psi^\Gamma)$ a *weak solution* to the Problem (P) if the energy inequality and the balance of net masses of Definition 7.1 are valid, and if the quantities ρ, J, r and $\hat{r}$, p and n^F obeying the Definitions (50) satisfy the relations

$$\begin{aligned}
&-\int_Q \rho\cdot\partial_t\psi - \int_Q (\rho\, v + J) : \nabla\psi\\
&\qquad = \int_\Omega \rho^0\cdot\psi(0) + \int_Q r\cdot\psi + \int_{S_T} (\hat{r} + J^0)\cdot\psi \quad \forall\, \psi \in C^1_c([0,T[;\, C^1(\overline{\Omega};\,\mathbb{R}^N)),
\end{aligned}\tag{63}$$

$$\begin{aligned}
&-\int_Q \varrho\, v\cdot\partial_t\eta - \int_Q \varrho\, v\otimes v : \nabla\eta - \int_Q p\,\mathrm{div}\,\eta + \int_Q \mathbb{S}(\nabla v) : \nabla\eta\\
&\qquad = \int_\Omega \varrho_0\, v^0\cdot\eta(0) - \int_Q n^F\,\nabla\phi\cdot\eta \quad \forall\, \eta \in C^1_c([0,T[;\, C^1_c(\Omega;\,\mathbb{R}^3)),
\end{aligned}\tag{64}$$

$$\bar{\chi}\int_Q \nabla\phi\cdot\nabla\zeta = \int_Q n^F\,\zeta \quad \forall\,\zeta \in L^1(0,T;\, W^{1,2}_\Gamma(\Omega)) \text{ and } \phi = \phi_0 \text{ as traces on }]0,T[\times\Gamma, \tag{65}$$

and if the identities (48) and (49) relating ϱ, q, R and R^Γ are valid.

This concept of weak solution is well defined owing to standard estimates.

7.2. Main theorems

Theorem 7.4. (Global-in-time existence) *Let $\Omega \in C^{0,1}$. Assume that the free energy function h satisfies (34) and (35) and that the mobility matrix M satisfies (36) and (37). Let $\Psi \in C^2(\mathbb{R}^s)$ and $\Psi^\Gamma \in C^2(\mathbb{R}^{s^\Gamma})$ be strictly convex, non-negative and satisfy (38). Assume that the initial data ρ^0 and v^0, and the boundary data μ^{ext}, ϕ_0 are non-degenerate in the sense of (42), and that one of the following conditions is valid:*

(1) $\alpha \geq 2$;
(2) $\frac{9}{5} \leq \alpha < 2$ *and* $r(\Omega,\,\Gamma) > \alpha'$;
(3) $\frac{3}{2} < \alpha < \frac{9}{5}$, $r(\Omega,\,\Gamma) > \alpha'$ *and the vectors* $m \in \mathbb{R}^N_+$ *and* $V \in \mathbb{R}^N_+$ *are parallel.*

Assume moreover that the vector $\bar{\rho}^0 := \int_\Omega \rho^0(x)\,\mathrm{d}x$ *of the initial net masses of the constituents has positive distance to the manifold* $\mathcal{M}_{crit}$ *of* (45). *Then, for* $T > 0$ *arbitrary, the problem* (P) *possesses a weak solution in the class* $\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$ *(sense of Definition* 7.3*).*

We can characterise the singular states of the system associated with species vanishing.

Theorem 7.5. *We adopt the same assumptions as in Theorem* 7.4*. For every weak solution to* (P)*, the compact set* $K_0 := \{t \in [0,T] \,:\, \min_{i=1,\ldots,N} \bar{\rho}_i(t) = 0\}$ *satisfies* $\lambda_1(K_0) = 0$*. For almost all* $t \in [0,T]\backslash K_0$*, the domain* Ω *possesses the disjoint decomposition* $\Omega = \mathcal{P}_t \cup \mathcal{V}_t \cup \mathcal{N}_t$ *where*

(1) $\mathcal{P}_t = \{x \in \Omega \,:\, \min_{i=1,\ldots,N} \rho_i(t,x) > 0\}$ *is a set where all components of the mixture are available;*
(2) $\mathcal{V}_t = \{x \in \Omega \,:\, \varrho(t,x) = 0\}$ *is a set occupied by a complete vacuum;*
(3) $\lambda_3(\mathcal{N}_t) = 0$.

If the initial net masses of the constituents belongs to the critical manifold, then it is possible that certain groups of species are completely consumed after finite time, and the solution then exists only up to this time. Afterwards, it might be necessary to restart the system with a smaller number of species.

Theorem 7.6. (Local-in-time existence) *We adopt the same assumptions as in Theorem* 7.4*, except that we require* $\bar{\rho}_0 \in \mathcal{M}_{crit}$*. Then, there are a time* $T_0 > 0$ *depending only on the data, and a maximal time* $T_0 \leq T^* \leq +\infty$ *such that for all* $t < T^*$*, there is a weak solution* $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma) \in \mathcal{B}(t,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$ *in the sense of Definition* 7.3 *to* (P_t)*. Moreover, the following alternative concerning* T^* *is valid:*

(1) *Either* $T^* = +\infty$*,*
(2) *Or there is* $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma) \in \bigcap_{t<T^*} \mathcal{B}(t,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$ *that weakly solves* (P_t) *for all* $t < T^*$*, such that* $\min_{i=1,\ldots,N} \bar{\rho}_i(t) > 0$ *for all* $t \in [0, T^*[$*, and such that*

$$\lim_{t\to T^*} \min_{i=1,\ldots,N} \bar{\rho}_i(t) = 0, \quad \liminf_{t\to T^*} \|q(t)\|_{L^1(\Omega;\,\mathbb{R}^{N-1})} = +\infty.$$

7.3. Structure of the next sections

Our plan for the next sections is as follows. According to the preliminary Sect. 6, the algebraic properties of Eq. (10) determines the analysis of the model. Our next Sect. 8 is therefore devoted to the proof of Proposition 6.1. After that, we shall turn our attention to the PDEs. In Sect. 9, we introduce thermodynamically consistent regularisations of the problem (P) for which it is easier to prove the solvability. For this larger class of problems, we then derive the energy and global mass balance identities (Sect. 9.3) and the resulting *a priori* estimates (Sect. 10). Section 11 deals in particular with *a priori* estimates for the variable q, one of the most demanding part of the analysis. In order to pass to the limit with the numerous nonlinearities of the system, it is necessary to obtain compactness statements for the principal variables (Sect. 12). With this apparatus at hand, we are able to complete the proof of the main theorems in Sect. 13 and 14 devoted to existence.

8. The natural variables: algebraic statements

As far as the mass transfer part of the problem (P) is concerned, the natural estimates resulting from the energy identity arise for the total mass density ϱ and for a $N-1$ dimensional reduction of the vector μ, its projection on $\mathbb{1}^\perp$. In this section, we describe the solution mapping for the nonlinear algebraic equation (10) in these variables. In particular, this section provides the rigorous derivation of the statements announced in Sect. 6.

8.1. The case of a general free energy

The algebraic relation between partial mass densities ρ and chemical potentials μ is given by

$$\mu_i = \partial_{\rho_i} h(\rho_1, \ldots, \rho_N) \quad \text{for } i = 1, \ldots, N. \tag{66}$$

In the isothermal case we can forget about the temperature-dependence, so $h = h(\rho)$. Using tools of convex analysis, we immediately obtain that the relation (66) is invertible if h is a function of Legendre type on $\mathbb{R}^N_+$, meaning that (cf. [32], chapter 26)

- $\rho \mapsto h(\rho)$ is strictly convex and continuously differentiable in $\mathbb{R}^N_+$;
- $|\nabla_\rho h(\rho^m)| \to +\infty$ for all $\{\rho^m\}_{m\in\mathbb{N}}$ such that $\operatorname{dist}(\rho^m, \partial\mathbb{R}^N_+) \to 0$ (h is *essentially smooth*).

Lemma 8.1. *Let $h \in C^2(\mathbb{R}^N_+) \cap C(\mathbb{R}^N_{0,+})$ be a function of Legendre type on $\mathbb{R}^N_+$. Let $D^*_h \subseteq \mathbb{R}^N$ be the image $\nabla_\rho h(\mathbb{R}^N_+)$, that is $D^*_h = \{\mu \in \mathbb{R}^N \,:\, \exists\, \rho \in \mathbb{R}^N_+,\ \mu = \nabla_\rho h(\rho)\}$. Then, the convex conjugate of h, denoted by h^*, is a well-defined strictly convex function on D^*_h, and it satisfies $h^* \in C^2(D^*_h)$. Moreover, the relation (66) is valid for $\mu \in D^*_h$ and $\rho \in \mathbb{R}^N_+$ if and only if $\rho = \nabla_\mu h^*(\mu)$.*

Proof. The claim follows from the Theorem 26.5 of [32]. □

Next we investigate the possibility to introduce 'mixed' coordinates to describe the set of solutions to (66). Let $\xi^1, \ldots, \xi^N \in \mathbb{R}^N$ be a basis of $\mathbb{R}^N$ such that $\xi^N := \mathbb{1}$. Choose $\eta^1, \ldots, \eta^N \in \mathbb{R}^N$ such that $\xi^i \cdot \eta^j = \delta^j_i$, $i, j = 1, \ldots, N$. We define $\Pi : \mathbb{R}^N \to \mathbb{R}^{N-1}$ and $\mathcal{E} : \mathbb{R}^{N-1} \to \mathbb{R}^N$ as in Proposition 6.1.

Corollary 8.2. *Under the assumptions of Lemma 8.1, we define a set $\mathscr{D} \subseteq \mathbb{R}_+ \times \mathbb{R}^{N-1}$ via*

$$\mathscr{D} := \left\{(s,\, q) \in \mathbb{R}_+ \times \mathbb{R}^{N-1} \,:\, \exists t \in \mathbb{R},\ \mathcal{E}q + t\,\mathbb{1} \in D^*_h \text{ and } \mathbb{1} \cdot \nabla h^*(\mathcal{E}q + t\,\mathbb{1}) = s\right\}.$$

Then, $\mathscr{D}$ is open, and there is a function $\mathscr{M} \in C^1(\mathscr{D})$, $(s,\, q) \mapsto \mathscr{M}(s,\, q)$, such that if (66) holds with $\mu \in D^*_h$ and $\rho \in \mathbb{R}^N_+$, then

$$\mu = \sum_{i=1}^{N-1} (\Pi\mu)_i\, \xi^i + \mathscr{M}(\rho \cdot \mathbb{1},\, \Pi\mu)\; \mathbb{1} = (\mathcal{E} \circ \Pi)\mu + \mathscr{M}(\rho \cdot \mathbb{1},\, \Pi\mu)\; \mathbb{1}.$$

The derivatives of $\mathscr{M}$ satisfy the identities

$$\partial_s \mathscr{M}(\rho \cdot \mathbb{1},\, q) = \frac{1}{D^2 h^*(\mu)\mathbb{1} \cdot \mathbb{1}}, \quad \partial_{q_j} \mathscr{M}(\rho \cdot \mathbb{1},\, q) = -\,\frac{D^2 h^*(\mu)\mathbb{1} \cdot \xi^j}{D^2 h^*(\mu)\mathbb{1} \cdot \mathbb{1}} \quad \textit{for } j = 1, \ldots, N-1.$$

Proof. Define an open set $\mathcal{U} \subset \mathbb{R}^{N-1} \times \mathbb{R}$ via

$$\mathcal{U} := \{(q,\, t) \in \mathbb{R}^{N-1} \times \mathbb{R} \,:\, \mathcal{E}q + t\,\mathbb{1} \in D^*_h\}.$$

We define a function $G : \mathcal{U} \times \mathbb{R}_+ \to \mathbb{R}$ via $G(q,\, t,\, s) := \mathbb{1} \cdot \nabla_\mu h^*(\mathcal{E}q + t\,\mathbb{1}) - s$. We compute the partial derivatives and we use the strict convexity of $D^2 h^*$ to show that

$$\partial_t G(q,\, t,\, s) = D^2 h^*(\mathcal{E}q + t\,\mathbb{1})\,\mathbb{1} \cdot \mathbb{1} > 0,\ \ \partial_{q_j} G(q,\, t,\, s) = D^2 h^*(\mathcal{E}q + t\,\mathbb{1})\,\xi^j \cdot \mathbb{1}.$$

Consider now the solution manifold for $G = 0$ in $\mathcal{U} \times \mathbb{R}_+$. Since $G_t > 0$, we obtain from the implicit function theorem that there is $\mathscr{M} \in C^1(\mathscr{D})$

$$G(q,\, t,\, s) = 0 \text{ if and only if } t = \mathscr{M}(s,\, q).$$

In particular, $\partial_s \mathscr{M} = G_t^{-1}(q,\, t,\, s)$ and $\partial_q \mathscr{M} = -G_q/G_t$.

Assume now that (66) is valid for $\mu \in D^*_h$ and $\rho \in \mathbb{R}^N_+$. We express $\mu = \sum_{i=1}^{N-1} (\mu \cdot \eta^i)\,\xi^i + (\mu \cdot \eta^N)\,\mathbb{1}$. Then, $G(\Pi\mu,\, \mu \cdot \eta^N,\, \rho \cdot \mathbb{1}) = 0$ so that $\mu \cdot \eta^N = \mathscr{M}(\rho \cdot \mathbb{1},\, \Pi\mu)$. □

Corollary 8.3. *Assumptions as in Corollary 8.2. Then, there is a bijection $\mathscr{R} : C^1(\mathscr{D}; \mathbb{R}^N_+)$ such that (66) is valid for $\mu \in D^*_h$ and $\rho \in \mathbb{R}^N_+$ if and only if $\mu \cdot \eta^N = \mathscr{M}(\rho \cdot \mathbb{1},\, \Pi\mu)$ and $\rho = \mathscr{R}(\rho \cdot \mathbb{1},\, \Pi\mu)$.*

Proof. For $(s,\, q) \in \mathscr{D}$, we define $\mathscr{R}(s,\, q) := \nabla_\mu h^*(\mathcal{E}\, q + \mathscr{M}(s,\, q)\, \mathbb{1})$. We may compute that

$$\partial_{q_j}\mathscr{R}_i(s,\, q) = D^2h^* e^i \cdot \xi^j - \frac{D^2h^*e^i \cdot \mathbb{1}\, D^2h^*\xi^j \cdot \mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}, \quad \partial_s\mathscr{R}_i(s,\, q) = \frac{D^2h^*e^i\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}. \tag{67}$$

In these formula, D^2h^* is evaluated at $\mu = \mathcal{E}q + \mathscr{M}(s,q)\,\mathbb{1}$. In order to prove that $\mathscr{R}$ is a bijection, it is sufficient to show that $d\mathscr{R}$ is invertible. Let $X = (r,\, q) \in \mathbb{R}\times\mathbb{R}^{N-1}$ arbitrary. Then, $d\mathscr{R}\, X = 0$ means that for $i = 1, \ldots, N$ one has

$$e^i \cdot D^2h^* \left(\mathcal{E}q - \mathbb{1}\left(\frac{r + D^2h^*\mathbb{1}\cdot\mathcal{E}q}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\right)\right) = 0.$$

The uniform invertibility of D^2h^* yields $\mathcal{E}q = \mathbb{1}\left(\frac{r+D^2h^*\mathbb{1}\cdot\mathcal{E}q}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\right)$. We now multiply this identity with $\eta^1, \ldots, \eta^{N-1}$, and since $\eta^j \cdot \mathbb{1} = 0$ for $j = 1, \ldots, N-1$, it follows that $q_1, \ldots, q_{N-1} = 0$. Therefore, also $r = 0$. This proves that $\mathscr{R}$ is bijective.

To prove the claimed equivalence, suppose first that (66) is valid. Applying Corollary 8.2, we find that $\mu = (\mathcal{E}\circ\Pi)\mu + \mathscr{M}(\rho\cdot\mathbb{1},\, \Pi\mu)\,\mathbb{1}$. Thus, $\mu\cdot\eta^N = \mathscr{M}(\rho\cdot\mathbb{1},\, \Pi\mu)$. The definition of $\mathscr{R}$ then yields $\nabla_\rho h(\rho) = \mu = \nabla_\rho h(\mathscr{R}(\varrho,\, \Pi\mu))$, showing that $\rho = \mathscr{R}(\varrho,\, \Pi\mu)$.

Reversely, if $\rho = \mathscr{R}(\varrho,\, \Pi\mu)$ and $\mu\cdot\eta^N = \mathscr{M}(\rho\cdot\mathbb{1},\, \Pi\mu)$, then the definition of $\mathscr{R}$ yields $\rho = \nabla_\mu h^*(\mathcal{E}\Pi\mu + \mu\cdot\eta^N\,\mathbb{1}) = \nabla_\mu h^*(\mu)$, proving that (66) is valid. □

The pressure function The pressure is given by the formula $p := -h + \sum_{i=1}^N \rho_i\,\mu_i$. We immediately see under (66) that $p = h^*(\mu)$ where h^* is the convex conjugate of h. We define a function $P : \mathscr{D} \to \mathbb{R}$ via $P(s,\, q) := h^*(\mathcal{E}\, q + \mathscr{M}(s,\, q)\,\mathbb{1})$.

Lemma 8.4. *Let $(s,\, q) \in \mathscr{D}$. Then, $P \in C^1(\mathscr{D})$ satisfies*

$$\partial_s P(s,\, q) = \frac{s}{D^2h^*\mathbb{1}\cdot\mathbb{1}}, \quad \partial_{q_j}P(s,\, q) = \xi^j\cdot\nabla_\mu h^* - s\,\frac{D^2h^*\mathbb{1}\cdot\xi^j}{D^2h^*\mathbb{1}\cdot\mathbb{1}} \quad \text{for } j = 1, \ldots, N-1.$$

In these formula, D^2h^* is evaluated at $\mu = \mathcal{E}q + \mathscr{M}(s,q)\,\mathbb{1}$.

Proof. Define $\mu := \mathcal{E}\, q + \mathscr{M}(s,\, q)\,\mathbb{1}$ and $\rho = \nabla_\mu h^*(\mu)$. Then,

$$\partial_s P(s,\, q) = \mathbb{1}\cdot\nabla_\mu h^*(\mu)\,\mathscr{M}_s(s,\, q) = \rho\cdot\mathbb{1}\,\mathscr{M}_s(s,\, q),$$
$$\partial_{q_j}P(s,\, q) = \xi^j\cdot\nabla_\mu h^*(\mu) + \mathbb{1}\cdot\nabla_\mu h^*(\mu)\mathscr{M}_{q_j}(s,\, q) = \rho\cdot\xi^j + \rho\cdot\mathbb{1}\,\mathscr{M}_{q_j}(s,\, q),$$

and the claim follows from Corollary 8.2. □

8.2. Special constitutive choice of the free energy

For special choices of the free energy, we can find more explicit formula than Lemma 8.1. Under the conditions (18), (19), (20) the relation (66) reads

$$\mu_i = c_i + \bar{V}_i\, F'(\bar{V}\cdot\rho) + \frac{1}{m_i}\ln y_i \quad i = 1, \ldots, N, \tag{68}$$

where $c_1, \ldots, c_N \in \mathbb{R}$ are constants related to the reference states, and $y_i = \rho_i/(m_i\sum_j(\rho_j/m_j))$ is the number fraction. Recall that $\bar{V}_i = V_i/m_i$. Note that the free energy $h = h^{\text{ref}} + h^{\text{mech}} + h^{\text{mix}}$ satisfies the assumptions of Lemma 8.1 if we assume that the function $F \in C^2(\mathbb{R}_+)\cap C(\mathbb{R}_{0,+})$ is of Legendre type on $\mathbb{R}_+$. At first we want to characterise the set D_h^* and we need a preliminary Lemma.

Lemma 8.5. *There is a function $f \in C^1(\mathbb{R}^N)$ such that, if (68) is valid for $\mu \in \mathbb{R}^N$ and $\rho \in \mathbb{R}^N_+$, then $F'(\bar{V}\cdot\rho) = f(\mu)$. Moreover, the function f satisfies the following inequalities*

$$c\,(\max_i \mu_i - \max_i c_i) \le f(\mu) \le C_1\,(\max_i \mu_i - \min_i c_i) + C_2\ln N\,, \qquad |\nabla_\mu f(\mu)| \le C_1, \tag{69}$$

where c, C_i $(i = 1, 2)$ are positive constants depending on V and m.

Proof. Define a function $G : \mathbb{R}^N \times \mathbb{R} \to \mathbb{R}$, $(\mu, t) \mapsto G(\mu, t)$ via

$$G(\mu, t) := \sum_{i=1}^{N} \exp\left(m_i\,(\mu_i - c_i) - V_i\,t\right) - 1.$$

For $\mu \in \mathbb{R}^N$, it is readily verified that $\lim_{t\to-\infty} G(\mu, t) = +\infty$ and that $\lim_{t\to+\infty} G(\mu, t) = -1$. Since $G_t(\mu, t) < 0$, the solution manifold to $G(\mu, t) = 0$ is a hyper-surface $\{(\mu, f(\mu)) : \mu \in \mathbb{R}^N\}$ where $\partial_i f(\mu) = -G_t^{-1}(\mu, f(\mu))\, G_{\mu_i}(\mu, f(\mu))$. Easy computations show that

$$\partial_i f(\mu) = m_i\, \frac{\exp\left(m_i\,(\mu_i - c_i) - V_i\, f(\mu)\right)}{\sum_{j=1}^{N} V_j\, \exp\left(m_j\,(\mu_j - c_j) - V_j\, f(\mu)\right)}. \tag{70}$$

In particular, $|\nabla_\mu f| \leq \max m / \min V$. Moreover, if $G(\mu, t) = 0$, then setting

$$y_i = \exp\left(m_i\,(\mu_i - c_i) - V_i\,t\right),$$

we see that $\mu_i = c_i + (V_i/m_i)\,t + (1/m_i)\,\ln y_i$ for $i = 1, \ldots, N$. Since $y \in]0, 1[^N$ and $y \cdot \mathbb{1} = 1$, the estimates (69) easily follow. □

We are now ready to prove an inversion formula for the relation (68).

Corollary 8.6. *Assume that the function $F \in C^2(\mathbb{R}_+) \cap C(\mathbb{R}_{0,+})$ is of Legendre type on $\mathbb{R}_+$. Define $D_h^* := \nabla_\rho h(\mathbb{R}^N_+)$. Then, $D_h^* = \{\mu \in \mathbb{R}^N : f(\mu) \in F'(\mathbb{R}_+)\}$. If $\mu \in D_h^*$, then*

$$\partial_i h^*(\mu) = m_i\, ([F']^{-1} \circ f)(\mu)\, \frac{\exp\left(m_i\,(\mu_i - c_i) - V_i\, f(\mu)\right)}{\sum_{j=1}^{N} V_j\, \exp\left(m_j\,(\mu_j - c_j) - V_j\, f(\mu)\right)} = \partial_i (F^* \circ f)(\mu), \tag{71}$$

where F^* is the Legendre transform of F.

Proof. If $\mu \in D_h^*$, then there is $\rho \in \mathbb{R}^N_+$ such that $\mu = \nabla_\rho h(\rho)$. Thus, (68) is valid, and Lemma 8.5 shows that $F'(\bar{V} \cdot \rho) = f(\mu)$. Thus, $f(\mu) \in F'(\mathbb{R}_+)$ and this first yields the inclusion $D_h^* \subseteq \{\mu \in \mathbb{R}^N : f(\mu) \in F'(\mathbb{R}_+)\}$. In order to prove the reverse inclusion, consider $\mu \in \mathbb{R}^N$ such that $f(\mu) \in F'(\mathbb{R}_+)$. Define

$$g(\mu) := [F']^{-1} \circ f(\mu), \quad \rho_i := m_i\, g(\mu)\, \frac{\exp\left(m_i\,(\mu_i - c_i) - V_i\, f(\mu)\right)}{\sum_{j=1}^{N} V_j\, \exp\left(m_j\,(\mu_j - c_j) - V_j\, f(\mu)\right)}.$$

We easily show that $\nabla_\rho h(\rho) = \mu$. Use of (70) yields

$$\partial_i h^*(\mu) = g(\mu)\, \partial_i f(\mu) = \partial_i (F^* \circ f)(\mu).$$

□

Lemma 8.7. *Adopt the same assumptions as in Corollary 8.6, and moreover assume that F fulfils (35). Then, $\nabla_\mu h^* \in C^1(D_h^*)$, and for $i, j = 1, \ldots, N$ there holds*

$$D^2 h^*_{i,j}(\nabla_\rho h(\rho)) = m_i\, \rho_j\, \delta_i^j + \frac{\rho_i\, \rho_j}{\rho \cdot \bar{V}}\, \left(\frac{1}{\rho \cdot \bar{V}\, F''(\rho \cdot \bar{V})} + \frac{n \cdot V^2}{\rho \cdot \bar{V}} - (V_i + V_j)\right), \tag{72}$$

with $n \cdot V^2 := \sum_{i=1}^{N} V_i^2\, n_i$. There are further constants C_0, C_1 independent on ρ such that

$$|D^2 h^*(\nabla_\rho h(\rho))| \leq C_1\, \rho \cdot \mathbb{1} \tag{73}$$

$$D^2 h^*(\nabla_\rho h(\rho))\, \mathbb{1} \cdot \mathbb{1} \geq C_0 / F''(\rho \cdot \mathbb{1}). \tag{74}$$

Proof. By direct computation starting from (71), we obtain (72). This entails

$$\begin{aligned} |D^2 h^*_{i,j}(\nabla_\rho h(\rho))| &\leq \rho_i\, \left(m_i + \frac{m_j}{\min V}\, \left(\frac{1}{\rho \cdot \bar{V}\, F''(\rho \cdot \bar{V})} + \frac{(\max V)^2}{\min V} + 2\, \max V\right)\right) \\ &\leq C\, \rho_i\, \left(1 + \frac{1}{\rho \cdot \bar{V}\, F''(\rho \cdot \bar{V})}\right). \end{aligned}$$

The function $s\,F''(s)$ is asymptotically equivalent to $s\,s^{-1} = \text{const}$ near zero (cf. (35)) and to $s\,s^{\alpha-2} = s^{\alpha-1}$ for s large. Thus, there is a constant $c_0 > 0$ such that $\inf_{s\in\mathbb{R}_+} s\,F''(s) \geq c_0$, and (73) follows. Further

$$D^2h^*\mathbb{1}\cdot e^i = \frac{\rho_i\,\rho\cdot\mathbb{1}}{F''(\rho\cdot\bar{V})\,(\rho\cdot\bar{V})^2} + \rho_i\left(m_i + \frac{\rho\cdot\mathbb{1}\,n\cdot V^2}{(\rho\cdot\bar{V})^2} - \frac{V_i\,\rho\cdot\mathbb{1}}{\rho\cdot\bar{V}} - \frac{\rho\cdot V}{\rho\cdot\bar{V}}\right).$$

Hence,

$$\begin{aligned}\sum_{i,j=1}^{N} D^2h^*_{j,i} &= \frac{(\rho\cdot\mathbb{1})^2}{(\rho\cdot\bar{V})^2\,F''(\rho\cdot\bar{V})} + m\cdot\rho + \frac{(\rho\cdot\mathbb{1})^2\,V^2\cdot n}{(\rho\cdot\bar{V})^2} - 2\,\frac{\rho\cdot V\,\rho\cdot\mathbb{1}}{\rho\cdot\bar{V}}\\ &= \frac{(\rho\cdot\mathbb{1})^2}{(\rho\cdot\bar{V})^2\,F''(\rho\cdot\bar{V})} + \left(\sqrt{m\cdot\rho} - \frac{\rho\cdot\mathbb{1}\,\sqrt{V^2\cdot n}}{\rho\cdot\bar{V}}\right)^2 + 2\,\frac{\rho\cdot\mathbb{1}}{\rho\cdot\bar{V}}\,(\sqrt{m\cdot\rho}\,\sqrt{V^2\cdot n} - V\cdot\rho). \end{aligned} \tag{75}$$

The estimate (74) is a consequence of (75) and of the Cauchy–Schwarz inequality: we can express $V_i\,\rho_i = (V_i\,\sqrt{n_i})\,(m_i\,\sqrt{n_i})$. In (74), we further make use of $F''(\rho\cdot\bar{V}) \geq F''(c\,\varrho) \geq \tilde{c}\,F''(\varrho)$ (cf. (35)). □

As corollaries of Lemma 8.7, note that the functions $\mathscr{M}$ of Corollary 8.2, $\mathscr{R}_i$ of Corollary 8.3, and P of Lemma 8.4 all belong to $\in C^1(\mathscr{D})$ and satisfy, for all $(s,\,q)\in\mathscr{D}$, the following inequalities:

$$\begin{aligned}\frac{1}{C_1\,s} \leq \partial_s\mathscr{M}(s,\,q) \leq \frac{F''(s)}{C_0},\quad |\partial_q\mathscr{M}(s,\,q)| \leq \frac{C_1}{C_0}\,s\,F''(s),\\ |\partial_s\mathscr{R}(s,\,q)| \leq \frac{C_1}{C_0}\,s\,F''(s),\quad |\partial_q\mathscr{R}(s,\,q)| \leq C_1\,s\,(1 + \frac{C_1}{C_0}\,s\,F''(s)),\\ \frac{1}{C_1} \leq \partial_s P(s,\,q) \leq \frac{s\,F''(s)}{C_0},\quad |\partial_q P(s,\,q)| \leq C\,s\,(1 + s\,F''(s)).\end{aligned} \tag{76}$$

Remark 8.8. For the applicability of our approximation methods, we are restricted to the case that $D^*_h = \mathbb{R}^N$. In view of Corollary 8.6 this is basically the case if F' is surjective. In this case, $\mathscr{D} = \mathbb{R}_+\times\mathbb{R}^{N-1}$ and there is no state-constraint on μ. Due to the bounds (76), the functions $\mathscr{M}$, $\mathscr{R}_i$ and P are globally Lipschitz continuous on $[0,\,r]\times\mathbb{R}^{N-1}$ for all $r < +\infty$.

Remark 8.9. In the case that the growth exponent of the function F is less than $9/5$, we rely in the analysis of the PDE system on the *convexity* of the function $s \mapsto P(s,\,q)$ at fixed q. We are able to establish this property only in the very special case that P is a function of the total mass density. We note the following trivial observation: Define P as in Lemma 8.4 and assume that the vectors $V\in\mathbb{R}^N_+$ and $m\in\mathbb{R}^N_+$ are parallel. Then, P depends only on the first variable.

9. Approximate solutions

9.1. The regularisation strategy

The regularisation strategy, though not mass conservative, will be chosen *thermodynamically consistent*, since it consists in two essential steps:

(1) A positive definite regularisation of the mobility matrix M;
(2) A convex regularisation of the free energy function h.

The method involves three levels associated with positive parameter, say σ, δ and τ. We first modify the mobility matrix M in order to ensure ellipticity and allow a control on $\nabla\mu$

$$M_\sigma(\rho) = M(\rho) + \sigma\,\mathrm{Id}.$$

The δ-regularisation consists in increasing the growth of the (mechanical) free energy modifying the function F that occurs in the definition of $h^{\rm mech}$ via $F(\rho\cdot\bar V) \rightsquigarrow F(\rho\cdot\bar V) + \delta\,(\rho\cdot\bar V)^{\alpha_\delta}$, $\alpha_\delta > 3$. If the original growth exponent of F is larger than 3, this step can be omitted. We denote h_δ the corresponding free energy function, that is

$$h_\delta(\rho) := h(\rho) + \delta\,\left(\rho\cdot\bar V\right)^{\alpha_\delta}. \tag{77}$$

The τ-regularisation is a stabilisation for the vector of chemical potentials. It consists in modifying the function h^* (or $(h_\delta)^*$) via

$$h^*_{\delta,\tau}(X) := (h_\delta)^*(X) + \tau\sum_{i=1}^N \omega(X_i), \tag{78}$$

where $\omega\in C^2(\mathbb{R})$ is a convex and increasing function for which we impose the growth conditions

$$\begin{aligned} c_0\,(\sqrt{|s^-|} + |s^+|^{\alpha'}) \le \omega'(s)\,s - \omega(s) &\le c_1\,(1+\sqrt{|s^-|} + |s^+|^{\alpha}) \\ \omega'(s) &\le c_2\,(1+\omega'(s)\,s-\omega(s))^{1/\alpha}. \\ \omega''(s) &\le c_3\,\omega'(s) \end{aligned} \tag{79}$$

For example, we may choose the function

$$\omega(s) := \begin{cases} -2\sqrt{|s|} & \text{for } s\le -1 \\ \frac14\,s^2 + \frac32\,s - \frac34 & \text{for } -1 < s < 1\,, \\ \frac{1}{2\alpha'\,(\alpha'-1)}\,s^{\alpha'} + (2-\frac{1}{2(\alpha'-1)})\,s + \frac{1}{2\alpha(\alpha'-1)} - 1 & \text{otherwise}\end{cases} \quad \alpha' := \frac{\alpha}{\alpha-1},$$

which satisfies these assumptions. The choice of the regularisation ω is by no means unique, the constants in the latter relation are determined from simple interpolation conditions. Essential for our purposes is in fact only the sublinear growth for $s\to-\infty$ that is compatible with global convexity. The function $h^*_{\tau,\delta}$ is twice differentiable and strictly convex. Making use of the strict convexity, we easily show that the mapping $\nabla h^*_{\tau,\delta}:\mathbb{R}^N\to\mathbb{R}^N_+$ is bijective. Interpreting (78) as Legendre transform, we introduce a regularised free energy function via

$$h_{\tau,\delta} := \text{ convex conjugate of the function } h^*_{\tau,\delta} = (h^*_{\tau,\delta})^*, \tag{80}$$

which is a twice differentiable convex function on $\mathbb{R}^N_+$. The main motivation for this construction is that the new free energy function has improved coercivity properties over the variables ρ and μ as exposed in the following statement.

Lemma 9.1. *Let the original free energy function h satisfy*

$$c_0\,|\rho|^{\alpha_0} - c_1 \le h(\rho) \le C_0\,|\rho|^{\alpha_0} + C_1, \quad \textit{for all } \rho\in\mathbb{R}^N_+,$$

with constants $3/2 < \alpha_0 < +\infty$ and $0 < c_0, c_1, C_0, C_1 < +\infty$. Let $\alpha = \alpha_\delta > 3$ be the regularisation exponent of (77), and ω a function satisfying (79). Define

$$\Phi_\omega(X) := \sum_{i=1}^N \omega'(X_i)\,X_i - \omega(X_i) \quad \textit{for } X\in\mathbb{R}^N. \tag{81}$$

Then, there are $\tilde c_0, \tilde c_1 > 0$, $C_2 > 0$, and $\tau_0(\alpha,\alpha_0) > 0$ such that, if $\tau\le\tau_0$,

(1) $h_{\tau,\delta}(\rho) \ge \tilde c_0\,(|\rho|^{\alpha_0} + \delta\,|\rho|^\alpha + \tau\,\Phi_\omega(\mu)) - \tilde c_1$;
(2) $|D^2 h^*_{\tau,\delta}(\mu)|/\varrho \le C_2$,

for all $\rho\in\mathbb{R}^N_+$ and $\mu\in\mathbb{R}^N$ connected by the identity $\rho = \nabla_\mu h^*_{\tau,\delta}(\mu)$.

Proof. The definition (80) implies that $h_{\tau,\delta}(\nabla h^*_{\tau,\delta}(X)) = h_\delta(\nabla(h_\delta)^*(X)) + \tau\,\Phi_\omega(X)$. By assumption, ρ and μ are related via $\rho = \nabla_\mu h^*_{\tau,\delta}(\mu) = \nabla_\mu (h_\delta)^*(\mu) + \tau\,\omega'(\mu)$, and we obtain for the regularised free energy the identity

$$\begin{aligned} h_{\tau,\delta}(\rho) &= h_\delta(\nabla(h_\delta)^*(\mu)) + \tau\,\Phi_\omega(\mu) = h_\delta(\rho - \tau\,\omega'(\mu)) + \tau\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) \\ &= h(\rho - \tau\,\omega'(\mu)) + \delta\,((\rho - \tau\,\omega'(\mu))\cdot \bar V)^\alpha + \tau\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)). \end{aligned}$$

On the other hand, the condition (79) ensures that $\omega'(\mu_i) \le c_2\,(1 + \omega'(\mu_i)\,\mu_i - \omega(\mu_i))^{1/\alpha}$. For $\alpha > 1$, denote by $\underline{c}(\alpha)$, $\bar c(\alpha)$ two constants such that $|a-b|^\alpha \ge \underline{c}(\alpha)\,a^\alpha - \bar c(\alpha)\,b^\alpha$ for all $a,\, b > 0$. Then,

$$\begin{aligned} ((\rho - \tau\,\omega'(\mu))\cdot\bar V)^\alpha &\ge (\min \bar V)^\alpha\,(\varrho - \tau\,|\omega'(\mu)|_1)^\alpha \\ &\ge (\min\bar V)^\alpha\,\Big(\underline{c}(\alpha)\,\varrho^\alpha - \bar c(\alpha)\,c_2^\alpha\,\tau^\alpha\,(\sum_{i=1}^N (1 + \omega'(\mu_i)\,\mu_i - \omega(\mu_i))^{1/\alpha})^\alpha\Big) \\ &\ge (\min\bar V)^\alpha\,\underline{c}(\alpha)\,\varrho^\alpha - (\min\bar V)^\alpha\,\bar c(\alpha)\,c_2^\alpha\,\tau^\alpha\,N^\alpha\,(1 + \Phi_\omega(\mu)). \end{aligned}$$

Hence, we find positive numbers $\tilde c$, $\hat c$ and C depending only on α, $\bar V$ and N such that

$$h_{\tau,\delta}(\rho) \ge h(\rho - \tau\,\omega'(\mu)) + \tilde c\,\delta\,|\rho|^\alpha + (1 - \hat c\,\delta\,\tau^{\alpha-1})\,\tau\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) - C.$$

If we assume that $\hat c\,\delta\,\tau^{\alpha-1} \le 1/4$, then

$$h_{\tau,\delta}(\rho) \ge h(\rho - \tau\,\omega'(\mu)) + \tilde c\,\delta\,|\rho|^\alpha + \frac{3}{4}\,\tau\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) - C.$$

We next use $h(\rho - \tau\,\omega'(\mu)) \ge c_0\,(\varrho - \tau\,|\omega'(\mu)|_1)^{\alpha_0} - c_1$. By similar arguments, and since $\alpha_0 < \alpha$, the claim (1) follows.

To prove (2), observe that $\varrho = \sum_{i=1}^N \partial_{\mu_i} h^*_{\tau,\delta}(\mu)$. For $X \in \mathbb{R}^N$, recall moreover that $\partial_i h^*_{\tau,\delta}(X) = \partial_i (h_\delta)^*(X) + \tau\,\omega'(X_i)$ (cp. (78)). Hence, $D^2_{i,j} h^*_{\tau,\delta}(X) = D^2_{i,j}(h_\delta)^*(X) + \tau\,\omega''(X_i)\,\delta_{i,j}$. Making use of (73) and of the definition of $h^*_{\delta,\tau}$

$$\frac{|D^2(h_\delta)^*(\mu)|}{\varrho} \le C_1\,\frac{\mathbb{1}\cdot\nabla(h_\delta)^*(\mu)}{\varrho} = C_1\,\frac{\varrho - \tau\,\sum_{i=1}^N \omega'(\mu_i)}{\varrho} \le C_1.$$

Moreover, owing to the choice of ω, there is a positive constant c_3 such that $\omega''(X_i) \le c_3\,\omega'(X_i)$ for all $X \in \mathbb{R}^N$ (cf. (79)), and therefore,

$$\frac{\tau\,\omega''(\mu_i)}{\varrho} = \frac{\tau\,\omega''(\mu_i)}{\mathbb{1}\cdot\nabla(h_\delta)^*(\mu) + \tau\,\sum_{i=1}^N \omega'(\mu_i)} \le c_3.$$

We define $C_2 := C_1 + c_3$, proving (2). □

9.2. Approximation scheme

For the existence proof, we embeds the problem (P) into a larger class of (approximate) problems $(P_{\tau,\sigma,\delta})$ characterised by an elliptic diffusion matrix M_σ and a regularised free energy $h_{\tau,\delta}$. Since in this approach it is possible to control the entire vector μ, a solution vector consists of the entries μ, v and ϕ.

In order to define the concept of solution, we introduce also in this case a natural class $\mathcal{B}$ for the approximate solutions. If $\delta,\,\sigma,\,\tau>0$, we say that $(\mu,\,v,\,\phi)$ belongs to $\mathcal{B}(T,\,\Omega,\,\alpha,\,N,\,\Psi,\,\Psi^\Gamma)$ if and only if

$$\mu\in W^{1,0}_2(Q;\,\mathbb{R}^N)\text{ and }(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)\in\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$$

with (82)

$$\varrho:=\nabla_\mu h^*_{\tau,\delta}(\mu)\cdot\mathbb{1},\quad q:=\Pi\,\mu,\quad R:=\bar R(\gamma\cdot\mu),\quad R^\Gamma:=\hat R^\Gamma(t,x,\hat\gamma\cdot\mu).$$

Replacing in $[(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)}$ the norm of q in $W^{1,0}_2(Q;\,\mathbb{R}^{N-1})$ with the full norm $\|\mu\|_{W^{1,0}_2(Q;\,\mathbb{R}^N)}$, we introduce the natural 'norm' $[(\mu,\,v,\,\phi)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,N,\,\Psi,\,\Psi^\Gamma)}$.

We say that $(\mu,\,v,\,\phi)$ satisfies the approximate energy (in)equality if and only if the corresponding vector $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$ satisfies the energy (in)equality of Definition 7.1, with free energy function $h_{\tau,\delta}$ and mobility matrix M_σ. For $\delta,\,\sigma,\,\tau>0$, we call weak solution to the problem $(P_{\tau,\,\sigma,\,\delta})$ a vector $(\mu,\,v,\,\phi)$ subject to the energy inequality and such that the quantities

$$\begin{aligned}&\rho=\nabla_\mu h^*_{\tau,\delta}(\mu),\qquad J=-M_\sigma(\rho)\,(\nabla\mu+\bar Z\,\nabla\phi),\\ &r=\sum_{k=1}^s\hat\gamma^k\,\bar R_k(\gamma^1\cdot\mu,\ldots,\gamma^s\cdot\mu),\qquad \hat r=\sum_{k=1}^{\hat s^\Gamma}\hat\gamma^k\,\hat R^\Gamma_k(t,x,\,\hat\gamma^1\cdot\mu,\ldots,\hat\gamma^{\hat s^\Gamma}\cdot\mu),\\ &p=h^*_{\tau,\delta}(\mu),\qquad n^F=\rho\cdot\bar Z,\end{aligned}\tag{83}$$

fulfil the identities (63), (65) and, instead of (64),

$$\begin{aligned}&-\int_Q\varrho\,v\cdot\partial_t\eta-\int_Q\varrho\,v\otimes v\,:\,\nabla\eta-\int_Q p\,\operatorname{div}\eta+\int_Q\mathbb{S}(\nabla v)\,:\,\nabla\eta\\ &\quad=\int_\Omega\varrho_0\,v^0\cdot\eta(0)-\int_Q n^F\,\nabla\phi\cdot\eta+\int_Q(\sum_{i=1}^N J^i\cdot\nabla)\eta\cdot v\quad\forall\,\eta\in C^1_c([0,T[;\,C^1_c(\Omega;\mathbb{R}^3)).\end{aligned}\tag{84}$$

Since the second definition in (83) in general implies that $\sum_{i=1}^N J^i\neq 0$, it is necessary to add this contribution in the momentum equation (84) in order to preserve the energy identity.

The existence of approximate solutions for the regularised scheme is not a trivial problem, because there is no monotone or pseudo-monotone structure inherent to the diffusion. We carry over this technical step in Sect. 14 by means of a time-continuous Galerkin method. It turns out that for parameters $\delta,\,\sigma>0$ and $\tau\geq 0$, weak solutions to $(P_{\tau,\sigma,\delta})$ exist and develop no vacuum.

9.3. Derivation of the global energy and mass balance identities

In this paragraph, we motivate the thermodynamically consistent approximations $(P_{\tau,\sigma,\delta})$ by deriving the natural *energy identity*. The derivation assumes here only formal character, meaning that the existence of a solution with increased regularity is assumed to perform the calculations. A rigorous proof of the existence claim for $(P_{\tau,\sigma,\delta})$ with energy *inequality* is, due to its technicality, postponed to Sect. 14.

Proposition 9.2. *Assume that there are vector fields $\mu\in C^{0,1}([0,T]\times\Omega;\,\mathbb{R}^N)$, $v\in C^{0,1}([0,T]\times\Omega;\,\mathbb{R}^3)$ and $\phi\in L^\infty([0,T];\,C^{0,1}(\Omega))$ that satisfy, together with their associate variables ρ, J, r, $\hat r$, p, n^F defined in (83), the relations (63), (65), (84) and the initial and boundary conditions*

$$\mu(0)=\mu^0\in C^{0,1}(\Omega;\,\mathbb{R}^N),\quad v(0)=v^0\in C^{0,1}(\Omega;\,\mathbb{R}^3)\ \textit{in}\ \Omega,$$
$$\phi=\phi_0\in C^{0,1}([0,T]\times\Omega))\ \textit{on}\ ]0,T[\times\Gamma,\quad v=0\ \textit{on}\ [0,T]\times\partial\Omega.$$

We define $\rho^0 = \nabla_\mu h^*_{\tau,\delta}(\mu^0)$. Then, for all $t \in]0,T[$, the vector (μ, v, ϕ) satisfies the energy equality (51) *with free energy function $h_{\tau,\delta}$ and mobility matrix M_σ.*

Proof. Due to the additional regularity assumed, it is fairly standard to show that (63), (65), (84) imply in every $t \in]0,T[$ that

$$\int_\Omega \partial_t\rho\cdot\psi - \sum_{i=1}^N \int_\Omega (\rho_i\, v + J^i)\cdot\nabla\psi^i = \int_\Omega r\cdot\psi + \int_\Gamma (\hat{r} + J^0)\cdot\psi, \tag{85}$$

$$\int_\Omega \varrho\,(\partial_t v + (v\cdot\nabla)v)\cdot\eta + \int_\Omega \mathbb{S}(\nabla v) : \nabla\eta - \int_\Omega p\,\operatorname{div}\eta = -\int_\Omega \left\{\left(\sum_{i=1}^N J^i\cdot\nabla\right) v + n^F\,\nabla\phi\right\}\cdot\eta, \tag{86}$$

$$\bar{\chi}\int_\Omega \nabla\phi\cdot\nabla\zeta = \int_\Omega n^F\,\zeta, \tag{87}$$

for all $\psi \in W^{1,1}(\Omega;\, \mathbb{R}^N)$, all $\eta \in W^{1,1}_0(\Omega;\, \mathbb{R}^3)$ and for all $\zeta \in W^{1,1}_\Gamma(\Omega)$.

We insert $\psi = \mu(t)$ into (85). The definition of ρ implies that $\sum_{i=1}^N \rho_i\,\nabla\mu_i = \nabla h^*_{\tau,\delta}(\mu) = \nabla p$. Moreover, it yields $\mu = \nabla_\rho h_{\tau,\delta}(\rho)$, and therefore $\partial_t\rho\cdot\mu = \partial_t h_{\tau,\delta}(\rho)$. It follows that

$$\partial_t \int_\Omega h_{\tau,\delta}(\rho) - \int_\Omega \left(v\cdot\nabla p + \sum_{i=1}^N J^i\cdot\nabla\mu_i\right) = \int_\Omega r\cdot\mu + \int_\Gamma (\hat{r} + J^0)\cdot\mu. \tag{88}$$

We choose $\psi = \bar{Z}\,\phi(t)$ in (85). Recall that $r\cdot\bar{Z} = 0$, because $\gamma^k\cdot\bar{Z} = 0$ for every reaction vector (elementary charge conservation, see (4)). Thus,

$$\int_\Omega \partial_t n^F\,\phi - \int_\Omega \left(n^F\,v\cdot\nabla\phi + \sum_{i=1}^N J^i\,\bar{Z}_i\cdot\nabla\phi\right) = \int_\Gamma (\hat{r} + J^0)\cdot\bar{Z}\,\phi_0. \tag{89}$$

We differentiate (87) in time, and we choose $\zeta = \phi(t) - \phi_0(t)$, This entails

$$\int_\Omega \partial_t n^F\,\phi = \int_\Omega \partial_t n^F\,\phi_0 + \frac{\bar{\chi}}{2}\,\partial_t \int_\Omega |\nabla\phi|^2 - \bar{\chi}\int_\Omega \nabla\phi_t\cdot\nabla\phi_0. \tag{90}$$

Thus, (89) and (90) yield

$$\begin{aligned}\frac{\bar{\chi}}{2}\,\partial_t \int_\Omega |\nabla\phi|^2 - \int_\Omega \left(n^F\,v\cdot\nabla\phi + \sum_{i=1}^N J^i\,\bar{Z}_i\cdot\nabla\phi\right)&\\ = \int_\Gamma (\hat{r} + J^0)\cdot\bar{Z}\,\phi_0 + \bar{\chi}\int_\Omega \nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega \partial_t n^F\,\phi_0.&\end{aligned} \tag{91}$$

If we now add (91) to (88), it follows that

$$\begin{aligned}&\partial_t \int_\Omega \{h_{\tau,\delta}(\rho) + \frac{\bar{\chi}}{2}\,|\nabla\phi|^2\} - \int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi) - \int_\Omega \sum_{i=1}^N J^i\cdot(\nabla\mu_i + \bar{Z}_i\,\nabla\phi)\\ &\quad - \int_\Omega r\cdot\mu - \int_\Gamma \hat{r}\cdot\mu = \int_\Gamma (J^0\cdot\mu + (J^0 + \hat{r})\cdot\bar{Z}\,\phi_0) + \bar{\chi}\int_\Omega \nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega \partial_t n^F\,\phi_0.\end{aligned} \tag{92}$$

Next we choose $\eta = v(t)$ in (86), which shows that

$$\frac{1}{2}\int_\Omega (\varrho\,\partial_t v^2 + \varrho\,(v\cdot\nabla)v^2) + \int_\Omega \mathbb{S}(\nabla v) : \nabla v + \int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi) = -\frac{1}{2}\int_\Omega \sum_{i=1}^N J^i\cdot\nabla v^2. \tag{93}$$

For $\psi = |v(t)|^2\,\mathbb{1}$ in (85), observing that $r\cdot\mathbb{1} = 0 = \hat{r}\cdot\mathbb{1}$ by definition, it follows that $\int_\Omega \partial_t\varrho\, v^2 - \int_\Omega(\varrho\, v + \sum_{i=1}^N J^i)\cdot\nabla v^2 = 0$, which directly entails

$$\int_\Omega \varrho\,\partial_t v^2 + \int_\Omega \varrho\, v\cdot\nabla v^2 + \int_\Omega \sum_{i=1}^N J^i\cdot\nabla v^2 = \partial_t \int_\Omega \varrho\, v^2\,.$$

Thus, (93) now yields

$$\frac{1}{2}\,\partial_t\int_\Omega \varrho\, v^2 + \int_\Omega \mathbb{S}(\nabla v) : \nabla v + \int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi) = 0. \tag{94}$$

We add (94) to (92) and obtain that

$$\begin{aligned}\partial_t \int_\Omega \{\frac{1}{2}\,\varrho\, v^2 + h_{\tau,\delta}(\rho) + \frac{\bar{\chi}}{2}\,|\nabla\phi|^2\} + \int_\Omega \mathbb{S}(\nabla v) : \nabla v - \int_\Omega J : D - \int_\Omega r\cdot\mu - \int_\Gamma \hat{r}\cdot\mu \\ = \int_\Gamma (J^0\cdot\mu + (J^0+\hat{r})\cdot\bar{Z}\,\phi_0) + \bar{\chi}\int_\Omega \nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega \partial_t n^F\,\phi_0.\end{aligned}$$

We integrate over time and are done. □

The proof of the global mass conservation identities (53) is comparatively simpler. It suffices to insert $\psi = e^i$ for $i = 1,\ldots,N$ into (85).

Proposition 9.3. *We adopt the assumptions of Proposition 9.2. Then, for all $t\in[0,T]$*

$$\bar{\rho}(t) = \bar{\rho}^0 + \int_0^t \left\{\int_\Omega r + \int_\Gamma (\hat{r} + J^0)\right\}(s)\,ds.$$

10. A priori estimates directly resulting from the energy equality

In this section, we derive *a priori* estimates on solutions to the problem (P) that result from the energy identity. In order to include in our considerations both approximation scheme and limit problem, we consider generic free energy functions for which there are $c_1 > 0$, $c_2 \geq 0$ and $C_i \geq 0$, $i = 1,2,3$ and $\tau > 0$ such that for all $\rho\in\mathbb{R}^N_+$

$$c_1\,|\rho|^\alpha + \tau\,\Phi_\omega[\nabla h(\rho)] - c_2 \leq h(\rho) \leq C_1\,|\rho|^\alpha + C_2\,\tau\,\Phi_\omega[\nabla h(\rho)] + C_3. \tag{95}$$

In view of Lemma 9.1, the growth condition (95) are precisely the ones to expect from the chosen stabilisation. Moreover, we consider mobility matrices $M_\sigma = M(\rho) + \sigma\,\mathrm{Id}$, $\sigma\geq 0$, such that M satisfies (36) and (37). We commence with a few standard estimates.

Proposition 10.1. *Let $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)$ satisfy the energy inequality of Definition 7.1 with free energy function h and mobility matrix M fulfilling (95), (36), (37). Then, there is a number $C_0 > 0$ depending only on Ω, T, on the constants c_i, C_i in the conditions (95), and on the quantity*

$$\begin{aligned}\mathcal{B}_0 := \|\rho^0\|_{L^\alpha(\Omega)} + \tau\,\|\Phi_\omega(\mu^0)\|_{L^1(\Omega)} + \|\sqrt{\varrho_0}\,v^0\|_{L^2(\Omega)} + \|\phi_0\|_{L^\infty(Q)} \\ + \|\phi_0\|_{L^\infty(0,T;\,W^{1,2}(\Omega))} + \|\phi_{0,t}\|_{W^{1,0}_2(Q)} + \|\phi_{0,t}\|_{L^{\alpha'}(Q)} + \|\jmath\|_{L^\infty(S;\,\mathbb{R}^{\hat{s}^\Gamma})},\end{aligned} \tag{96}$$

such that, with ρ, J, etc. obeying Definitions (50) or (83),

$$\begin{aligned}
&\|\rho\|_{L^{\infty,\alpha}(Q)} + \tau\, \|\Phi_\omega(\mu)\|_{L^{\infty,1}(Q)} + \|\sqrt{\varrho}\, v\|_{L^{\infty,2}(Q)} + \|\nabla\phi\|_{L^{\infty,2}(Q)} \leq C_0,\\
&\|v\|_{W^{1,0}_2(Q)} + \|\nabla q\|_{L^2(Q)} \leq C_0,\\
&\|D^R\|_{L_\Psi(Q)} + \|\hat{D}^{\Gamma,R}\|_{L_{\hat{\Psi}^\Gamma}(S)} \leq C_0,\\
&\sum_{i=1}^N \|J^i\|_{L^{2,\frac{2\alpha}{1+\alpha}}(Q)} + [-R]_{L_{\Psi^*}(Q)} + [-R^\Gamma]_{L_{(\hat{\Psi}^\Gamma)^*}(S)} \leq C_0,\\
&\sqrt{\sigma}\, \|\nabla\mu\|_{L^2(Q)} + \min\{\sigma,\, \tau^2\}\, \|\mu\|_{L^{2,3}(Q)} \leq C_0,\\
&\|\mathbb{1}\cdot J\|_{L^2(Q)} \leq C_0\, \sqrt{\sigma}, \quad \|\tau\, \omega'(\mu)\|_{L^{\infty,\alpha}(Q)} \leq C_0\, \tau^{1/\alpha'}.
\end{aligned}$$

Proof. Due to the property (95),

$$\int_\Omega h(\rho)(t) \geq c_1 \int_\Omega |\rho(t)|^\alpha + \tau \int_\Omega \Phi_\omega(\mu(t)) - c_2\, |\Omega|.$$

For general velocity fields $v \in W^{1,2}(\Omega;\mathbb{R}^3)$, we invoke (17) to see that

$$\int_\Omega \mathbb{S}(\nabla v) \,:\, \nabla v = \int_\Omega \frac{\eta}{2}\, |D(v) - \frac{2}{3}\, \operatorname{div} v\, \mathrm{Id}|^2 + \int_\Omega (\lambda + \frac{2}{3}\,\eta)\, (\operatorname{div} v)^2.$$

In the case that $v = 0$ on $\partial\Omega$, integration by parts directly yields

$$\int_\Omega \mathbb{S}(\nabla v) \,:\, \nabla v = \int_\Omega (\eta\, |\nabla v|^2 + (\lambda+\eta)\, (\operatorname{div} v)^2).$$

For estimating the right hand of the energy identity

$$\begin{aligned}
\left|\int_\Omega n^F(t)\, \phi_0(t)\right| &\leq |\bar{Z}| \int_\Omega |\rho(t)|\, |\phi_0(t)| \leq \frac{c_1}{2} \int_\Omega |\rho(t)|^\alpha + c \int_\Omega |\phi_0(t)|^{\alpha'},\\
\left|\bar{\chi} \int_\Omega \nabla\phi(t)\cdot\nabla\phi_0(t)\right| &\leq \frac{\bar{\chi}}{4} \int_\Omega |\nabla\phi(t)|^2 + c \int_\Omega |\nabla\phi_0(t)|^2.
\end{aligned}$$

Owing to similar standard considerations

$$\begin{aligned}
\left|\int_{Q_t} \{n^F\, \phi_{0,t} - \bar{\chi}\, \nabla\phi\cdot\nabla\phi_{0,t}\}\right| &\leq \int_0^t \{\|n^F\|_{L^\alpha(\Omega)}\, \|\phi_{0,t}\|_{L^{\alpha'}(\Omega)} + \bar{\chi}\, \|\nabla\phi\|_{L^2(\Omega)}\, \|\nabla\phi_{0,t}\|_{L^2(\Omega)}\}\\
&\leq \int_0^t \{\|n^F\|^\alpha_{L^\alpha(\Omega)} + \bar{\chi}\, \|\nabla\phi\|^2_{L^2(\Omega)}\} + C \int_0^t \{\|\phi_{0,t}\|^{\alpha'}_{L^{\alpha'}(\Omega)} + \|\nabla\phi_{0,t}\|^2_{L^2(\Omega)}\}.
\end{aligned}$$

The Young inequality further implies that

$$-\int_{S_t} R^\Gamma_k\, \hat{\gamma}^k\cdot\bar{Z}\,\phi_0 \leq \int_{S_t} (\hat{\Psi}^\Gamma)^*(t,x,\, -\tfrac{1}{4}\, R^\Gamma) + \int_{S_t} \hat{\Psi}^\Gamma(t,x,\, 4\,\phi_0\, (\hat{\gamma}^1\cdot\bar{Z}, \ldots,\, \hat{\gamma}^{\hat{s}^\Gamma}\cdot\bar{Z})).$$

Since $(\hat{\Psi}^\Gamma)^*(t,x,\,-\frac{1}{4}\,R^\Gamma) = (\hat{\Psi}^\Gamma)^*(t,x,\,\frac{1}{4}\,(-R^\Gamma) + \frac{3}{4}\,0)$, convexity implies that

$$-\int_{S_t} R^\Gamma_k\,\hat{\gamma}^k \cdot \bar{Z}\,\phi_0 \le \frac{1}{4}\int_{S_t}(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma) + \int_{S_t}\hat{\Psi}^\Gamma(t,x,\,4\,\phi_0\,(\hat{\gamma}^1\cdot\bar{Z},\ldots,\,\hat{\gamma}^{\hat{s}^\Gamma}\cdot\bar{Z}))$$
$$= \frac{1}{4}\int_{S_t}(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma) + C_0(\|\phi_0\|_{L^\infty([0,T]\times\Gamma)}).$$

Recall that J^0 possesses the representation (43), and therefore

$$\int_{S_t} J^0\cdot\mu \le \int_{S_t}\hat{\Psi}^\Gamma(t,x,\,\tfrac{1}{4}\,\hat{D}^{\Gamma,\mathrm{R}}) + \int_{S_t}(\hat{\Psi}^\Gamma)^*(t,x,\,4\,\jmath) \le \frac{1}{4}\int_{S_t}\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathrm{R}}) + C_0(\|\jmath\|_{L^\infty(S)}).$$

Due to convex duality

$$\Psi(D^{\mathrm{R}}) + (\Psi)^*(-\bar{R}(D^{\mathrm{R}})) = -\sum_{k=1}^{s}\bar{R}_k(D^{\mathrm{R}})\,\gamma^k\cdot\mu,$$
$$\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathrm{R}}) + (\hat{\Psi}^\Gamma)^*(t,x,\,-\bar{R}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathrm{R}})) = -\sum_{k=1}^{\hat{s}^\Gamma}\bar{R}^\Gamma_k(t,x,\,\hat{D}^{\Gamma,\mathrm{R}})\,\hat{\gamma}^k\cdot\mu.$$

Thus, for all $t\in]0,T[$, the dissipation inequality implies that

$$\int_\Omega\left\{\frac{1}{2}\,\varrho\,v^2 + \frac{\bar{\chi}}{4}\,|\nabla\phi|^2 + \frac{c_1}{2}\,|\rho|^\alpha + \tau\,\Phi_\omega(\mu)\right\}(t)$$
$$+\int_{Q_t}\left\{\eta\,|\nabla v|^2 + (\lambda+\eta)\,(\operatorname{div} v)^2 - \sum_{i=1}^N J^i\cdot D^i + (\Psi(D^{\mathrm{R}}) + (\Psi)^*(-R))\right\}$$
$$+\frac{1}{2}\int_{S_t}\{\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathrm{R}}) + (\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)\} \le C_0 + C\int_0^t\{\|\rho\|^\alpha_{L^\alpha(\Omega)} + \bar{\chi}\,\|\nabla\phi\|^2_{L^2(\Omega)}\}.$$

Owing to the thermodynamical consistency, we (at least) obtain that $\sum_{i=1}^N J^i\cdot D^i \le 0$. Moreover, $\lambda+\frac{2}{3}\,\eta\ge 0$ implies $\mathbb{S}(\nabla v)\,:\,\nabla v\ge 0$. Exploiting the Gronwall Lemma, we thus obtain bounds for the quantities $\|\sqrt{\varrho}\,v\|_{L^{\infty,2}(Q)}$, $\|\nabla\phi\|_{L^{\infty,2}(Q)}$ and $\|\rho\|_{L^{\infty,\alpha}(Q)}$ and $\tau\,\|\Phi_\omega(\mu)\|_{L^{\infty,1}(Q)}$. It next follows that

$$\int_\Omega\left\{\frac{1}{2}\,\varrho\,v^2 + \frac{1}{4}\,\bar{\chi}\,|\nabla\phi|^2 + \frac{c_1}{2}\,|\rho|^\alpha + \tau\,\Phi_\omega(\mu)\right\}(t)$$
$$+\int_{Q_t}\left\{\eta\,|\nabla v|^2 + (\lambda+\eta)\,(\operatorname{div} v)^2 - \sum_{i=1}^N J^i\cdot D^i + (\Psi(D^{\mathrm{R}}) + (\Psi)^*(-R))\right\}$$
$$+\frac{1}{2}\int_{S_t}\{\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathrm{R}}) + (\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)\} \le C_0(T).$$

Since $\lambda+\frac{2}{3}\,\eta\ge 0$ this in turn implies bounds for $\|\operatorname{div} v\|_{L^2(Q)}$, and for $\|\nabla v\|_{L^2(Q)}$. Moreover, the production factors R and R^Γ are bounded in Orlicz classes

$$[-R]_{L_{(\Psi)^*}(Q;\mathbb{R}^s)} + [-R^\Gamma]_{L_{(\hat{\Psi}^\Gamma)^*}(S_T;\mathbb{R}^{\hat{s}^\Gamma})} \le C_0,$$

whereas the reaction driving forces satisfy $[D^{\mathrm{R}}]_{L_\Psi(Q;\mathbb{R}^s)} + [\hat{D}^{\Gamma,\mathrm{R}}]_{L_{\hat{\Psi}^\Gamma}(S_T;\mathbb{R}^{\hat{s}^\Gamma})} \le C_0$. It remains to exploit the dissipation due to diffusion and the driving forces $D^1,\ldots,D^N$. At first we note that $-\sum_{i=1}^N J^i\cdot D^i =$

$\sum_{i,j} M_{i,j}\, D^i\cdot D^j$. For $i=1,\ldots,N$ the Cauchy–Schwarz inequality and the growth condition (37) on M (or M_σ) imply that

$$|J^i| = |\sum_{j=1}^N M_{i,j}\, D^j| \le (MD\,:\,D)^{1/2}\,(Me^i\cdot e^i)^{1/2} \le (\sqrt{\sigma}+\sqrt{\lambda})\,(1+|\rho|)^{1/2}\,(MD\,:\,D)^{1/2}.$$

Therefore, we obtain for the diffusion fluxes that

$$\|J^i(t)\|_{L^{\frac{2\alpha}{1+\alpha}}(\Omega)} \le c\,\|MD\,:\,D(t)\|_{L^1(\Omega)}^{1/2}\,(1+\|\rho(t)\|_{L^\alpha(\Omega)}^{1/2}) \le C_0\,\|MD\,:\,D(t)\|_{L^1(\Omega)}^{1/2}.$$

It follows that $\|J^i\|_{L^{2,2\alpha/(1+\alpha)}(Q)} \le c\,(\int_Q MD\,:\,D)^{1/2} \le C_0$.

We finally want to obtain estimates on the gradients of the (relative) chemical potentials. Here, we make use of the Assumption (37) that yields

$$-\sum_{i=1}^N J^i\cdot D^i = \sum_{i,j=1}^N M_{i,j}\, D^i\cdot D^j \ge \underline{\lambda}\,|P_{\mathbb{1}^\perp}\, D|^2\,,$$

where $P_{\mathbb{1}^\perp}$ is the orthogonal projection on the space $\mathbb{1}^\perp$. Due to additive splitting of the driving force $D^i = \nabla\mu_i + \bar{Z}_i\,\nabla\phi$, we can obtain that

$$-\sum_{i=1}^N J^i\cdot D^i \ge (\underline{\lambda}/2)\,|P_{\mathbb{1}^\perp}\nabla\mu|^2 - 3\,\underline{\lambda}\,\left|\bar{Z}\right|^2\,|\nabla\phi|^2.$$

We make use of the identity $P_{\mathbb{1}^\perp}\mu = \sum_{i=1}^{N-1} q_i\,P_{\mathbb{1}^\perp}\xi^i$. Due to the choice of $\xi^1,\ldots,\xi^{N-1}$, the vectors $P_{\mathbb{1}^\perp}\xi^1,\ldots,P_{\mathbb{1}^\perp}\xi^{N-1}$ are a basis of $\mathbb{1}^\perp$. Thus, there is a constant depending only on the choice of the projector Π such that $|P_{\mathbb{1}^\perp}\nabla\mu|^2 \ge c_\Pi\,|\nabla q|^2$. This entails $|\nabla q|^2 \le c\,(-\sum_{i=1}^N J^i\cdot D^i + |\nabla\phi|^2)$, proving that $\|\nabla q\|_{L^2(Q)} \le C_0$. Since $M_\sigma D\cdot D \ge \sigma\, D^2$, we also see that

$$C_0 \ge -\sum_{i=1}^N \int_Q J^i\cdot D^i \ge \frac{\sigma}{2}\int_Q |\nabla\mu|^2 - 3\,\sigma\,\left|\bar{Z}\right|\,\|\nabla\phi\|_{L^2(Q)}^2,$$

which yields the bound for $\sqrt{\sigma}\,\|\nabla\mu\|_{L^2(Q)}$. Moreover,

$$\|\mathbb{1}\cdot J\|_{L^2(Q)} = \sigma\,\|\mathbb{1}\cdot D\|_{L^2(Q)} \le c\,\sqrt{\sigma}\,(\sqrt{\sigma}\,\|\nabla\mu\|_{L^2(Q)} + \sqrt{\sigma}\,\|\nabla\phi\|_{L^2(Q)}).$$

Due to the conditions (79), we verify that $|\omega'|^\alpha \le c\,(1+\Phi_\omega)$ and this directly yields

$$\|\tau\,\omega'(\mu)\|_{L^{\infty,\alpha}(Q)} \le c\,\tau^{1/\alpha'}\,\|\tau\,(\Phi_\omega(\mu)+1)\|_{L^{\infty,1}(Q)}^{\frac{1}{\alpha}} \le \tau^{1/\alpha'}\,C_0.$$

At last we can verify that the function $w=\sqrt{1+|\mu|}$ possesses a distributional gradient in $L^2(Q)$ and, making use also of the growth property of Φ_ω, we prove the bound

$$\|\nabla w\|_{L^2(Q)} \le \frac{1}{2}\,\|\nabla\mu\|_{L^2(Q)} \le C_0\,\sigma^{-1/2},$$
$$\|w\|_{L^{\infty,1}(Q)} \le |\Omega| + \|\sqrt{|\mu|}\|_{L^{\infty,1}(Q)} \le c\,(1+\|\Phi_\omega(\mu)\|_{L^{\infty,1}(Q)}) \le C_0\,\tau^{-1}.$$

Hence, the Sobolev embedding theorems and its extensions yield $\|w\|_{L^{2,6}(Q)} \le C_{\sigma,\tau}$. □

Lemma 10.2. *We adopt the assumptions of Proposition 10.1. Assume moreover that for almost all $t\in\,]0,T[$, the electrical potential $\phi\in L^\infty(0,T;\,W^{1,2}(\Omega))$ satisfies*

$$-\bar{\chi}\,\triangle\phi(t) = n^F(t)\ \text{in}\ [W^{1,2}_\Gamma(\Omega)]^*,\quad \phi(t)=\phi_0(t)\ \text{as traces on}\ \Gamma,$$

with $\phi_0 \in L^\infty(Q) \cap L^\infty(0,T;\, W^{1,\beta}(\Omega))$, $\beta = \min\{r(\Omega, \Gamma),\, \frac{3\alpha}{(3-\alpha)^+}\}$. *Then,*

$$\|\phi\|_{L^\infty(Q)} \leq \|\phi_0\|_{L^\infty(Q)} + c\,\|\rho\|_{L^{\infty,\alpha}(Q)},$$
$$\|\phi\|_{L^\infty(0,T;\,W^{1,\beta}(\Omega))} \leq c\,(\|\phi_0\|_{L^\infty(0,T;\,W^{1,\beta}(\Omega))} + \|\rho\|_{L^{\infty,\alpha}(Q)}).$$

Moreover, $\|n^F\,\nabla\phi\|_{L^{\infty,\,\frac{\beta\alpha}{\beta+\alpha}}(Q)} \leq \|n^F\|_{L^{\infty,\alpha}(Q)}\,\|\nabla\phi\|_{L^{\infty,\beta}(Q)}$ *whenever* $\beta \geq \alpha'$.

Proof. We only need to recall that $\alpha > 3/2$ and the definition of the exponent $r(\Omega, \Gamma) \geq 2$ (see (40)). The estimates for ϕ are standard consequences of second order elliptic theory, whereas the bound for $n^F\,\nabla\phi$ follows from the Hölder inequality. □

Next we can derive the uniform continuity estimate that results from the mass balance equations.

Proposition 10.3. *Assumptions of Proposition 10.1. If* $\bar{\rho}$ *satisfies the identity of Definition (53), then* $[\bar{\rho}]_{C_{\Phi^*}([0,T])} \leq C_0$.

Proof. Let $0 \leq t_1 < t_2 \leq T$. Note that by assumption $\bar{\rho}(t_2) - \bar{\rho}(t_1) = \int_{t_1}^{t_2}\{\int_\Omega r + \int_\Gamma (\hat{r} + J^0)\}$. We note that

$$\left|\int_{t_1}^{t_2}\int_\Omega r_i\right| = \left|\int_{t_1}^{t_2}\int_\Omega R\cdot\gamma_i\right| \leq \sup_{[-R]_{L_{\Psi^*}} \leq C_0}\left|\int_{t_1}^{t_2}\int_\Omega R\cdot\gamma\right|.$$

We argue similarly with the other right-hand side terms. Recall the definition of the natural class $\mathcal{B}$ to show that $|\bar{\rho}(t_2) - \bar{\rho}(t_1)| \leq \bar{C}_0\,\Phi^*(t_1,\, t_2)$. □

In the course of the proofs, we shall also need bounds of more technical nature obtained via Hölder and Sobolev inequalities. We denote α the growth exponent of the function h at infinity and $\beta := \min\{r(\Omega,\,\Gamma),\, 3\alpha/(3-\alpha)^+\}$ the optimal regularity of the electric field.

Lemma 10.4. *We assume that the bounds in Proposition 10.1 are valid. Then,*

$$\|\varrho\, v\|_{L^{2,\frac{6\alpha}{6+\alpha}}(Q)} \leq c\,\|\varrho\|_{L^{\infty,\alpha}(Q)}\,\|v\|_{W^{1,0}_2(Q)} \leq C_0,$$
$$\|\varrho\, v\|_{L^{\infty,\frac{2\alpha}{1+\alpha}}(Q)} \leq \|\sqrt{\varrho}\, v\|_{L^{\infty,2}(Q)}\,\|\varrho\|^{1/2}_{L^{\infty,\alpha}(Q)} \leq C_0,$$
$$\|\varrho\, v^2\|_{L^{1,\frac{3\alpha}{3+\alpha}}(Q)} \leq c\,\|\varrho\|_{L^{\infty,\alpha}(Q)}\,\|v\|^2_{W^{1,0}_2(Q)} \leq C_0,$$
$$\|\varrho\, v^2\|_{L^{\frac{5\alpha-3}{3\alpha}}(Q)} \leq c\,\|\varrho\, v^2\|^{(2\alpha-3)/(5\alpha-3)}_{L^{\infty,1}(Q)}\,\|\varrho\, v^2\|^{(3\alpha)/(5\alpha-3)}_{L^{1,\frac{3\alpha}{3+\alpha}}(Q)} \leq C_0,$$
$$\left\|\sum_{i=1}^N J^i\, v\right\|_{L^{1,3/2}(Q)} \leq \left\|\sum_{i=1}^N J^i\right\|_{L^2(Q)}\|v\|_{L^{2,6}(Q)} \leq C_0\,\sqrt{\sigma}.$$

Further, we shall need an improved bound on the pressure. This is also fairly standard and, therefore, we postpone the proof to the appendix.

Lemma 10.5. *Assume that the relation (84) is valid:*

- *If* $\alpha > 3$, *then* $\|p\|_{L^{1+1/\alpha}(Q)} \leq C_0$;
- *If* $3/2 < \alpha \leq 3$, $r(\Omega,\,\Gamma) > \alpha'$ *and* $\mathbb{1}\cdot J \equiv 0$, *then* $\|p\|_{L^{1+\frac{2}{3}-\frac{1}{\alpha}}(Q)} \leq C_0$.

The only piece of information still missing in order to obtain a bound in the natural class is the estimate on the vector q. This is the object of the next section.

11. A priori estimates for the (relative) chemical potentials

In this section, we show that a combination between the estimates on the reaction driving forces D^{R}, $D^{\Gamma,\mathrm{R}}$, the control on the gradient of the relative potentials $(q_1, \ldots, q_{N-1}) = \Pi\mu$ (cf. Proposition 10.1) and the balance of total mass (Proposition 9.3) allows to control also the L^2-norm of these functions in the sense of the natural class $\mathcal{B}$.

The starting point is a given pair $(\varrho, q) \in L^{\infty,\alpha}(Q) \times L^1(Q; \mathbb{R}^{N-1})$. We define $\rho := \mathscr{R}(\varrho, q)$, $\bar{\rho} := \int_\Omega \rho \, \mathrm{d}x$ and $\mu := \mathcal{E}q$ (see Sect. 8). An essential ingredient of the proof is the balance of total mass valid for all $t \in]0, T[$ implying, with the linear space W of (44),

$$\bar{\rho}(t) \in \{\bar{\rho}^0\} \oplus \mathrm{span}\{\gamma^1, \ldots, \gamma^s, \hat{\gamma}^1, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}\} = \{\bar{\rho}^0\} \oplus W. \tag{97}$$

At every point where $\varrho > 0$, we may resort to the representations

$$\partial_{\rho_i} h(\rho) = c_i + \bar{V}_i \, F'(\rho \cdot \bar{V}) + \frac{1}{m_i} \ln y_i, \tag{98}$$

$$\begin{aligned} \mu_i - \mu_k &= \mathcal{E}q \cdot (e^i - e^k) = (\mathcal{E}q + \mathscr{M}(\varrho, q) \, \mathbb{1}) \cdot (e^i - e^k) \\ &= c_i - c_k + (\bar{V}_i - \bar{V}_k) \, F'(\rho \cdot \bar{V}) + \left(\frac{1}{m_i} \ln y_i - \frac{1}{m_k} \ln y_k \right). \end{aligned} \tag{99}$$

Here, $y_i = (\rho_i / m_i) / \sum_j (\rho_j / m_j)$.

We commence stating an obvious estimate, that results from Proposition 10.1.

Lemma 11.1. *Define $P_W : \mathbb{R}^N \to W$ the orthogonal projection on the subspace W. There is C depending only on Ω such that*

$$\|P_W \mu\|_{L^2(Q)} + \|P_W \mu\|_{L^2(S)} \leq C \, (1 + \|\nabla q\|_{L^2(Q)} + [D^R]_{L_\Psi(Q)} + [\hat{D}^{\Gamma,R}]_{L_{\hat{\Psi}^\Gamma}(S)}).$$

Proof. Consider the vectors $\gamma^k \in \mathbb{R}^N$, $k \in \{1, \ldots, s\}$ associated with the bulk reactions. Since we assume (38), then obviously $\|\mu \cdot \gamma\|_{L^2(\Omega)}$ is controlled by $[D^{\mathrm{R}}]_{L_\Psi(\Omega; \mathbb{R}^s)}$. Since $\gamma^k \cdot \mathbb{1} = 0$ for all k, there is a constant $c_{W,\Pi}$ depending on W and the choice of the projector Π such that $|\nabla(\gamma \cdot \mu)| \leq c_{W,\Pi} \, |\nabla \Pi \mu|$. We also obtain (trace theorem) that $\|\mu \cdot \gamma\|_{L^2(\Gamma)} \leq C \, \|\mu \cdot \gamma\|_{W^{1,2}(\Omega)}$. Thus,

$$\begin{aligned} \|\mu \cdot \gamma\|_{L^2(S)} &\leq C \, (\|\nabla \Pi \mu\|_{L^2(Q; \mathbb{R}^{(N-1) \times 3})} + \|D^{\mathrm{R}}\|_{L^2(Q; \mathbb{R}^s)}) \\ &\leq C \, (\|\nabla \Pi \mu\|_{L^2(Q; \mathbb{R}^{(N-1) \times 3})} + c_\Psi \, [D^{\mathrm{R}}]_{L_\Psi(Q; \mathbb{R}^s)}) \leq C_0. \end{aligned}$$

We analogously observe that $|\mu \cdot \hat{\gamma}|$ is controlled by $|\hat{D}^{\Gamma,\mathrm{R}}|$, which is bounded by the data in $L_{\hat{\Psi}^\Gamma}$ and, due to (38), also in $L^2(]0, T[\times \Gamma)$. We make use of the fact that $\|\mu \cdot \hat{\gamma}\|_{L^2(\Omega)} \leq C \, (\|\nabla(\mu \cdot \hat{\gamma})\|_{L^2(\Omega)} + \|\mu \cdot \hat{\gamma}\|_{L^2(]0,T[\times \Gamma)})$, and the claim follows. ☐

We next setup a preliminary tool for the main estimate of this section.

Lemma 11.2. *Let $\epsilon > 0$. For $u \in L^1(\Omega)$, define*

$$A_\epsilon(u) := \{x \in \Omega \, : \, u(x) < \epsilon^{-1}\}, \; B_\epsilon(u) := \{x \in \Omega \, : \, u(x) > -\epsilon^{-1}\}.$$

For all $\delta > 0$, there is $C^* = C^*(\delta)$ depending only on Ω such that for all $u \in W^{1,1}(\Omega)$

$$\begin{aligned} &\min\{\lambda_3(A_\epsilon(u)), \, \lambda_3(B_\epsilon(u))\} \geq \delta \\ \Longrightarrow \; & \\ &\|u\|_{L^1(\Omega)} \leq C^*(\delta) \, (\|\nabla u\|_{L^1(\Omega)} + \tfrac{1}{\epsilon} \max\{\lambda_3(A_\epsilon(u)), \, \lambda_3(B_\epsilon(u))\}). \end{aligned}$$

Proof. We at first show that for all $\delta > 0$, there is $c = c(\delta)$ depending only on Ω such that

$$\|u\|_{L^1(\Omega)} \leq c(\delta) \left(\|\nabla u\|_{L^1(\Omega)} + \max\left\{\int_A |u^+|, \int_B |u^-|\right\}\right)$$
$$\text{for all } u \in W^{1,1}(\Omega), \quad \text{for all } A,\, B \subset \Omega \text{ such that } \min\{|A|,\, |B|\} \geq \delta. \tag{100}$$

Otherwise, there is $\delta_0 > 0$ such that for all $j \in \mathbb{N}$, one finds $u_j \in W^{1,1}(\Omega)$ and $A_j,\, B_j \subset \Omega$, $|A_j|,\, |B_j| \geq \delta_0$ and

$$\|u_j\|_{L^1(\Omega)} \geq j \left(\|\nabla u_j\|_{L^1(\Omega)} + \max\left\{\int_{A_j} |u_j^+|, \int_{B_j} |u_j^-|\right\}\right).$$

Consider $\bar{u}_j := u_j/\|u_j\|_{L^1(\Omega)}$. Then, $\|\bar{u}_j\|_{W^{1,1}(\Omega)} \leq \|\nabla \bar{u}_j\|_{L^1(\Omega)} + 1 \leq j^{-1} + 1$. Consequently, there are a subsequence (no new labels) and a limiting element $\bar{u} \in L^1(\Omega)$ such that $\bar{u}_j \to \bar{u}$ strongly in $L^1(\Omega)$. But since $\nabla \bar{u}_j \to 0$ strongly in $L^1(\Omega)$, $\bar{u}$ must be a constant. Since also $\bar{u}^+\,|A_j| + |\bar{u}^-|\,|B_j| \to 0$, it obviously follows that $\bar{u} \equiv 0$. Thus, $1 = \|\bar{u}_j\|_{L^1(\Omega)} \to 0$, a contradiction.

For $u \in L^1(\Omega)$, we apply (100) with the choices

$$A := \{x \in \Omega \,:\, u(x) < \epsilon^{-1}\},\ B := \{x \in \Omega \,:\, u(x) > -\epsilon^{-1}\}.$$

It follows that either $\min\{|A|,\, |B|\} < \delta$ or that

$$\|u\|_{L^1(\Omega)} \leq c(\delta) \left(\|\nabla u\|_{L^1(\Omega)} + \max\left\{\int_A |u^+|, \int_B |u^-|\right\}\right) \leq c(\delta)\,(\|\nabla u\|_{L^1(\Omega)} + \frac{1}{\epsilon}\,\max\{|A|,\, |B|\}).$$

□

We define $\tilde{s} := \dim W$, and we choose $b^1, \ldots, b^{\tilde{s}} \in W$ to be some basis of W. We call a selection $S \subseteq \{1, \ldots, N\}$ *critical* if the span of the vectors $P_S(b^1), \ldots, P_S(b^{\tilde{s}})$ is a true subspace of $P_S(\mathbb{R}^N)$. For all critical selections, the manifold $W_S := \operatorname{span}\{P_S(b^1), \ldots, P_S(b^{\tilde{s}})\} \oplus P_{S^c}(\mathbb{R}^N)$ has at most dimension $N - 1$.

The critical manifold is defined via (45).

Theorem 11.3. *Assume that* $\bar{\rho}(t) \in \{\bar{\rho}_0\} \oplus W$ *for all* $t \in [0, T]$. *Let* $\tilde{s} = \dim W$ *and* $b^1, \ldots, b^{\tilde{s}}$ *be a basis of* W. *Then, if* $\operatorname{dist}(\bar{\rho}_0,\, \mathcal{M}_{crit}) > 0$, *the estimate*

$$\|q\|_{L^2(Q;\,\mathbb{R}^{N-1})} \leq c\,(k_0\,T^{\frac{1}{2}} + \|(b^1 \cdot \mu, \ldots, b^{\tilde{s}} \cdot \mu)\|_{L^2(Q;\,\mathbb{R}^{\tilde{s}})} + c_0^*\,\|\nabla q\|_{L^2(Q;\,\mathbb{R}^{(N-1)\times 3})})$$

is valid. Here, c_0^* *and* k_0 *depend on* $\operatorname{dist}(\bar{\rho}_0,\, \mathcal{M}_{crit})$.

Proof. For $t \in]0, T[$, we define $r_0(t) := \sum_{k=1}^{\tilde{s}} \|b^k \cdot \mu(t)\|_{L^1(\Omega)}$, and $d_0(t) := \|\nabla q(t)\|_{L^1(\Omega)}$.

Preliminary Consider the function $\hat{q}_i := \mu_i - \max_{j=1,\ldots,N} \mu_j$ for $i = 1, \ldots, N$. Then, $\hat{q} \leq 0$ componentwise.

Moreover, $\hat{q}_i$ possesses the generalised gradient $\nabla \hat{q}_i = \sum_{i_0=1}^N \nabla(\mu_i - \mu_{i_0})\,\chi_{B_{i_0}}$, where the set B_{i_0} obeys the definition $B_{i_0} := \{x \in \Omega \,:\, \mu_{i_0} = \max_{j=1,\ldots,N} \mu_j\}$. Recall that, for all $i \neq i_0$, the vector $e^i - e^{i_0}$ belongs to $\operatorname{span}\{\eta^1, \ldots, \eta^{N-1}\}$. Therefore, we can show that

$$\int_\Omega |\nabla \hat{q}_i(t)| = \sum_{i_0=1}^N \int_{B_{i_0}} |\nabla(\mu_i - \mu_{i_0})(t)| \leq c \sum_{i_0=1}^N \int_{B_{i_0}} |\nabla q(t)| = c\,d_0(t).$$

First step Now, exploiting Lemma 11.2 with $u = \hat{q}_i$ (recall that $\hat{q}_i^+ = 0$ for $i = 1, \ldots, N$), we obtain for $\delta,\, \epsilon > 0$ and $t \in]0, T[$ the alternative

$$\|\hat{q}_i(t)\|_{L^1(\Omega)} \leq C^*(\delta)\,(d_0(t) + \epsilon^{-1}\,\lambda_3(\Omega))$$

or

$$\lambda_3(\{x\,:\,\hat{q}_i(t,\,x) \geq -\tfrac{1}{\epsilon}\}) < \delta. \tag{101}$$

Due to the definitions of $\hat{q}$, i_0 and to the Assumption (99), there holds, in $B_{i_0} \subseteq \Omega$,

$$\hat{q}_i = c_i - c_{i_0} + (\bar{V}_i - \bar{V}_{i_0})\,F'(\bar{V}\cdot\rho) + (\tfrac{1}{m_i}\,\ln y_i - \tfrac{1}{m_{i_0}}\,\ln y_{i_0}).$$

Hence,

$$\ln y_i \leq \tfrac{m_i}{m_{i_0}}\,\ln y_{i_0} + m_i\,\big(\hat{q}_i + 2\,|c|_\infty + \sup_{j,k=1,\ldots N} |\bar{V}_j - \bar{V}_k|\,|F'(\bar{V}\cdot\rho)|\big). \tag{102}$$

We define $\epsilon_0 := \frac{1}{8\,|c|_\infty}$, $a_0 := \sup_{j,k=1,\ldots N} |\bar{V}_j - \bar{V}_k|$. For $0 < \epsilon \leq \epsilon_0$ and $t \in]0, T[$, we also define

$$A_\epsilon(t) := \{x\,:\,|F'(\bar{V}\cdot\rho(t,x))| \leq 1/(4a_0\epsilon)\}.$$

Due to the inequality (102), the set inclusion

$$\{x\,:\,\hat{q}_i(t,\,x) < -\tfrac{1}{\epsilon}\} \cap A_\epsilon(t) \subseteq \{x\,:\,y_i(t,\,x) \leq e^{-\frac{m_i}{2\,\epsilon}}\} \tag{103}$$

is valid. We next observe that the set $\Omega\backslash A_\epsilon(t)$ can be decomposed via

$$\begin{aligned}\Omega\backslash A_\epsilon(t) &= C_\epsilon^+(t) \cup C_\epsilon^-(t),\\ C_\epsilon^-(t) &:= \{x\,:\,F'(\bar{V}\cdot\rho(t,x)) \leq -1/(4a_0\epsilon)\},\\ C_\epsilon^+(t) &:= \{x\,:\,F'(\bar{V}\cdot\rho(t,x)) \geq 1/(4a_0\epsilon)\}.\end{aligned}$$

Due to the asymptotic behaviour of the function F' (see (35)), there are $\epsilon_1 > 0$ and $\bar{k}_1,\, \bar{k}_2 > 0$ depending only on F and a_0 such that

$$x \in C_\epsilon^-(t) \Rightarrow \ln(\bar{V}\cdot\rho(t,x)) \leq -\frac{\bar{k}_1}{\epsilon} \text{ and } x \in C_\epsilon^+(t) \Rightarrow (\bar{V}\cdot\rho(t,x))^{\alpha-1} \geq \frac{\bar{k}_2}{\epsilon}.$$

In particular, it follows that

$$C_\epsilon^- \subseteq \{x\,:\,\max_{i=1,\ldots,N} \rho_i(t,x) \leq \tfrac{1}{\min \bar{V}}\,e^{-\frac{\bar{k}_1}{\epsilon}}\}. \tag{104}$$

Thus, invoking (103) and (104), we obtain that

$$\begin{aligned}&\{x\,:\,\hat{q}_i(t,\,x) < -\tfrac{1}{\epsilon}\} \cap (\Omega\backslash C_\epsilon^+(t))\\ &\subseteq \{x\,:\,y_i(t,\,x) \leq e^{-\frac{m_i}{2\,\epsilon}}\} \cup \{x\,:\,\max_{i=1,\ldots,N} \rho_i(t,x) \leq \tfrac{1}{\min \bar{V}}\,e^{-\frac{\bar{k}_1}{\epsilon}}\}.\end{aligned} \tag{105}$$

On the other hand, we readily see that

$$\lambda_3(C_\epsilon^+(t)) \leq \|\varrho\|^\alpha_{L^{\infty,\alpha}(Q)}\,(\max \bar{V})^\alpha\,\left(\frac{\epsilon}{\bar{k}_2}\right)^{\alpha'}. \tag{106}$$

Thus, if $\lambda_3(\{x\,:\,\hat{q}_i(t,\,x) \geq -\frac{1}{\epsilon}\}) \leq \delta$, we can invoke (105) and (106) to see that

$$\begin{aligned}&\lambda_3(\{x\,:\,y_i(t,x) \leq e^{-\frac{m_i}{2\,\epsilon}}\} \cup \{x\,:\,\max_{i=1,\ldots,N} \rho_i(t,x) \leq \tfrac{1}{\min \bar{V}}\,e^{-\frac{\bar{k}_1}{\epsilon}}\})\\ &\qquad \geq \lambda_3(\Omega) - \delta - \|\varrho\|^\alpha_{L^{\infty,\alpha}(Q)}\,(\max \bar{V})^\alpha\,\left(\frac{\epsilon}{\bar{k}_2}\right)^{\alpha'}.\end{aligned}$$

For all $0 < \epsilon < \min\{\epsilon_0, \epsilon_1\}$ and $0 < \delta$, we therefore obtain from the latter and from (101) that

$$\begin{aligned}&\|\hat{q}_i(t)\|_{L^1(\Omega)} > C^*(\delta)\,(d_0(t) + \epsilon^{-1}\,\lambda_3(\Omega))\\ \Longrightarrow&\\ &\lambda_3(\Big\{x\,:\,y_i(t,x) \leq e^{-\frac{m_i}{2\,\epsilon}}\Big\} \cup \Big\{x\,:\,\max_{i=1,\ldots,N} \rho_i(t,x) \leq \tfrac{1}{\min \bar{V}}\,e^{-\frac{\bar{k}_1}{\epsilon}}\Big\}) \geq \lambda_3(\Omega) - \delta - C_0\,\epsilon^{\alpha'}.\end{aligned}$$

The second inequality would further imply that

$$\begin{aligned}\int_\Omega \rho_i(t) \leq& \int_{\{x\,:\,y_i(t,x)\leq e^{-\frac{m_i}{2\,\epsilon}}\}} \rho_i + \int_{\{x\,:\,\max_{i=1,\ldots,N}\,\rho_i(t,x)\leq \frac{1}{\min \bar{V}}\,e^{-\frac{k_1}{\epsilon}}\}} \rho_i + \|\rho_i\|_{L^{\infty,\alpha}(Q)}\,(\delta + C_0\,\epsilon^{\alpha'})^{\frac{1}{\alpha'}}\\ &\leq m_i\,e^{-\frac{m_i}{2\,\epsilon}}\,\|n\|_{L^{\infty,1}(\Omega)} + \tfrac{1}{\min \bar{V}}\,e^{-\frac{\bar{k}_1}{\epsilon}}\,\lambda_3(\Omega) + \|\rho_i\|_{L^{\infty,\alpha}(Q)}\,(\delta + C_0\,\epsilon^{\alpha'})^{\frac{1}{\alpha'}}.\end{aligned}$$

For all $0 < \epsilon < \min\{\epsilon_0, \epsilon_1\}$ and $0 < \delta$, we therefore can conclude that

$$\|\hat{q}_i(t)\|_{L^1(\Omega)} > C^*(\delta)\,(d_0(t) + \epsilon^{-1}\lambda_3(\Omega)) \quad\Longrightarrow\quad \bar{\rho}_i(t) \leq C_0\,\left(\delta^{\frac{1}{\alpha'}} + \max\left\{\epsilon,\, e^{-\frac{C_1}{\epsilon}}\right\}\right), \tag{107}$$

where C_0, C_1 are certain constants depending on the data, but independent on q and ρ.

Second step Let $t \in]0, T[$. Consider $i_1 \in \{1, \ldots, N\}$. Then, we claim that there are constants c_0, $c_1 > 0$, depending only on the vectors $b^1, \ldots, b^{\tilde{s}}$, and a critical index set $J \supset \{i_1\}$ such that

$$\inf_{j\in J} \|\hat{q}_j(t)\|_{L^1(\Omega)} \geq c_0\,(\|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} - c_1\,r_0(t)). \tag{108}$$

We prove this claim inductively. Let us at first describe the induction step. Suppose that $K \subset \{1, \ldots, N\}$ is any non-critical index set. Then, by the definition of such a set, there are for all $k \in K$ coefficients $\lambda^k_1, \ldots, \lambda^k_{\tilde{s}}$ such that

$$P_K(e^k) = \sum_{\ell=1}^{\tilde{s}} \lambda^k_\ell\,P_K(b^\ell) = \sum_{\ell=1}^{\tilde{s}} \lambda^k_\ell\,b^\ell - \sum_{\ell=1}^{\tilde{s}} \lambda^k_\ell\,P_{K^c}(b^\ell).$$

Hence, scalar multiplication with $\hat{q}$ yields

$$\|\hat{q}_k\|_{L^1(\Omega)} \leq \sup_{\ell=1,\ldots,\tilde{s}} |\lambda^k_\ell|\,(r_0(t) + \tilde{s}\,\sup_{\ell=1,\ldots,\tilde{s}} |b^\ell|_\infty\,\max_{j\in K^c} \|\hat{q}_j\|_{L^1(\Omega)}).$$

Choosing $k \in K$ such that $\|\hat{q}_k\|_{L^1(\Omega)} = \max_{j\in K} \|\hat{q}_j\|_{L^1(\Omega)}$ and $\ell \in K^c$ such that $\max_{j\in K^c} \|\hat{q}_j\|_{L^1(\Omega)} = \|\hat{q}_\ell\|_{L^1(\Omega)}$, it follows that

$$\|\hat{q}_\ell\|_{L^1(\Omega)} \geq \frac{1}{\tilde{s}\,|b|_\infty\,|\lambda|_\infty}\,(\max_{j\in K} \|\hat{q}_j\|_{L^1(\Omega)} - |\lambda|_\infty\,r_0(t)).$$

Suppose now that for the non-critical selection $K \supseteq \{i_1\}$ of cardinality $m \geq 1$, we already know that there are positive constants $c_0(m)$, $c_1(m)$ such that

$$\min_{j\in K} \|\hat{q}_j\|_{L^1(\Omega)} \geq c_0(m)\,\|\hat{q}_{i_1}\|_{L^1(\Omega)} - c_1(m)\,r_0(t). \tag{109}$$

Then, invoking the two latter inequalities, the strictly larger selection $K(m+1) = K \cup \{\ell\}$ satisfies

$$\begin{aligned}\min_{j\in K(m+1)} \|\hat{q}_j\|_{L^1(\Omega)} &= \min\{\min_{j\in K} \|\hat{q}_j\|_{L^1(\Omega)},\, \|\hat{q}_\ell\|_{L^1(\Omega)}\}\\ &\geq \min\{c_0(m),\, \tfrac{1}{\tilde{s}\,|b|_\infty\,|\lambda|_\infty}\}\,\|\hat{q}_{i_1}\|_{L^1(\Omega)} - \max\{c_1(m),\, \tfrac{|\lambda|_\infty}{\tilde{s}\,|b|_\infty\,|\lambda|_\infty}\}\,r_0(t).\end{aligned}$$

We apply this inductively starting from the selection $K(1) = \{i_1\}$. If $K(1)$ is critical, we are done already. Otherwise, since K consists of only the one element i_1, it satisfies (109) with $c_0(1) = 1$ and $c_1(1) = 0$. Thus, we find some strictly larger selection $K(2)$ satisfying (109) again. After a finite number of steps, we must reach some critical selection $J \supseteq \{i_1\}$, proving the subclaim (108).

Now, assume that for parameters $0 < \epsilon < \min\{\epsilon_0, \epsilon_1\}$ and $0 < \delta$ the inequality

$$\|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} > \tfrac{1}{c_0}\, (C^*(\delta)\, (d_0(t) + \epsilon^{-1}\, \lambda_3(\Omega)) + c_1\, r_0(t))$$

is valid with the constants c_0, c_1 from (108). Then, there is a critical selection $J \supseteq \{i_1\}$ such that

$$\inf_{j\in J} \|\hat{q}_j(t)\|_{L^1(\Omega)} > C^*(\delta)\, (d_0(t) + \epsilon^{-1}\, \lambda_3(\Omega)).$$

Employing the first step of the proof (cf. (107)) then yields

$$\max_{j\in J} \bar{\rho}_j(t) \le C_0\, (\delta^{\frac{1}{\alpha'}} + \max\{\epsilon,\, e^{-\frac{C_1}{\epsilon}}\}).$$

Thus, we have proved the new alternative

$$\begin{aligned} &\|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} > \tfrac{1}{c_0}\, (C^*(\delta)\, (d_0(t) + \epsilon^{-1}\, \lambda_3(\Omega)) + c_1\, r_0(t)) \\ &\quad\Longrightarrow \\ &\max_{j\in J} \bar{\rho}_j(t) \le C_0\, (\delta^{\frac{1}{\alpha'}} + \max\{\epsilon,\, e^{-\frac{C_1}{\epsilon}}\}), \quad \text{for a critical selection } J \supseteq \{i_1\}. \end{aligned} \tag{110}$$

Third step By assumption $\text{dist}(\bar{\rho}_0,\, \mathcal{M}_{\text{crit}}) > 0$. As we assume that $\bar{\rho}(t) \in \bar{\rho}^0 \oplus W$, there holds $P_S(\bar{\rho}(t)) \in P_S(\bar{\rho}^0) \oplus W_S$ for every selection S. For every critical selection J, the definition (45) implies that $|P_J(\bar{\rho}(t))| \ge \text{dist}(\bar{\rho}_0,\, M_{\text{crit}}) > 0$. This in turn implies that

$$\max_{j\in J} \bar{\rho}_j(t) \ge N^{-1}\, \text{dist}(\bar{\rho}_0,\, M_{\text{crit}}).$$

Thus, there are $\delta_0 > 0$ and $\bar{\epsilon}_0 > 0$ depending only on $\text{dist}(\bar{\rho}_0,\, M_{\text{crit}})$ such that the hypothesis in (110) yields a contradiction for all $\delta \le \delta_0$ and $0 < \epsilon \le \min\{\epsilon_0,\, \epsilon_1,\, \bar{\epsilon}_0\}$. With $d_0 := \text{dist}(\bar{\rho}_0,\, M_{\text{crit}})$, one indeed may choose

$$\delta_0 = \min\{1,\, (\tfrac{d_0}{4NC_0})^{\alpha'}\},\ \bar{\epsilon}_0 := \min\{\tfrac{d_0}{4NC_0},\, \frac{C_1}{|\ln \frac{d_0}{4NC_0}|}\}.$$

Conclusion We define $k := C^*(\frac{\delta_0}{2})\, \epsilon^{-1}\, \lambda_3(\Omega)$. For $k \ge k_0 = C^*(\frac{\delta_0}{2})\, \lambda_3(\Omega)\, [\min\{\epsilon_0,\, \epsilon_1,\, \bar{\epsilon}_0\}]^{-1}$, the alternative (110) implies that the set

$$\{t \,:\, c_0\, \|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} - C^*(\tfrac{\delta_0}{2})\, d_0(t) - c_1\, r_0(t) \ge k\}$$

has measure zero. Hence,

$$c_0\, \|\hat{q}_{i_1}\|_{L^{2,1}(Q)} - C^*(\tfrac{\delta_0}{2})\, \|d_0\|_{L^2(0,T)} - c_1\, \|r_0\|_{L^2(0,T)} \le k_0\, T^{\frac{1}{2}}.$$

Lemma 11.1 provides the bound for r_0 and, since we control the gradients of q in $L^{2,2}(Q)$, the claim now follows easily. □

If the vector of initial net initial masses $\bar{\rho}_0$ is on the critical manifold, then the argument of Theorem 11.3 does not apply, and can prove only a local-in-time version of the estimate.

Lemma 11.4. *Assume that* (97) *is valid. Define*

$$T^* := \inf\{t \in [0,T] \,:\, \min_{i=1,\dots,N} \bar{\rho}_i(t) = 0\}.$$

Then, there is a time $T_0 > 0$ depending on $\mathcal{B}_0$ (cf. (96)) and on $\inf_{i=1,\dots,N} \bar{\rho}_i^0$ such that $T^* \ge T_0$, and $\|q\|_{L^2(Q_t;\mathbb{R}^{N-1})} \le C_{0,t}$ for all $t < T^*$.

Proof. We recall Proposition 10.3, and we see that $|\bar{\rho}(t) - \bar{\rho}^0| \le \tilde{C}_0\, \Phi^*(t,0)$ for all $t \in [0,T]$. Thus, if T_0 is such that $\inf_{i=1,\dots,N} \bar{\rho}_i^0 - \tilde{C}_0\, \Phi^*(T_0,0) \ge c_0 > 0$, we obtain that $\inf_{i=1,\dots,N} \bar{\rho}_i(t) > c_0$ for all $t \in [0,T_0]$. Due to the first step of the proof of Theorem 11.3, relation (107), it then follows that

$$\|\hat{q}_i(t)\|_{L^1(\Omega)} \le C^*(\tfrac{\delta_0}{2})\, (d_0(t) + \epsilon^{-1}\, \lambda_3(\Omega)),$$

almost everywhere on $[0,\, T_0]$ for all $i = 1, \dots, N$, δ_0 appropriate, and all $\epsilon \le \min\{\epsilon_0,\, \epsilon_1\}$. □

12. Compactness

Our aim in this section is to derive a general compactness tool in order to pass to the limit with approximate solutions to the problem (P). We will discuss here the passage to the limit with the parameters δ and σ. The limit passage for $\tau \to 0$ can be dealt with comparably simpler methods: see Sect. 14. Since we do not want to specify with which of the approximation parameters—δ or σ—we pass to the limit, we will consider families indexed by a generic parameter $\epsilon > 0$.

We thus study compactness for a 'solution family' $\{(\varrho_\epsilon,\, q^\epsilon,\, v^\epsilon,\, \phi_\epsilon,\, R^\epsilon,\, R^{\Gamma,\epsilon})\}_{\epsilon>0}$ which might for example correspond to free energy functions $\{h_\epsilon\}_{\epsilon>0}$ and mobility matrices $\{M_\epsilon\}_{\epsilon>0}$. In this section, our minimal assumptions are that $h_\epsilon(\rho) \geq c_0\,|\rho|^\alpha - c_1$ for all $\rho \in \mathbb{R}^N_+$, and that $M_\epsilon \xi \cdot \xi \geq \underline{\lambda}\,|P_{\mathbb{1}^\perp}\xi|^2$ for all $\xi \in \mathbb{R}^N$. These conditions are satisfied with constants $\alpha > 3/2$, c_0, c_1 and $\underline{\lambda}$ independent of ϵ.

Moreover, for both limits of interest $(\sigma,\, \delta \to 0)$, we can assume the validity of a representation

$$\partial_{\rho_i} h_\epsilon(\rho) = c_i + F'_\epsilon(\bar{V}\cdot\rho)\,\bar{V}_i + \frac{1}{m_i}\ln y_i, \tag{111}$$

where $F_\epsilon(s) = F(s) + \epsilon\, s^{\alpha_\epsilon}$. Here, F is a function of Legendre type on $\mathbb{R}_+$, with surjective derivative. The map $\mathscr{R} = \mathscr{R}^\epsilon \in C^1(]0, +\infty[\times\mathbb{R}^{N-1};\, \mathbb{R}^N)$, introduced in Corollary 8.3 to reparametrise the densities, satisfies the estimates (76) with uniform constants. Remark 8.8 thus shows that the family $\{\mathscr{R}^\epsilon\}_{\epsilon>0}$ is bounded uniformly in $C^{0,1}([0,\, r]\times\mathbb{R}^{N-1})$ for all $r < +\infty$. Hence, as $\epsilon \to 0$,

$$\mathscr{R}^\epsilon \to \mathscr{R} \text{ uniformly on compact subsets of } [0,\, +\infty[\times\mathbb{R}^{N-1}, \tag{112}$$

where $\mathscr{R} \in C^1(\mathbb{R}_+\times\mathbb{R}^{N-1}) \cap C(\mathbb{R}_{0,+}\times\mathbb{R}^{N-1})$ corresponds to the limit free energy ($\epsilon = 0$ in (111)).

In order to obtain the compactness, we shall need the information on distributional time-derivatives contained in the system (63), (64) (or (84) instead). For technical reasons, it is convenient to express these information in an older (though elementary) fashion (see [24], Lemma 5.1 for the inspiring precursor of all Aubin–Lions-type techniques). For the sake of brevity, we introduce an auxiliary vector $\mathcal{A}$ associated with the solution vector $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)$ and the auxiliary quantities (50), (83) via

$$\mathcal{A} := (J,\, \varrho\, v,\, r,\, \hat{r},\, \nabla v,\, \varrho\, v\otimes v,\, v\otimes(\mathbb{1}\cdot J),\, p,\, n^F\,\nabla\phi) \in [L^1(Q)]^a, \tag{113}$$

where $a = 5N + 34$ is the number of scalar components of the vector $\mathcal{A}$. Due to the structure of the weak formulation, the identities

$$\begin{pmatrix} \int\limits_\Omega \rho^\epsilon(t)\cdot\psi \\ \int\limits_\Omega \varrho_\epsilon(t)\, v^\epsilon(t)\cdot\eta \end{pmatrix} = \begin{pmatrix} \int\limits_\Omega \rho^0\cdot\psi \\ \int\limits_\Omega \varrho_0(t)\, v^0\cdot\eta \end{pmatrix} + \begin{pmatrix} \int\limits_0^t\int\limits_\Omega \sum_{j=0,1} \mathscr{L}^{1,j}(\mathcal{A}^\epsilon)\cdot D^j\psi \\ \int\limits_0^t\int\limits_\Omega \sum_{j=0,1} \mathscr{L}^{2,j}(\mathcal{A}^\epsilon)\cdot D^j\eta \end{pmatrix}, \tag{114}$$
$$\forall\, t\in[0,T], \quad \forall\, (\psi,\, \eta) \in C^1_c(\Omega;\, \mathbb{R}^N)\times C^1_c(\Omega;\, \mathbb{R}^3)\,.$$

are valid. Here, $\mathscr{L}^{i,j}(\mathcal{A})$, $i, j = 1, 2$ are certain linear combinations with bounded coefficients of the entries of the vector $\mathcal{A}$. The following observation is elementary.

Remark 12.1. Consider a family $\{(\varrho_\epsilon,\, q^\epsilon,\, v^\epsilon,\, \phi_\epsilon,\, R^\epsilon,\, R^{\Gamma,\epsilon})\}_{\epsilon>0}$ which satisfies a uniform bound in the class $\mathcal{B}(T,\, \Omega,\, \alpha,\, N-1,\, \Psi,\, \Psi^\Gamma)$. Define and auxiliary quantity $\mathcal{A}^\epsilon$ in the fashion of (113). If the representation (114) is valid, then there is a subsequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ such that for almost all $t\in[0,T]$ the sequences $\{\rho_{\epsilon_n}(t)\}_{n\in\mathbb{N}}$ and $\{\varrho_{\epsilon_n}\, v^{\epsilon_n}(t)\}_{n\in\mathbb{N}}$ converge as distribution in Ω.

Proof. Define $w^\epsilon := (\rho^\epsilon,\, \varrho_\epsilon\, v^\epsilon)$, and let Y be the Banach space $W^{1,\infty}_0(\Omega;\, \mathbb{R}^N)\times W^{1,\infty}_0(\Omega;\, \mathbb{R}^3)$. Obviously, the identity (114) implies the bound $\|\partial_t w^\epsilon\|_{L^1(0,T;\, Y^*)} \leq C_0\, \sup_{\epsilon\in[0,1]}\|\mathcal{A}^\epsilon\|_{[L^1(Q)]^a}$. Moreover, for arbitrary $0 < t_1 < t_2 < T$, the family $\{\int\limits_{t_1}^{t_2} w^\epsilon(t)\,dt\}_{\epsilon>0}$ is uniformly bounded in $L^{2\alpha/(1+\alpha)}(\Omega)$ (second bound in Lemma 10.4), hence compact in Y^*.

We invoke Lemma 4 and Theorem 1 of [33] to show that w^ϵ is in a compact subset of $L^p(0,T;\,Y^*)$ for all $1 \leq p < +\infty$. Hence, we find $w \in L^1(0,T;\,Y^*)$ and can extract a subsequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ such that $w^{\epsilon_n} \to w \in L^1(0,T;\,Y^*)$ and $w^{\epsilon_n}(t) \to w(t)$ in Y^* for almost all $t \in]0,T[$. □

At first we need to extract weakly convergent sub-sequences.

Lemma 12.2. *Consider a family* $\{(\varrho_\epsilon,\, q^\epsilon,\, v^\epsilon,\, \phi_\epsilon,\, R^\epsilon,\, R^{\Gamma,\epsilon})\}_{\epsilon>0}$ *which satisfies a uniform bound in the class* $\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$. *Define auxiliary quantities* ρ^ϵ, J_ϵ, r^ϵ, $\hat{r}^\epsilon$, p_ϵ, n^F_ϵ *and* $\mathcal{A}^\epsilon$ *in the fashion of* (50) *(or* (83)*) and* (113). *Assume that* (114) *is valid. Assume that for almost all* $t \in]0,T[$, $\phi_\epsilon(t)$ *satisfies in the weak sense* $-\bar{\chi}\,\triangle\phi_\epsilon(t) = \bar{Z}\cdot\rho^\epsilon(t)$ *in* Ω *with the boundary conditions* $\nu\cdot\nabla\phi_\epsilon(t) = 0$ *on* Σ *and* $\phi_\epsilon(t) = \phi_0(t)$ *on* Γ. *Then, there are*

$$\rho \in L^{\infty,\alpha}(Q;\,\mathbb{R}^N_+), \quad J \in L^{2,\frac{2\alpha}{1+\alpha}}(Q;\,\mathbb{R}^{N\times 3}), \quad -R \in L_\Psi(Q;\,\mathbb{R}^s), \quad -R^\Gamma \in L_{\hat{\Psi}^\Gamma}(S;\,\mathbb{R}^{\hat{s}^\Gamma}),$$
$$v \in W^{1,0}_2(Q;\,\mathbb{R}^3), \quad p \in L^{\infty,1}(Q) \cap L^{\min\{1+\frac{1}{\alpha},\,\frac{5}{3}-\frac{1}{\alpha}\}}(Q), \quad \phi \in L^\infty(Q) \cap L^\infty(0,T;\,W^{1,\beta}(\Omega)),$$

and a subsequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ *such that as* $n \to \infty$*:*

$$\begin{aligned}
&\rho^{\epsilon_n} \to \rho \text{ weakly in } L^\alpha(Q;\,\mathbb{R}^N),\\
&\rho^{\epsilon_n}(t) \to \rho(t) \text{ weakly in } L^\alpha(\Omega;\,\mathbb{R}^N) \quad \text{for almost all } t \in [0,T],\\
&\bar{\rho}^{\epsilon_n} \to \bar{\rho} \text{ strongly in } C([0,T];\,\mathbb{R}^N),\\
&J_{\epsilon_n} \to J \text{ weakly in } L^{2,\frac{2\alpha}{1+\alpha}}(Q;\,\mathbb{R}^{N\times 3}),\\
&R^{\epsilon_n} \to R \text{ weakly in } L^1(Q;\,\mathbb{R}^s),\; R^{\Gamma,\epsilon_n} \to R^\Gamma \text{ weakly in } L^1(S;\,\mathbb{R}^{\hat{s}^\Gamma}),\\
&v^{\epsilon_n} \to v \text{ weakly in } W^{1,0}_2(Q;\,\mathbb{R}^3),\\
&p_{\epsilon_n} \to p \text{ weakly in } L^{1+\min\{\frac{1}{\alpha},\,\frac{2}{3}-\frac{1}{\alpha}\}}(Q),\\
&\phi_{\epsilon_n} \to \phi \text{ strongly in } W^{1,0}_2(Q),\\
&\bar{Z}\cdot\rho^{\epsilon_n}\,\nabla\phi_{\epsilon_n} \to \bar{Z}\cdot\rho\,\nabla\phi \text{ weakly in } L^1(Q;\,\mathbb{R}^3),\\
&\varrho_{\epsilon_n}\, v^{\epsilon_n} \to \varrho\, v \text{ weakly in } L^{2,\frac{6\alpha}{6+\alpha}}(Q;\,\mathbb{R}^3),\\
&(\varrho_{\epsilon_n}\, v^{\epsilon_n})(t) \to \varrho(t)\, v(t) \text{ weakly in } L^{\frac{2\alpha}{1+\alpha}}(\Omega;\,\mathbb{R}^3) \quad \text{for almost all } t \in [0,T],\\
&\varrho_{\epsilon_n}\, v^{\epsilon_n} \otimes v^{\epsilon_n} \to \varrho\, v \otimes v \text{ weakly in } L^{\frac{5\alpha-3}{3\alpha}}(Q;\,\mathbb{R}^{3\times 3}).
\end{aligned}$$

Proof. Using the bounds in the natural class $\mathcal{B}$, we at first extract a subsequence such that

$$\begin{aligned}
&\rho^{\epsilon_n} \to \rho \text{ weakly in } L^\alpha(Q;\,\mathbb{R}^N), \quad \bar{\rho}^{\epsilon_n} \to \bar{\rho} \text{ strongly in } C([0,T];\,\mathbb{R}^N),\\
&J_{\epsilon_n} \to J \text{ weakly in } L^{2,\frac{2\alpha}{1+\alpha}}(Q;\,\mathbb{R}^{N\times 3}),\\
&R^{\epsilon_n} \to R \text{ weakly in } L^1(Q;\,\mathbb{R}^s), \quad R^{\Gamma,\epsilon_n} \to R^\Gamma \text{ weakly in } L^1(S;\,\mathbb{R}^{\hat{s}^\Gamma}),\\
&v^{\epsilon_n} \to v \text{ weakly in } W^{1,0}_2(Q;\,\mathbb{R}^3), \quad p_{\epsilon_n} \to p \text{ weakly in } L^{1+\min\{\frac{1}{\alpha},\,\frac{2}{3}-\frac{1}{\alpha}\}}(Q),\\
&\varrho_{\epsilon_n}\, v^{\epsilon_n} \to \xi \text{ weakly in } L^{2,\frac{6\alpha}{6+\alpha}}(Q;\,\mathbb{R}^3), \qquad \varrho_{\epsilon_n}\, v^{\epsilon_n} \otimes v^{\epsilon_n} \to \tilde{\xi} \text{ weakly in } L^{\frac{5\alpha-3}{3\alpha}}(Q;\,\mathbb{R}^{3\times 3}),\\
&\phi_{\epsilon_n} \to \phi \text{ weakly } W^{1,0}_2(Q), \quad n^F_{\epsilon_n}\,\nabla\phi_{\epsilon_n} \to k_L \text{ weakly in } L^1(Q;\,\mathbb{R}^3).
\end{aligned}$$

We now make use of the identity (114) via Remark 12.1. Thus, for all $t \in [0,T]$, we realise that the entire sequence $\{\rho^{\epsilon_n}(t)\}$ converges as distributions. Since it is uniformly bounded in $L^\alpha(\Omega)$, we obtain that $\{\rho^{\epsilon_n}(t)\}$ weakly converges in $L^\alpha(\Omega)$. The limit must be identical with $\rho(t)$ for almost all $t \in [0,T]$. Thus, making use of Remark 12.3 hereafter, $\rho^{\epsilon_n} \to \rho$ strongly in $[W^{1,0}_2(Q)]^*$, and this allows to show that $\varrho^{\epsilon_n}\, v^{\epsilon_n} \to \varrho\, v$ as distributions in Q. Clearly $\xi = \varrho\, v$.

Next we define $\phi(t) \in W^{1,2}(\Omega)$ to be the unique weak solution to the problem $-\bar{\chi}\,\triangle\phi(t) = \bar{Z}\cdot\rho(t)$ with the boundary conditions $-\nu\cdot\nabla\phi(t) = 0$ on Σ and $\phi(t) = \phi_0(t)$ on Γ. Due to Remark 12.3 we can verify, for almost all $t \in]0,T[$, the strong convergence $\phi_{\epsilon_n}(t) \to \phi(t)$ in $W^{1,2}(\Omega)$. Thus, it also follows that $\bar{Z}\cdot\rho^{\epsilon_n}\,\nabla\phi_{\epsilon_n} \to \bar{Z}\cdot\rho\,\nabla\phi$ weakly in $L^1(Q)$, implying that $k_L = n^F\,\nabla\phi$. Remark 12.1 implies that $\varrho_{\epsilon_n}(t)\,v^{\epsilon_n}(t)$ converges as distributions to $\varrho(t)\,v(t)$ for almost all $t \in]0,T[$, and therefore also weakly in $L^{2\alpha/(1+\alpha)}(\Omega)$. Since $2\alpha/(1+\alpha) > 6/5$, it also follows $\varrho_{\epsilon_n}\,v^{\epsilon_n} \to \varrho\,v$ strongly in $[W^{1,0}_2(Q)]^*$. This in turn allows to show that $\varrho_{\epsilon_n}\,v^{\epsilon_n}\otimes v^{\epsilon_n} \to \varrho\,v\otimes v$ as distributions, that means $\tilde{\xi} = \varrho\,v\otimes v$. □

Remark 12.3.
- Let $1 \le p \le +\infty$. Let $\mathcal{K} : L^p(\Omega) \to W^{1,p}(\Omega)$ be a bounded, compact operator. Assume that $\{u_n\}_{n\in\mathbb{N}} \subset L^p(Q)$ is a sequence such that $u_n(t) \to u(t)$ weakly in $L^p(\Omega)$ for almost all $t \in]0,T[$. Then, $\mathcal{K}(u_n(t)) \to \mathcal{K}(u(t))$ strongly in $W^{1,p}(\Omega)$ for almost all $t \in]0,T[$.
- If $v_n \to v$ weakly in $W^{1,0}_2(Q)$ and $u_n(t) \to u(t)$ strongly in $[W^{1,2}(\Omega)]^*$ for almost all $t \in]0,T[$, then $u_n\,v_n \to u\,v$ weakly in $L^1(Q)$.

We next can obtain the strong convergence of the velocity field. This result is in principle known (see [28], page 9).

Corollary 12.4. *Assumptions of Lemma 12.2. Then, there is a subsequence such that $\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v|^2$ converges to zero strongly in $L^1(Q)$ and pointwise almost everywhere in Q.*

Proof. Consider a sequence $\{v^m\}$ of smooth vector fields such that $v^m \to v$ in $W^{1,0}_2(Q;\mathbb{R}^3)$ for $m \to \infty$. Due to Lemma 12.2, $\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v^m|^2$ is readily seen to converge to $\varrho\,|v - v^m|^2$ weakly in $L^1(Q)$ for $n \to \infty$. On the other hand, using the continuity of the embedding $W^{1,2}(\Omega) \subset L^r(\Omega)$ for $r \le 6$, we show for all $\alpha \ge 3/2$ that

$$\|\varrho\,|v - v^m|^2\|_{L^1(Q)} \le \|\varrho\|_{L^{\infty,\alpha}(Q)}\,\|v - v^m\|^2_{L^{2,\,2\alpha/(\alpha-1)}(Q)} \le c\,\|\varrho\|_{L^{\infty,\alpha}(Q)}\,\|v - v^m\|^2_{W^{1,0}_2(Q)}.$$

With similar arguments

$$\begin{aligned}\|\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v^m|^2\|_{L^1(Q)} \ge&\frac{1}{2}\,\|\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v|^2\|_{L^1(Q)} - \|\varrho_{\epsilon_n}\,|v^m - v|^2\|_{L^1(Q)}\\ \ge&\frac{1}{2}\,\|\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v|^2\|_{L^1(Q)} - c\,\|\varrho_{\epsilon_n}\|_{L^{\infty,\alpha}(Q)}\,\|v - v^m\|^2_{W^{1,0}_2(Q)}.\end{aligned}$$

Thus, $\limsup_{n\to\infty}\|\varrho_{\epsilon_n}\,|v^{\epsilon_n} - v|^2\|_{L^1(Q)} \le C_0\,\|v - v^m\|^2_{W^{1,0}_2(Q)}$. Letting $m \to +\infty$, the claim follows. □

12.1. Conditional compactness statements

We now can prove the conditional compactness of the family $\{\rho^\epsilon\}_{\epsilon>0}$. We will need the following auxiliary statements.

Lemma 12.5. *Consider a family $\{\mathscr{R}^\epsilon\}_{\epsilon>0} \subset C(\mathbb{R}_{0,+}\times\mathbb{R}^{N-1};\mathbb{R}^N_+)$ fulfilling (112). For $x \in \mathbb{R}_+\times\mathbb{R}^{N-1}$, we denote $x = (x_1,\,\bar{x})$. Let $K \subset L^1(\Omega;\mathbb{R}^N)$ be a weakly sequentially compact set, and $K^* \subset L^1(\Omega)$ a sequentially compact set. Let $\phi^1,\,\phi^2,\ldots \in C^\infty(\overline{\Omega})$ be a countable, dense subset of $C(\overline{\Omega};\mathbb{R}^N)$.*

For all $\delta > 0$, there are $C(\delta) > 0$, $m(\delta) \in \mathbb{N}$ such that, for all $0 < \epsilon_1,\,\epsilon_2 \le 1/m(\delta)$

$$\begin{aligned}&\|\mathscr{R}^{\epsilon_1}(w^1) - \mathscr{R}^{\epsilon_2}(w^2)\|_{L^1(\Omega)}\\ &\quad\le \delta\left(1 + \sum_{i=1,2}\|\bar{w}^i\|_{W^{1,1}(\Omega)}\right) + C(\delta)\sum_{i=1}^m\left|\int_\Omega(\mathscr{R}^{\epsilon_1}(w^1) - \mathscr{R}^{\epsilon_2}(w^2))\cdot\phi^i\right|\end{aligned}$$

for all $w^1,\,w^2 \in L^1(\Omega;\mathbb{R}_+\times\mathbb{R}^{N-1})$ such that

$$\mathscr{R}^{\epsilon_i}(w^i) \in K,\quad w^i_1 \in K^*,\quad \bar{w}_i \in W^{1,1}(\Omega;\mathbb{R}^{N-1})\quad \textit{for } i = 1,2.$$

Proof. Clearly, it is sufficient to prove the existence of $C(\delta)$ and $m(\delta)$ and, for all $0 < \epsilon_1, \epsilon_2 \leq 1/m(\delta)$, the inequality

$$\|\mathscr{R}^{\epsilon_1}(w^1) - \mathscr{R}^{\epsilon_2}(w^2)\|_{L^1(\Omega)} \leq \delta \sum_{i=1,2} \|\bar{w}^i\|_{W^{1,1}(\Omega)} + C(\delta) \sum_{i=1}^{m} \left| \int_\Omega (\mathscr{R}^{\epsilon_1}(w^1) - \mathscr{R}^{\epsilon_2}(w^2)) \cdot \phi^i \right|$$

for all $w^1, w^2 \in L^1(\Omega; \mathbb{R}_+ \times \mathbb{R}^{N-1})$ such that $\mathscr{R}^{\epsilon_i}(w^i) \in K$, $w_1^i \in K^*$ and $\bar{w}^i \in W^{1,1}(\Omega; \mathbb{R}^{N-1})$ for $i = 1, 2$ and such that $\|\mathscr{R}^{\epsilon_1}(w^1) - \mathscr{R}^{\epsilon_2}(w^2)\|_{L^1(\Omega)} \geq \delta$. We argue by contradiction. If the latter claim is not true, there is $\delta_0 > 0$ such that for all $n \in \mathbb{N}$ and $i = 1, 2$, we can find $0 < \epsilon_{i,n} < 1/n$, $w^{i,n} \in L^1(\Omega; \mathbb{R}_+ \times \mathbb{R}^{N-1})$ such that $\mathscr{R}^{\epsilon_{i,n}}(w^{i,n}) \in K$, $w_1^{i,n} \in K^*$, $\bar{w}^{i,n} \in W^{1,1}(\Omega; \mathbb{R}^{N-1})$ $(i = 1, 2)$ satisfying the properties

$$\|\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n})\|_{L^1(\Omega)} \geq \delta_0 \sum_{i=1,2} \|\bar{w}^{i,n}\|_{W^{1,1}(\Omega)} + n \sum_{i=1}^{n} \left| \int_\Omega (\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n})) \cdot \phi^i \right| \tag{115}$$

$$\|\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n})\|_{L^1(\Omega)} \geq \delta_0. \tag{116}$$

Since we assume that $\mathscr{R}^{\epsilon_{i,n}}(w^{i,n}) \in K$ for $i = 1, 2$ and since K is a bounded set of $L^1(\Omega)$, we obtain first that $\|\bar{w}^{i,n}\|_{W^{1,1}(\Omega)} \leq C$ for all $n \in \mathbb{N}$. Thus, we can extract a subsequence that we not relabel such that for almost all $x \in \Omega$ there exists $\bar{w}^i(x) := \lim_{n\to\infty} \bar{w}^{i,n}(x)$.

Moreover, as $w_1^{i,n} \in K^*$, we can extract a subsequence such that $w_1^{i,n} \to w_1^i$ strongly in $L^1(\Omega)$ and almost everywhere in Ω. Consequently, we obtain for a subsequence and for $i = 1, 2$ that

$$w^{i,n} \to w^i := (w_1^i, \bar{w}^i) \text{ strongly in } L^1(\Omega; \mathbb{R}^N) \text{ and a. e. in } \Omega.$$

Now using that $\mathscr{R}^{\epsilon_{i,n}}(w^{i,n}) \in K$, we can pass to a subsequence again to see that $\mathscr{R}^{\epsilon_{i,n}}(w^{i,n}) \to u^i$ weakly in $L^1(\Omega; \mathbb{R}^N)$ for $i = 1, 2$. The property (112) and the pointwise convergence of $w^{i,n}$ yield $u^i = \mathscr{R}(w^i)$. We next use the second implication of (115), that is,

$$\sum_{i=1}^{n} \left| \int_\Omega (\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n})) \cdot \phi^i \right| \leq c\, n^{-1},$$

so that $\mathscr{R}(w^1) = \mathscr{R}(w^2)$ almost everywhere in Ω. Hence, $\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n}) \to 0$ weakly in $L^1(\Omega)$ and pointwise. This implies that $\mathscr{R}^{\epsilon_{1,n}}(w^{1,n}) - \mathscr{R}^{\epsilon_{2,n}}(w^{2,n}) \to 0$ strongly in $L^1(\Omega)$ and that the condition (116) is violated. □

We now state and prove our main compactness tool.

Corollary 12.6. *Consider a sequence* $\{\mathscr{R}^{\epsilon_n}\}_{n\in\mathbb{N}} \subset C(\mathbb{R}_{0,+} \times \mathbb{R}^{N-1}; \mathbb{R}^N_+)$ *fulfilling* (112). *For* $n \in \mathbb{N}$, *let* $w^n : [0, T] \to L^1(\Omega; \mathbb{R}_+ \times \mathbb{R}^{N-1})$ *be continuous. Assume that* $\bigcup_{n\in\mathbb{N}} \bigcup_{t\in[0,T]} \{w_1^n(t)\}$ *is compact in* $L^1(\Omega)$, *and that there is* C_1 *independent on* n *such that* $\|\bar{w}^n\|_{L^1(Q;\mathbb{R}^{N-1})} + \|\nabla \bar{w}^n\|_{L^1(Q;\mathbb{R}^{N-1})} \leq C_1$. *Assume moreover that* $\|\mathscr{R}^{\epsilon_n}(w^n)\|_{L^{\infty,\alpha}(Q;\mathbb{R}^{N-1})} \leq C_1$, *and that the sequence* $\{\mathscr{R}^{\epsilon_n}(w^n(t))\}_{n\in\mathbb{N}}$ *converges as distributions in* Ω *for almost all* t.

Then, there is a subsequence (no new labels) for which there exists $\rho(t, x) := \lim_{n\to\infty} \mathscr{R}^{\epsilon_n}(w^n(t, x))$ *for almost all* $(t, x) \in Q$, *and* $\mathscr{R}^{\epsilon_n}(w^n(t, x)) \to \rho$ *strongly in* $L^1(Q; \mathbb{R}^N)$.

Proof. For simplicity let $\mathscr{R}^n := \mathscr{R}^{\epsilon_n}$. For $n \in \mathbb{N}$, the assumptions imply that $\mathscr{R}^n(w^n(t)) \in L^\alpha(\Omega; \mathbb{R}^N)$ for all $t \in [0, T]$. We define $K \subset L^1(\Omega; \mathbb{R}^N)$ via $K := \bigcup_{n\in\mathbb{N}} \bigcup_{t\in[0,T]} \{\mathscr{R}^n(w^n(t))\}$ By assumption K is bounded in $L^\alpha(\Omega)$ and thus also weakly sequentially compact in $L^1(\Omega)$.

By assumption again, the set $K^* := \bigcup_{n\in\mathbb{N}}\bigcup_{t\in[0,T]}\{w_1^n(t)\}$ is compact in $L^1(\Omega)$. For $\delta > 0$, we find the constants $C(\delta)$ and $m(\delta) \in \mathbb{N}$ according to Lemma 12.5. For all $n \in \mathbb{N}$ such that $\epsilon_n < 1/m(\delta)$, we apply the inequality of this Lemma with $\epsilon_1 = \epsilon_n$, $\epsilon_2 = \epsilon_{n+p}$, $w^1 = w^n(t)$ and $w^2 := w^{n+p}(t)$ ($p \in \mathbb{N}$ arbitrary). For $t \in [0,T]$ it follows that

$$\begin{aligned}\|\mathscr{R}^n(w^n(t)) - \mathscr{R}^{n+p}(w^{n+p}(t))\|_{L^1(\Omega)} &\le \delta\left(1 + \|\bar{w}^n(t)\|_{W^{1,1}(\Omega)} + \|\bar{w}^{n+p}(t)\|_{W^{1,1}(\Omega)}\right)\\ &\quad + C(\delta)\sum_{i=1}^m \left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \mathscr{R}^{n+p}(w^{n+p}(t)))\cdot\phi^i\right|. \end{aligned} \tag{117}$$

We integrate the relation (117) over the set $]0,T[$ and this yields

$$\begin{aligned}\|\mathscr{R}^n(w^n) - \mathscr{R}^{n+p}(w^{n+p})\|_{L^1(Q)} &\le \delta\,(T + 2\sup_n \|\bar{w}^n\|_{W_1^{1,0}(Q)})\\ &\quad + C(\delta)\sum_{i=1}^m \int_0^T \left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \mathscr{R}^{n+p}(w^{n+p}(t)))\cdot\phi^i\right|\\ &\le \delta\,(T + C) + C(\delta)\sum_{i=1}^m \int_0^T \left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \mathscr{R}^{n+p}(w^{n+p}(t)))\cdot\phi^i\right|.\end{aligned}$$

The vector fields $\mathscr{R}^n(w^n)$ weakly converges in $L^1(\Omega;\,\mathbb{R}^N)$ for almost all t to some element $\rho \in L^{\infty,\alpha}(Q;\,\mathbb{R}^N)$. Invoking the triangle inequality,

$$\int_0^T \left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \mathscr{R}^{n+p}(w^{n+p}(t)))\cdot\phi^i\right| \le 2\sup_{k\ge n}\int_0^T \left|\int_\Omega (\mathscr{R}^k(w^k(t)) - \rho(t))\cdot\phi^i\right|.$$

It follows that

$$\sup_{p\ge 0}\|\mathscr{R}^n(w^n) - \mathscr{R}^{n+p}(w^{n+p})\|_{L^1(Q)} \le \delta\,(T + C) + 2\,C(\delta)\sum_{i=1}^m \sup_{k\ge n}\int_0^T \left|\int_\Omega (\mathscr{R}^k(w^k(t)) - \rho(t))\cdot\phi^i\right|.$$

Due to the uniform bound in $L^{\infty,\alpha}$, the functions $g_n(t) := \int_\Omega (\mathscr{R}^n(w^n(t)) - \rho(t))\cdot\phi^i$ are uniformly bounded in $L^\infty(0,T)$ independently on n. Hence, invoking the Fatou Lemma

$$\begin{aligned}\limsup_{n\to\infty}\sup_{k\ge n}\int_0^T \left|\int_\Omega (\mathscr{R}^k(w^k(t)) - \rho(t))\cdot\phi^i\right| &= \limsup_{n\to\infty}\int_0^T \left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \rho(t))\cdot\phi^i\right|\\ &\le \int_0^T \limsup_{n\to\infty}\left|\int_\Omega (\mathscr{R}^n(w^n(t)) - \rho(t))\cdot\phi^i\right|.\end{aligned}$$

The vector fields $\mathscr{R}^n(w^n(t))$ weakly converges in $L^1(\Omega)$ for almost all t. Hence, the right-hand is zero in the latter inequality, and $\limsup_{n\to\infty}\sup_{k\ge n}\int_0^T \left|\int_\Omega (\mathscr{R}^k(w^k(t)) - \rho(t))\cdot\phi^i\right| = 0$. It next follows that

$$\limsup_{n\to\infty}\sup_{p\ge 0}\|\mathscr{R}^n(w^n) - \mathscr{R}^{n+p}(w^{n+p})\|_{L^1(Q)} \le \delta\,(T + C)$$

and, since δ is arbitrary, $\limsup_{n\to\infty}\sup_{p\ge 0}\|\mathscr{R}^n(w^n) - \mathscr{R}^{n+p}(w^{n+p})\|_{L^1(Q)} = 0$. This means that $\{\mathscr{R}^n(w^n)\}$ is a Cauchy sequence in $L^1(Q)$. In particular, we can extract a subsequence such that $\lim_{n\to+\infty}\mathscr{R}^n(w^n)$ exists almost everywhere in Q. □

Corollary 12.7. *We adopt the same assumptions as in Lemma 12.2, and we assume moreover that the family of the total mass densities* $\{\varrho_\epsilon(t)\}_{\epsilon\geq 0,\, t\in]0,T[}$ *is compact in* $L^1(\Omega)$*. Assume further that the family of transformations* $\{\mathscr{R}^\epsilon\}_{\epsilon>0}$ *fulfils (112). Then,* $\rho^{\epsilon_n} \to \rho$ *strongly in* $L^1(Q;\, \mathbb{R}^N)$*. Moreover, for almost all* $(t,\, x) \in Q$ *such that* $\varrho(t,\, x) > 0$*, there exists* $q(t,\, x) := \lim_{n\to\infty} q^{\epsilon_n}(t,\, x)$*. The identity* $\rho = \mathscr{R}(\varrho,\, q)$ *is valid at almost every point of the set* $Q^+(\varrho) = \{(t,\, x)\, :\, \varrho(t,\, x) > 0\}$*.*

Proof. We consider a subsequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ fulfilling the convergence properties of Lemma 12.2. We define $w^n = (\varrho_{\epsilon_n},\, q^{\epsilon_n})$, and verify easily that all requirements of Corollary 12.6 are satisfied. We apply this Corollary to first show that $\rho^{\epsilon_n} = \mathscr{R}^{\epsilon_n}(\varrho_{\epsilon_n},\, q^{\epsilon_n})$ converges strongly in $L^1(Q)$ and pointwise almost everywhere.

In order to also show that $\{q^{\epsilon_n}\}$ converges strongly, we resort to the representation (111) and to the definition of $\mathscr{R}^{\epsilon_n}$. For $k = 1, \ldots, N-1$, they yield

$$q_k^{\epsilon_n} = \eta^k \cdot \nabla_\rho h_{\epsilon_n}(\mathscr{R}^{\epsilon_n}(\varrho_{\epsilon_n},\, q^{\epsilon_n})) = \eta^k \cdot (c + F'_{\epsilon_n}(\rho^{\epsilon_n}\cdot \bar{V})\, \bar{V} + \frac{1}{m}\ln y^{\epsilon_n}). \tag{118}$$

As $\{\eta^1, \ldots, \eta^{N-1}\}$ are chosen to form a basis of $\{\mathbb{1}\}^\perp$, we can represent for $i \neq j$ arbitrary the vector $e^i - e^j$ with a linear combination of the $\sum_{k=1}^{N-1} a_k^{i,j}\, \eta^k$, hence

$$\frac{1}{m_i}\ln y_i^{\epsilon_n} - \frac{1}{m_j}\ln y_j^{\epsilon_n} = c_j - c_i + (\bar{V}_j - \bar{V}_i)\, F'_{\epsilon_n}(\rho^{\epsilon_n}\cdot\bar{V}) + a^{i,j}\cdot q^{\epsilon_n}.$$

We now choose j as the indice associated with the largest number fraction, which implies that $|(1/m_j) \ln y_j^{\epsilon_n}| \leq \ln N/\min m$. For $i = 1, \ldots, N$, we deduce the inequality

$$|\ln y_i^{\epsilon_n}| \leq C\,(1 + |F'_{\epsilon_n}(\rho^{\epsilon_n}\cdot\bar{V})| + |q^{\epsilon_n}|).$$

Recall that $F_\epsilon(s) = F(s) + \epsilon\, s^\alpha$ with $\alpha > 3$, while F is associated with a growth exponent $\alpha_0 \leq \alpha$. We multiply with $\min\{\varrho_{\epsilon_n},\, 1\}$ and, using the growth conditions (35) for F and the uniform bounds for ρ^{ϵ_n} in L^{∞,α_0}, for $\epsilon_n\, \varrho_{\epsilon_n}^\alpha$ in $L^{\infty,1}$, and for q^{ϵ_n} in L^2, it follows that

$$\|\min\{\varrho_{\epsilon_n},\, 1\}\, \ln y_i^{\epsilon_n}\|_{L^{\min\{\alpha',2\}}(Q)} \leq C_0. \tag{119}$$

Since $y_i^{\epsilon_n} = \rho_i^{\epsilon_n}/(m_i \sum_j(\rho_j^{\epsilon_n}/m_j))$ converges pointwise, we can choose a subsequence such that min $\{\varrho_{\epsilon_n},\, 1\}\, \ln y_i^{\epsilon_n} \to \min\{\varrho,\, 1\}\, \ln y_i$ strongly in $L^1(Q)$ and pointwise almost everywhere in Q.

Making use of (118), we then verify that

$$\min\{\varrho_{\epsilon_n},\, 1\}\, q_k^{\epsilon_n} \to \min\{\varrho,\, 1\}\, \eta^k \cdot (c + F'(\rho\cdot\bar{V})\,\bar{V} + \frac{1}{m}\ln y) \text{ pointwise a. e. in } Q.$$

It remains to observe that $(\min\{\varrho_{\epsilon_n},\, 1\} - \min\{\varrho,\, 1\})\, |q^{\epsilon_n}|$ is uniformly bounded in $L^2(Q)$ and tends to zero in $L^1(Q)$, to show that $\lim_{n\to\infty} q^{\epsilon_n}(t,x)$ exists for almost all (t,x) such that $\varrho(t,x) > 0$. □

In order to pass to the limit in the boundary reaction terms, we also discuss the strong convergence of the relative chemical potentials on the boundary $]0,T[\times\Gamma$.

Lemma 12.8. *Assumptions of Corollary 12.7. Then, for almost every* $(t,\, x) \in S^+(\varrho)$*, there exists* $q(t,\, x) := \lim_{n\to\infty} q^{\epsilon_n}(t,\, x)$*.*

Proof. By definition, the surface $S^+(\varrho)$ is relatively open and possesses an open neighbourhood U in Q such that $|U \cap \{(t,x)\, :\, \varrho(t,\, x) = 0\}| = 0$. Thus, for $(t_0,\, x^0) \in S^+(\varrho)$ arbitrary, there is $R > 0$ such that the cube $Q_R(t_0, x^0)$ with radius $R > 0$ and centred at $(t_0,\, x^0)$ is contained in U. For all $\epsilon > 0$, there is a constant $c = c(\Omega,\, \epsilon)$ such that

$$\|u\|_{L^1(\Gamma_R(x^0))} \leq \epsilon\, \|\nabla u\|_{L^1(\Omega_R(x^0))} + c(\epsilon,\, \Omega)\, \|u\|_{L^1(\Omega_R(x^0))} \quad \text{for all } u \in W^{1,1}(\Omega).$$

Here, Γ_R and Ω_R denote the intersection of Γ and Ω with $Q_R(x^0)$, the three-dimensional cube with radius R centred at x^0. With the help of this inequality, we obtain for almost all $t \in]t_0 - R,\, t_0 + R[$ that

$$\|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Gamma\cap Q_R(x^0))} \leq \epsilon\, (\|\nabla q^{\epsilon_n}(t)\|_{L^1(\Omega)} + \|\nabla q(t)\|_{L^1(\Omega)}) + c(\epsilon,\, \Omega)\, \|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Omega\cap Q_R(x^0))}.$$

Integrating in time, it follows that

$$\int_{t_0-R}^{t_0+R} \|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Gamma_R(x^0))} \,\mathrm{d}t \le C_0\,\epsilon + c(\epsilon,\,\Omega) \int_{t_0-R}^{t_0+R} \|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Omega_R(x^0))} \,\mathrm{d}t$$

Now as $(]t_0 - R,\, t_0 + R[\times\Omega) \cap Q_R(x^0))$ is a subset of U, Corollary 12.7 implies that $\int_{t_0-R}^{t_0+R} \|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Omega_R(x^0))} \,\mathrm{d}t \to 0$. Hence, $\limsup_{n\to\infty} \int_{t_0-R}^{t_0+R} \|q^{\epsilon_n}(t) - q(t)\|_{L^1(\Gamma_R(x^0))} \,\mathrm{d}t = 0$. □

It remains to enlighten the global convergence property of the variables $\{q^{\epsilon_n}\}$ inclusively of the set where vacuum possibly occurs. The following statement is a simple consequence of the *a priori* estimates, so we might spare the proof for the sake of being concise.

Lemma 12.9. *Under the same assumptions as in Corollary 12.7, there is a subsequence such that $q^{\epsilon_n} \to q$ weakly in $W^{1,0}_2(Q)$.*

With the help of the compactness statement, we can now identify all remaining weak limits.

Corollary 12.10. *Assumptions as in Corollary 12.7. Let J, p, r and $\hat{r}$ denote the weak limit of J^{ϵ_n}, p_{ϵ_n}, r^{ϵ_n} and $\hat{r}^{\epsilon_n}$ constructed in Lemma 12.2. Then, for almost all $t \in]0,T[$, the following identities are valid:*

$$J = -M(\rho)\,(\nabla\mathcal{E}\,q + \bar{Z}\,\nabla\phi), \qquad p = P(\varrho,\,q),$$

$$r = \sum_{k=1}^{s} \gamma^k\,\bar{R}_k(D^R) \text{ with } D^R_k = \gamma^k \cdot \mathcal{E}q \text{ in } Q^+(\varrho),$$

$$\hat{r} = \sum_{k=1}^{\hat{s}^\Gamma} \hat{\gamma}^k\,\hat{R}^\Gamma_k(t, x,\,\hat{D}^{\Gamma,R}) \text{ with } \hat{D}^{\Gamma,R}_k = \hat{\gamma}^k \cdot \mathcal{E}q \text{ on } S^+(\varrho).$$

Proof. Exploiting the convergence properties stated in Corollary 12.7 and Lemma 12.2, we see that

$$J_{\epsilon_n} = -M(\rho^{\epsilon_n})\,(\nabla\mathcal{E}q^{\epsilon_n} + \bar{Z}\,\nabla\phi_{\epsilon_n}) \to -M(\rho)\,(\nabla\mathcal{E}\,q + \bar{Z}\,\nabla\phi)$$

weakly in $L^{2,\frac{2\alpha}{1+\alpha}}(Q)$. Since $P_{\epsilon_n} \to P$ on compact subsets of $[0,\,\infty[\times\mathbb{R}^{N-1}$, the pointwise convergence of $\{\rho^{\epsilon_n}\}$ and $\{q^{\epsilon_n}\}$ yield $P_{\epsilon_n}(\varrho_{\epsilon_n},\,q^{\epsilon_n}) \to P(\varrho,\,q)$ pointwise in $Q^+(\varrho)$, while $|P_{\epsilon_n}(\varrho_{\epsilon_n},\,q^{\epsilon_n})| \le c\,\varrho^\alpha_{\epsilon_n} \to 0$ pointwise in $Q\backslash Q^+(\varrho)$. The other claims are proved similarly. □

We now resume the results of the section formulating our main (conditional) convergence statement.

Proposition 12.11. *Consider a family $\{(\varrho_\epsilon,\,q^\epsilon,\,v^\epsilon,\,\phi_\epsilon,\,R^\epsilon,\,R^{\Gamma,\epsilon})\}_{\epsilon>0}$ which satisfies a uniform bound in the class $\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$. Assume the condition (112) for the family $\{\mathscr{R}^\epsilon\}_{\epsilon>0}$, the condition (114) on the time derivatives, and that $\{\varrho_\epsilon\} \subset C([0,T];\,L^1(\Omega))$ with $\{\varrho_\epsilon(t)\}_{t\in[0,T],\,\epsilon>0}$ compact in $L^1(\Omega)$. Then, there are a limiting element $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma) \in \mathcal{B}$ and a subsequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ such that all convergence properties stated in Lemma 12.2, Corollary 12.4, Corollary 12.7, Lemma 12.8, Lemma 12.9 and Corollary 12.10 are valid.*

We finally note an important consequence of Proposition 12.11 concerning the lower semi-continuity of the energy identity.

Corollary 12.12. *Assumptions of Proposition 12.11. Let $\{(\varrho_\epsilon,\,q^\epsilon,\,v^\epsilon,\,\phi_\epsilon,\,R^\epsilon,\,R^{\Gamma,\epsilon})\}_{\epsilon>0}$ satisfy for $\epsilon > 0$ the energy inequality with mobility matrix $M_\epsilon \ge M$, and free energy functions h_ϵ having the property*

$$\rho^\epsilon \to \rho \in \mathbb{R}^N_{0,+} \Longrightarrow \liminf_{\epsilon\to 0} h_\epsilon(\rho^\epsilon) \ge h(\rho).$$

Then, the limiting element $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$ constructed in Proposition 12.11 satisfies the energy inequality with free energy function h and mobility matrix M.

The proof is rather obvious. For the limit passage $\delta \to 0$, the free energies $\{h_\delta\}_{\delta>0}$ converge uniformly on compact subsets of $\overline{\mathbb{R}}_+^N$ (see (77)). For the limit passage $\tau \to 0$, we use that the family $\{h_\tau\}_{\tau>0}$ is constructed via convex duality (see (80)) and that the dual functions h_τ^* converge uniformly on compact subsets of $\mathbb{R}^N$ (see (78)).

12.2. Compactness of the total mass density

We showed that boundedness in the energy class together with the existence of weak time derivatives implies the compactness of the solution vector if the condition $\{\varrho_\epsilon(t)\} \subseteq K^*$ for all t is satisfied, where K^* is a fixed compact of $L^1(\Omega)$. Using an extension of the method of Lions for the compressible Navier–Stokes operator, we can show that this condition is satisfied for the approximation schemes of interest to us. We in fact show the compactness in $C([0,T];\, L^1(\Omega))$, which is a stronger statement.

Proposition 12.13. *Consider a family $\{(\varrho_\epsilon,\, q^\epsilon,\, v^\epsilon,\, \phi_\epsilon,\, R^\epsilon,\, R^{\Gamma,\epsilon})\}_{\epsilon>0} \subset \mathcal{B}$ which is uniformly bounded in the natural class $\mathcal{B}(T,\, \Omega,\, \alpha,\, N-1,\, \Psi,\, \Psi^\Gamma)$ and satisfies the assumptions of Lemma 12.2. Let $\{\bar{J}^\epsilon\}_{\epsilon>0} \subset L^2(Q;\, \mathbb{R}^3)$ be a family of perturbations such that $\bar{J}^\epsilon \to 0$ strongly in $L^2(Q)$ as $\epsilon \to 0$ and such that*

$$\begin{cases} \limsup_{\epsilon\to 0} \|(\bar{J}^\epsilon \cdot \nabla \ln \varrho_\epsilon)^+\|_{L^1(Q)} = 0 & \text{if } \alpha > 3, \\ \bar{J}^\epsilon \equiv 0 & \text{if } \frac{3}{2} < \alpha \le 3. \end{cases}$$

Suppose that the identities

$$-\int_Q \varrho_\epsilon\, \partial_t \psi - \int_Q (\varrho_\epsilon\, v^\epsilon + \bar{J}^\epsilon) \cdot \nabla \psi = \int_\Omega \varrho_0\, \psi(0), \tag{120}$$

$$-\int_Q \varrho_\epsilon\, v^\epsilon \cdot \partial_t \eta - \int_Q \varrho_\epsilon\, v^\epsilon \otimes v^\epsilon : \nabla \eta - \int_Q p_\epsilon\, \operatorname{div} \eta + \int_Q \mathbb{S}(\nabla v^\epsilon) : \nabla \eta$$
$$= \int_\Omega \varrho_0\, v^0 \cdot \eta(0) + \int_Q (\bar{J}^\epsilon \cdot \nabla)\eta \cdot v^\epsilon - \int_Q n_\epsilon^F\, \nabla \phi_\epsilon \cdot \eta\,, \tag{121}$$

are valid for all $\psi \in C_c^1([0,T[;\, C^1(\overline{\Omega}))$ and all $\eta \in C_c^1([0,T[;\, C_c^1(\Omega;\, \mathbb{R}^3))$. Assume that either $\alpha \ge 9/5$, or that $3/2 < \alpha < 9/5$ and the vectors $\bar{V}$ and 1^N are parallel. Then, for every sequence $\{\epsilon_n\}_{n\in\mathbb{N}}$, the sequence $\{\varrho_{\epsilon_n}\}_{n\in\mathbb{N}}$ is compact in $C([0,T];\, L^1(\Omega))$.

Insiders in mathematical fluid dynamics will directly conclude from the representation of the pressure $p = P(\varrho,\, q)$, with P increasing in ϱ and with ∇q controlled, that the total mass density must be compact. For readers less familiar with the Lions theory, a sketch of the proofs allowing for independent reading is given in the appendix, section B.

13. Existence of solutions

Weak solutions to (P) are defined in the spirit of viscosity solutions by passing to the limit $\sigma \to 0$ and then $\delta \to 0$ in the approximation scheme $(P_{\tau=0,\sigma,\delta})$.

Proposition 13.1. *We adopt the assumptions of Theorems 7.4, 7.6. For $\sigma > 0$ and $\delta > 0$ assume that there is $(\mu^{\sigma,\delta},\, v^{\sigma,\delta},\, \phi_{\sigma,\delta}) \in \mathcal{B}(T,\, \Omega,\, \alpha,\, N,\, \Psi,\, \Psi^\Gamma)$, subject to the energy inequality and to the global conservation of partial masses, that weakly solves $(P_{\tau=0,\sigma,\delta})$. Then, (P) possesses a weak solution (as stated in Theorems 7.4, 7.6).*

Proof. We first show the claim under the assumptions of Theorem 7.4 (Global existence).

The validity of the mass conservation identity (63) implies that the vector of net masses $\bar{\rho}^{\sigma,\delta} \in C_{\Phi^*}([0,T];\,\mathbb{R}^N)$ satisfies

$$\bar{\rho}^{\sigma,\delta}(t) \in \{\bar{\rho}^0\} \oplus W \quad \text{for all } t \in [0,T].$$

We apply the bounds in Sects. 10 (statements 10.1–10.5) and 11 (Theorem 11.3), and we obtain that

$$\begin{aligned}[][(\varrho_{\sigma,\delta},\, q^{\sigma,\delta},\, v^{\sigma,\delta},\, \phi_{\sigma,\delta},\, R^{\sigma,\delta},\, R^{\Gamma,\sigma,\delta})]_{\mathcal{B}(T,\,\Omega,\,\alpha_\delta,\,N-1,\,\Psi,\,\Psi^\Gamma)} \leq C(\delta,\mathcal{B}_0),\\ [(\varrho_{\sigma,\delta},\, q^{\sigma,\delta},\, v^{\sigma,\delta},\, \phi_{\sigma,\delta},\, R^{\sigma,\delta},\, R^{\Gamma,\sigma,\delta})]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)} \leq C(\mathcal{B}_0).\end{aligned} \tag{122}$$

Here, we distinguish the regularisation exponent $\alpha_\delta > 3$ and the original growth exponent $3/2 < \alpha < +\infty$ of the free energy function.

Moreover, time integration in (63) and (84) means that (114) is valid.

We fix $\delta > 0$. By construction, the condition $\alpha_\delta > 3$ is valid. With the help of Lemma A.2 in the appendix, we verify that

$$\|((\mathbb{1}\cdot J^{\sigma,\delta})\cdot\nabla\ln\varrho_{\sigma,\delta})^+\|_{L^1(Q)} \to 0 \quad \text{for } \sigma \to 0. \tag{123}$$

As the bounds (76) imply that (112) is valid, Proposition 12.13 applied with $\bar{J}^\sigma := \mathbb{1}\cdot J^\sigma$ now guarantees that the family $\{\varrho_{\sigma,\delta}\}_{\sigma>0}$ is compact in $C([0,T];\,L^1(\Omega))$. It remains to apply Proposition 12.11 in order to obtain the convergence to a weak solution $(\varrho_\delta,\, q^\delta,\, v^\delta,\, \phi_\delta,\, R^\delta,\, R^{\Gamma,\delta}) \in \mathcal{B}(T,\,\Omega,\,\alpha_\delta,\,N-1,\,\Psi,\,\Psi^\Gamma)$ to $(P_{\tau=0,\sigma=0,\delta})$.

For the passage to the limit $\delta \to 0$ the reasoning is the same. The second of the bounds (122) is available. Since there is no perturbation $\bar{J}^\delta$ in the mass conservation equation, Proposition 12.13 guaranties at once the uniform in time compactness in $C([0,T];\,L^1(\Omega))$ of $\{\varrho_\delta\}_{\delta>0}$, and Proposition 12.11 guarantees the convergence to a weak solution to (P).

In order to prove the additional claims of Theorem 7.5 concerning the singularities, we recall the inequality $\|\min\{\varrho_{\sigma,\delta},\,1\}\ln y_i^{\sigma,\delta}\|_{L^{\min\{\alpha',2\}}(Q)} \leq C_0$ (derivation in (119)), where $y_i^{\sigma,\delta}$ are the associated number fractions. With the pointwise convergence of the densities and Fatou's Lemma, this inequality always implies that the limiting number fractions are strictly positive almost everywhere outside of the vacuum set.

It remains to discuss the case of Theorem 7.6 about local-in-time existence. Due to Proposition 10.3, $[\bar{\rho}^{\sigma,\delta}]_{C_{\Phi^*}([0,T];\,\mathbb{R}^N)} \leq C_0$. We can extract sub-sequences such that $\rho^{\sigma,\delta}$ converges weakly in $L^\alpha(Q)$, and $\bar{\rho}^{\sigma,\delta}$ converges uniformly on $[0,T]$. We define a time $T^*_{\sigma,\delta}$ via

$$T^*_{\sigma,\delta} = \inf\{t \in [0,T[\,:\, \inf_{i=1,\ldots,N} \bar{\rho}_i^{\sigma,\delta}(t) = 0\}.$$

We know that $T^*_{\sigma,\delta} \geq T_0 > 0$ where T_0 is fixed by the data (cf. Lemma 11.4). At first we can extract a subsequence such that $T^*_{\sigma,\delta} \to T^*$. Due to the continuity of $\bar{\rho}$, we see that $0 = \inf \bar{\rho}^{\sigma,\delta}(T^*_{\sigma,\delta}) \to \inf \bar{\rho}(T^*)$.

Consider now $T' \in [0,\, T^*[$ arbitrary. Then, for all $\sigma \leq \sigma_0(T^*-T')$, and $\delta \leq \delta_0(T^*-T')$, we establish the estimates (122) with T replaced by T'. We then finish the proof as for Theorem 7.4 with T replaced by T'. By definition, we now have $\lim_{T'\to T^*} \min_{i=1,\ldots,N} \bar{\rho}_i(T') = 0$. Hence, there must exist an index i_1 such that $\bar{\rho}_{i_1}(T^*) = 0$. For $t < T^*$, we then consider the function $\hat{q}_{i_1} = \mu_{i_1} - \max_{i=1,\ldots,N}\mu_i \leq 0$. We can introduce constants

$$\bar{a}_0 := \frac{1}{2|\Omega|}\int_\Omega \varrho_0, \quad \bar{b}_0 = \left(\frac{|\Omega|}{2\|\varrho\|_{L^{\infty,\alpha}(Q)}}\int_\Omega \varrho_0\right)^{\alpha'} \tag{124}$$

and show that the set $A_0(t) := \{x \in \Omega \,:\, \varrho(t,x) \geq \bar{a}_0\}$ satisfies $\lambda_3(A_0(t)) \geq \bar{b}_0$ for all $t \in]0,T[$. Since $\lambda_3(\{x \in \Omega \,:\, \varrho(t,x) \geq k\}) \leq C_0/k$, we easily construct a set $A_1(t) := \{x \in \Omega \,:\, \bar{a}_1 \geq \varrho(t,x) \geq \bar{a}_0\}$ such that $\lambda_3(A_1(t)) \geq \bar{b}_0/2$ for all $t \in]0,T[$. Now observe that $x \in A_1(t)$ implies $|F'(\bar{V} \cdot \rho(t,x))| \leq C(F, \bar{a}_0, \bar{a}_1)$. Thus, for $t \in]0,T[$ and $x \in A_1(t)$

$$\tfrac{1}{\max m} \ln \tfrac{1}{N} - |\bar{V}|\, C(F, \bar{a}_0, \bar{a}_1) - \|c\|_\infty \leq \max_{i=1,\ldots,N} \mu_i \leq |\bar{V}|\, C(F, \bar{a}_0, \bar{a}_1) + \|c\|_\infty.$$

For $t \in]0,T[$ and $x \in A_1(t)$ it follows that $\hat{q}_{i_1}(t,x) \leq \frac{1}{m_{i_1}} \ln \rho_{i_1}(t,x) + \tilde{C}(F, \bar{a}_0, \bar{a}_1)$. Due to the Jensen inequality

$$\tfrac{1}{\lambda_3(A_1(t))} \int_{A_1(t)} |\hat{q}_{i_1}| \geq \frac{1}{m_{i_1}} \ln \frac{1}{\frac{1}{\lambda_3(A_1(t))} \int_{A_1(t)} \rho_{i_1}} - \tilde{C}.$$

In this way, we easily see that $\liminf_{t \to T^*} \|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} = +\infty$. □

Due to Proposition 13.1, it is sufficient to prove the solvability of the problem $(P_{\tau=0,\sigma,\delta})$ in order to complete the proof of the existence theorems. We are going to carry over this last step by means of a Galerkin approximation described hereafter.

14. Galerkin approximation for $(P_{\tau=0,\sigma,\delta})$

We choose

(1) A countable, linearly independent system $\eta^1, \eta^2, \ldots \in W^{1,\infty}_0(\Omega; \mathbb{R}^3)$ dense in $W^{1,2}_0(\Omega; \mathbb{R}^3)$, in order to approximate the variable v;
(2) A countable, linearly independent system $\zeta^1, \zeta^2, \ldots \in W^{1,\infty}_\Gamma(\Omega)$ dense in $W^{1,2}_\Gamma(\Omega)$, in order to approximate the variable ϕ;

In order to approximate the variables μ, we need a countable system $\psi^1, \psi^2, \ldots$ of $W^{1,\infty}(\Omega; \mathbb{R}^N)$ dense in $W^{1,2}(\Omega; \mathbb{R}^N)$. For technical reasons, we have to require additional properties of this set. For $n \in \mathbb{N}$, and $i, j \in \{1, \ldots, n\}$ such that $i \leq j$, we introduce the products $\tilde{\eta}^{i,j} = \eta^i \cdot \eta^j$ with $\eta^1, \ldots, \eta^n$ from (1). By means of an obvious renumbering, we denote these functions $\tilde{\eta}^s$ for $s = 1, \ldots, n\,(n+1)/2$. For all $n \in \mathbb{N}$, we assume that there is $p = p(n) > n$ such that the following additional conditions are valid

$$\begin{cases} \mathbb{1} \in \operatorname{span}\{\psi^1, \ldots, \psi^p\} & \\ \tilde{\eta}^s\, \mathbb{1} \in \operatorname{span}\{\psi^1, \ldots, \psi^p\} & \text{for all } s = 1, \ldots, n\,(n+1)/2 \\ \phi_0\, \bar{Z},\, \zeta^s\, \bar{Z} \in \operatorname{span}\{\psi^1, \ldots, \psi^p\} & \text{for all } s = 1, \ldots, n. \end{cases} \tag{125}$$

Obvious corollaries of this property are

$$\begin{cases} v \in \operatorname{span}\{\eta^1, \ldots, \eta^n\} \Longrightarrow |v|^2\, \mathbb{1} \in \operatorname{span}\{\psi^1, \ldots, \psi^{p(n)}\} \\ \tilde{\phi} \in \operatorname{span}\{\zeta^1, \ldots, \zeta^n\} \Longrightarrow (\tilde{\phi} + \phi_0)\, \bar{Z} \in \operatorname{span}\{\psi^1, \ldots, \psi^{p(n)}\}. \end{cases} \tag{126}$$

For $n \in \mathbb{N}$, we are looking for approximate solutions

$$\mu^n \in C^1([0,T];\, W^{1,\infty}(\Omega; \mathbb{R}^N)),\ v^n \in C^1([0,T];\, W^{1,\infty}_0(\Omega; \mathbb{R}^3)),\ \phi_n \in C^1([0,T];\, W^{1,\infty}(\Omega)) \tag{127}$$

following the ansatz

$$\mu^n = \sum_{\ell=1}^{p(n)} a_\ell(t)\, \psi^\ell(x), \quad v^n = \sum_{\ell=1}^{n} b_\ell(t)\, \eta^\ell(x), \quad \phi_n = \phi_0 + \sum_{\ell=1}^{n} c_\ell(t)\, \zeta^\ell(x). \tag{128}$$

where the vector fields $a = a^{(n)} \in C^1([0,T]; \mathbb{R}^p)$, $b = b^{(n)} \in C^1([0,T]; \mathbb{R}^n)$ and $c = c^{(n)} \in C^1([0,T]; \mathbb{R}^n)$ are to determine.

Our approximation scheme is $(P_{\tau,\sigma,\delta})$ as described in Sect. 9. We choose $\tau = 1/n$, and we project this scheme on the Galerkin space. In order to state approximate equations, we need to recall the definition (80) the free energy functions $h_{\tau,\delta}$. In this point, we introduce the abbreviation

$$\mathscr{R}^*(\mu) = \mathscr{R}^*_n(\mu) := \nabla_\mu h^*_{\tau,\delta}(\mu) = \nabla_\mu (h_\delta)^*(\mu) + \frac{1}{n}\,\omega'(\mu). \tag{129}$$

In order to approximate Eq. (25), we consider for $s \in \{1,\ldots,p(n)\}$ the equations

$$\begin{aligned}\int_\Omega \partial_t \mathscr{R}^*(\mu^n)\cdot\psi^s &= \int_\Omega ((\mathscr{R}^*(\mu^n)\,v^n + J^n)\cdot\nabla\psi^s + r(\mu^n)\cdot\psi^s) + \int_\Gamma (\hat{r}(\mu^n) + J^0)\cdot\psi^s,\\ J^n &= -M(\mathscr{R}^*(\mu^n))\,(\nabla\mu^n + \bar{Z}\,\nabla\phi_n).\end{aligned} \tag{130}$$

Introduce a matrix-valued mapping $\mu \mapsto A^1(\mu) = \{a_{i,j}(\mu)\}_{i,j=1,\ldots,p(n)}$ via

$$a_{i,j}(\mu) := \int_\Omega \mathscr{R}^*_{\ell,\mu_s}(\mu)\,\psi^j_\ell\,\psi^i_s = \int_\Omega (D^2_{l,s}h^*_\delta(\mu) + \frac{1}{n}\,\omega''(\mu_s)\,\delta_{s,\ell})\,\psi^j_\ell\,\psi^i_s. \tag{131}$$

Owing to the convexity of h^*_δ and of the function ω, we see that $A^1(\mu)$ is symmetric and positive semi-definite. Due to the ansatz (128) for μ^n, we can now express (130) in the equivalent form

$$\begin{aligned}&A^1(\mu^n(t))\,a'(t) = F^1(a(t),\,b(t),\,c(t)),\\ &\quad F^1_s := \int_\Omega (\mathscr{R}^*(\mu^n)\,v^n + J^n)\cdot\nabla\psi^s + \int_\Omega r(\mu^n)\cdot\psi^s + \int_\Gamma (\hat{r}(\mu^n) + J^0)\cdot\psi^s.\end{aligned}$$

In order to approximate Eq. (84), we consider for $s \in \{1,\ldots,n\}$ the equations

$$\begin{aligned}\int_\Omega \mathscr{R}^*(\mu^n)\cdot\mathbb{1}\,\partial_t v^n\cdot\eta^s &= -\int_\Omega \mathscr{R}^*(\mu^n)\cdot\mathbb{1}\,(v^n\cdot\nabla)v^n\cdot\eta^s + \int_\Omega h^*_{\tau_n,\delta}(\mu^n)\,\operatorname{div}\eta^s\\ &\quad - \int_\Omega \mathbb{S}(\nabla v^n)\,:\,\nabla\eta^s - \int_\Omega (\sum_{i=1}^N J^{n,i}\cdot\nabla)v^n\cdot\eta^s - \int_\Omega \bar{Z}\cdot\mathscr{R}^*(\mu^n)\,\nabla\phi_n\cdot\eta^s.\end{aligned} \tag{132}$$

Introduce $\mu \mapsto A^2(\mu) = \{a^{(2)}_{i,j}(\mu)\}_{i,j=1,\ldots,n}$

$$a^{(2)}_{i,j}(\mu) := \int_\Omega \mathscr{R}^*(\mu)\cdot\mathbb{1}\,\eta^i\cdot\eta^j = \int_\Omega (\nabla_\mu h^*_\delta(\mu) + \frac{1}{n}\,\omega'(\mu^n))\cdot\mathbb{1}\,\eta^i\cdot\eta^j\,. \tag{133}$$

Owing to the non-negativity of $\nabla_\mu h^*_\delta$ and of ω', we see that $A^2(\mu)$ is symmetric and positive semi definite. Due to the ansatz (128) for v^n and μ^n, we can express (132) in the equivalent form

$$\begin{aligned}&A^2(\mu^n(t))\,b'(t) = F^2(a(t),\,b(t),\,c(t)),\\ &\quad F^2_s := -\int_\Omega \mathscr{R}^*(\mu^n)\cdot\mathbb{1}\,(v^n\cdot\nabla)v^n\cdot\eta^s + \int_\Omega h^*_{\tau_n,\delta}(\mu^n)\,\operatorname{div}\eta^s\\ &\quad\quad - \int_\Omega \mathbb{S}(\nabla v^n)\cdot\nabla\eta^s - \int_\Omega (\sum_{i=1}^N J^{n,i}\cdot\nabla)v^n\cdot\eta^s - \int_\Omega \bar{Z}\cdot\mathscr{R}^*(\mu^n)\,\nabla\phi^n\cdot\eta^s.\end{aligned}$$

In order to determine ϕ_n, we use the ansatz $\phi_n = \tilde{\phi}_n + \phi_0$ and we consider the projection onto $\operatorname{span}\{\zeta^1,\ldots,\zeta^n\}^*$ of the Poisson equation, that is

$$\bar{\chi}\int_\Omega \nabla\tilde{\phi}_n\cdot\nabla\zeta^i = -\bar{\chi}\int_\Omega \nabla\phi_0\cdot\nabla\zeta^i + \int_\Omega \bar{Z}\cdot\mathscr{R}^*(\mu^n)\,\zeta^i. \tag{134}$$

We make use of the ansatz (128) for ϕ_n, and we see that the vector $c_1, \dots c_n$ can be determined via for a linear system $A\,c = f$ where

$$A_{i,j} := \bar{\chi} \int\limits_{\Omega} \nabla\zeta^i \cdot \nabla\zeta^j \quad \text{for } i, j = 1, \dots, n,$$

$$f_i := -\bar{\chi} \int\limits_{\Omega} \nabla\phi_0 \cdot \nabla\zeta^i + \int\limits_{\Omega} \bar{Z} \cdot \mathscr{R}^*(\mu^n)\,\zeta^i \quad \text{for } i = 1, \dots, n.$$

Since the matrix A is by assumption invertible, we obtain that $c = A^{-1} f =: \tilde{f}(a)$.

Overall, the Galerkin approximation (130), (132), (134) has the form

$$\begin{pmatrix} A^1(a(t)) & 0 \\ 0 & A^2(a(t)) \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix} = \begin{pmatrix} F^1(a(t), b(t), \tilde{f}(a(t))) \\ F^2(a(t), b(t), \tilde{f}(a(t))) \end{pmatrix}. \tag{135}$$

We consider the initial conditions

$$a(0) = a^{0,n} \in \mathbb{R}^p, \quad b(0) = b^{0,n} \in \mathbb{R}^n. \tag{136}$$

Here, we require for the reason of consistency that

$$\mu^{0,n} := \sum_{\ell=1}^{p(n)} a_\ell^{0,n}\,\psi^\ell \to \mu^0 := \nabla_\rho h_\delta(\rho^0) \text{ in } L^1(\Omega;\, \mathbb{R}^N),$$

$$v^{0,n} := \sum_{\ell=1}^{n} b_\ell^{0,n}\,\eta^\ell \to v^0 \text{ in } L^1(\Omega;\, \mathbb{R}^3) \text{ as } n \to \infty.$$

We moreover assume that $\|\mu^{0,n}\|_{L^\infty(\Omega)} \le C_0$ which, by definition, implies for $i = 1, \dots, N$ that

$$\rho_i^{0,n} := \mathscr{R}_i^*(\mu^{0,n}) \ge c_0(n) > 0 \text{ everywhere in } \Omega. \tag{137}$$

At first we can obtain local existence for the problem (135), (136).

Proposition 14.1. *There is $\epsilon = \epsilon(n,\, a^{0,n},\, b^{0,n})$ such that the problem (135), (136) possesses a solution in $C^1([0,\, \epsilon];\, \mathbb{R}^p \times \mathbb{R}^n)$.*

Proof. Recall (137). Consider the matrix $A^1(\mu^0) = \int_\Omega D^2_{\ell,s} h^*_{\tau_n,\delta}(\mu^0)\,\psi^j_\ell\,\psi^i_s$ (cf. (131)). Owing to the strict convexity of $h^*_{\tau_n,\delta}$ on compact sets, $A^1(\mu^0)$ is positive definite and therefore invertible, and $\|[A^1(\mu^0)]^{-1}\| \le C(a^0,\, n)$. The matrix $A^2(\mu^0)$ (cf. (133)) is uniformly invertible because $\nabla_\mu h^*_{\tau_n,\delta}$ is strictly positive on compact subsets of $\mathbb{R}^N_+$, and $\|[A^2(\mu^0)]^{-1}\| \le C(a^0,\, n)$.

The block-diagonal matrix A in (135) satisfies $\det A = \det A^1\, \det A^2$. Thus, A is invertible at a^0, b^0, and standard perturbation arguments yield the claim. □

Next we want establish a continuation property for the solution, and we need *a priori* estimates.

Proposition 14.2. *Assume that the approximate system (135), (136) possesses a solution $(a,\, b) \in C^1([0,\, T^*[;\, \mathbb{R}^p \times \mathbb{R}^n)$ for a $T^* > 0$. Then, μ^n, v^n and ϕ_n satisfy the energy identity with free energy $h_{\tau_n,\delta}$ and mobility matrix M_σ.*

Proof. We apply the ideas of Proposition 9.2. We can multiply (130) with μ^n. Due to the additional property (125) and to (126) on the system $\{\psi^1, \dots, \psi^p\}$, we can also multiply (130) with $\bar{Z}\,\phi_n$. Second, we multiply (132) with v^n. Due again to the additional property (125) and to (126) we can also choose $|v^n|^2\,\mathbb{1}$ as a test function in (130). The claim follows. □

Next we verify a continuation criterion.

Proposition 14.3. *Under the assumptions of Proposition 14.2, there is a constant $C(n)$ independent on time such that $\|\mu^n\|_{L^\infty([0,T^*]\times\Omega)} + \|v^n\|_{L^\infty([0,T^*]\times\Omega)} + \|\phi_n\|_{L^\infty([0,T^*]\times\Omega)} \leq C(n)$.*

Proof. We want to obtain a L^∞ bound for μ^n. By construction, for $t \in]0, T^*[$ arbitrary,

$$c\,\frac{1}{n}\sum_{i=1}^N \int_\Omega \sqrt{|\mu_i^n(t)|} \leq \frac{1}{n}\int_\Omega \Phi_\omega(\mu^n) \leq C_0.$$

Now we prove: There is $c = c(n)$ such that $|x|_{L^\infty}^{1/2} \leq c\,\||x\cdot\psi|^{1/2}\|_{L^1(\Omega)}$ for all $x \in \mathbb{R}^p$. Otherwise there is for each $j \in \mathbb{N}$ a $x^j \in \mathbb{R}^p$ such that $|x^j|_\infty^{1/2} \geq j\,\||x^j\cdot\psi|^{1/2}\|_{L^1(\Omega)}$. Thus, $\||\bar{x}^j\cdot\psi|^{1/2}\|_{L^1(\Omega)} \leq j^{-1}$ with $\bar{x}^j = x^j/|x^j|_{L^\infty}$. For a subsequence, $\bar{x}^j \to \bar{x}$ in $\mathbb{R}^p$, $|\bar{x}|_\infty = 1$. But since $\||\bar{x}\cdot\psi|^{1/2}\|_{L^1(\Omega)} = 0$, we obtain that $\bar{x}\cdot\psi = 0$ in Ω, and due to the choice of the system $\{\psi^1, \ldots, \psi^p\}$, it follows that $\bar{x} = 0$, a contradiction. Hence,

$$\|\mu^n(t)\|_{L^\infty(\Omega)}^{1/2} \leq k(n)\,|a(t)|_\infty^{1/2} \leq k(n)\,c(n)\,\||\mu^n(t)|^{1/2}\|_{L^1(\Omega)} \leq \frac{C(n)}{\tau_n}\,C_0$$

and this implies that $\|\mu^n\|_{L^\infty([0,T^*]\times\Omega)} \leq C(n)$. The properties of $\mathscr{R}^*$ entail

$$\inf_{i=1,\ldots,N}\ \inf_{[0,T^*]\times\Omega} \mathscr{R}_i^*(\mu^n) \geq c(n) > 0.$$

From the bound $\int_\Omega \mathscr{R}^*(\mu^n(t))\cdot\mathbb{1}\,|v^n(t)|^2 \leq C_0$, we obtain that $\|v^n\|_{L^\infty([0,T^*]\times\Omega)} \leq C_0\,c(n)^{-1}$. Analogously, $\int_\Omega |\nabla\phi_n(t)|^2 \leq C_0$ implies that $\|\nabla\phi_n\|_{L^\infty([0,T^*]\times\Omega)} \leq C(n)$, and since $\phi_n = \phi_0$ on $[0,T^*]\times\Gamma$, the claim follows. □

Corollary 14.4. *Let $T > 0$. Then, the approximate system (135), (136) possesses a solution $(a, b) \in C^1([0,T]; \mathbb{R}^p \times \mathbb{R}^n)$.*

Proof. Owing to Proposition 14.1, there is $T^* > 0$ such that (135), (136) possesses a solution $(a, b) \in C^1([0, T^*]; \mathbb{R}^p \times \mathbb{R}^n)$. Since $\|\mu^n\|_{L^\infty([0,T^*]\times\Omega)} \leq C(n)$, we have $\inf_{i=1,\ldots,N}\inf_{[0,T^*]\times\Omega}\mathscr{R}_i^*(\mu^n) \geq c(n)$, hence the matrix $A^1(\mu^n(t))$ (cp. (131)) is invertible for all $t \in [0, T^*]$ with $\|[A^1(\mu^n(t))]^{-1}\| \leq C(n)$. The matrix $A^2(\mu^n(t))$ (cf. (133)) is likewise invertible, and the norm of the inverse satisfies a uniform bound $\|[A^2(\mu^n(t))]^{-1}\| \leq C(n)$ on $[0,T^*]$. Due to Proposition 14.3, the functions $\mu^n(T^*)$, $v^n(T^*)$ and $\phi_n(T^*)$ belong to $L^\infty(\Omega)$ and their norm in this space is bounded independently on t.

Thus, the problem (135), with initial data $(a(T^*), b(T^*))$ possesses solution in an interval $[T^*, T^* + \epsilon(n)]$, and the claim follows reiterating this argument. □

Proposition 14.5. *Let $n \in \mathbb{N}$ and $T > 0$. The Galerkin approximation (130), (132), (134), possesses a solution with the regularity (127) such that the dissipation inequality is valid with free energy function $h_{\tau_n,\delta}$ and mobility matrix M_σ.*

Uniform estimates

We define $\tau_n := 1/n$ and

$$\rho^n := \mathscr{R}_n^*(\mu^n) = \nabla_\mu(h_\delta)^*(\mu^n) + \frac{1}{n}\,\omega'(\mu^n), \quad p_n := h_{\tau_n,\delta}^*(\mu^n).$$

The family $\{\mu^n, v^n, \phi_n\}_{n\in\mathbb{N}}$ satisfies the bounds of Proposition 10.1 and Lemma 10.4 due to the energy identity. Since $\mathbb{1} \in \text{span}\{\psi^1, \ldots, \psi^p\}$, the balance of net masses is also valid, hence also the bound of Proposition 10.3. In order to obtain a uniform bound for $\{p_n\}$, we make use of the identity $\nabla p_n = \sum_{i=1}^N \partial_{\mu_i} h_{\tau_n,\delta}^*(\mu^n)\,\nabla\mu_i^n = \sum_{i=1}^N \rho_i^n\,\nabla\mu_i^n$. It implies that

$$\|\nabla p_n\|_{L^{2,\frac{2\alpha}{1+\alpha}}(Q)} \leq \|\rho^n\|_{L^{\infty,\alpha}(Q)}\,\|\nabla\mu^n\|_{L^2(Q)} \leq C_0\,\sigma^{-1/2}. \tag{138}$$

We combine with the bound for $\{p_n\}$ in $L^{\infty,1}(Q)$ to obtain, via the Sobolev embedding, that $\{p_n\}$ is bounded in $L^{2,6\alpha/(3+\alpha)}(Q)$.

With the uniform estimate for $\{\nabla\phi_n\}$ in $L^{\infty,2}(Q)$, we bound $\{\bar{Z}\cdot\rho^n\,\nabla\phi_n\}$ in $L^{\infty,2\alpha/(\alpha+2)}(Q)$.

In order to extract weakly convergent subsequences for all relevant quantities, it remains only to show that the norms $\|\mu^n\|_{L^2(Q)}$ are bounded independently on n. We next sketch the arguments to obtain this bound. We consider perturbed mass densities

$$r^n := \nabla_\mu (h_\delta)^*(\mu^n) = \rho^n - \frac{1}{n}\,\omega'(\mu^n).$$

Owing to Proposition 10.1, $\|r^n-\rho^n\|_{L^{\infty,\alpha}(Q)} = \tau_n\,\|\omega'(\mu^n)\|_{L^{\infty,\alpha}(Q)} \leq C_0\,n^{-1/\alpha'}$. The approximate vector of net masses $\bar{\rho}^n \in C^1([0,T];\mathbb{R}^N)$ defined via $\bar{\rho}^n(t) = \int_\Omega \rho^n(t)\,\mathrm{d}x$ satisfies by assumption $\bar{\rho}^n(0)\to\rho^0$ for $n\to\infty$. Therefore, for every $\epsilon>0$ we find $n_0(\epsilon)$ such that for all $n\geq n_0$

$$\bar{\rho}^n(t) \in B_\epsilon(\bar{\rho}^0)\oplus W = B_\epsilon(\bar{\rho}^0)\oplus \mathrm{span}\{\gamma^1,\ldots,\gamma^s,\,\hat{\gamma}^1,\ldots,\hat{\gamma}^{\hat{s}^\Gamma}\}.$$

Hence, the quantities $\bar{r}^n(t) := \int_\Omega r^n(t)\,\mathrm{d}x$ fulfil $\bar{r}^n(t)\in B_{\epsilon+c\,n^{-\alpha'}}(\bar{\rho}^0)\oplus W$ for all $n\geq n_0$. For all $\epsilon>0$ and $n_0\in\mathbb{N}$ such that $\epsilon + c\,n_0^{-\alpha'}\leq \frac{1}{2}\,\mathrm{dist}(\bar{\rho}^0,\,\mathcal{M}_{\mathrm{crit}})$, the distance of $\bar{r}^n(t)$ to the critical manifold remains strictly positive. The definition (129) implies that $\mu^n = \nabla_\rho h_\delta(r^n)$, which means that (cf. (98), (111))

$$\mu_i^n = c_i + F_\delta'(r^n\cdot\bar{V})\,\bar{V} + \frac{1}{m_i}\,\ln\tilde{y}_i^n, \tag{139}$$

where $\tilde{y}_i^n = r_i^n/(m_i\sum_j(r_j^n/m_j))$ are the associated fractions. This is the structure required to apply Theorem 11.3 (cf. (98)). Hence, a uniform estimate is available in $L^2(Q;\mathbb{R}^{N-1})$ for the relative chemical potentials $(\eta^1\cdot\mu^n,\ldots,\eta^{N-1}\cdot\mu^n)$.

To obtain an estimate for the complete vector μ, we choose the index i associated with the largest fraction $\tilde{y}_i^n\geq 1/N$. By means of (139), we see that $\max_i\mu_i^n\geq c_0 + F_\delta'(r^n\cdot\bar{V})\,\bar{V}_i$. Obviously, we also can state that $\max_i\mu_i^n\leq c_1\,(1+|F_\delta'(r^n\cdot\bar{V})|)$. Thus, employing the growth conditions (34) and(35), there are sets $A_n(t)\subseteq\Omega$ and constants $a_0,\,b_0>0$ such that $\lambda_3(A_n(t))\geq a_0$ and $|\max_i\mu_i^n(t,x)|\leq b_0$ almost everywhere on $A_n(t)$. We do not detail this construction here, referring to the relations (124) and the proof of Lemma A.1 for similar ideas. Applying Lemma 11.2, and using the fact that $\|\nabla\mu^n\|_{L^2(Q)}\leq C_0\,\sigma^{-1/2}$, we obtain the bound $\|\max\mu^n\|_{L^2(Q)}\leq C(a_0)\,(\sigma^{-1/2}+b_0)$.

Passage to the limit $n\to\infty$

Due to the condition (125), we can multiply Eq. (130) with $\psi = v^n\cdot\eta^s\,\mathbb{1}$, $s\in\{1,\ldots,n\}$ arbitrary. We obtain that

$$\int_\Omega \partial_t\varrho_n\,v^n\cdot\eta^s - \int_\Omega \varrho_n\,v^n\cdot\nabla(v^n\cdot\eta^s) = \int_\Omega (\mathbb{1}\cdot J^n)\cdot\nabla(v^n\cdot\eta^s).$$

Thus, it follows that

$$\begin{aligned}\int_\Omega \partial_t(\varrho_n\,v^n)\cdot\eta^s - \int_\Omega \varrho_n\,\partial_t v^n\cdot\eta^s - \int_\Omega \varrho_n\,(v^n\cdot\nabla)v^n\cdot\eta^s - \int_\Omega \varrho_n\,(v^n\otimes v^n) : \nabla\eta^s \\ = \int_\Omega (\mathbb{1}\cdot J^n)\cdot\nabla(v^n\cdot\eta^s).\end{aligned}$$

Rearranging terms

$$\int_\Omega \partial_t(\varrho_n\, v^n)\cdot\eta^s - \int_\Omega \varrho_n\,(v^n\otimes v^n)\,:\,\nabla\eta^s - \int_\Omega (\mathbb{1}\cdot J^n)\cdot\nabla(v^n\cdot\eta^s)$$
$$= \int_\Omega \varrho_n\,(\partial_t v^n + (v^n\cdot\nabla)v^n)\cdot\eta^s.$$

Making use of the latter identity and of (132)

$$\int_\Omega \partial_t(\varrho_n\, v^n)\cdot\eta^s - \int_\Omega \varrho_n\,(v^n\otimes v^n)\cdot\nabla\eta^s = \int_\Omega p_n\,\operatorname{div}\eta^s - \int_\Omega \mathbb{S}(\nabla v^n)\cdot\nabla\eta^s$$
$$+ \int_\Omega (\sum_{i=1}^N J^{n,i}\cdot\nabla)\eta^s\cdot v^n - \int_\Omega \bar{Z}\cdot\rho^n\,\nabla\phi_n\cdot\eta^s. \tag{140}$$

Due to the identities (130) and (140) we obtain for all $t\in[0,T]$ the representation

$$\begin{pmatrix} \int_\Omega \rho^n(t)\cdot\psi \\ \int_\Omega \varrho_n(t)\,v^n(t)\cdot\eta \end{pmatrix} = \begin{pmatrix} \int_\Omega \rho^0\cdot\psi \\ \int_\Omega \varrho_0(t)\,v^0(t)\cdot\eta \end{pmatrix} + \begin{pmatrix} \int_0^t\int_\Omega \sum_{j=0,1}\mathscr{L}^{1,j}(\mathcal{A}^n)\cdot D^j\psi \\ \int_\Omega \sum_{j=0,1}\mathscr{L}^{2,j}(\mathcal{A}^n)\cdot D^j\eta \end{pmatrix}$$

for all $t\in[0,T]$ and for all $(\psi,\,\eta)\in\operatorname{span}\{\psi^1,\ldots,\,\psi^{p(n)}\}\times\operatorname{span}\{\eta^1,\ldots,\eta^n\}$.

Here, $\mathscr{L}_{i,j}(\mathcal{A}^n)$ are linear combinations in $\mathcal{A}$ naturally defined by the right-hands of (130) and (132). Since the systems $\operatorname{span}\{\psi^1,\ldots,\,\psi^{p(n)}\}$ and $\operatorname{span}\{\eta^1,\ldots,\eta^n\}$ are dense in C^1 for $n\to\infty$, we easily show that there is a subsequence such that $\rho^n(t)$ and $\varrho_n(t)\,v^n(t)$ converge as distributions for all $t\in]0,T[$. Thus, the conclusions of Lemma 12.2 are valid and we can produce a limit element $(\mu,\,v,\,\phi)$. In particular, the limit $\phi\in L^\infty(0,T;\,W^{1,2}(\Omega))$ is a weak solution to $-\bar{\chi}\,\triangle\phi=\bar{Z}\cdot\rho$ in Q with $\nu\cdot\nabla\phi=0$ on $]0,T[\times\Sigma$ and $\phi=\phi_0$ on $]0,T[\times\Gamma$. Hence, the estimates of Lemma 10.2 apply, with which it is proved that $(\mu,\,v,\,\phi)\in\mathcal{B}(T,\,\Omega,\,\alpha,\,N,\,\Psi,\,\Psi^\Gamma)$.

In order to obtain the strong convergence of the sequence, we make use of the identity $\nabla\rho^n = D^2h^*_{\tau_n,\delta}(\mu^n)\,\nabla\mu^n$. We can show that $|D^2h^*_{\tau_n,\delta}(\mu^n)|\le C\,\varrho_n$ (cf. proof of Lemma A.2, relation (2)). Hence, as in (138), we see that $\|\nabla\rho_n\|_{L^{2,2\alpha/(1+\alpha)}(Q)}\le C_0\,\sigma^{-1/2}$. With this uniform bound on the spatial gradient and the distributional convergence for all t, we conclude from standard arguments that $\{\rho^n\}$ converges strongly in $L^1(Q;\,\mathbb{R}^N)$.

Then, owing to the uniform bound $\|\mu^n\|_{L^2(Q)}\le C_0$, we can show that $\mu:=\lim_{n\to\infty}\mu^n$ exists almost everywhere in Q. Here, we start from the representation (139) and repeat the argument of Corollary 12.7. We obtain pointwise convergence in the whole of Q because the vacuum can be excluded for $\sigma>0$ (see the estimate in Lemma A.1).

It remains to identify $(\mu,\,v,\,\phi)\in\mathcal{B}(T,\,\Omega,\,\alpha,\,N,\,\Psi,\,\Psi^\Gamma)$ as a weak solution to the problem $(P_{\tau=0,\sigma,\delta})$. Passage to the limit in the energy identity is unproblematic if it is relaxed to an inequality (see Corollary 12.12).

Passage to the limit in the integral identities is also straightforward up to one instance: The sequence $\mathbb{1}\cdot J^n\otimes v^n$ does not satisfy a better uniform bound than in $L^{1,3/2}(Q;\mathbb{R}^{3\times3})$. However, recall that $\mathbb{1}\cdot J^n = \sigma\,(\nabla\sum_{i=1}^N\mu_i^n+\sum_{i=1}^N\bar{Z}_i\,\nabla\phi_n)$. Thus, for a test function $\zeta\in C^2_c(Q)$, $k\in\{1,\ldots,N\}$ and $\ell=1,2,3$

$$\int_Q \mathbb{1}\cdot J^n_k\,v^n_\ell\cdot\nabla\zeta = -\sigma\int_Q\sum_{i=1}^N\mu_i^n\,\partial_k(v^n_\ell\cdot\nabla\zeta)+\sigma\sum_{i=1}^N\bar{Z}_i\int_Q\partial_k\phi_n\,v^n_\ell\cdot\nabla\zeta.$$

Since $\mu^n \to \mu$ strongly in $L^2(Q)$, we then can show that

$$\int_Q \mathbb{1} \cdot J_k^n \, v_\ell^n \cdot \nabla\zeta \to - \sigma \int_Q \sum_{i=1}^N \mu_i \, \partial_k (v_\ell \cdot \nabla\zeta) + \sigma \sum_{i=1}^N \bar{Z}_i \int_Q \partial_k \phi \, v_\ell \cdot \nabla\zeta = \int_Q \mathbb{1} \cdot J_k \, v_\ell \cdot \nabla\zeta.$$

Thus $\mathbb{1} \cdot J^n \otimes v^n \to \mathbb{1} \cdot J \otimes v$ as distributions.

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Appendix A. Proofs of some auxiliary statements

A.1. Proof of Lemma 10.5

The proof relies on the availability of a solution operator to the problem

$$\operatorname{div} X = f \text{ in } \Omega, \quad X = 0 \text{ on } \partial\Omega, \tag{141}$$

for all f having mean value zero over Ω, so that for all $1 < q < +\infty$ the estimates

$$\|X\|_{W^{1,q}(\Omega)} \leq c_q \, \|f\|_{L^q(\Omega)}, \quad \|X\|_{L^q(\Omega)} \leq c_q \, \|f\|_{[W_0^{1,q'}(\Omega)]^*} \tag{142}$$

are valid. For details about the solution operator, see among others [15], section 3.1.

Due to the natural estimates, the density satisfies a bound in $L^{\infty,\alpha}(Q)$. We begin with the case $\alpha > 3$. For all $\eta \in C_c^1([0,T[; C_c^1(\Omega; \mathbb{R}^3))$ the function p obeys

$$\int_Q p \operatorname{div} \eta = - \int_Q \varrho \, v \cdot \partial_t \eta - \int_Q \varrho \, v \otimes v \, : \, \nabla\eta + \int_Q \mathbb{S}(\nabla v) \, : \, \nabla\eta$$
$$- \int_Q (\sum_{i=1}^N J^i \cdot \nabla)\eta \cdot v - \int_\Omega \varrho_0 \, v^0 \cdot \eta(0) + \int_Q n^F \, \nabla\phi \cdot \eta.$$

We make use of the estimates

$$
\begin{aligned}
\Big|\int_Q \varrho\, v\cdot\eta_t\Big| &\le \|\varrho\, v\|_{L^{2,\,\frac{6\alpha}{6+\alpha}}(Q)}\,\|\eta_t\|_{L^{2,\,\frac{6\alpha}{5\alpha-6}}(Q)},\\
\Big|\int_Q \varrho\, v\otimes v\,:\,\nabla\eta\Big| &\le \|\varrho\, v^2\|_{L^{1,\,\frac{3\alpha}{3+\alpha}}(Q)}\,\|\nabla\eta\|_{L^{\infty,\,\frac{3\alpha}{2\alpha-3}}(Q)},\\
\Big|\int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta\Big| &\le c\,\|\nabla v\|_{L^2(Q)}\,\|\nabla\eta\|_{L^2(Q)},\\
\Big|\int_Q (\sum_{i=1}^N J^i_\sigma\cdot\nabla)\eta\cdot v\Big| &\le \Big\|\sum_{i=1}^N J^i_\sigma\, v\Big\|_{L^{1,3/2}(Q)}\,\|\nabla\eta\|_{L^{\infty,3}(Q)},\\
\Big|\int_Q n^F\,\nabla\phi\cdot\eta\Big| &\le \|n^F\,\nabla\phi\|_{L^{\infty,1}(Q)}\,\|\eta\|_{L^{1,\infty}(Q)} \le c\,\|n^F\,\nabla\phi\|_{L^{\infty,1}(Q)}\|\eta\|_{L^\infty(0,T;\,W^{1,\alpha}(\Omega))}.
\end{aligned}
\tag{143}
$$

Let $t\in]0,T[$ and consider according to (141) a solution to the problem

$$\operatorname{div} X = \varrho(t)-\bar\varrho(t) \text{ in } \Omega, \quad X=0 \text{ on } \partial\Omega.$$

Since $\bar\varrho(t)=\|\varrho_0\|_{L^1(\Omega)}$ for all t as a consequence of (63), (142) yields

$$\|X\|_{W^{1,\alpha}(\Omega)} \le c\,(\|\varrho(t)\|_{L^\alpha(\Omega)}+\|\varrho_0\|_{L^1(\Omega)}).$$

The identity (63) also implies that

$$-\int_Q \varrho\,\partial_t\psi = \int_Q \varrho\, v\cdot\nabla\psi + \int_Q \sum_{i=1}^N J^i\cdot\nabla\psi = 0 \quad \text{for all } \psi\in C^1_c(0,T;\,C^1(\overline{\Omega})),$$

and since we assume $\alpha>3$, this yields

$$\|\varrho_t\|_{L^2(0,T;\,[W^{1,2}(\Omega)]^*)} \le \|\varrho\, v\|_{L^2(Q)} + \|\sum_{i=1}^N J^i\|_{L^2(Q)} \le C_0.$$

The properties (142) hence imply that $\|X_t\|_{L^2(Q)}\le c\,\|\varrho_t\|_{L^2(0,T;\,[W^{1,2}(\Omega)]^*)}\le C_0$. Owing to the inequalities $6\alpha/(5\alpha-6)<2$ and $3\alpha/(2\alpha-3)<\alpha$, we see with the help of the bounds (143) that $|\int_Q p\,\operatorname{div} X|\le C_0$. Thus, $\int_Q p\,\varrho\le C_0$, and since $\varrho\ge c\,p^{1/\alpha}$ the claim follows.

If $\alpha\le 3$, then we assume that $\mathbb{1}\cdot J=0$ and, for all $\eta\in C^1_c([0,T[;\,C^1_c(\Omega;\mathbb{R}^3))$, p satisfies

$$\int_Q p\,\operatorname{div}\eta = -\int_Q \varrho\, v\cdot\partial_t\eta - \int_Q \varrho\, v\otimes v\,:\,\nabla\eta + \int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta - \int_\Omega \varrho_0\, v^0\cdot\eta(0) + \int_Q n^F\,\nabla\phi\cdot\eta.$$

We apply the estimates (143) for the right-hand except for the last one. The exponent β of (58) satisfies $\beta\ge\min\{3,\, r(\Omega,\Gamma)\}>\alpha'$ by assumption. Hence, $\beta\alpha/(\beta+\alpha)>1$. Since $3\alpha/(2\alpha-3)\ge 3$, and since $W^{1,3}(\Omega)$ is continuously embedding in $L^q(\Omega)$ for all $q<+\infty$,

$$\Big|\int_Q n^F\,\nabla\phi\cdot\eta\Big| \le \|n^F\,\nabla\phi\|_{L^{\frac{\beta\alpha}{\beta+\alpha}}(Q)}\,\|\eta\|_{L^{\frac{\beta\alpha}{\beta\alpha-\beta-\alpha}}(Q)} \le C_0\,\|\eta\|_{L^\infty(0,T;\,W^{1,\,\frac{3\alpha}{2\alpha-3}}(\Omega))}.$$

It can be shown using (63) that ϱ is a solution to the continuity equation in the sense of *renormalised solutions* (see [28] or [15]) and that, for all $s > 0$ and $\psi \in C^1_c(0, T; C^1(\overline{\Omega}))$

$$-\int_Q \varrho^s \, \partial_t \psi = \int_Q \varrho^s \, v \cdot \nabla \psi + (1-s) \int_Q \rho^s \, \operatorname{div} v \, \psi.$$

Defining $r := 2\alpha/(2s+\alpha)$

$$\|\varrho^s(t) \, \operatorname{div} v(t)\|_{L^r(\Omega)} \leq \|\operatorname{div} v(t)\|_{L^2(\Omega)} \, \|\varrho(t)\|^s_{L^\alpha(\Omega)} \leq C_0 \, \|\operatorname{div} v(t)\|_{L^2(\Omega)}.$$

Thus, $\|\varrho^s \, \operatorname{div} v\|_{L^{2,r}(Q)} \leq C_0$. Moreover, defining $\tilde{r} = 6\alpha/(6s+\alpha)$

$$\|\varrho(t)^s \, v(t)\|_{L^{\tilde{r}}(\Omega)} \leq \|\varrho(t)\|^s_{L^\alpha(\Omega)} \, \|v(t)\|_{L^6(\Omega)} \leq C_0 \, \|v(t)\|_{L^6(\Omega)},$$

and this shows that $\|\varrho^s \, v\|_{L^{2,\tilde{r}}(Q)} \leq C_0$, $\tilde{r} = 6\alpha/(6s+\alpha)$. Making use of the Sobolev inequality

$$\left| \int_Q \varrho^s \, \psi_t \right| \leq C_0 \, (\|\nabla \psi\|_{L^{2,\tilde{r}'}(Q)} + \|\psi\|_{L^{2,r'}(Q)}) \leq C_0 \, \|\psi\|_{L^2(0,T;\, W^{1,\frac{6\alpha}{5\alpha-6s}}(\Omega))}.$$

For the choice $s = \frac{2}{3}\alpha - 1$, it follows that $\|(\varrho^s)'\|_{L^2(0,T;\, [W^{1,6\alpha/(6+\alpha)}(\Omega)]^*)} \leq C_0$. Now we consider a solution to the problem $\operatorname{div} X = \varrho^s(t) - \bar{\varrho}^s(t)$ in Ω with $X = 0$ on $\partial\Omega$. Hence, $\|X\|_{L^\infty(0,T;\, W^{1,3\alpha/(2\alpha-3)}(\Omega))} \leq C_0$ and $\|X_t\|_{L^{2,6\alpha/(5\alpha-6)}(Q)} \leq C_0$ due to the properties (142). We see again that $\int_Q p \, \operatorname{div} X$ is finite, and Lemma 10.5 is proved.

A.2. Special estimates for $\sigma > 0$ and $\tau > 0$

In the case $\sigma > 0$, the dissipation inequality provides $\sqrt{\sigma} \, \|\nabla \mu\|_{L^2(Q)} \leq C_0$, hence a gradient bound for *all* coordinates of the vector μ. We recall that we can always express $\rho = \nabla_\mu h^*_{\tau,\delta}(\mu)$. Hence, $\nabla \rho = (\nabla \mu \cdot D^2 h^*_{\tau,\delta}(\mu))$, and the inequalities (73) or Lemma 9.1, (2), imply that

$$|\nabla \rho| \leq C \, \varrho \, |\nabla \mu|, \tag{144}$$

where C is independent of all approximation parameters.

Lemma A.1. *Assume $\sigma > 0$. Then, $\|\ln \varrho\|_{W^{1,0}_2(Q)} \leq C_0 \, \sigma^{-1/2}$.*

Proof. Due to the global mass conservation $\|\varrho(t)\|_{L^1(\Omega)} = M_0$ for all $t \in]0, T[$, we find parameter $\epsilon_0 > 0$, $\delta_0 > 0$ depending only on the data such that, for all $t \in]0, T[$,

$$|\{x \in \Omega \, : \, \epsilon_0^{-1} \geq \varrho(t) \geq \epsilon_0\}| \geq \delta_0.$$

Let $1 > \gamma > 0$. Due to (144), $|\nabla \ln(\varrho + \gamma)| \leq C \, |\nabla \mu|$. Thus, $\sqrt{\sigma} \, \|\nabla \ln(\varrho + \gamma)\|_{L^2(Q)} \leq C$. Applying (100) (see the proof of Lemma 11.2)

$$\int_\Omega |\ln(\varrho(t) + \gamma)| \leq C^*(\delta_0) \left(\|\nabla \ln(\varrho(t) + \gamma)\|_{L^1(\Omega)} + \ln \frac{1}{\epsilon_0} \right).$$

We integrate in time and obtain that $\|\ln(\varrho + \gamma)\|_{L^{2,1}(Q)} \leq C_0 \, (1 + \sigma^{-1/2})$. We let $\gamma \to 0$, and obtain a control on $\|\ln \varrho\|_{L^{2,1}(Q)}$. Due to (144) and the Sobolev embedding, the claim follows. □

Lemma A.1 allows to show the following statement.

Lemma A.2. *Assume $\sigma > 0$. Then, $\|((\mathbb{1} \cdot J^\sigma) \cdot \nabla \ln \varrho_\sigma)^+\|_{L^1(Q)} \leq C_0 \, \sqrt{\sigma}$.*

Proof. For a while we are now going to forget about the δ indices. We compute that

$$\nabla \ln \varrho_\sigma = \varrho_\sigma^{-1} \sum_{i,j=1}^N D^2_{i,j} h^*_\tau(\mu^\sigma) \nabla \mu^\sigma_j = \frac{D^2 h^*_\tau \mathbb{1}\cdot \mathbb{1}}{N\, \varrho_\sigma} \nabla (\mu^\sigma \cdot \mathbb{1}) + \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1} \cdot \xi^\ell}{\varrho_\sigma} \nabla(\mu^\sigma \cdot \xi^\ell),$$

where $\xi^1, \ldots, \xi^{N-1}$ are chosen as to form an orthonormal basis of $\mathbb{1}^\perp$. Thus, introducing for $k = 1, \ldots, N$ the driving forces $D_k := \nabla \mu^\sigma_k + \bar{Z}_k \nabla \phi_\sigma$, we obtain that

$$\nabla \ln \varrho_\sigma = \frac{D^2 h^*_\tau \mathbb{1}\cdot \mathbb{1}}{N\, \varrho_\sigma} (\mathbb{1}\cdot D) + \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot \xi^\ell}{\varrho_\sigma} (\xi^\ell \cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot \bar{Z}}{\varrho_\sigma} \nabla \phi_\sigma.$$

Making use of the identity $-\sum_{i=1}^N J^{i,\sigma} = \sigma\, (\mathbb{1}\cdot D)$

$$\begin{aligned} -\sum_{i=1}^N J^{i,\sigma} \cdot \nabla \ln \varrho_\sigma = \sigma\, & \frac{D^2 h^*_\tau \mathbb{1}\cdot \mathbb{1}}{N\, \varrho_\sigma} (\mathbb{1}\cdot D)^2 \\ & - \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot \xi^\ell}{\varrho_\sigma} \left(\sum_{i=1}^N J^{i,\sigma}\right) \cdot (\xi^\ell \cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot \bar{Z}}{\varrho_\sigma} \left(\sum_{i=1}^N J^{i,\sigma} \cdot \nabla \phi_\sigma\right) \\ & \geq - \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot \xi^\ell}{\varrho_\sigma} \left(\sum_{i=1}^N J^{i,\sigma}\right) \cdot (\xi^\ell \cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot \bar{Z}}{\varrho_\sigma} \left(\sum_{i=1}^N J^{i,\sigma} \cdot \nabla \phi_\sigma\right). \end{aligned} \tag{145}$$

Since $|\xi^\ell \cdot D| \leq c\, |\Pi\, D| \leq c \sqrt{MD\cdot D}$ for $\ell = 1, \ldots, N-1$, it follows that

$$\left\| \left(\sum_{i=1}^N J^{i,\sigma}\right) \cdot (\xi^\ell \cdot D) \right\|_{L^1(Q)} \leq \left\| \sum_{i=1}^N J^{i,\sigma} \right\|_{L^2(Q)} \|\Pi\, D\|_{L^2(Q)} \leq C_0 \sqrt{\sigma},$$

$$\left\| \left(\sum_{i=1}^N J^{i,\sigma}\right) \cdot \nabla \phi_\sigma \right\|_{L^1(Q)} \leq \left\| \sum_{i=1}^N J^{i,\sigma} \right\|_{L^2(Q)} \|\nabla \phi_\sigma\|_{L^2(Q)} \leq C_0 \sqrt{\sigma}.$$

We invoke Lemma 9.1, (2), and find a constant C_2 such that $|D^2 h^*_\tau(\mu^\sigma)|/\varrho_\sigma \leq C_2$. Together with (145), this implies that $\|((\mathbb{1}\cdot J^\sigma)\cdot \nabla \ln \varrho_\sigma)^+\|_{L^1(Q)} \leq C_0\, \tilde{C}_1 \sqrt{\sigma}$. □

Appendix B. Compactness of the total mass density

In Sect. 12, we showed that boundedness in the energy class together with the existence of weak time derivatives implies the compactness of the solution vector if the condition $\varrho_\epsilon(t) \in K^*$ is satisfied, where K^* is a fixed compact of $L^1(\Omega)$. The aim of the present section is to give readers enough insights into the proof of Proposition 12.13 as to allow independent reading of the paper. We commence with a preliminary remark.

Remark B.1. Under the assumptions of Proposition 12.13, we apply Lemma 12.2 and we find a weakly convergent subsequence and limiting elements such that

$$-\int_Q \varrho\, (\partial_t \psi + (v\cdot \nabla)\psi) = \int_\Omega \varrho_0\, \psi(0), \tag{146}$$

$$-\int_Q \varrho\, v\, (\partial_t \eta + (v\cdot \nabla)\eta) - \int_Q p\, \operatorname{div} \eta + \int_Q \mathbb{S}(\nabla v) : \nabla \eta = \int_\Omega \varrho_0\, v^0 \cdot \eta(0) - \int_Q n^F\, \nabla \phi \cdot \eta, \tag{147}$$

for all $\psi \in C^1_c([0,T[;\, C^1(\overline{\Omega}))$ and for all $\eta \in C^1_c([0,T[;\, C^1_c(\Omega;\, \mathbb{R}^3))$.

There is a branching in the proof: We consider separately the cases $\alpha > 3$ and $3/2 < \alpha \leq 3$.

B.1. The case $\alpha > 3$

We are going to establish after Lions convergence properties associated with the effective viscous flux $p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n}$. Here, we abbreviate $\eta' := \lambda + 2\eta > 0$.

Lemma B.2. *Let p, v and ϱ denote the same weak limits as in Remark B.1. Then,*

$$(p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n})\, \varrho_{\epsilon_n} \to (p - \eta' \operatorname{div} v)\, \varrho \text{ as distributions in } Q.$$

Proof. Let $\zeta \in C^1_c(0,T)$. Consider for $t \in]0,T[$ the weak solution $\psi_\epsilon \in W^{1,2}(\Omega)$ to the auxiliary problem $-\triangle \psi_\epsilon = \varrho_\epsilon(t)\, \zeta(t)$ in Ω with $\psi_\epsilon = 0$ on $\partial\Omega$. Then, $\|\psi_\epsilon\|_{L^\infty(0,T;\, W^{2,\alpha}_{\text{loc}}(\Omega))} \leq c_\zeta\, \|\varrho_\epsilon\|_{L^\infty(0,T;\, L^\alpha(\Omega))}$. Moreover, due to (120), the time-derivative $u = \partial_t \psi_\epsilon$ is a weak solution to

$$-\triangle u = (\varrho_\epsilon(t)\, \zeta(t))_t = \zeta(t)\, (-\operatorname{div}(\varrho_\epsilon\, v^\epsilon + \bar{J}^\epsilon)) + \varrho_\epsilon(t)\, \zeta'(t), \quad u = 0 \text{ on } \partial\Omega.$$

Hence, since $6\alpha/(6+\alpha) \geq 2$ for $\alpha > 3$

$$\|\partial_t \psi_\epsilon\|_{L^2(0,T;\, W^{1,2}(\Omega))} \leq c_\zeta\, (\|\varrho_\epsilon\, v^\epsilon\|_{L^2(Q)} + \|\bar{J}^\epsilon\|_{L^2(Q)} + \|\varrho_\epsilon\|_{L^{2,6/5}(Q)}) \leq c_\zeta\, C_0.$$

For $\varphi \in C^1_c(\Omega)$ arbitrary, we consider the field $X^\epsilon := -\varphi\, \nabla \psi_\epsilon$. Then,

$$\|\partial_t X^\epsilon\|_{L^2(Q)} \leq C_0, \quad \|\nabla X^\epsilon\|_{L^{\infty,\alpha}(Q)} \leq c_\varphi\, \|\psi_\epsilon\|_{L^\infty(0,T;\, W^{2,\alpha}(\operatorname{supp}\varphi))} \leq C_0.$$

Define $\psi \in W^{1,2}(\Omega)$ to be the weak solution to the auxiliary Problem $-\triangle \psi = \varrho_\epsilon(t)\, \zeta(t)$ in $[W^{1,2}_0(\Omega)]^*$. Then, it is readily proved (use Remark 12.3) for $X = -\nabla\psi\, \varphi$ that

$$X^\epsilon \to X \text{ strongly in } L^2(Q), \quad \partial_t X^\epsilon \to \partial_t X \text{ weakly in } L^2(Q),$$
$$\nabla X^\epsilon \to \nabla X \text{ weakly in } L^\alpha(Q).$$

Since $2 > 6\alpha/(5\alpha - 6)$ and $\alpha > 3\alpha/(2\alpha - 3)$ (this is exactly the case for $\alpha > 3$), we can show that the assumptions of Lemma B.3 after this proof are satisfied. Thus,

$$\varrho_\epsilon\, v^\epsilon \cdot \partial_t X^\epsilon + \varrho_\epsilon\, v^\epsilon \otimes v^\epsilon : \nabla X^\epsilon \to \varrho\, v \cdot \partial_t X + \varrho\, v \otimes v : \nabla X \text{ weakly in } L^1(Q).$$

Moreover,

$$\begin{aligned}
\int_Q \mathbb{S}(\nabla v^\epsilon) : \nabla X^\epsilon &= \eta \int_Q D(\nabla v^\epsilon) : \nabla X^\epsilon + \lambda \int_Q \operatorname{div} v^\epsilon \operatorname{div} X^\epsilon \\
&= -\eta \int_Q v^\epsilon \cdot \triangle X^\epsilon - \eta \int_Q v^\epsilon \cdot \nabla(\operatorname{div} X^\epsilon) + \lambda \int_Q \operatorname{div} v^\epsilon \operatorname{div} X^\epsilon \\
&= \eta \int_Q v^\epsilon \cdot \operatorname{curl}\operatorname{curl} X^\epsilon - 2\eta \int_Q v^\epsilon \cdot \nabla(\operatorname{div} X^\epsilon) + \lambda \int_Q \operatorname{div} v^\epsilon \operatorname{div} X^\epsilon \\
&= \eta \int_Q \operatorname{curl} v^\epsilon \cdot \operatorname{curl} X^\epsilon + (\lambda + 2\eta) \int_Q \operatorname{div} v^\epsilon \operatorname{div} X^\epsilon.
\end{aligned}$$

Hence, in view of the choice of X^ϵ,

$$\int_Q \mathbb{S}(\nabla v^\epsilon) : \nabla X^\epsilon = \eta' \int_Q \operatorname{div} v^\epsilon\, \varrho_\epsilon\, \zeta + \int_Q \{\eta' \operatorname{div} v^\epsilon\, \nabla\psi_\epsilon \cdot \nabla\varphi + \eta \operatorname{curl} v^\epsilon \cdot (\nabla\psi_\epsilon \times \nabla\varphi)\}.$$

We also note that $\int_Q p_\epsilon \operatorname{div} X^\epsilon = \int_Q p_\epsilon\, \varrho_\epsilon\, \varphi\, \zeta - \int_Q p_\epsilon\, \nabla\psi_\epsilon \cdot \nabla\varphi$. Moreover,

$$\left| \int_Q (\bar{J}^\epsilon \cdot \nabla) X^\epsilon \cdot v^\epsilon \right| \leq \|\bar{J}^\epsilon\|_{L^2(Q)}\, \|\nabla X^\epsilon\|_{L^{\infty,3}(Q)}\, \|v^\epsilon\|_{L^{2,6}(Q)} \to 0.$$

Multiplying the Navier–Stokes equation with X^ϵ and the limiting equation with X, we then easily obtain that $\int_Q \zeta\,\varphi\,(p_\epsilon - \eta'\,\operatorname{div} v^\epsilon)\,\varrho_\epsilon \to \int_Q \zeta\,\varphi\,(p - \eta'\,\operatorname{div} v)\,\varrho$. □

The following Lemma recalls the fundamental technical observations due to Lions ([28], page 17–21) about the compensated compactness of the acceleration terms (see also [15], section 3.4).

Lemma B.3. *Assumptions of Proposition 12.13. Let* $a > 6\alpha/(5\alpha - 6)$ *and* $b > \max\{2, 3\alpha/(2\alpha - 3)\}$. *Consider* $\{X^\epsilon\}_{\epsilon>0},\, X \subset L^2(Q;\,\mathbb{R}^3)$ *such that for* $\epsilon \to 0$

$$X^\epsilon \to X \text{ strongly in } L^2(Q;\,\mathbb{R}^3), \quad \partial_t X^\epsilon \to \partial_t X \text{ weakly in } L^{2,a}(Q;\mathbb{R}^3)$$
$$\nabla X^\epsilon \to \nabla X \text{ weakly in } L^b(Q;\mathbb{R}^9).$$

Then, $\varrho_\epsilon\, v^\epsilon \cdot \partial_t X^\epsilon + \varrho_\epsilon\, v^\epsilon \otimes v^\epsilon : \nabla X^\epsilon \to \varrho\, v \cdot \partial_t X + \varrho\, v \otimes v : \nabla X$ *weakly in* $L^1(Q)$.

We next use an important property of our regularisation.

Lemma B.4. *Let* ϱ_ϵ *satisfy* (120). *Then,* $\varrho_\epsilon \in C([0,T];\, L^1(\Omega))$, *and for all* $t \in [0,T]$

$$\int_\Omega \varrho_\epsilon(t)\,\ln \varrho_\epsilon(t) - \int_\Omega \varrho_0\,\ln \varrho_0 + \int_0^t \int_\Omega \varrho_\epsilon\,\operatorname{div} v^\epsilon \le \|(\bar{J}^\epsilon \cdot \nabla \ln \varrho_\epsilon)^+\|_{L^1(Q)}. \tag{148}$$

Denote ϱ *a weak limit of* $\{\varrho_{\epsilon_n}\}$. *Then,* $\varrho \in C([0,T];\, L^1(\Omega))$ *and for all* $t \in [0,T]$

$$\int_\Omega \varrho(t)\,\ln \varrho(t) - \int_\Omega \varrho_0\,\ln \varrho_0 + \int_0^t \int_\Omega \varrho\,\operatorname{div} v = 0. \tag{149}$$

Proof. Owing to Lemma A.1, we can rely for $\epsilon > 0$ on the fact that $\ln \varrho_\epsilon \in W^{1,0}_2(Q)$. Making use of well-known smoothing techniques in time, of which we spare the details here, we can multiply Eq. (120) with the function $1 + \ln \varrho_\epsilon$. If follows for almost all $t \in]0,T[$ that

$$\int_\Omega (\varrho_\epsilon(t)\,\ln \varrho_\epsilon(t) - \varrho_0\,\ln \varrho_0) + \int_0^t \int_\Omega \varrho_\epsilon\,\operatorname{div} v^\epsilon - \int_0^t \int_\Omega \bar{J}^\epsilon \cdot \nabla \ln \varrho_\epsilon = 0.$$

The first claim (148) follows. The second claim (149) follows from the fact that ϱ is a renormalised solution to (146). This was shown in [28] (for instance on page 14, see also [27], Lemma 2.3) and [15], section 3.5. In order to state (148), (149) for all $t \in [0,T]$, we need that ϱ^ϵ and ϱ belong to $C([0,T];\, L^1(\Omega))$. This was proved in [28], page 23. □

The compactness of the mass density will follow from a last observation. Comparable ideas are to find for instance in [28], section 8.5.

Lemma B.5. *If* p, v *and* ϱ *denote the weak limits according to Remark* B.1 *then, for all* $\zeta \in C^1(\overline{Q})$ *such that* $\zeta \ge 0$ *in* Q, *there holds*

$$\liminf_{n\to\infty} \int_Q p_{\epsilon_n}\,\varrho_{\epsilon_n}\,\zeta \ge \int_Q p\,\varrho\,\zeta + c_0 \liminf_{n\to\infty} \int_Q (\varrho_{\epsilon_n} - \varrho)^2\,\zeta.$$

Proof. We note that $p_{\epsilon_n} = P_{\epsilon_n}(\varrho_{\epsilon_n},\, q^{\epsilon_n})$ with the functions P_{ϵ_n} of Lemma 8.4. Due to the estimates (76), we can rely on the property

$$P_{\epsilon_n} \to P \text{ uniformly on compact subsets of } [0,\, +\infty[\times\mathbb{R}^{N-1}. \tag{150}$$

Moreover, due to Lemma 8.4, $\partial_s P_{\epsilon_n} \geq c_0$. For arbitrary non-negative $u \in C^1(\overline{Q})$, we therefore obtain that $(P_{\epsilon_n}(\varrho_{\epsilon_n}, q^{\epsilon_n}) - P_{\epsilon_n}(u, q^{\epsilon_n}))\,(\varrho_{\epsilon_n} - u) \geq c_0\,(\varrho_{\epsilon_n} - u)^2$. Hence,

$$\liminf_{n\to\infty} \int_Q p_{\epsilon_n}\, \varrho_{\epsilon_n}\, \zeta - \int_Q p\, u\, \zeta \geq \liminf_{n\to\infty} \int_\Omega P_{\epsilon_n}(u, q^{\epsilon_n})\,(\varrho_{\epsilon_n} - u)\,\zeta + c_0 \liminf_{n\to\infty} \int_Q (\varrho_{\epsilon_n} - u)^2\,\zeta.$$

Since $\nabla P_{\epsilon_n}(u, q^{\epsilon_n}) = \partial_s P_{\epsilon_n}(u, q^{\epsilon_n})\,\nabla u + \sum_{j=1}^{N-1} \partial_{q_j} P_{\epsilon_n}(u, q^{\epsilon_n})\,\nabla q_j^{\epsilon_n}$, Lemma 8.4 and the estimates (76) imply that

$$|\nabla P_{\epsilon_n}(u, q^{\epsilon_n})| \leq c\,\{|u|^{\alpha-1}\,|\nabla u| + |u|^\alpha\,|\nabla q^{\epsilon_n}|\}.$$

It follows that $\|\nabla P_{\epsilon_n}(u, q^{\epsilon_n})\|_{L^2(Q)} \leq C_u\, C_0$. Since moreover $|P_{\epsilon_n}(u, q^{\epsilon_n})| \leq C\,|u|^\alpha$, there is $a = a_u \in L^\infty(Q) \cap W_2^{1,0}(Q)$ and a subsequence such that

$$P_{\epsilon_n}(u, q^{\epsilon_n}) \to a \text{ weakly in } W_2^{1,0}(Q).$$

We easily show that $\int_Q P_{\epsilon_n}(u, q^{\epsilon_n})\,(\varrho_{\epsilon_n} - u)\,\zeta \to \int_Q a\,(\varrho - u)\,\zeta$. Note that the inequality $P_{\epsilon_n}(u, q^{\epsilon_n}) \leq c\,|u|^\alpha$ implies that $|a| \leq c\,|u|^\alpha$. We obtain that

$$\liminf_{n\to\infty} \int_Q p_{\epsilon_n}\, \varrho_{\epsilon_n}\, \zeta - \int_Q p\, u\, \zeta \geq \int_Q a\,(\varrho - u)\,\zeta + c_0 \liminf_{n\to\infty} \int_Q (\varrho_{\epsilon_n} - u)^2\,\zeta.$$

It suffices now to approximate ϱ in $L^{1+\alpha}(Q)$ with functions u of $C^1(\overline{Q})$. □

Lemma B.6. *Assumptions of Proposition 12.13 for $\alpha > 3$. Then, for every sequence $\{\epsilon_n\}_{n\in\mathbb{N}}$ such that the convergence properties of Remark B.1 are valid:*

1. *$\varrho_{\epsilon_n}(t) \to \varrho(t)$ strongly in $L^1(\Omega)$ for all $t \in]0, T[$.*
2. *The family $\bigcup_{n\in\mathbb{N}}\{\varrho_{\epsilon_n}\}$ is sequentially compact in $C([0, T];\, L^1(\Omega))$.*

Proof. We consider an arbitrary sequence of times $\{t_n\}_{n\in\mathbb{N}} \subset]0, T[$ such that $t_n \to t^*$ for $n \to \infty$. We choose for $j \in \mathbb{N}$ a non-negative function $f_j \in C^1(\mathbb{R})$ with the following properties

$$f_j(s) \begin{cases} = 0 & \text{for } s \leq j^{-1} \\ \in [0, 1] & \text{for } s \in [j^{-1},\, 2j^{-1}]\,, \quad |f_j'(s)| \leq c\,j. \\ = 1 & \text{for } s \geq 2\,j^{-1} \end{cases}$$

We define functions $\zeta_{j,n} \in C_c^1(Q)$ via $\zeta_{j,n}(t, x) := f_j(t_n - t)\, f_j(\text{dist}(x, \partial\Omega))$. Note that $\zeta_{j,n} \to \zeta_j := f_j(t^* - t)\, f_j(\text{dist}(x, \partial\Omega))$ uniformly in Q for $n \to \infty$. Moreover, $|\nabla_4 \zeta_{j,n}| \leq c\,j$ and

$$\|\zeta_{j,n} - \chi_{[0,t_n]}\,\chi\Omega\|_{L^{2,\frac{2\alpha}{\alpha-2}}(Q)} \leq c\,(j)^{-\frac{1}{2}-\frac{\alpha-2}{2\alpha}}\,. \tag{151}$$

We then rephrase

$$\int_Q p_{\epsilon_n}\, \varrho_{\epsilon_n}\, \zeta_{j,n} = \int_Q (p_{\epsilon_n} - \eta' \,\text{div}\, v^{\epsilon_n})\, \varrho_{\epsilon_n}\, \zeta_{j,n}$$
$$+ \eta' \int_Q \text{div}\, v^{\epsilon_n}\, \varrho_{\epsilon_n}\,(\zeta_{j,n} - \chi_{[0,t_n]}\,\chi\Omega) + \eta' \int_{Q_{t_n}} \text{div}\, v^{\epsilon_n}\, \varrho_{\epsilon_n}.$$

With $o_n := \|(\bar{J}^{\epsilon_n} \cdot \nabla \ln \varrho_{\epsilon_n})^+\|_{L^1(Q)}$, the identity (148) yields

$$\eta' \int_\Omega (\varrho_{\epsilon_n}(t_n) \ln \varrho_{\epsilon_n}(t_n) - \varrho_0 \ln \varrho_0) + \int_Q p_{\epsilon_n} \varrho_{\epsilon_n} \zeta_{j,n}$$
$$\leq \int_Q (p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n}) \varrho_{\epsilon_n} \zeta_{j,n} + \eta' \int_Q \operatorname{div} v^{\epsilon_n} \varrho_{\epsilon_n} (\zeta_{j,n} - \chi_{[0,t_n]} \chi\Omega) + o_n.$$

Moreover, owing to (149),

$$\eta' \int_\Omega (\varrho(t^*) \ln \varrho(t^*) - \varrho_0 \ln \varrho_0) + \int_Q p \varrho \zeta_{j,n} = \int_Q (p - \eta' \operatorname{div} v) \varrho \zeta_{j,n} + \eta' \int_Q \operatorname{div} v \varrho (\zeta_{j,n} - \chi_{[0,t^*]} \chi\Omega).$$

Thus, subtracting the two latter identities

$$\eta' \int_\Omega (\varrho_{\epsilon_n}(t_n) \ln \varrho_{\epsilon_n}(t_n) - \varrho(t^*) \ln \varrho(t^*)) + \int_Q (p_{\epsilon_n} \varrho_{\epsilon_n} - p \varrho) \zeta_{j,n}$$
$$\leq \int_Q ((p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n}) \varrho_{\epsilon_n} - (p - \eta' \operatorname{div} v) \varrho) \zeta_{j,n}$$
$$+ \eta' \int_Q \operatorname{div} v^{\epsilon_n} \varrho_{\epsilon_n} (\zeta_{j,n} - \chi_{[0,t_n]} \chi\Omega) - \eta' \int_Q \operatorname{div} v \varrho (\zeta_{j,n} - \chi_{[0,t^*]} \chi\Omega) + o_n. \tag{152}$$

Due to (151), we can bound

$$\left| \int_Q \operatorname{div} v^{\epsilon_n} \varrho_{\epsilon_n} (\zeta_{j,n} - \chi_{[0,t_n]} \chi\Omega) \right| \leq \| \operatorname{div} v^{\epsilon_n} \varrho_{\epsilon_n} \|_{L^{2,\frac{2\alpha}{2+\alpha}}(Q)} \|\zeta_{j,n} - \chi_{[0,t_n]} \chi\Omega\|_{L^{2,\frac{2\alpha}{\alpha-2}}(Q)} \leq C_0 \, j^{-1+1/\alpha}.$$

Moreover, we easily show that $\|\zeta_{j,n} - \chi_{[0,t^*]} \chi\Omega\|_{L^{2,\frac{2\alpha}{\alpha-2}}(Q)} \leq c \, j^{-1+1/\alpha} + |t_n - t^*|^{1/2}$, and therefore

$$\left| \int_Q \operatorname{div} v \varrho (\zeta_{j,n} - \chi_{[0,t^*]} \chi\Omega) \right| \leq C_0 (j^{-1+1/\alpha} + |t_n - t^*|^{1/2}).$$

Since $\zeta_{n,j} \to \zeta_j$ uniformly in Q, Lemma B.2 implies that

$$\lim_{n\to\infty} \int_Q ((p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n}) \varrho_{\epsilon_n} - (p - \eta' \operatorname{div} v) \varrho) \zeta_{j,n}$$
$$= \lim_{n\to\infty} \int_Q ((p_{\epsilon_n} - \eta' \operatorname{div} v^{\epsilon_n}) \varrho_{\epsilon_n} - (p - \eta' \operatorname{div} v) \varrho) \zeta_j = 0.$$

Further, Lemma B.5 implies that

$$\lim_{n\to\infty} \int_Q (p_{\epsilon_n} \varrho_{\epsilon_n} - p \varrho) \zeta_{j,n} = \lim_{n\to\infty} \int_Q (p_{\epsilon_n} \varrho_{\epsilon_n} - p \varrho) \zeta_j \geq c_0 \lim_{n\to\infty} \int_Q (\varrho_{\epsilon_n} - \varrho)^2 \zeta_j$$
$$= c_0 \lim_{n\to\infty} \int_Q (\varrho_{\epsilon_n} - \varrho)^2 (\zeta_j - \chi_{[0,t^*]} \chi\Omega) + c_0 \lim_{n\to\infty} \int_{Q_{t^*}} (\varrho_{\epsilon_n} - \varrho)^2$$
$$\geq c_0 \lim_{n\to\infty} \int_{Q_{t^*}} (\varrho_{\epsilon_n} - \varrho)^2 - \limsup_{n\to\infty} \|\varrho_{\epsilon_n} - \varrho\|^2_{L^{\infty,\alpha}(Q)} \left(\frac{1}{j}\right)^{1+\frac{\alpha-2}{\alpha}}.$$

For a certain $r > 0$, it follows from (152) that

$$\eta' \limsup_{n\to\infty} \int\limits_{\Omega} (\varrho_{\epsilon_n}(t_n) \ln \varrho_{\epsilon_n}(t_n) - \varrho(t^*) \ln \varrho(t^*)) + c_0 \liminf_{n\to\infty} \int\limits_{Q_{t^*}} (\varrho_{\epsilon_n} - \varrho)^2 \leq C_0 \, j^{-r}, \tag{153}$$

where we also use the assumption that $\lim_{n\to\infty} o_n = 0$. Since $\varrho_{\epsilon_n} \in C([0,T];\, \mathcal{D}^*(\Omega))$, we show easily that $\varrho_{\epsilon_n}(t_n) \to \varrho(t^*)$ as distributions in Ω, and this added to (153) yields

$$\varrho_{\epsilon_n}(t_n) \to \varrho(t^*) \text{ strongly in } L^1(\Omega). \tag{154}$$

We now deduce both claims of the Lemma.

In order to establish (1), we choose $t_n = t \in [0,T]$ fixed. Then, due to (154), we see that $\varrho_{\epsilon_n}(t) \to \varrho(t)$ strongly in $L^1(\Omega)$. The claim (1) follows

In order to prove (2), we observe that $\varrho_{\epsilon_n} \in C([0,T];\, L^1(\Omega))$ for all $n \in \mathbb{N}$ and that also $\varrho \in C([0,T];\, L^1(\Omega))$. This was observed in Lemma B.4. If $\bigcup_{n\in\mathbb{N}}\{\varrho_{\epsilon_n}\}$ is not compact in $C([0,T];\, L^1(\Omega))$, we find $\delta_0 > 0$ and a subsequence $\{n_k\}$ such that $\max_{t\in[0,T]} \|\varrho_{\epsilon_{n_k}}(t) - \varrho(t)\|_{L^1(\Omega)} \geq \delta_0$, hence also a $t_k \in [0,T]$ such that $\|\varrho_{\epsilon_{n_k}}(t_k) - \varrho(t_k)\|_{L^1(\Omega)} \geq \delta_0$. We can always extract a subsequence such that $t_k \to t^* \in [0,T]$, an applying the result (154), it follows that $\varrho_{\epsilon_{n_k}}(t_k) \to \varrho(t^*)$ strongly in $L^1(\Omega)$. □

B.2. The case $3/2 < \alpha \leq 3$

If we cannot rely on the condition $\alpha > 3$, additional technical problems occur. Nevertheless, the passage to the limit can be carried over using an extension of the method of Lions ($\alpha \geq 9/5$, [28], Chapter 5) and Feireisl, Novotný and Petzeltová ($3/2 < \alpha < 9/5$, [15]) . Here, we have to assume that the approximate solutions satisfy global mass conservation exactly (the perturbation $\bar{J}^\epsilon$ in (120), (121) vanishes). In particular, it holds that

$$-\int\limits_{Q} \varrho_\epsilon \, (\partial_t \psi + (v^\epsilon \cdot \nabla)\psi) = \int\limits_{\Omega} \varrho_0 \, \psi(0) \quad \text{for all } \psi \in C^1_c([0,T[;\, C^1(\overline{\Omega})). \tag{155}$$

Lemma B.2 and the further reasoning have to be modified. Here, we will stick to the approach of Feireisl, Novotný and Petzeltová in [15]. One introduces for $k \in \mathbb{N}$ the cut-off function

$$T_k(\varrho_\epsilon) := \min\{\varrho_\epsilon,\, k\}.$$

It is possible to extract a subsequence (which might be a different one for all values of k), and to find $a_k \in L^\infty(Q)$ such that $T_k(\varrho_\epsilon) \to a_k$ weakly in $L^p(Q)$ for all $1 < p < \infty$. Exploiting the a priori bounds, it follows that

$$\|T_k(\varrho_\epsilon)(t) - \varrho_\epsilon(t)\|_{L^1(\Omega)} \leq (|\{x \,:\, \varrho_\epsilon(t,x) \geq k\}|^{1/\alpha'} \, \|\varrho_\epsilon\|_{L^\alpha(\Omega)} \leq C_0 \left(\frac{1}{k}\right)^{\frac{\alpha}{\alpha'}},$$

so that $\|a_k(t) - \varrho(t)\|_{L^1(\Omega)} \leq C_0 \; (k)^{-\alpha/\alpha'}$. Thus, a_k is an approximation of ϱ. Now, the arguments of [15], Lemma 4.4 allow to prove that the limit ϱ is also a renormalised solution to (146), and to obtain the following statement.

Lemma B.7. *Let ϱ_ϵ satisfy (155). Define*

$$L_k(\varrho) := \begin{cases} \varrho \, \ln \varrho & \text{if } \rho \leq k \\ \varrho \, \ln k + \varrho - k & \text{otherwise} \end{cases}$$

Then, for all $\epsilon > 0$, the function ϱ_ϵ belongs to $C([0,T];\, L^1(\Omega))$ and for all $t \in [0,T]$

$$\int_\Omega L_k(\varrho_\epsilon)(t) - \int_\Omega L_k(\varrho_0) + \int_0^t \int_\Omega T_k(\varrho_\epsilon)\,\operatorname{div} v^\epsilon = 0.$$

Denote ϱ the weak limit of $\{\varrho_{\epsilon_n}\}$. Then, $\varrho \in C([0,T];\, L^1(\Omega))$ and for all $t \in [0,T]$

$$\int_\Omega L_k(\varrho)(t) - \int_\Omega L_k(\varrho_0) + \int_0^t \int_\Omega T_k(\varrho)\,\operatorname{div} v = 0.$$

Proof. We can reproduce the proof [15], Lemma 4.4 (see also the section 4.6) one to one. □

With the same method as in Lemma B.2, one moreover proves

Lemma B.8. *Let p, v and ϱ denotes the weak limits according to Remark B.1. Then, for one subsequence possibly depending on k*

$$(p_{\epsilon_n} - \eta'\,\operatorname{div} v^{\epsilon_n})\,T_k(\varrho_{\epsilon_n}) \to (p - \eta'\,\operatorname{div} v)\,a_k \text{ weakly in } L^1(Q).$$

We next can establish the essential property of Lemma B.5 also if $\alpha \le 3$.

Lemma B.9. *For all $t \in [0,T]$ there holds:*

$$\limsup_{n\to\infty} \int_{Q_t} (p_{\epsilon_n}\,T_k(\varrho_{\epsilon_n}) - p\,a_k) \ge c_0\,\limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_{\epsilon_n}) - a_k)^2.$$

If $\{P_{\epsilon_n}\}$ is moreover a family of convex functions of ϱ (see Remark 8.9), then

$$\limsup_{n\to\infty} \int_{Q_t} p_{\epsilon_n}\,T_k(\varrho_{\epsilon_n}) \ge \int_{Q_t} p\,T_k(\varrho) + c_0\,\limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_{\epsilon_n}) - T_k(\varrho))^2.$$

Proof. For arbitrary non-negative $u \in C^1(\overline{Q})$, we have

$$(P_{\epsilon_n}(\varrho_{\epsilon_n},\, q^{\epsilon_n}) - P_{\epsilon_n}(u,\, q^{\epsilon_n}))\,(T_k(\varrho_{\epsilon_n}) - T_k(u)) \ge c_0\,(T_k(\varrho_{\epsilon_n}) - T_k(u))^2.$$

As in the proof of Lemma B.5, we use that the functions $P_{\epsilon_n}(u,\, q^{\epsilon_n})$ have a bounded gradient in $L^2(Q)$ for fixed u. Exploiting the weak convergence $p_{\epsilon_n} \rightharpoonup p$ and $T_k(\varrho_{\epsilon_n}) \rightharpoonup a_k$, we can show that

$$\limsup_{n\to\infty} \int_{Q_t} p_{\epsilon_n}\,T_k(\varrho_{\epsilon_n}) - \int_{Q_t} p\,T_k(u) \ge \int_{Q_t} \beta(u)\,(a_k - T_k(u)) + c_0\,\limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_{\epsilon_n}) - T_k(u))^2.$$

Here, $\beta(u)$ denote a weak limit of $P_{\epsilon_n}(u,\, q^{\epsilon_n})$. Since $a_k \le k$ almost everywhere in Q, it is possible to represent $a_k = T_k(a_k)$. Therefore, we can approximate a_k with functions $T_k(u)$, $u \in C^1(\overline{Q})$, and it follows that

$$\limsup_{n\to`\infty} \int_{Q_t} p_{\epsilon_n}\,T_k(\varrho_{\epsilon_n}) - \int_{Q_t} p\,a_k \ge c_0\,\limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_{\epsilon_n}) - a_k)^2.$$

If P is a *convex* function depending only on ϱ, then we follow [15], Lemma 4.3. □

At last we mention the equivalent of Lemma B.6.

Lemma B.10. *1. $\varrho_{\epsilon_n}(t) \to \varrho(t)$ strongly in $L^1(\Omega)$ for almost all $t \in]0,T[$.*
2. The family $\bigcup_{n\in\mathbb{N}}\{\varrho_{\epsilon_n}\}$ is sequentially compact in $C([0,T];\, L^1(\Omega))$.

Proof. We have

$$\int\limits_{Q_{t_n}} p_{\epsilon_n}\, T_k(\varrho_{\epsilon_n}) = \int\limits_{Q_{t_n}} (p_{\epsilon_n} - \eta'\, \operatorname{div} v^{\epsilon_n})\, T_k(\varrho_{\epsilon_n}) + \eta' \int\limits_{Q_{t_n}} \operatorname{div} v^{\epsilon_n}\, T_k(\varrho_{\epsilon_n})$$
$$= \int\limits_{Q_{t_n}} (p_{\epsilon_n} - \eta'\, \operatorname{div} v^{\epsilon_n})\, T_k(\varrho_{\epsilon_n}) - \eta' \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n}(t_n)) - L_k(\varrho_0)).$$

Invoking Lemmas B.7 and B.8

$$\limsup_{n\to\infty} \int\limits_{Q_t} p_{\epsilon_n}\, T_k(\varrho_{\epsilon_n})$$
$$= \int\limits_{Q_t} (p - \eta'\, \operatorname{div} v)\, a_k - \eta' \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n}(t_n)) - L_k(\varrho_0))$$
$$= \int\limits_{Q_t} p\, a_k - \eta' \int\limits_{Q_t} \operatorname{div} v\, (a_k - T_k(\varrho)) - \eta' \int\limits_{Q_t} \operatorname{div} v\, T_k(\varrho) - \eta' \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n}(t_n)) - L_k(\varrho_0))$$
$$= \int\limits_{Q_t} p\, a_k - \eta' \int\limits_{Q_t} \operatorname{div} v\, (a_k - T_k(\varrho)) + \eta' \left(\int\limits_{\Omega} L_k(\varrho(t)) - \liminf_{n\to\infty} \int\limits_{\Omega} L_k(\varrho_{\epsilon_n}(t_n)) \right).$$

From Lemma B.9, we obtain the inequality

$$c_0 \limsup_{n\to\infty} \int\limits_{Q_t} (T_k(\varrho_{\epsilon_n}) - a_k)^2 + \eta' \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n})(t_n) - L_k(\varrho)(t)) \leq -\eta' \int\limits_{Q_t} \operatorname{div} v\, (a_k - T_k(\varrho)).$$

Now we distinguish two cases, according to whether the density satisfies a bound in $L^2(Q)$. If $\alpha \geq 9/5$, the density is bounded in $L^2(Q)$, hence the right-hand of the latter relation converges to zero for $k \to \infty$. If $\alpha < 9/5$, but the function P is convex in the first argument, there is the stronger statement

$$c_0 \limsup_{n\to\infty} \int\limits_{Q_t} (T_k(\varrho_{\epsilon_n}) - T_k(\varrho))^2 + \eta' \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n})(t_n) - L_k(\varrho)(t)) \leq -\eta' \int\limits_{Q_t} \operatorname{div} v\, (a_k - T_k(\varrho)).$$

Thus, using that both terms on the left-hand are non-negative

$$c_0 \limsup_{n\to\infty} \int\limits_{Q_t} (T_k(\varrho_{\epsilon_n}) - T_k(\varrho))^2 \leq -\eta' \int\limits_{Q_t} \operatorname{div} v\, (a_k - T_k(\varrho)) = -\eta' \lim_{n\to\infty} \int\limits_{Q_t} \operatorname{div} v\, (T_k(\varrho_{\epsilon_n}) - T_k(\varrho))$$
$$\leq |\eta'|\, \|\operatorname{div} v\|_{L^2(Q)} \limsup_{n\to\infty} \|T_k(\varrho_{\epsilon_n}) - T_k(\varrho)\|_{L^2(Q_t)}.$$

This shows that $c_0\, \|a_k - T_k(\varrho)\|_{L^2(Q_t)} \leq |\eta'|\, \|\operatorname{div} v\|_{L^2(Q)}$. If $3/2 < \alpha < 9/5$ and if P depends only on ϱ, we thus can prove that $a_k - T_k(\varrho)$ is uniformly bounded in $L^2(Q)$, and converges at least weakly to zero in this space. Thus, in both cases, it follows that

$$c_0 \limsup_{k\to\infty} \limsup_{n\to\infty} \int\limits_{Q_t} (T_k(\varrho_{\epsilon_n}) - a_k)^2 + \liminf_{k\to\infty} \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon})(t_n) - \varrho(t)\, \ln \varrho(t))$$
$$= c_0 \limsup_{k\to\infty} \limsup_{n\to\infty} \int\limits_{Q_t} (T_k(\varrho_{\epsilon_n}) - a_k)^2 + \liminf_{k\to\infty} \liminf_{n\to\infty} \int\limits_{\Omega} (L_k(\varrho_{\epsilon_n})(t_n) - L_k(\varrho)(t)) \leq 0. \tag{156}$$

Now we introduce, for $k > 2$ and $n \in \mathbb{N}$, the variables $u_{k,\epsilon}$ such that $u_{k,\epsilon_n} \, \ln u_{k,\epsilon_n} = L_k(\varrho_{\epsilon_n})$. Denoting ψ the inverse of the function $t \mapsto t \, \ln t$ in the range $[2, +\infty]$, we have

$$\varrho_{\epsilon_n} - u_{k,\epsilon_n} = \begin{cases} 0 & \text{if } \varrho_{\epsilon_n} \leq k, \\ \varrho_{\epsilon_n} - \psi(\varrho_{\epsilon_n} \, \ln k + \varrho_{\epsilon_n} - k) & \text{otherwise.} \end{cases}$$

Thus,

$$\|u_{k,\epsilon_n}(t) - \varrho_{\epsilon_n}(t)\|_{L^1(\Omega)} \leq (\|\varrho_{\epsilon_n}(t)\|_{L^\alpha(\Omega)} + \|\varrho(t)\|_{L^\alpha(\Omega)}) \, k^{-\alpha}. \tag{157}$$

We make use of the latter to show that

$$u_{k,\epsilon_n}(t_n) = u_{k,\epsilon_n}(t_n) - \varrho_{\epsilon_n}(t_n) + \varrho_{\epsilon_n}(t_n) \to \varrho(t) \text{ as distributions for } k, n \to \infty.$$

It follows that $\liminf_{k,\, n\to\infty} \int_\Omega u_{k,\epsilon_n}(t_n) \, \ln u_{k,\epsilon_n}(t) \geq \int_\Omega \varrho(t) \, \ln \varrho(t)$. Using the definition of u_{k,ϵ_n} and (156), we conclude that the equality sign is valid, showing that $u_{k,\epsilon}(t) \to \varrho(t)$ strongly in $L^1(\Omega)$, and thus due to (157) also that $\varrho_{\epsilon_n}(t_n) \to \varrho(t)$ strongly in $L^1(\Omega)$. The claims follow using the same argument as in Lemma B.6. □

Appendix C. The boundary reduction

We prove that the boundary conditions (28), (29), (30) allow to compute the flux of the electrolytic species as a function of a $(N-1)$-dimensional reduction of the vector μ from the bulk and of the data. We make use of the algebraic equations

$$r^\Gamma - (M^\Gamma + M^{\Gamma,\text{ext}}) \, \mu^\Gamma = -M^\Gamma \, \mu - M^{\Gamma,\text{ext}} \mu^{\text{ext}}, \tag{158}$$

which result from (28), (29), (30), in order to eliminate the occurrences of the surface potentials μ^Γ. Note that (158) makes sense if we reinterpret, via trivial extension, the matrices M^Γ and $M^{\Gamma,\text{ext}}$ as positive semi-definite elements of $\mathbb{R}^{N^\Gamma \times N^\Gamma}_{\text{sym}}$. The vectors μ and μ^{ext} are trivially extended as well according to the scheme $\mu \rightsquigarrow (\mu, 0) \in \mathbb{R}^N \times 0^{N^{\text{ext}}}$ and $\mu^{\text{ext}} \rightsquigarrow (0, \mu^{\text{ext}}) \in 0^N \times \mathbb{R}^{N^{\text{ext}}}$. For the sake of simplicity, we do not introduce explicitly these operators by means of additional symbols.

For the solution to (158), a linear subspace $\mathcal{V} := \text{span}\{\gamma_\Gamma^1, \ldots, \gamma_\Gamma^{s^\Gamma}\} \oplus \text{R}(M^{\Gamma,\text{ext}}) \oplus \text{R}(M^\Gamma)$ is introduced. We introduce

- The numbers $d^\Gamma = \dim \mathcal{V}$ and $\hat{s}^\Gamma := \dim \text{R}(M^\Gamma) \leq d^\Gamma$;
- The positive eigenvalues $\lambda_1, \ldots, \lambda_{\hat{s}^\Gamma}$ with orthonormal eigenvectors $b^1, \ldots, b^{\hat{s}^\Gamma}$ of M^Γ;
- Vectors $b_{\hat{s}^\Gamma+1}, \ldots, b_{d^\Gamma} \in \mathbb{R}^{N^\Gamma}$ such that $\{b_1, \ldots, b_{d^\Gamma}\}$ is a basis for $\mathcal{V}$;
- The abbreviation $d^{\text{ext}} = \text{rk}\, M^{\text{ext}}$, the nonzero eigenvalues $\lambda_1^{\text{ext}}, \ldots, \lambda_{d^{\text{ext}}}^{\text{ext}}$ with orthonormal eigenvectors $e^1, \ldots, e^{d^{\text{ext}}} \in \mathbb{R}^{N^\Gamma}$ of $M^{\Gamma,\text{ext}}$.

The latter notations imply that $M^{\Gamma,\text{ext}}_{i,j} = \sum_{k=1}^{d^{\text{ext}}} \lambda_k^{\text{ext}} \, e_i^k \, e_j^k$ for $i, j = 1, \ldots, N^\Gamma$. Recalling now that $\{b^1, \ldots, b^{d^\Gamma}\}$ is a basis of $\mathcal{V}$, there are coefficients $\{A_{j,\ell}\}_{j=1\ldots,s^\Gamma,\ \ell=1,\ldots,d^\Gamma}$ and $\{\tilde{A}_{j,\ell}\}_{j=1\ldots,d^{\text{ext}},\ \ell=1,\ldots,d^\Gamma}$ such that

$$\gamma_\Gamma^j = \sum_{\ell=1}^{d^\Gamma} A_{j,\ell} \, b^\ell, \quad e^j = \sum_{\ell=1}^{d^\Gamma} \tilde{A}_{j,\ell} \, b^\ell. \tag{159}$$

Employing these notations and properties, we see that

$$r^\Gamma - (M^\Gamma + M^{\Gamma,\text{ext}}) \, \mu^\Gamma = \sum_{k=1}^{d^\Gamma} b^k \left(\sum_{j=1}^{s^\Gamma} A_{j,k} \, R^{\Gamma,j} - \sum_{j=1}^{d^{\text{ext}}} \tilde{A}_{j,k} \, \lambda_j^{\text{ext}} \, e^j \cdot \mu^\Gamma \right) - \sum_{k=1}^{\hat{s}^\Gamma} b^k \, \lambda_k \, b^k \cdot \mu^\Gamma.$$

Moreover, there is a representation

$$-M^{\Gamma,\mathrm{ext}}\,\mu^{\mathrm{ext}} = \sum_{k=1}^{d^\Gamma}\left(\sum_{j=1}^{d^{\mathrm{ext}}}\tilde{A}_{j,k}\,\lambda_j^{\mathrm{ext}}\,e^j\cdot\mu^{\mathrm{ext}}\right)\,b^k =: \sum_{k=1}^{d^\Gamma} w_k\,b^k. \tag{160}$$

Due to the two latter relations, (158) is equivalent to

$$\begin{cases}\sum_{j=1}^{s^\Gamma}A_{j,k}\,R^{\Gamma,j}-\sum_{j=1}^{d^{\mathrm{ext}}}\tilde{A}_{j,k}\,\lambda_j^{\mathrm{ext}}\,e^j\cdot\mu^\Gamma-\lambda_k\,b^k\cdot\mu^\Gamma = w_k-\lambda_k\,b^k\cdot\mu & \text{for } k=1,\ldots,\hat{s}^\Gamma,\\ \sum_{j=1}^{s^\Gamma}A_{j,k}\,R^{\Gamma,j}-\sum_{j=1}^{d^{\mathrm{ext}}}\tilde{A}_{j,k}\,\lambda_j^{\mathrm{ext}}\,e^j\cdot\mu^\Gamma = w_k & \text{for } k=\hat{s}^\Gamma+1,\ldots,d^\Gamma.\end{cases} \tag{161}$$

Choose Ψ^Γ from (22). We introduce an auxiliary potential $\tilde{\Psi}\in C^2(\mathbb{R}^{d^\Gamma})$ via

$$\tilde{\Psi}(X) := \Psi^\Gamma(A\,X)+\frac{1}{2}\sum_{k=1}^{d^{\mathrm{ext}}}\lambda_k^{\mathrm{ext}}(\tilde{A}_k\cdot X)^2+\frac{1}{2}\sum_{i=1}^{\hat{s}^\Gamma}\lambda_i\,X_i^2.$$

With $X=(b^1\cdot\mu^\Gamma,\ldots,b^{d^\Gamma}\cdot\mu^\Gamma)\in\mathbb{R}^{d^\Gamma}$ and $Y:=(b^1\cdot\mu,\ldots,b^{\hat{s}^\Gamma}\cdot\mu)\in\mathbb{R}^{\hat{s}^\Gamma}$ the identities (161) are valid if and only if

$$-\partial\tilde{\Psi}(X) = w-\overline{\mathcal{D}}\,Y. \tag{162}$$

Here, $\overline{\mathcal{D}}\in\mathbb{R}^{d^\Gamma\times\hat{s}^\Gamma}$ is the rectangular matrix

$$\overline{\mathcal{D}} = \begin{pmatrix}\mathcal{D}\\0\end{pmatrix},\quad \mathcal{D}=\mathrm{diag}(\lambda_1,\ldots,\lambda_{\hat{s}^\Gamma})\in\mathbb{R}^{\hat{s}^\Gamma\times\hat{s}^\Gamma}. \tag{163}$$

It can be verified that $\tilde{\Psi}$ is strictly convex on $\mathbb{R}^{d^\Gamma}$ and the following statement is then obvious.

Lemma C.1. *The solution to Eq. (161) at the point* $X=(b^1\cdot\mu^\Gamma,\ldots,b^{d^\Gamma}\cdot\mu^\Gamma)\in\mathbb{R}^{d^\Gamma}$ *and* $Y:=(b^1\cdot\mu,\ldots,b^{\hat{s}^\Gamma}\cdot\mu)\in\mathbb{R}^{\hat{s}^\Gamma}$ *is given by* $X=\partial\tilde{\Psi}^*(\overline{\mathcal{D}}\,Y-w)$.

In view of Lemma C.1, the flux J_ν in (28) possesses the equivalent representation

$$J_\nu = \sum_{i=1}^{\hat{s}^\Gamma}\lambda_i\,(b^i\cdot\mu-b^i\cdot\mu^\Gamma)\,b^i = \sum_{i=1}^{\hat{s}^\Gamma}\lambda_i\,(Y_i-\partial_i\tilde{\Psi}^*(\overline{\mathcal{D}}\,Y-w))\,b^i,$$

in which $Y=(b^1\cdot\mu,\ldots,b^{\hat{s}^\Gamma}\cdot\mu)\in\mathbb{R}^{\hat{s}^\Gamma}$. We introduce a potential $\hat{\Psi}^\Gamma\in C^2(\mathbb{R}^{\hat{s}^\Gamma}\times\mathbb{R}^{d^\Gamma})$ via

$$\hat{\Psi}^\Gamma(Y,\,w) := \frac{1}{2}\,\mathcal{D}Y\cdot Y-\tilde{\Psi}^*(\overline{\mathcal{D}}\,Y-w)+\tilde{\Psi}^*(-w)+\overline{\mathcal{D}}\,Y\cdot\partial\tilde{\Psi}^*(-w). \tag{164}$$

Then, at the point $Y=(b^1\cdot\mu,\ldots,b^{\hat{s}^\Gamma}\cdot\mu)$ we obtain the equivalence

$$J_\nu = \sum_{i=1}^{\hat{s}^\Gamma}(\partial_{Y_i}\hat{\Psi}^\Gamma(Y,\,w)-(\overline{\mathcal{D}}\,\partial\tilde{\Psi}^*(-w))_i)\,b^i. \tag{165}$$

We reinterpret the identity (165) by defining

- A modified reaction rate vector field $\hat{R}^\Gamma\in C^1(\mathbb{R}^{\hat{s}^\Gamma}\times\mathbb{R}^{d^\Gamma})$ via $\hat{R}^\Gamma(Y,\,w) := -\partial_Y\hat{\Psi}^\Gamma(Y,\,w)$,
- Modified reaction vectors $\hat{\gamma}^k := b^k$ and driving forces $\hat{D}_k^{\Gamma,\mathrm{R}} := \hat{\gamma}^k\cdot\mu$ for $k=1,\ldots,\hat{s}^\Gamma$.

Lemma C.2. *Making use of the potential* $\hat{\Psi}^\Gamma$ *from (164), we define*

$$\hat{r} := \sum_{k=1}^{\hat{s}^\Gamma}\hat{R}_k^\Gamma(\hat{D}^{\Gamma,R},\,w)\,\hat{\gamma}^k = -\sum_{k=1}^{\hat{s}^\Gamma}\partial_Y\hat{\Psi}_k^\Gamma(\hat{D}^{\Gamma,R},\,w)\,\hat{\gamma}^k,\quad J^0 := \sum_{i=1}^{\hat{s}^\Gamma}\jmath_i(w)\,\hat{\gamma}^i,$$

with $w_k := \sum_{j=1}^{d^{ext}}\tilde{A}_{j,k}\,\lambda_j^{ext}\,e^j\cdot\mu^{ext}$ *for* $k=\ldots,d^\Gamma$ *and* $\jmath_i(w) := \lambda_i\,\partial_i\tilde{\Psi}^*(-w)$ *for* $i=1,\ldots,\hat{s}^\Gamma$. *Then, the conditions (28), (29), (30) imply that* $J_\nu=-\hat{r}-J^0$.

It remains to show that $\hat{r}$ has the desired structure of a reaction term.

Proposition C.3. *Assume that* $\Psi^\Gamma \in C^2(\mathbb{R}^{s^\Gamma})$ *is a strictly convex, non-negative potential satisfying* (38). *Assume that* M^Γ *and* $M^{\Gamma,ext}$ *are positive semi definite elements of* $\mathbb{R}^{N^\Gamma\times N^\Gamma}_{sym}$. *Let* $\hat{s}^\Gamma := \operatorname{rk} M^\Gamma$. *We define the reduced potential* $\hat{\Psi}^\Gamma$ *via* (164). *Then,* $\hat{\Psi}^\Gamma \in C^1(\mathbb{R}^{\hat{s}^\Gamma}\times\mathbb{R}^{d^\Gamma})$ *is non-negative, and the function* $Y \mapsto \hat{\Psi}^\Gamma(Y, w)$ *is of class* $C^2(\mathbb{R}^{\hat{s}^\Gamma})$*, strictly convex and coercive for all* $w \in \mathbb{R}^{d^\Gamma}$.

Proof. Due to the representation (164), $\hat{\Psi}^\Gamma$ is of class C^1 and even of class C^2 in the first variable. The second derivative $D^2\hat{\Psi}^\Gamma$ is given by

$$D^2\hat{\Psi}^\Gamma = \mathcal{D} - \overline{\mathcal{D}}^\mathsf{T}\, D^2\tilde{\Psi}^*(\overline{\mathcal{D}}\,Y - w))\,\overline{\mathcal{D}}.$$

Due to convex conjugation, the identity $D^2\tilde{\Psi}^*(\mathcal{D}\,Y - w) = [D^2\tilde{\Psi}(X)]^{-1}$ is valid at the point $X = \partial\tilde{\Psi}^*(\overline{\mathcal{D}}\,Y - w)$. The definition of $\tilde{\Psi}$ induces $D^2\tilde{\Psi}(X) = D^2\tilde{\Psi}^1(X) + \widetilde{\mathcal{D}}$. Here, we denote by $\widetilde{\mathcal{D}} \in \mathbb{R}^{d^\Gamma\times d^\Gamma}$ the matrix $\operatorname{diag}(\lambda_1,\ldots,\lambda_{\hat{s}^\Gamma},0,\ldots,0)$, and $\tilde{\Psi}^1 := \Psi^\Gamma(A\,X) + \frac{1}{2}\sum_{k=1}^{d^{\text{ext}}}\lambda_k^{\text{ext}}(\tilde{A}_k\cdot X)^2$.

Therefore, $D^2\hat{\Psi}^\Gamma(Y, w) = \mathcal{D} - \overline{\mathcal{D}}^\mathsf{T}\,[D^2\tilde{\Psi}^1(X) + \widetilde{\mathcal{D}}]^{-1}\,\overline{\mathcal{D}}$. By definition (recall also the definitions (159) of the matrices A and $\tilde{A}$), for $\eta \in \mathbb{R}^{d^\Gamma}$ arbitrary

$$\begin{aligned} D^2\tilde{\Psi}^1(X)\eta\cdot\eta &= D^2\Psi^\Gamma(A\,X)\,A\eta\cdot A\eta + \frac{1}{2}\sum_{i=1}^{d^{\text{ext}}}\lambda_i^{\text{ext}}\,(\tilde{A}\eta)_i^2 \\ &\geq \inf\{\lambda_{\min}(D^2\Psi^\Gamma),\,\lambda_1^{\text{ext}},\ldots,\lambda_{d^{\text{ext}}}^{\text{ext}}\}\,(|A\eta|^2 + |\tilde{A}\eta|^2) \geq c_0\,|\eta|^2, \end{aligned}$$

where we make use of the Assumption (38). The latter estimate and elementary arguments yield $\lambda_{\min}(D^2\hat{\Psi}^\Gamma) \geq c_0\,\lambda_{\min}(\mathcal{D})/(c_0 + \lambda_{\max}(\mathcal{D}))$. ☐

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Wolfgang Dreyer, Pierre-Étienne Druet, Paul Gajewski and Clemens Guhlke
Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
e-mail: pierre-etienne.druet@wias-berlin.de

Wolfgang Dreyer
e-mail: wolfgang.dreyer@wias-berlin.de

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