Weierstraß-Institut
für Angewandte Analysis und Stochastik
Leibniz-Institut im Forschungsverbund Berlin e. V.

Preprint ISSN 2198-5855

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

Part II: Approximation and *a priori* estimates

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submitted: May 5, 2017

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No. 2396
Berlin 2017

2010 *Mathematics Subject Classification.* 35Q35, 76T30, 78A57, 35Q30, 76N10, 35M33, 35D30, 35B45.

2008 *Physics and Astronomy Classification Scheme.* 82.45.Gjk, 82.45.Mp, 82.60.Lf.

Key words and phrases. Electrolyte, electrochemical interface, chemical reaction, compressible fluid, Navier-Stokes equations, advection-diffusion-reaction equations, PDE system of mixed-type, a-priori estimates, weak solution.

Edited by
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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 model takes into account the elastic deformation of the medium that induces an inherent coupling of mass and momentum transport. 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 kernel. In this paper, which continues the investigation of [DDGG17a], we derive for thermodynamically consistent approximation schemes the natural uniform estimates associated with the dissipations. Our results essentially improve our former study [DDGG16], in particular the *a priori* estimates concerning the relative chemical potentials.

1 Introduction

This paper is the second part of an investigation devoted to the mathematical analysis of an improved Nernst-Planck-Poisson system first proposed in [DGM13] and extended in [DGL14, DGM15]. In the first part of this investigation (see [DDGG17a]), we have exposed the model and presented a survey of the main results. In this paper we deal with the rigorous derivation and the technical framework concerning:

- The reformulation of the problem in natural variables following the original ideas of [DGM13];
- The construction of thermodynamically consistent approximation schemes that preserve the natural dissipation mechanisms;
- The *a priori* estimates for the system.

In particular, we will identify the *relative chemical potentials* as natural variables in the mass transfer equations. For these variables, we prove a complex estimate valid for very general structures of the diffusion tensor and of the bulk and boundary chemical reactions (see Theorem 3.1 below). The estimate relies on an *initial compatibility condition* which was first introduced in [DDGG16] and represents a new concept in the analysis of systems subject to chemical reactions. The method is absolutely new and deserves attention in its own right. It essentialy simplifies and improves our former approach in [DDGG16].

DOI 10.20347/WIAS.PREPRINT.2396

The model. We consider a bounded domain $\Omega \subset \mathbb{R}^3$ representing an electrolyte. The boundary of Ω possesses a disjoint decomposition $\partial\Omega = \Gamma \cup \Sigma$: The surface Γ represents an *active surface*, a one-sided interface between the electrolyte and an external material (electrode). The surface Σ is an inert outer wall. The electrolyte is a compressible mixture of $N \in \mathbb{N}$ species $\mathrm{A}_1, \ldots, \mathrm{A}_\mathrm{N}$ with mass densities $\rho_1, \ldots, \rho_N$. Each species A_i is a carrier of atomic mass $m_i \in \mathbb{R}_+$, charge $z_i \in \mathbb{Z}$ and possesses a reference specific volume $V_i \in \mathbb{R}_+$. We assume that the system is isothermal. Following [DDGG16, DDGG17a], the mixture obeys in $]0, T[\times\Omega$ the following system of partial differential equations

$$\frac{\partial \rho_i}{\partial t} + \mathrm{div}(\rho_i\, v + J^i) = r_i \qquad \text{for } i = 1, \ldots, N \tag{1}$$

$$\frac{\partial \varrho\, v}{\partial t} + \mathrm{div}(\varrho\, v \otimes v - \mathbb{S}^{\text{visc}}) + \nabla p = -n^F\, \nabla\phi \tag{2}$$

$$-\epsilon_0\,(1+\chi)\,\triangle\phi = n^F \qquad . \tag{3}$$

Here, v denotes the *barycentric velocity* of the mixture, while for $i = 1, \ldots, N$ the quantities J^i and r_i denote the dissipative diffusion flux, and the mass production due to chemical reactions for the ith constituent. In the momentum balance (2), we have introduced the total bulk mass density $\varrho := \sum_{i=1}^N \rho_i$, the viscous stress tensor $\mathbb{S}^{\text{visc}}$, the pressure p, and the Lorentz force $-n^F\,\nabla\phi$ for a quasi-static approximation of the electro-dynamical phenomena. The function n^F is the density of free charges. Moreover, ϵ_0 is the Gauss constant, while χ denote the dielectric susceptibility of the medium assumed constant as well.

In order to formulate constitutive equations for the quantities J, r and p, the free energy of the system must be specified. Following [DDGG17a] (see [DGM13] for the original breakthrough), we assume that its density $\varrho\psi$ is given in the form $\varrho\psi = h(\theta,\, \rho)$, where the function h is defined via

$$\begin{aligned} h(\theta,\, \rho) &= \sum_{i=1}^N \rho_i\, \mu_i^{\text{ref}} + h^{\text{mech}}(\rho) + h^{\text{mix}}(\theta,\, \rho) \\ h^{\text{mech}} &= K\ F(\sum_{i=1}^N n_i\, V_i) \\ h^{\text{mix}} &= k_B\ \theta\, \sum_{i=1}^N n_i\, \sum_{i=1}^N y_i\, \ln y_i \end{aligned} \tag{4}$$

Here μ_i^{ref} $(i = 1, \ldots, N)$ are constants related to certain reference states of the pure constituents. The *number densities* or *concentrations* $n_1, \ldots, n_N$ of the constituents are defined via $n_i := \rho_i/m_i$ $(i = 1, \ldots, N)$. The mechanical free energy is an increasing function of the dimensionless quantity $\sum_{i=1}^N n_i\, V_i =: n \cdot V$ (a 'volume density' for the mixture). The constant $K > 0$ is the compression modulus of the mixture. In the definiton of the mixing-entropy, k_B denotes the Boltzmann constant and θ is the absolute temperature assumed constant. The quantity $\sum_{i=1}^N n_i$ is the *total number density* and $y_i := n_i/(\sum_{i=1}^N n_i)$ $(i = 1, \ldots, N)$ are the *number fractions* summing up to one.

The chemical potentials of the mixture are defined via

$$\mu_i = \partial_{\rho_i} h(\theta,\, \rho_1, \ldots, \rho_N) \text{ for } i = 1, \ldots, N\,. \tag{5}$$

Thus, under the particular constitutive assumption (4)

$$\mu_i = c_i + K\, \tfrac{V_i}{m_i}\, F'(n \cdot V) + \tfrac{k_B\,\theta}{m_i}\, \ln y_i \text{ for } i = 1, \ldots, N\,, \tag{6}$$

where $c_1, \ldots, c_N$ are certain constants. The following constitutive equations and definitions are assumed:

$$J^i = -\sum_{j=1}^N M_{i,j}\, D^j \quad \text{for } i = 1, \ldots, N\,, \tag{7a}$$

$$D^j := \nabla\left(\frac{\mu_j}{\theta}\right) + \frac{1}{\theta}\,\frac{z_j}{m_j}\,\nabla\phi \quad \text{for } j = 1, \ldots, N \tag{7b}$$

$$r_i = -\sum_{k=1}^s \partial_{D^{\mathsf{R}}_k}\Psi(D^{\mathsf{R}}_1, \ldots, D^{\mathsf{R}}_s)\,\gamma^k_i\,, \qquad D^{\mathsf{R}}_k := \gamma^k\cdot\mu \tag{7c}$$

$$\mathbb{S}^{\text{visc}}(\nabla v) = \eta\, D(v) + \lambda\, \operatorname{div} v\, \text{Id} \tag{7d}$$

$$p = -h(\theta,\, \rho) + \sum_{i=1}^N \mu_i\,\rho_i \tag{7e}$$

$$n^F = \sum_{i=1}^N \tfrac{z_i}{m_i}\,\rho_i \tag{7f}$$

In (7a), M is a symmetric, positive semi definite $N\times N$ matrix called the mobility matrix, while $D \in \mathbb{R}^{N\times 3}$ is the diffusion driving force. In (7c), $s \in \mathbb{N}\cup\{0\}$ is the number of chemical reactions. The vector $\gamma^k \in \mathbb{R}^N$ ($k = 1, \ldots, s$) does not as usual denote the stoichiometric vector $\gamma^{\text{stoi},k} \in \mathbb{Z}^N$ associated with the reactions. For reasons of notation we set $\gamma^k := \gamma^{\text{stoi},k}_i\, m_i$ for $i = 1, \ldots, N$ and $k = 1, \ldots, s$. The reaction potential Ψ is defined on $\mathbb{R}^s$ and assumed convex (plausible examples in [DDGG17a]). The entries of the vector $D^{\mathsf{R}} \in \mathbb{R}^s$ are called reaction driving forces. The assumption (7d) is the usual expression for the Newtonian viscous stress tensor: Here $D(v) = (\partial_i v_j + \partial_j v_i)_{i,j=1,\ldots,3}$ while $\eta > 0$ and $\lambda + \frac{2}{3}\,\eta \geq 0$ are the coefficients of shear and bulk viscosity. The constitutive assumption (7e) for the pressure is called the Gibbs-Duhem equation, while (7f) is actually the definition of the free charge density.

The equations (1), (2), (3) with the constitutive equations (7) based on the choice (4) of the free energy density are the constituent parts of a generalised model of Poisson–Nernst–Planck type first proposed in [DGM13] and extensively developed in [DGL14], [DGM15] and [Guh14]. This model provides a general description of electrolytes in the presence of electrochemical interfaces for non equilibrium situations. In this paper, the focus is on mathematical analysis and we will consider for the system (1), (2), (3) simplified boundary conditions. At first we assume no velocity slip, and Dirichlet conditions for the electrical potential on the active boundary

$$v = 0 \text{ on }]0, T[\times\partial\Omega \tag{8}$$

$$\phi = \phi_0 \text{ on }]0, T[\times\Gamma, \quad \nabla\phi\cdot\nu = 0 \text{ on }]0, T[\times\Sigma\,. \tag{9}$$

At second, for the diffusion-reaction equations we assume for $i = 1, \ldots, N$ that

$$J^i\cdot\nu + \hat{r}_i = -J^0_i \tag{10a}$$

$$\hat{r}_i := \sum_{k=1}^{\hat{s}^\Gamma} \hat{R}^\Gamma_k(t,\, x,\, \hat{\gamma}^1\cdot\mu, \ldots,\, \hat{\gamma}^{\hat{s}^\Gamma}\cdot\mu)\,\hat{\gamma}^k_i \tag{10b}$$

$$J^0_i := \sum_{k=1}^{\hat{s}^\Gamma} \jmath_k(t,\, x)\,\hat{\gamma}^k_i\,. \tag{10c}$$

The boundary conditions describe the reaction and adsorption of contituents on the active surface $]0,T[\times\Gamma$ in contact with an external bulk. The meaning of the number $\hat{s}^\Gamma \in \mathbb{N}\cup\{0\}$ and of the vectors $\hat{\gamma}^1,\ldots,\hat{\gamma}^{\hat{s}^\Gamma} \in \mathbb{R}^N$ have been explained in the modelling part of the paper [DDGG17a]. Both are related to the boundary reaction and adsorption phenomena. In particular, each vector $\hat{\gamma}^k$ satisfies $\sum_{i=1}^N \hat{\gamma}^k_i = 0$. In other words, it is orthogonal to the vector $\mathbb{1} = 1^N = (1,\,1,\ldots,1) \in \mathbb{R}^N$. The vector field $\hat{R}^\Gamma$ defining the reaction rates is derived from a potential $\hat{\Psi}^\Gamma :]0,T[\times\Gamma\times\mathbb{R}^{\hat{s}^\Gamma} \to \mathbb{R}_{0,+}$ via

$$\hat{R}^\Gamma(t,\,x,\,D) = \nabla_D\hat{\Psi}^\Gamma(t,\,x,\,D) \text{ for } (t,x)\in]0,T[\times\Gamma,\; D\in\mathbb{R}^{\hat{s}^\Gamma}\,.$$

Following [DDGG17a], the potential $\hat{\Psi}^\Gamma$ is convex in the D variable, and $\nabla_D\hat{\Psi}^\Gamma(t,\,x,\,0) = 0$. In (10), the coefficients $\jmath \in [0,T]\times\Gamma \to \mathrm{span}\{\hat{\gamma}^1,\ldots,\hat{\gamma}^{\hat{s}^\Gamma}\}$ are given.

2 Assumptions on the data and preliminaries.

Notations 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.

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

Moreover we define the vector $\mathbb{1} := 1^N := (1,\,1,\ldots,1) \in \mathbb{R}^N$, and the vectors of quotients of charge and mass, and of volume and mass

$$\frac{z}{m} := (\tfrac{z_1}{m_1},\,\tfrac{z_2}{m_2},\ldots,\tfrac{z_N}{m_N})\in\mathbb{R}^N,\quad \frac{V}{m} := (\tfrac{V_1}{m_1},\tfrac{V_2}{m_2},\ldots,\tfrac{V_N}{m_N})\in\mathbb{R}^N\,.$$

Using these conventions, we have a. o. the identities

$$\varrho = \mathbb{1}\cdot\rho,\quad n^F = \frac{z}{m}\cdot\rho,\quad n\cdot V = \rho\cdot\frac{V}{m} \text{ etc.}$$

The diffusion fluxes $J^1,\ldots,J^N$ span a rectangular matrix $J = \{J^i_j\}\in\mathbb{R}^N\times\mathbb{R}^3$. 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 $\gamma = \{\gamma^k_i\}\in\mathbb{R}^s\times\mathbb{R}^N$. 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 $\hat{\gamma}^1,\ldots,\hat{\gamma}^{\hat{s}^\Gamma}$ span a rectangular matrix $\hat{\gamma} = \{\hat{\gamma}^k_i\}\in\mathbb{R}^{\hat{s}^\Gamma}\times\mathbb{R}^N$.

Since we assume overall that $\theta = \text{const}$, we write $h(\rho)$ for $h(\theta,\,\rho)$.

The analysis presuposes restrictions of mathematical nature to the data.

(1) **Free energy:** In (4), we assume that the function F belongs to $C^2(\mathbb{R}_+)\cap C(\mathbb{R}_{0,+})$ and is convex. We assume that there are $\frac{3}{2} < \alpha < +\infty$ and constants $0 < c_0,\,c_1$ such that

$$F(s) \geq c_0\,s^\alpha - c_1 \quad \text{for all } s > 0\,. \tag{11}$$

In the neighbourhood of zero, we assume that $F(s)$ behaves like $s\,\ln s$: There are constants positive constants $k_0 < k_1$ and $s_0 > 0$ such that

$$\frac{k_0}{s} \leq F''(s) \leq \frac{k_1}{s} \quad \text{for all } s\in]0,s_0]\,. \tag{12}$$

As explained in the papers [DDGG16], [DDGG17a] we crucially need that $F' : \mathbb{R}_+ \to \mathbb{R}$ is a surjective map in order to obtain an unconstrained PDE system.

(2) **Mobility matrix:** We assume that the mobility matrix M is given by a mapping $\overline{M}(\rho)$ of the mass densities. The mapping $\overline{M}$ is defined on $\mathbb{R}^N_+$ and it maps into the set of symmetric, positive semi definite $N \times N$ matrices. Throughout the paper, we assume that $\overline{M}$ is mass conservative, that is

$$\overline{M}(\rho)\mathbb{1} = 0 \text{ for all } \rho \in \mathbb{R}^N_+ \,. \tag{13}$$

Moreover we assume that the entries of $\overline{M}(\rho)$ are continuous functions with at most linear–growth. In this paper we restrict ourselves to the assumption that M has rank $N-1$ independently on ρ: Denoting $0 = \lambda_1(M) \leq \lambda_2(M) \leq \ldots \leq \lambda_N(M)$ the eigenvalues of the matrix M, we assume that there are positive constants $0 < \underline{\lambda} \leq \overline{\lambda}$ such that

$$\underline{\lambda} \leq \lambda_i(\overline{M}(\rho)) \leq \overline{\lambda}\,(1+|\rho|) \quad \text{for all } i = 2,3,\ldots,N,\ \rho \in \mathbb{R}^N_+ \,. \tag{14}$$

(3) **Reaction rates:** We assume that the reaction rates are derived from a strictly convex, non-negative potential $\Psi \in C^2(\mathbb{R}^s)$. Moreover, Ψ satisfies

$$\Psi(0) = 0, \qquad \frac{\Psi(D^{\mathsf{R}})}{|D^{\mathsf{R}}|} \to +\infty \text{ for } |D^{\mathsf{R}}| \to \infty \,. \tag{15}$$

Similarly, we require that the boundary reaction rates are derived from a strictly convex, non-negative potential $\hat{\Psi}^\Gamma \in L^\infty([0,T]\times\Gamma;\, C^2(\mathbb{R}^{\hat{s}^\Gamma}))$ such that

$$\hat{\Psi}^\Gamma(t,x,\,0) = 0 \ \text{ for (almost) all } (t,x) \in [0,T]\times\Gamma \,. \tag{16}$$

For simplicity we explicitly require at least linear growth of the reaction rates (uniformly quadratic growth of the potentials)

$$\inf_{D^{\mathsf{R}}\in\mathbb{R}^s} \lambda_{\min}(D^2\Psi(D^{\mathsf{R}})) > 0, \ \operatorname*{essinf}_{(t,x)\in[0,T]\times\Gamma}\ \inf_{D^{\Gamma,\mathsf{R}}\in\mathbb{R}^{\hat{s}^\Gamma}} \lambda_{\min}(D^2\Psi^\Gamma(t,\,x,\,D^{\Gamma,\mathsf{R}})) > 0 \,. \tag{17}$$

(4) **Domain:** The domain $\Omega \subset \mathbb{R}^3$ possesses a boundary of class $\mathcal{C}^{0,1}$. In connection with the optimal regularity of the solution to the Poisson equation with mixed-boundary conditions, we need to introduce a further exponent $r(\Omega,\,\Gamma)$ as the largest number in the range $]2,+\infty[$ such that

$$\begin{aligned} -\triangle u = f \text{ in } [W^{1,\beta'}_\Gamma(\Omega)]^* &\text{ implies } u \in W^{1,\beta}_\Gamma(\Omega) \\ &\text{for all } f \in [W^{1,\beta'}_\Gamma(\Omega)]^* \text{ and all } \beta \in]r',\,r[\,. \end{aligned} \tag{18}$$

With the α from (11), we require that

$$\alpha' := \frac{\alpha}{\alpha-1} < r \,. \tag{19}$$

(5) **Initial and boundary data:** We assume sufficient (not optimal) regularity

$$\begin{aligned} \rho^0 &\in L^\infty(\Omega;\,(\mathbb{R}_+)^N) \\ v^0 &\in L^\infty(\Omega;\,\mathbb{R}^3) \\ \phi_0 &\in L^\infty(0,T;\,W^{1,r}(\Omega)) \cap L^\infty(]0,T[\times\Omega) \\ \partial_t\phi_0 &\in W^{1,0}_2(]0,T[\times\Omega) \cap L^{\alpha'}(]0,T[\times\Omega) \\ \jmath &\in L^\infty(]0,T[\times\Gamma;\,\mathbb{R}^{\hat{s}^\Gamma}) \,. \end{aligned} \tag{20}$$

Moreover we assume as a compatibility condition the validity in the weak sense of $-\epsilon_0\,(1+\chi)\,\triangle\phi_0(0) = \frac{z}{m}\cdot\rho^0$.

Functional classes: We make use of standard Sobolev spaces. Moreover, the vectorial Orlicz classes $L_{\Psi}(Q;\, \mathbb{R}^s)$ and $L_{\Psi^*}(Q_T;\, \mathbb{R}^s)$ are then well known. We make use of the notation

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

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 $\hat{D}^{\Gamma,\mathsf{R}} :\, S \to \mathbb{R}^{\hat{s}^{\Gamma}}$ such that

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

Let us recall (see [DDGG16] for a detailed construction) that there is a non-negative function $\Phi^* \in C([0,T]^2)$, $\Phi^*(t,\, t) = 0$ constructed from the functions Ψ, $\hat{\Psi}^{\Gamma}$ such that the variable

$$\bar{\rho} := \int_{\Omega} \rho = \int_{\Omega} \mathscr{R}(\varrho,\, q)\,, \tag{21}$$

satisfies the estimate $[\bar{\rho}]_{C_{\Phi^*}([0,T];\,\mathbb{R}^N)} := \sup_{t_1,\, t_2 \in [0,T]} \frac{|\bar{\rho}(t_1) - \bar{\rho}(t_2)|}{\Phi^*(t_1,\, t_2)} < +\infty$.

Formulation of the weak problem. Following [DDGG16], [DDGG17a] a solution vector to the initial boundary value problem (1), (2), (3), (7), (8), (9), (10) with 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). Since we want to account for the possibility of vacuum, the productions factors are not everywhere functions of these components only. Thus we also introduce $R :\, Q \to \mathbb{R}^s$ and $R^{\Gamma} :\, S \to \mathbb{R}^{\hat{s}^{\Gamma}}$ as variables. For a vector $(\varrho,\, q,\, v,\, \phi,\, R,\, R^{\Gamma})$, we recover all variables of the system via

$$\rho = \mathscr{R}(\varrho,\, q) \tag{22a}$$

$$J = -M(\rho)\, D, \qquad D := \nabla\mathcal{E}\, q + \frac{z}{m}\, \nabla\phi \tag{22b}$$

$$r = \sum_{k=1}^{s} \gamma^k\, R_k, \qquad D^{\mathsf{R}}_k := \gamma^k \cdot \mathcal{E}q \text{ for } k = 1, \ldots, s \tag{22c}$$

$$\hat{r} = \sum_{k=1}^{\hat{s}^{\Gamma}} \hat{\gamma}^k\, R^{\Gamma}_k, \qquad \hat{D}^{\Gamma,\mathsf{R}}_k := \hat{\gamma}^k \cdot \mathcal{E}q \text{ for } k = 1, \ldots, \hat{s}^{\Gamma} \tag{22d}$$

$$p = P(\varrho,\, q) \tag{22e}$$

$$n^F = \rho \cdot \frac{z}{m}\,. \tag{22f}$$

For $q \in \mathbb{R}^{N-1}$, we denote $\mathcal{E}\, q := \sum_{i=1}^{N-1} q_i\, \xi^i$, where $\xi^1, \ldots, \xi^{N-1} \in \mathbb{R}^N$ are fixed vectors that are extendable via 1^N to a basis of $\mathbb{R}^N$ (details below in Section 4). The vector fieds $\mathscr{R}$ and the pressure function P are associated with (5), (6), and are likewise constructed in Section 4. We next state the main properties of weak solutions.

(1) **Energy conservation:** 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

(22) satisfy for almost all $t \in]0, T[$

$$
\begin{aligned}
&\int_\Omega \left\{\frac{1}{2}\,\varrho\, v^2 + \frac{1}{2}\,\epsilon_0\,(1+\chi)\,|\nabla\phi|^2 + h(\rho)\right\}(t)\\
&\quad + \int_{Q_t} \left\{\mathbb{S}(\nabla v)\,:\,\nabla v + M\,D\cdot D + (\Psi(D^{\mathsf{R}}) + \Psi^*(-R))\right\}\\
&\quad + \int_{S_t} \{\hat{\Psi}^\Gamma(\cdot,\,\hat{D}^{\Gamma,\mathsf{R}}) + (\hat{\Psi}^\Gamma)^*(\cdot,\,-R^\Gamma)\}\\
&\overset{(<)}{=} \int_\Omega \left\{\frac{1}{2}\,\varrho_0\,|v^0|^2 + \frac{1}{2}\,\epsilon_0\,(1+\chi)\,|\nabla\phi_0(0)|^2 + h(\rho^0)\right\}\\
&\int_{Q_t} \left\{n^F\,\phi_{0,t} - \epsilon_0\,(1+\chi)\,\nabla\phi\cdot\nabla\phi_{0,t}\right\} - \int_\Omega \left\{n^F\,\phi_0 - \epsilon_0\,(1+\chi)\,\nabla\phi\cdot\nabla\phi_0\right\}\Big|_0^t\\
&+ \int_{S_t} ((\hat{r} + J^0)\cdot\frac{z}{m}\,\phi_0 + J^0\cdot\mathcal{E}q)\,. \qquad (23)
\end{aligned}
$$

(2) **Balance of total partial masses:** We say that $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$ satisfies the *balance of total partial masses* if the vector field (cf. (21)) is subject to

$$
\bar{\rho}(t) = \bar{\rho}^0 + \int_0^t \left\{\int_\Omega r + \int_\Gamma (\hat{r} + J^0)\right\}(s)\,ds \quad \text{for all } t \in [0,T]\,. \qquad (24)
$$

with $\bar{\rho}^0 := \int_\Omega \rho^0\,dx$.

(3) **Natural class:** We say that $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma)$ belongs to the class $\mathcal{B}(T,\,\Omega,\,\alpha, \operatorname{rk} M,\,\Psi,\,\Psi^\Gamma)$ if and only if the number

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

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

(4) **Weak solution:** We call a vector $(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma) \in \mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)$ *weak solution* to the Problem (P) if the energy inequality and the balance of partial total masses are

valid, and if the quantities ρ, J, r and $\hat{r}$, p and n^F obeying the definitions (22) satisfy the relations

$$
\begin{aligned}
& - \int_Q \rho \cdot \psi_t - \int_Q (\rho_i\, v + J^i) \cdot \nabla \psi_i && (25)\\
& \quad = \int_\Omega \rho^0 \cdot \psi(0) + \int_Q r \cdot \psi + \int_{S_T} (\hat{r} + J^0) \cdot \psi \qquad \forall\, \psi \in C^1_c([0,T[;\, C^1(\overline{\Omega};\, \mathbb{R}^N)) \\
& - \int_Q \varrho\, v \cdot \eta_t - \int_Q \varrho\, v \otimes v \,:\, \nabla \eta - \int_Q p\, \operatorname{div} \eta + \int_Q \mathbb{S}(\nabla v) \,:\, \nabla \eta && (26)\\
& \quad = \int_\Omega \varrho_0\, v^0 \cdot \eta(0) - \int_Q n^F\, \nabla \phi \cdot \eta \qquad \forall\, \eta \in C^1_c([0,T[;\, C^1_c(\Omega;\, \mathbb{R}^3)) \\
& \epsilon_0\, (1+\chi) \int_Q \nabla \phi \cdot \nabla \zeta = \int_Q n^F\, \zeta \qquad \forall\, \zeta \in L^1(0,T;\, W^{1,2}_\Gamma(\Omega))\,, && (27)
\end{aligned}
$$

$\phi = \phi_0$ as traces on $]0,T[\times \Gamma$

and if r and $\hat{r}$ obey their representation (7c), (10b) in the vacuum free sets $Q^+(\varrho)$ and $S^+(\varrho)$ ([DDGG17a, DDGG17b] for details).

3 Main estimate

We will prove that the boundedness in the class $\mathcal{B}$ is a natural property of weak solutions. For one part, the *a priori* bounds result from standard methods (Gronwall Lemma) or from known properties of the Navier-Stokes equations (pressure estimate). However, our estimate on the q variable is original. The dissipation due to diffusion allows only to control ∇q while the reactions provide a control only for the projection on the space

$$W := \operatorname{span}\left\{\gamma^1, \ldots, \gamma^s,\, \hat{\gamma}^1, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}\right\}. \tag{28}$$

Call *selection* S of cardinality $|S| \leq N$ a subset $\{i_1, \ldots, i_{|S|}\}$ of $\{1, \ldots, N\}$ such that $i_1 \leq \ldots \leq i_{|S|}$. 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

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

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 selection $\{1, \ldots, N\} \backslash S$. It can easily be shown that the manifold

$$\mathcal{M}_{\text{crit}} := \mathbb{R}^N_+ \cap \bigcup_{S \subset \{1,\ldots,N\},\ S \text{ critical}} W_S \times P_{S^\perp}(\mathbb{R}^N) \tag{29}$$

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

Theorem 3.1. *Assume that* $\bar{\rho}(t) \in \{\bar{\rho}_0\} \oplus W$ *for all* $t \in [0,T]$ *(cf.* (24)*). Let* $\tilde{s} := \dim W$ *and* $b^1, \ldots, b^{\tilde{s}}$ *be a basis of* W*. Then, if* $\operatorname{dist}(\bar{\rho}_0,\, \mathcal{M}_{\text{crit}}) > 0$*, 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, where c^*_0 *and* k_0 *depend on* $\operatorname{dist}(\bar{\rho}_0,\, \mathcal{M}_{\text{crit}})$.

The critical manifold was first introduced in [DDGG16] and is a new concept in the analysis of systems with chemical reactions.

Our plan is as follows. The properties of the nonlinear algebraic equation (5) determine the analysis of the model. Our next Section 4 is devoted to the solution of these equations *in the natural variables* of the mass transfer problem. The natural variables are, on the one hand, the total mass density $\varrho = \sum_{i=1}^N \rho_i$ and, on the other hand, a $N-1$ dimensional reduction of the vector μ that we shall denote $q := \Pi\mu$. The variable $q \in \mathbb{R}^{N-1}$, that we call vector of the relative chemical potentials, is constructed via a projection of the vector μ onto $\mathbb{1}^{\perp} := \{X \in \mathbb{R}^N \, : \, \sum_{i=1}^N X_i = 0\}$. The reader is referred to the Section 6 of [DDGG17a] or to [DDGG16] for more background.

After that, we shall turn our attention to the Pde s. In the Section 5 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 (Section 6) and the resulting *a priori* estimates (Section 7). The Section 8 deals in particular with the proof of Theorem 3.1.

4 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 (5) in these variables. In particular, this section provides the rigorous derivation of the statements announced in the Section 6 of [DDGG17a]. For the proofs we mainly follow the lines of the former study [DDGG16].

4.1 The case of a general free energy

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

$$\mu_i = \partial_i h(\rho_1, \ldots, \rho_N) \text{ for } i = 1, \ldots, N \, . \tag{30}$$

In the isothermal case we can forget about the temperature-dependence, and $h = h(\rho)$. Using tools of convex analysis, we immediately obtain that the relation (30) is invertible if h is convex and smooth. In the remainder of the paper we always denote $\mathbb{R}^N_+ = (\mathbb{R}_+)^N = \{X \in \mathbb{R}^N \, : \, X_i > 0 \text{ for } i = 1, \ldots, N\}$, and $\mathbb{R}^N_{0,+} = (\mathbb{R}_{0,+})^N = \{X \in \mathbb{R}^N \, : \, X_i \geq 0 \text{ for } i = 1, \ldots, N\}$.

Lemma 4.1. *Let $h \in C^2(\mathbb{R}^N_+) \cap C(\mathbb{R}^N_{0,+})$ be convex. Let $D^*_h \subseteq \mathbb{R}^N$ be the set $\mathrm{Image}(\nabla h; \, \mathbb{R}^N_+)$, that is $D^*_h = \{\mu \in \mathbb{R}^N \, : \, \exists \, \rho \in \mathbb{R}^N_+, \, \mu = \nabla h(\rho)\}$. Then, the Legendre transform of h, denoted h^*, is a well-defined proper convex function on D^*_h, and it satisfies $h^* \in C^2(D^*_h)$. Moreover the relation* (30) *is valid for $\mu \in D^*_h$ and $\rho \in \mathbb{R}^N_+$ if and only if $\rho = \nabla h^*(\mu)$.*

Proof. Since $h \in C(\mathbb{R}^N_{0,+})$, it is a closed proper convex function in the sense of [Roc70]. The claim follows from the Theorem 26.5 of this book. □ □

Next we investigate the possibility to introduce 'mixed' coordinates to describe the set of solutions to (30). 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 $\xi^i \cdot \eta^j = \delta_i^j$, $i, j = 1, \ldots, N$. 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

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

Corollary 4.2. *Assumptions of Lemma 4.1. Let* $\xi^1, \ldots, \xi^N \in \mathbb{R}^N$ *be a basis of* $\mathbb{R}^N$ *such that* $\xi^N := \mathbb{1}$*. Define a set* $\mathscr{D} \subseteq \mathbb{R}_+ \times \mathbb{R}^{N-1}$ *via*

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

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* (30) *is valid for* $\mu \in D_h^*$ *and* $\rho \in \mathbb{R}^N_+$ *if and only if*

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

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

$$\partial_s \mathscr{M}(\rho \cdot \mathbb{1},\, q) = \frac{1}{D^2 h^*(\mu) \mathbb{1} \cdot \mathbb{1}}, \quad \partial_{q_j} \mathscr{M}(\rho \cdot \mathbb{1},\, q) = - \, \frac{D^2 h^*(\mu) \mathbb{1} \cdot \xi^j}{D^2 h^*(\mu) \mathbb{1} \cdot \mathbb{1}} \qquad j = 1, \ldots, N-1 \, . \tag{31}$$

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 $G(q,\, t,\, s) := \mathbb{1} \cdot \nabla h^*(\mathcal{E} q + t \, \mathbb{1}) - s$. 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 (30) 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 4.3. *Assumptions as in Corollary 4.2. Then there is a bijection* $\mathscr{R} : C^1(\mathscr{D};\, \mathbb{R}^N_+)$ *such that* (30) *is valid for* $\mu \in D_h^*$ *and* $\rho \in \mathbb{R}^N_+$ *if and only if* $\rho_i = \mathscr{R}_i(\rho \cdot \mathbb{1},\, \Pi\mu)$ *for* $i = 1, \ldots, N$.

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

$$\begin{aligned} \partial_{q_j}\mathscr{R}_i(s,\, q) &= D^2h^* e^i \cdot \xi^j - \frac{D^2h^* e^i \cdot \mathbb{1}\, D^2 h^* \xi^j \cdot \mathbb{1}}{D^2 h^* \mathbb{1} \cdot \mathbb{1}} \\ \partial_s \mathscr{R}_i(s,\, q) &= \frac{D^2 h^* e^i \cdot \mathbb{1}}{D^2 h^* \mathbb{1} \cdot \mathbb{1}}\,. \end{aligned} \tag{32}$$

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

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

The uniform invertibility of D^2h^* yields $\mathcal{E}q = \mathbb{1} \left(\frac{r + D^2 h^* \mathbb{1} \cdot \mathcal{E} q}{D^2 h^* \mathbb{1} \cdot \mathbb{1}} \right)$. 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 $r = 0$, and the claim follows. □ □

The pressure function. The pressure is given by the formula $p := -h + \sum_{i=1}^N \rho_i\, \mu_i$. We immediately see under (30) 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 4.4. *Let $(s,\, q) \in \mathscr{D}$. Then $P \in C^1(\mathscr{D})$ satisfies*

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

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 $\rho = \nabla h^*(\mu)$. Then

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

and the claim follows from the Corollary 4.2. □ □

4.2 Special constitutive choice of the free energy

For special choices of the free energy, we can find more explicit formula than Lemma 4.1. Under the conditions (4), the relation (30) reads

$$\mu_i = c_i + K\, \frac{V_i}{m_i}\, F'(V \cdot n) + \frac{k_B\, \theta}{m_i}\, \ln y_i \quad i = 1, \ldots, N\,, \tag{33}$$

where $c_1, \ldots, c_N \in \mathbb{R}$ are certain constants depending on the reference states, $\theta > 0$ is the absolute temperature assumed constant and k_B is the Boltzmann constant.

Note that the free energy $h = h^{\text{ref}} + h^{\text{mech}} + h^{\text{mix}}$ satisfies the assumptions of Lemma 4.1 if we assume that the function $F \in C^2(\mathbb{R}_+) \cap C(\mathbb{R}_{0,+})$ is convex. At first we want to characterise the set D_h^* and we need a preliminary Lemma.

Lemma 4.5. *There is a function $f \in C^1(\mathbb{R}^N)$ such that if the identity* (33) *is valid for $\mu \in \mathbb{R}^N$ and $n \in \mathbb{R}^N_+$ then $F'(V \cdot n) = f(\mu)$. Moreover, the function f satisfies the following inequalities*

$$\tfrac{\underline{m}}{K\,\overline{V}}\,(\sup_i \mu_i - \sup_i c_i) \leq f(\mu) \leq \tfrac{\overline{m}}{K\,\underline{V}}\,(\sup_i \mu_i - \inf_i c_i) + \tfrac{k_B\,\theta}{K\,\underline{V}}\,\ln N \tag{34}$$

and $|\nabla f| \leq \overline{m}/(\underline{V}\,K)$. For $V \in \mathbb{R}^N_+$ we here abbreviate $\underline{V} := \inf_{i=1,\ldots,N} V_i$ and $\overline{V} := \sup_{i=1,\ldots,N} V$.

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

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

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 curve $\{(\mu,\, f(\mu))\;:\; \mu \in \mathbb{R}^N\}$ where $\partial_i f(\mu) = -G_t^{-1}(\mu,\, f(\mu))\, G_{\mu_i}(\mu,\, f(\mu))$. Easy computations show that

$$\partial_i f(\mu) = \frac{m_i}{K}\, \frac{\exp\left(\frac{m_i\,(\mu_i - c_i) - K\,V_i\,f(\mu)}{k_B\,\theta}\right)}{\sum_{j=1}^N V_j\, \exp\left(\frac{m_j\,(\mu_j - c_j) - K\,V_j\,f(\mu)}{k_B\,\theta}\right)}\,. \tag{35}$$

In particular $|\nabla f| \leq \overline{m}\,\underline{V}\,K^{-1}$. Moreover, if $G(\mu,\, t) = 0$, then setting

$$y_i = \exp\left(\frac{m_i\,(\mu_i - c_i) - K\,V_i\,t}{k_B\,\theta}\right)\,,$$

we see that $\mu_i = c_i + K\,\frac{V_i}{m_i}\,t + \frac{k_B\,\theta}{m_i}\,\ln y_i$ for $i = 1, \ldots, N$. Since $y \in]0,1[^N$ and $y \cdot \mathbb{1} = 1$, the estimates (34) easily follow. □ □

We are now ready to prove an inversion formula for the relation (33).

Corollary 4.6. *Assume that the function $F \in C^2(\mathbb{R}_+) \cap C(\mathbb{R}_{0,+})$ is convex.*

Define $D^*_h := \operatorname{Image}(\nabla h;\, \mathbb{R}^N_+)$. Then $D^*_h = \{\mu \in \mathbb{R}^N \;:\; f(\mu) \in \operatorname{Image}(F',\, \mathbb{R}_+)\}$. If $\mu \in D^*_h$, then

$$\begin{aligned}\partial_i h^*(\mu) &= m_i\,([F']^{-1} \circ f)(\mu)\, \frac{\exp\left(\frac{m_i\,(\mu_i - c_i) - K\,V_i\,f(\mu)}{k_B\,\theta}\right)}{\sum_{j=1}^N V_j\, \exp\left(\frac{m_j\,(\mu_j - c_j) - K\,V_j\,f(\mu)}{k_B\,\theta}\right)} \\ &= \partial_i(F^* \circ f)(\mu)\,.\end{aligned} \tag{36}$$

with $F^* =$ Legendre transform of F.

Proof. If $\mu \in D^*_h$, then there is $\rho \in \mathbb{R}^N_+$ such that $\mu = \nabla h(\rho)$. Thus, (33) is valid, and Lemma 4.5 shows that $F'(\frac{V}{m} \cdot \rho) = f(\mu)$. Thus, $f(\mu) \in \operatorname{Image}(F',\, \mathbb{R}_+)$ and this first yields the inclusion $D^*_h \subseteq \{\mu \in \mathbb{R}^N \;:\; f(\mu) \in \operatorname{Image}(F',\, \mathbb{R}_+)\}$. In order to prove the reverse inclusion, consider $\mu \in \mathbb{R}^N$ such that $f(\mu) \in \operatorname{Image}(F',\, \mathbb{R}_+)$. Denote

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

We easily show that $\nabla h(\rho) = \mu$. Making use of (35), we see that

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

□ □

Lemma 4.7. *Assumptions of Corollary 4.6. Assume moreover* (12). *Then* $\nabla h^* \in C^1(D_h^*)$*. For* $i,\, j = 1, \ldots, N$

$$D^2 h^*_{i,j}(\nabla h(\rho)) = \frac{m_i\, \rho_j\, \delta_i^j}{k_B\, \theta} + \frac{\rho_i\, \rho_j}{n\cdot V}\, \left(\frac{1}{K\, n\cdot V\, F''(n\cdot V)} + \frac{V^2\cdot n}{k_B\, \theta\, n\cdot V} - \frac{V_i + V_j}{k_B\, \theta}\right) \tag{37}$$

is valid with $V^2 \cdot n := \sum_{i=1}^N V_i^2\, n_i$*. There further holds*

$$|D^2 h^*(\nabla h(\rho))| \leq C_1\, \rho \cdot \mathbb{1} \tag{38}$$

$$D^2 h^*(\nabla h(\rho))\, \mathbb{1}\cdot \mathbb{1} \geq C_0\, \frac{1}{K\, F''(\rho\cdot \mathbb{1})}\,. \tag{39}$$

Proof. By direct computation starting from (36) we obtain (37). This entails

$$\begin{aligned}|D^2 h^*_{i,j}(\nabla h(\rho))| &\leq \rho_i\, \left(\frac{m_i}{k_B\, \theta} + \frac{m_j}{\underline{V}}\, \left(\frac{1}{K\, n\cdot V\, F''(n\cdot V)} + \frac{\overline{V}^2}{k_B\, \theta\, \underline{V}} + 2\, \frac{\overline{V}}{k_B\, \theta}\right)\right)\\ &\leq C\, \rho_i\, \left(1 + \frac{1}{K\, n\cdot V\, F''(n\cdot V)}\right)\,.\end{aligned}$$

The function $s\, F''(s)$ is asymptotically equivalent to $s\, s^{-1} = const$ near zero (cf. (12)) 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 (38) follows. Further

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

Thus

$$\begin{aligned}&\sum_{i,j=1}^N D^2 h^*_{j,i}\\ &= \frac{(\rho\cdot \mathbb{1})^2}{K\, (V\cdot n)^2\, F''(V\cdot n)} + \frac{1}{k_B\, \theta}\, \left(m\cdot \rho + \frac{(\rho\cdot \mathbb{1})^2\, V^2\cdot n}{(V\cdot n)^2} - 2\, \frac{\rho\cdot V\, \rho\cdot \mathbb{1}}{n\cdot V}\right)\\ &= \frac{(\rho\cdot \mathbb{1})^2}{K\, (V\cdot n)^2\, F''(V\cdot n)} + \frac{1}{k_B\, \theta}\, \left(\sqrt{m\cdot \rho} - \frac{\rho\cdot \mathbb{1}\, \sqrt{V^2\cdot n}}{V\cdot n}\right)^2\\ &\quad + \frac{2}{k_B\, \theta}\, \frac{\rho\cdot \mathbb{1}}{n\cdot V}\, (\sqrt{m\cdot \rho}\, \sqrt{V^2\cdot n} - V\cdot \rho)\,.\end{aligned} \tag{40}$$

The estimate (39) is a straightforward consequence of (40) and of the Cauchy-Schwarz inequality: we can express $V_i\, \rho_i = (V_i\, \sqrt{n_i})\, (m_i\, \sqrt{n_i})$.In (39), we further make use of $F''(n\cdot V) \geq F''(c\, \varrho) \geq \tilde{c}\, F''(\varrho)$ (cf. (12)). ☐ ☐

As corollaries of Lemma 4.7, note that the functions $\mathscr{M} \in C^1(\mathscr{D})$ of Corollary 4.2 and $P \in C^1(\mathscr{D})$ satisfy for all $(s,\, q) \in \mathscr{D}$ the following inequalities (cp. (31), Lemma 4.4):

$$\frac{1}{C_1\, s} \leq \partial_s \mathscr{M}(s,\, q) \leq \frac{K\, F''(s)}{C_0}\,,\ |\partial_q \mathscr{M}(s,\, q)| \leq \frac{C_1}{C_0}\, K\, s\, F''(s)$$

$$\frac{1}{C_1} \leq \partial_s P(q,\, s) \leq \frac{K\, s\, F''(s)}{C_0}\,,\ |\partial_{q_j} P(s,\, q)| \leq C\, s\, (1 + K\, s\, F''(s))\,.$$

Remark 4.8. *For the applicability of our approximation methods we are restricted to the case that $D_h^* = \mathbb{R}^N$. In view of the Corollary 4.6 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.*

Remark 4.9. *In the case that the polynomial growth 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 the Lemma 4.4 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.*

5 Approximate solutions. Regularisation strategy

For the existence theory we shall embed the problem (P) into a larger class of approximating, regularised problems that are easier to solve. These approximations (in the spirit of 'viscosity solutions') are constructed in such a way that the integrability of the entire vector of chemical potentials μ as main variable can be expected.

5.1 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 $\nabla\mu$

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

The $\delta-$regularisation consists in increasing the growth of the (mechanical) free energy modifying the function F that occurs in the definition of h^{mech} via $F(n \cdot V) \rightsquigarrow F(n \cdot V) + \delta\, (n \cdot V)^\alpha$, $\alpha > 3$. 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

$$h_\delta(\rho) := h(\rho) + \delta\, \left(\rho \cdot \tfrac{V}{m}\right)^\alpha \,. \tag{41}$$

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

$$h^*_{\delta,\tau}(X) := (h_\delta)^*(X) + \tau \sum_{i=1}^N \omega(X_i)\,, \tag{42}$$

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

$$\begin{aligned} c_0\,(\sqrt{|s^-|} + |s^+|^{\alpha'}) \leq \omega'(s)\, s - \omega(s) &\leq c_1\,(\sqrt{|s^-|} + |s^+|^{\alpha}) \\ \omega'(s) &\leq c_2\,(1 + \omega'(s)\, s - \omega(s))^{1/\alpha} \\ \omega''(s) &\leq c_3\, \omega'(s) \end{aligned} \tag{43}$$

For example, we may choose the function

$$\omega(s) := \begin{cases} -2\sqrt{|s|} & \text{for } s \leq -1 \\ \frac{1}{4}\,s^2 + \frac{3}{2}\,s - \frac{3}{4} & \text{for } -1 < s < 1 \\ \frac{1}{2\alpha'\,(\alpha'-1)}\,s^{\alpha'} + (2 - \frac{1}{2(\alpha'-1)})\,s + \frac{1}{2\alpha(\alpha'-1)} - 1 & \text{otherwise}\,. \end{cases}$$

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 sub linear growth for $s \to -\infty$ that guaranties convexity. The function $h^*_{\tau,\delta}$ is twice differentiable and convex. Making use of the convexity we easily show that the mapping $\nabla h^*_{\tau,\delta} \,:\, \mathbb{R}^N \to \mathbb{R}^N_+$ is bijective. Interpreting (42) as Legendre transform, we introduce a regularised free energy function via

$$h_{\tau,\delta} := \text{ convex conjugate of the function } h^*_{\tau,\delta} = (h^*_{\tau,\delta})^*\,, \tag{44}$$

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 5.1. *Let the original free energy function h satisfy*

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

with constants $3/2 < \alpha_0 < +\infty$ and $0 < c_0,\, c_1,\, C_0,\, C_1 < +\infty$. Let $\alpha > 3$ be the regularisation exponent of (41)*, and ω a function satisfying* (43)*. Define*

$$\Phi_\omega(X) := \sum_{i=1}^N \omega'(X_i)\,X_i - \omega(X_i) \text{ for } X \in \mathbb{R}^N\,. \tag{45}$$

Then there are $\tilde{c}_0,\, \tilde{c}_1 > 0$, and $\tau_0(\alpha,\, \alpha_0) > 0$ such that if $\tau \leq \tau_0$

$$h_{\tau,\delta}(\rho) \geq \tilde{c}_0\,(|\rho|^{\alpha_0} + \delta\,|\rho|^\alpha + \tau\,\Phi_\omega(\mu)) - \tilde{c}_1$$

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

Proof. The definition (44) 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

$$\rho := \nabla h^*_{\tau,\delta}(\mu) = \nabla(h_\delta)^*(\mu) + \tau\,\omega'(\mu)\,,$$

and we obtain for the regularised free energy the identity

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

Using the properties of $h_\delta(Y) = h(Y) + \delta\,(Y \cdot \frac{V}{m})^\alpha$, we obtain that

$$h_{\tau,\delta}(\rho) \geq h(\rho - \tau\,\omega'(\mu)) + \delta\,((\rho - \tau\,\omega'(\mu)) \cdot \tfrac{V}{m})^\alpha + \tau\,\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i))\,.$$

On the other hand, the condition (43) ensures that $\omega'(\mu_i) \leq c\,(1+\omega'(\mu_i)\,\mu_i - \omega(\mu_i))^{1/\alpha}$. For $\alpha > 1$, denote $\underline{c}(\alpha),\ \bar{c}(\alpha)$ two constants such that $|a-b|^\alpha \geq \underline{c}(\alpha)\,a^\alpha - \bar{c}(\alpha)\,b^\alpha$ for all $a,\,b > 0$. If follows that

$$
\begin{aligned}
h_{\tau,\delta}(\rho) &\geq h(\rho - \tau\,\omega'(\mu)) + c_2\,\delta\,|\rho - \tau\,\omega'(\mu))|^\alpha + \tau\,\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i))\\
&\geq h(\rho - \tau\,\omega'(\mu)) + \min\{c_2\,\delta,\,\underline{c}(\alpha)\}\,|\rho|^\alpha\\
&\qquad + \tau\,\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) - c_2\,\delta\,\tau^\alpha\,\bar{c}(\alpha)\,|\omega'(\mu)|^\alpha\\
&= h(\rho - \tau\,\omega'(\mu)) + \min\{c_2\,\delta,\,\underline{c}(\alpha)\}\,|\rho|^\alpha\\
&\qquad + (1 - c_2\,\delta\,\bar{c}(\alpha)\,\tau^{\alpha-1})\,\tau\,\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) - C\,.
\end{aligned}
$$

If we assume that $C\,\delta\,\tau^{\alpha-1} \leq 1/4$, then

$$
\begin{aligned}
&h_{\tau,\delta}(\rho)\\
&\quad \geq h(\rho - \tau\,\omega'(\mu)) + \min\{c_2\,\delta,\,\underline{c}(\alpha)\}\,|\rho|^\alpha + \frac{3}{4}\,\tau\,\sum_{i=1}^N (\mu_i\,\omega'(\mu_i) - \omega(\mu_i)) - C\,.
\end{aligned}
$$

Making use of the growth of the free energy h and analogous arguments, the claim follows. □

5.2 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

$$
\begin{aligned}
&(\varrho,\,q,\,v,\,\phi,\,R,\,R^\Gamma) \in \mathcal{B}(T,\,\Omega,\,\alpha,\,N-1,\,\Psi,\,\Psi^\Gamma)\\
&\qquad\qquad \text{with } \varrho := \nabla h^*_{\tau,\delta}(\mu)\cdot \mathbb{1} \text{ and } q := \Pi\,\mu,\\
&\qquad\qquad R_k = \bar{R}_k(D^{\mathsf{R}}),\quad D^{\mathsf{R}}_k := \gamma^k\cdot\mu \text{ for } k = 1,\ldots,s,\\
&\qquad\qquad R^\Gamma_k = \hat{R}^\Gamma_k(t,x,\,\hat{D}^{\Gamma,\mathsf{R}}),\quad \hat{D}^{\Gamma,\mathsf{R}}_k := \hat{\gamma}^k\cdot\mu \text{ for } k = 1,\ldots,\hat{s}^\Gamma\\
&\qquad\qquad \mu \in W^{1,0}_2(Q;\,\mathbb{R}^N)\,.
\end{aligned}
\tag{46}
$$

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 (23), with free energy function $h_{\tau,\delta}$ and mobility matrix M_σ. For $\delta > 0$, $\sigma > 0$ and $\tau \geq 0$ we call weak solution to the problem $(P_{\tau,\sigma,\delta})$ a vector $(\mu,\, v,\, \phi) \in \mathcal{B}$ subject to the energy inequality and such that the quantities

$$\begin{aligned}
\rho &= \nabla h^*_{\tau,\delta}(\mu)\\
J &= -M_\sigma(\rho)\, D, \quad D := \frac{\nabla \mu}{\theta} + \frac{1}{\theta}\,\frac{z}{m}\,\nabla\phi\\
r &= \sum_{k=1}^{s} \hat{\gamma}^k\, \bar{R}_k(D^{\mathsf{R}}), \quad D^{\mathsf{R}} = (\gamma^1\cdot\mu, \ldots, \gamma^s\cdot\mu)\\
\hat{r} &= \sum_{k=1}^{\hat{s}^\Gamma} \hat{\gamma}^k\, \hat{R}^\Gamma_k(t, x,\, \hat{D}^{\Gamma,\mathsf{R}}), \quad \hat{D}^{\Gamma,\mathsf{R}} = (\hat{\gamma}^1\cdot\mu, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}\cdot\mu)\\
p &= h^*_{\tau,\delta}(\mu)\\
n^F &= \rho\cdot\frac{z}{m}
\end{aligned} \tag{47}$$

satisfy the identities (25), (27), and instead of (26)

$$\begin{aligned}
&- \int_Q \varrho\, v\cdot\eta_t - \int_Q \varrho\, v\otimes v \,:\, \nabla\eta - \int_Q p\,\operatorname{div}\eta + \int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta \\
&= \int_\Omega \varrho_0\, v^0\cdot\eta(0) - \int_Q n^F\,\nabla\phi\cdot\eta - \int_Q (\sum_{i=1}^N J^i\cdot\nabla)\eta\cdot v \qquad \forall \eta\in C^1_c([0,T[;\, C^1_c(\Omega;\mathbb{R}^3))\,.
\end{aligned} \tag{48}$$

Since the definitions (47) imply that $\sum_{i=1}^N J^i \neq 0$, it is necessary to add this term in the momentum equation (48) in order to preserve the energy identity.

6 Derivation of the global energy and mass balance identities

In this section we derive the *energy identity* naturally associated with the problem (P). In the context of its thermodynamically consistent approximations $(P_{\tau,\sigma,\delta})$, the increased regularity of the solution is sufficient to derive an *identity*.

Proposition 6.1. *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* (47) *the relations* (25)*,* (48)*,* (27) *together with the conditions*

$$\begin{aligned}
\mu(0) = \mu^0 \in C^{0,1}(\Omega;\,\mathbb{R}^N), \quad v(0) = v^0\in C^{0,1}(\Omega;\,\mathbb{R}^3) \text{ in } \Omega\\
\phi = \phi_0 \in C^{0,1}([0,T]\times\Omega)) \text{ on }]0,T[\times\Gamma,\; v = 0 \text{ on } [0,T]\times\partial\Omega\,.
\end{aligned} \tag{49}$$

We define $\rho^0 = \nabla h^*_{\tau,\delta}(\mu^0)$*. Then, for all* $t\in]0,T[$*, the vector* $(\mu,\, v,\, \phi)$ *satisfies the approximate energy equality, that is, it satisfies the energy equality* (23) *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

$$\int_\Omega \partial_t\rho\cdot\psi - \int_\Omega (\rho_i\, v + J^i)\cdot\nabla\psi^i = \int_\Omega r\cdot\psi + \int_\Gamma (\hat{r}+J^0)\cdot\psi \tag{50}$$

$$\int_\Omega \varrho\,\partial_t v\cdot\eta + \int_\Omega \varrho\,(v\cdot\nabla)v\cdot\eta + \int_\Omega \mathbb{S}(\nabla v)\,:\,\nabla\eta - \int_\Omega p\,\operatorname{div}\eta$$
$$= -\int_\Omega (\sum_{i=1}^N J^i\cdot\nabla)v\cdot\eta - \int_\Omega n^F\,\nabla\phi\cdot\eta \tag{51}$$

$$\epsilon_0\,(1+\chi)\int_\Omega \nabla\phi\cdot\nabla\zeta = \int_\Omega n^F\,\zeta\,, \tag{52}$$

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 choose $\psi=\mu(t)$ in (50). The Lemma 4.4 implies that $\sum_{i=1}^N\rho_i\,\nabla\mu_i = \nabla h^*_{\tau,\delta}(\mu) = \nabla p$. Moreover, the definition of ρ yields $\mu=\nabla h_{\tau,\delta}(\rho)$ and therefore $\partial_t\rho\cdot\mu = \partial_t h_{\tau,\delta}(\rho)$. It follows that

$$\partial_t\int_\Omega h_{\tau,\delta}(\rho) - \int_\Omega\left(v\cdot\nabla p + \sum_{i=1}^N J^i\cdot\nabla\mu_i\right) = \int_\Omega r\cdot\mu + \int_\Gamma(\hat{r}+J^0)\cdot\mu\,. \tag{53}$$

We choose $\psi=\frac{z}{m}\,\phi$ in (50). Recall that $r\cdot\frac{z}{m}=0$, because $\gamma^k\cdot\frac{z}{m}=0$ for every reaction vector (atomic charge conservation). Thus

$$\int_\Omega \partial_t n^F\,\phi - \int_\Omega\left(n^F\,v\cdot\nabla\phi + \sum_{i=1}^N J^i\,\frac{z_i}{m_i}\cdot\nabla\phi\right) = \int_\Gamma(\hat{r}+J^0)\cdot\tfrac{z}{m}\,\phi_0\,. \tag{54}$$

We differentiate (52) in time, and we choose $\zeta=\phi(t)-\phi_0(t)$, This entails

$$\int_\Omega n^F_t\,\phi = \int_\Omega n^F_t\,\phi_0 + \frac{\epsilon_0\,(1+\chi)}{2}\,\partial_t\int_\Omega|\nabla\phi|^2 - \epsilon_0\,(1+\chi)\int_\Omega\nabla\phi_t\cdot\nabla\phi_0\,. \tag{55}$$

Thus, (54) and (55) yield

$$\frac{\epsilon_0\,(1+\chi)}{2}\,\partial_t\int_\Omega|\nabla\phi|^2 - \int_\Omega\left(n^F\,v\cdot\nabla\phi + \sum_{i=1}^N J^i\,\frac{z_i}{m_i}\cdot\nabla\phi\right)$$
$$= \int_\Gamma(\hat{r}+J^0)\cdot\tfrac{z}{m}\,\phi_0 + \epsilon_0\,(1+\chi)\int_\Omega\nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega n^F_t\,\phi_0\,. \tag{56}$$

If we now add (56) to (53), it follows that

$$\partial_t\int_\Omega\{h_{\tau,\delta}(\rho) + \frac{\epsilon_0\,(1+\chi)}{2}\,|\nabla\phi|^2\} - \int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi)$$
$$-\int_\Omega\sum_{i=1}^N J^i\cdot(\nabla\mu_i + \tfrac{z_i}{m_i}\cdot\nabla\phi) - \int_\Omega r\cdot\mu - \int_\Gamma\hat{r}\cdot\mu$$
$$= \int_\Gamma(J^0\cdot\mu + (J^0+\hat{r})\cdot\tfrac{z}{m}\,\phi_0) + \epsilon_0\,(1+\chi)\int_\Omega\nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega n^F_t\,\phi_0\,. \tag{57}$$

Next we choose $\eta=v(t)$ in (51), which shows that

$$\frac{1}{2}\int_\Omega(\varrho\,\partial_t v^2 + \varrho\,(v\cdot\nabla)v^2) + \int_\Omega\mathbb{S}(\nabla v)\,:\,\nabla v$$
$$+\int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi) = -\frac{1}{2}\int_\Omega\sum_{i=1}^N J^i\cdot\nabla v^2\,. \tag{58}$$

DOI 10.20347/WIAS.PREPRINT.2396

For $\psi = v^2\,\mathbb{1}$ in (50), 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

$$\int_\Omega \varrho\,\partial_t v^2 + \int_\Omega \varrho\, v\cdot\nabla v^2 + \int_\Omega \sum_{i=1}^N J^i\cdot\nabla v^2 = \partial_t \int_\Omega \varrho\, v^2\,, \tag{59}$$

Thus (58) yields

$$\frac{1}{2}\,\partial_t \int_\Omega \varrho\, v^2 + \int_\Omega \mathbb{S}(\nabla v)\,:\,\nabla v + \int_\Omega v\cdot(\nabla p + n^F\,\nabla\phi) = 0\,. \tag{60}$$

We add (60) to (57):

$$\begin{aligned}
&\partial_t \int_\Omega \{\frac{1}{2}\,\varrho\, v^2 + h_{\tau,\delta}(\rho) + \frac{\epsilon_0\,(1+\chi)}{2}\,|\nabla\phi|^2\} + \int_\Omega \mathbb{S}(\nabla v)\,:\,\nabla v\\
&\quad - \int_\Omega \theta\, J\cdot D - \int_\Omega r\cdot\mu - \int_\Gamma \hat{r}\cdot\mu\\
&\quad = \int_\Gamma (J^0\cdot\mu + (J^0+\hat{r})\cdot\tfrac{z}{m}\,\phi_0) + \epsilon_0\,(1+\chi)\int_\Omega \nabla\phi_t\cdot\nabla\phi_0 - \int_\Omega n_t^F\,\phi_0\,.
\end{aligned}$$

We integrate over time and are done. □ □

The proof of the global mass conservation identities is comparatively simpler. It suffices to insert $\psi = e^i$ for $i = 1,\ldots,N$ into (50).

Proposition 6.2. *Assumptions of Proposition 6.1. Then for all* $t\in[0,T]$

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

7 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 here consider generic free energy functions satisfying the following growth assumption: 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 $\rho\in\mathbb{R}^N_+$

$$c_1\,|\rho|^\alpha + \tau\,\Phi_\omega[\nabla h(\rho)] - c_2 \leq h(\rho) \leq C_1\,|\rho|^\alpha + C_2\,\tau\,\Phi_\omega[\nabla h(\rho)] + C_3\,. \tag{61}$$

Moreover we consider mobility matrices $M_\sigma = M(\rho) + \sigma\,\mathrm{Id}$, $\sigma\geq 0$, such that M satisfies (13) and (14). We commence with a few standard estimates.

Proposition 7.1. *Let* $(\varrho,\, q,\, v,\, \phi,\, R,\, R^\Gamma)$ *satisfy the energy inequality* (23) *with free energy function* h *satisfying* (61) *and mobility matrix* M *satisfying* (13), (14)*. Then, there is a number* $C_0 > 0$ *depending only on* Ω*, on the constants* c_i*,* C_i *in the conditions* (61)*, and on the quantity*

$$\begin{aligned}
\mathcal{B}_0 :=\ & \|\rho^0\|_{L^\alpha(\Omega)} + \tau\,\|\Phi_\omega(\mu^0)\|_{L^1(\Omega)} + \|\sqrt{\varrho_0}\,v^0\|_{L^2(\Omega)} + \|\phi_0\|_{L^\infty(Q)}\\
&+ \|\phi_0\|_{L^\infty(0,T;\,W^{1,2}(\Omega))} + \|\phi_{0,t}\|_{W^{1,0}_2(Q)} + \|\phi_{0,t}\|_{L^{\alpha'}(Q)} + \|\jmath\|_{L^\infty(S;\,\mathbb{R}^{\hat{s}\Gamma})}\,,
\end{aligned} \tag{62}$$

such that

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

Here the quantities ρ, J, etc. obey the definitions (22) *or* (47)*.*

Proof. Due to the assumption (61)

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

For general velocity fields $v \in W^{1,2}(\Omega;\,\mathbb{R}^3)$

$$\int_\Omega \mathbb{S}(\nabla v)\,:\,\nabla v = \int_\Omega \frac{\eta}{4}\,|D(v) - \frac{2}{3}\,\mathrm{div}\,v\,\mathsf{Id}|^2 + \int_\Omega (\lambda + \frac{2}{3}\,\eta)\,(\mathrm{div}\,v)^2\,.$$

In the case that $v = 0$ on $\partial\Omega$

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

For estimating the right hand of the energy identity

$$\begin{aligned}
\Big|\int_\Omega n^F(t)\,\phi_0(t)\Big| \leq \big|\tfrac{z}{m}\big| \int_\Omega |\rho|\,|\phi_0(t)| \leq \frac{c_1}{2} \int_\Omega |\rho|^\alpha + c \int_\Omega |\phi_0|^{\alpha'}\\
\Big|\epsilon_0\,(1+\chi) \int_\Omega \nabla\phi\cdot\nabla\phi_0\Big| \leq \frac{\epsilon_0\,(1+\chi)}{4} \int_\Omega |\nabla\phi(t)|^2 + c \int_\Omega |\nabla\phi_0|^2\,.
\end{aligned}$$

Owing to similar standard considerations

$$\begin{aligned}
&\Big|\int_{Q_t} \{n^F\,\phi_{0,t} - \epsilon_0\,(1+\chi)\,\nabla\phi\cdot\nabla\phi_{0,t}\}\Big|\\
&\leq \int_0^t \{\|n^F\|_{L^\alpha(\Omega)}\,\|\phi_{0,t}\|_{L^{\alpha'}(\Omega)} + \epsilon_0\,(1+\chi)\,\|\nabla\phi\|_{L^2(\Omega)}\,\|\nabla\phi_{0,t}\|_{L^2(\Omega)}\}\\
&\leq \int_0^t \{\|n^F\|^\alpha_{L^\alpha(\Omega)} + \epsilon_0\,(1+\chi)\,\|\nabla\phi\|^2_{L^2(\Omega)}\}\\
&\qquad + C \int_0^t \{\|\phi_{0,t}\|^{\alpha'}_{L^{\alpha'}(\Omega)} + \|\nabla\phi_{0,t}\|^2_{L^2(\Omega)}\}\,.
\end{aligned}$$

The Young inequality further implies that

$$\begin{aligned}
-\int_{S_t} R^\Gamma_k\,\hat{\gamma}^k\cdot\tfrac{z}{m}\,\phi_0 \leq & \int_{S_t} (\hat{\Psi}^\Gamma)^*(t,x,\,-\tfrac{1}{4}\,R^\Gamma)\\
&+ \int_{S_t} \hat{\Psi}^\Gamma(t,x,\,4\,\phi_0\,(\hat{\gamma}^1\cdot\tfrac{z}{m},\ldots,\,\hat{\gamma}^{\hat{s}^\Gamma}\cdot\tfrac{z}{m}))\,.
\end{aligned}$$

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

$$\begin{aligned}
-\int_{S_t} R_k^\Gamma\,\hat{\gamma}^k\cdot\tfrac{z}{m}\,\phi_0 \le & \frac{1}{4}\int_{S_t}(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)\\
&+\int_{S_t}\hat{\Psi}^\Gamma(t,x,\,4\,\phi_0\,(\hat{\gamma}^1\cdot\tfrac{z}{m},\ldots,\,\hat{\gamma}^{\hat{s}^\Gamma}\cdot\tfrac{z}{m}))\\
&=\frac{1}{4}\int_{S_t}(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)+C_0(\|\phi_0\|_{L^\infty([0,T]\times\Gamma)})\,.
\end{aligned}$$

Recall that J^0 possesses a representation $J^0=\sum_{k=1}^{\hat{s}^\Gamma}\jmath_k\,\hat{\gamma}^k$, and therefore

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

Due to convex duality

$$\Psi(D^{\mathsf{R}})+(\Psi)^*(-\bar{R}(D^{\mathsf{R}})) = -\sum_{k=1}^{s}\bar{R}_k(D^{\mathsf{R}})\,\gamma^k\cdot\mu$$

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

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

$$\begin{aligned}
&\int_\Omega\Big\{\frac{1}{2}\,\varrho\,v^2+\frac{\epsilon_0\,(1+\chi)}{4}\,|\nabla\phi|^2+\frac{c_1}{2}\,|\rho|^\alpha+\tau\,\Phi_\omega(\mu)\Big\}(t)\\
&\quad+\int_{Q_t}\Big\{\eta\,|\nabla v|^2+(\lambda+\eta)\,(\operatorname{div}v)^2-\theta\sum_{i=1}^N J^i\cdot D^i+(\Psi(D^{\mathsf{R}})+(\Psi)^*(-R))\Big\}\\
&\quad+\frac{1}{2}\int_{S_t}\{\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathsf{R}})+(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)\}\\
&\le C_0+C\int_0^t\{\|\rho\|_{L^\alpha(\Omega)}^\alpha+\epsilon_0\,(1+\chi)\,\|\nabla\phi\|_{L^2(\Omega)}^2\}
\end{aligned}$$

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

$$\begin{aligned}
&\int_\Omega\Big\{\frac{1}{2}\,\varrho\,v^2+\frac{1}{4}\,\epsilon_0\,(1+\chi)\,|\nabla\phi|^2+\frac{c_1}{2}\,|\rho|^\alpha+\tau\,\Phi_\omega(\mu)\Big\}(t)\\
&+\int_{Q_t}\Big\{\eta\,|\nabla v|^2+(\lambda+\eta)\,(\operatorname{div}v)^2-\theta\sum_{i=1}^N J^i\cdot D^i+(\Psi(D^{\mathsf{R}})+(\Psi)^*(-R))\Big\}\\
&+\frac{1}{2}\int_{S_t}\{\hat{\Psi}^\Gamma(t,x,\,\hat{D}^{\Gamma,\mathsf{R}})+(\hat{\Psi}^\Gamma)^*(t,x,\,-R^\Gamma)\}\le C_0(T)\,.
\end{aligned}$$

Since $\lambda + \frac{2}{3}\,\eta \geq 0$ 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

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

whereas the reaction driving forces satisfy

$$[D^{\mathsf{R}}]_{L_{\Psi}(Q;\mathbb{R}^s)} + [\hat{D}^{\Gamma,\mathsf{R}}]_{L_{\hat{\Psi}^{\Gamma}}(S_T;\mathbb{R}^{\hat{s}^{\Gamma}})} \leq C_0\,.$$

It remains to exploit the dissipation due to diffusion and the driving forces $D^1, \ldots, D^N$. At first we note that $-\theta \sum_{i=1}^N J^i \cdot D^i = \theta \sum_{i,j} M_{i,j}\, D^i \cdot D^j$. For $i = 1, \ldots, N$ the Cauchy-Schwarz inequality and the growth condition (14) on M (or M_σ) imply that

$$\begin{aligned}|J^i| = |\sum_{j=1}^N M_{i,j}\, D^j| &\leq (MD\cdot D)^{1/2}\,(Me^i\cdot e^i)^{1/2}\\ &\leq (\sqrt{\sigma} + \sqrt{\overline{\lambda}})\,(1+|\rho|)^{1/2}\,(MD\cdot D)^{1/2}\,.\end{aligned}$$

Therefore, we obtain for the diffusion fluxes that

$$\begin{aligned}\|J^i(t)\|_{L^{\frac{2\alpha}{1+\alpha}}(\Omega)} &\leq c\,\|MD\cdot D(t)\|_{L^1(\Omega)}^{1/2}\,(1+\|\rho(t)\|_{L^{\alpha}(\Omega)}^{1/2})\\ &\leq C_0\,\|MD\cdot D(t)\|_{L^1(\Omega)}^{1/2}\,.\end{aligned}$$

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

We finally want to obtain estimates on the gradients of the (relative) chemical potentials. Here we make use of the assumption (14) that yields

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

Here $P_{\mathbb{1}^\perp}$ the orthogonal projection on the space $\mathbb{1}^\perp$. Splitting the driving force $D^i = \theta^{-1}\,(\nabla\mu_i + \frac{z_i}{m_i}\,\nabla\phi)$, we can obtain that

$$-\theta\sum_{i=1}^N J^i\cdot D^i \geq \frac{\underline{\lambda}}{2\,\theta}\,|P_{\mathbb{1}^\perp}\nabla\mu|^2 - \frac{3\,\underline{\lambda}}{\theta}\,\left|\frac{z}{m}\right|^2\,|\nabla\phi|^2\,.$$

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 $|P_{\mathbb{1}^\perp}\nabla\mu|^2 \geq c_\Pi\,|\nabla q|^2$. This entails $|\nabla q|^2 \leq c\,(-\theta^2\,\sum_{i=1}^N J^i\cdot D^i + |\nabla\phi|^2)$, proving that $\|\nabla q\|_{L^2(Q)} \leq C_0$. Since $M_\sigma D\cdot D \geq \sigma\,D^2$

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

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

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

Due to the conditions (43), we verify that $|\omega'|^{\alpha} \leq (1+\Phi_{\omega})$ and this directly yields

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

At last we can verify, making use of the growth property of Φ_{ω} that the function $w = \sqrt{1+|\mu|}$ possesses a distributional gradient in $L^2(Q)$ and is bounded in $L^{\infty,1}(Q)$ via

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

Thus, $\|w\|_{L^{2,6}(Q)} \leq C_{\sigma,\tau}$. □ □

Lemma 7.2. *Assumptions of Proposition 7.1. Assume moreover that for almost all* $t\ \in]0,T[$*, the electrical potential* $\phi \in L^{\infty}(0,T;\, W^{1,2}(\Omega))$ *satisfies*

$$-\epsilon_0\,(1+\chi)\,\triangle \phi(t) = n^F(t) \text{ in } [W^{1,2}_{\Gamma}(\Omega)]^*, \quad \phi(t) = \phi_0(t) \text{ as traces on } \Gamma\,,$$

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*

$$\begin{aligned}
\|\phi\|_{L^{\infty}(Q)} &\leq \|\phi_0\|_{L^{\infty}(Q)} + c\, \|\rho\|_{L^{\infty,\alpha}(Q)}\\
\|\phi\|_{L^{\infty}(0,T;\, W^{1,\beta}(\Omega))} &\leq c\, (\|\phi_0\|_{L^{\infty}(0,T;\, W^{1,\beta}(\Omega))} + \|\rho\|_{L^{\infty,\alpha}(Q)})\,.
\end{aligned} \tag{63}$$

Moreover, if $\beta \geq \alpha'$

$$\|n^F\, \nabla \phi\|_{L^{\infty,\frac{\beta\alpha}{\beta+\alpha}}(Q)} \leq \|n^F\|_{L^{\infty,\alpha}(Q)}\, \|\nabla\phi\|_{L^{\infty,\beta}(Q)}\,. \tag{64}$$

Proof. We only need to recall that $\alpha > 3/2$ and the definition of the exponent $r(\Omega,\Gamma) \geq 2$ (see (18)). The estimates (63) are standard consequences of second order elliptic theory, whereas (64) follows from the Hölder inequality. □

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

Proposition 7.3. *Assumptions of Proposition 7.1. If* $\bar{\rho}$ *satisfies the identity of Definition* (24)*, 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

$$\left|\int_{t_1}^{t_2} \int_{\Omega} r_i\right| = \left|\int_{t_1}^{t_2} \int_{\Omega} R\cdot \gamma_i\right| \leq \sup_{i=1,\ldots,N,\, [-R]_{L_{\Psi^*}} \leq C_0} \left|\int_{t_1}^{t_2} \int_{\Omega} R\cdot \gamma_i\right|\,.$$

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 $\beta := \min\{r(\Omega,\,\Gamma),\, \frac{3\alpha}{(3-\alpha)^+}\}$ the optimal regularity of the electric field.

Lemma 7.4. *We assume that the bounds in the Proposition 7.1 and Lemma 7.2 are valid. Then*

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

Further we shall need an improved bound on the pressure. This is also fairly standard, and therefore we give the proof in the Appendix.

Lemma 7.5. *Assume that the relation* (25) *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.

8 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}, $D^{\Gamma,\mathrm{R}}$ and the control on the gradient of the relative potentials $(q_1, \ldots, q_{N-1}) = \Pi\mu$ (cf. Proposition 7.1) and the balance of total mass (Proposition 6.2) allows a control in time on 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 $\rho := \mathscr{R}(\varrho,\, q)$, and $\mu := \mathcal{E}q$ if $|q|$ is finite. An essential ingredient of the proof is the balance of total mass valid for all $t \in]0, T[$ implying

$$\bar{\rho}(t) \in \{\bar{\rho}^0\} \oplus \mathrm{span}\{\gamma^1, \ldots, \gamma^s,\, \hat{\gamma}^1, \ldots, \hat{\gamma}^{\hat{s}^\Gamma}\} =: \{\bar{\rho}^0\} \oplus W\,. \tag{65}$$

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

$$\partial_i h(\rho) = c_i + K\, \frac{V_i}{m_i}\, F'(\rho \cdot \tfrac{V}{m}) + k_B\, \theta\, \frac{1}{m_i}\, \ln y_i \tag{66}$$

$$\begin{aligned}\mu_i - \mu_k &= \mathcal{E}q \cdot (e^i - e^k) = (\mathcal{E}q + \mathscr{M}(\varrho,\, q)\, \mathbb{1}) \cdot (e^i - e^k) \\ &= c_i - c_k + K\left(\tfrac{V_i}{m_i} - \tfrac{V_k}{m_k}\right) F'(\rho \cdot \tfrac{V}{m}) + k_B\, \theta \left(\tfrac{1}{m_i}\, \ln y_i - \tfrac{1}{m_k}\, \ln y_k\right)\,.\end{aligned} \tag{67}$$

Let $\tilde{s} := \dim W$ and $b^1, \ldots, b^{\tilde{s}} \in W$ be a basis of W ($0 \leq \tilde{s} \leq s$).

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 $P_S(\mathbb{R}^N)$. The manifold $W_S := \mathrm{span}\{P_S(b^1), \ldots, P_S(b^{\tilde{s}})\} \oplus P_{S^c}(\mathbb{R}^N)$ has at most dimension $N-1$.

The critical manifold was first introduced in the paper [DDGG16] and is defined via (29). We commence stating an obvious estimate, that results from the Proposition 7.1.

Lemma 8.1. *Define $P_W : \mathbb{R}^N \to W$ the orthogonal projection on the subspace W. There is C depending only on Ω such that*

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

Proof. Consider at first a vector $\gamma^k \in \mathbb{R}^N$, $k \in \{1,\ldots,s\}$ associated with the bulk reactions. Since we assume at least quadratic growth of the potential Ψ (17), then obviously $\|\mu\cdot\gamma^k\|_{L^2(\Omega)} \leq [D^{\mathsf{R}}]_{L_\Psi(\Omega;\,\mathbb{R}^s)}$. By assumption, $\gamma^k\cdot\mathbb{1} = 0$ for all k. This means that there is a constant $c_{W,\Pi}$ depending on W and the choice of the projector Π such that $|\nabla(\gamma^k\cdot\mu)| \leq c_{W,\Pi}\,|\nabla\Pi\mu|$. We also obtain (trace theorem) that $\|\mu\cdot\gamma^k\|_{L^2(\Gamma)} \leq C\,\|\mu\cdot\gamma^k\|_{W^{1,2}(\Omega)}$. Thus

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

For $k \in \{1,\ldots,\hat{s}^\Gamma\}$, we analogously observe that $|\mu\cdot\hat{\gamma}^k| \leq |\hat{D}^{\Gamma,\mathsf{R}}|$ which is bounded by the data in $L_{\hat{\Psi}^\Gamma}$ and therefore in $L^2(]0,T[\times\Gamma)$ (17). We make use of the fact that $\|\mu\cdot\hat{\gamma}^k\|_{L^2(\Omega)} \leq C\left(\|\nabla(\mu\cdot\hat{\gamma}^k)\|_{L^2(\Omega)} + \|\mu\cdot\hat{\gamma}^k\|_{L^2(]0,T[\times\Gamma)}\right)$, and the claim follows. □

As a preliminary tool to the main estimate of this section, we have the following Lemma.

Lemma 8.2. *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 $\delta > 0$, there is $C^* = C^*(\delta)$ depending only on Ω such that for all $u \in W^{1,1}(\Omega)$

$$\min\{\lambda_3(A_\epsilon(u)),\, \lambda_3(B_\epsilon(u))\} \geq \delta$$

implies that

$$\|u\|_{L^1(\Omega)} \leq C^*(\delta)\left(\|\nabla u\|_{L^1(\Omega)} + \tfrac{1}{\epsilon}\max\{\lambda_3(A_\epsilon(u)),\, \lambda_3(B_\epsilon(u))\}\right).$$

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

$$\|u\|_{L^1(\Omega)} \leq c(\delta)\,\left(\|\nabla u\|_{L^1(\Omega)} + \max\left\{\int_A |u^+|,\, \int_B |u^-|\right\}\right) \tag{68}$$

for all $u \in W^{1,1}(\Omega)$, for all $A,\, B \subset \Omega$ such that $\min\{|A|,\,|B|\} \geq \delta\,.$

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 (68) 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

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

□

We now prove the main result 3.1. First we recall the statement.

Theorem 8.3. *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, where 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 for $i = 1, \ldots, N$ the function $\hat{q}_i := \mu_i - \max_{j=1,\ldots,N} \mu_j$. 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 $\operatorname{span}\{\xi^1, \ldots, \xi^{N-1}\}$. Therefore, we can show that

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

First step: Now, exploiting Lemma 8.2 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

$$\begin{cases}\|\hat{q}_i(t)\|_{L^1(\Omega)} \leq C^*(\delta)\,(d_0(t) + \epsilon^{-1}\,\lambda_3(\Omega))\\ \text{or}\\ \lambda_3(\{x \,:\, \hat{q}_i(t,\,x) \geq -\frac{1}{\epsilon}\}) < \delta\,.\end{cases} \tag{69}$$

Due to the definitions of $\hat{q}$, i_0 and (67), there holds in $B_{i_0} \subseteq \Omega$

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

Thus

$$\ln y_i \leq \tfrac{m_i}{m_{i_0}}\,\ln y_{i_0} + \tfrac{m_i}{k_B\,\theta}\,(\hat{q}_i + 2\,|c|_\infty + \sup_{j,k=1,\ldots N} |\tfrac{V_j}{m_j} - \tfrac{V_k}{m_k}|\,F'(\tfrac{V}{m}\cdot\rho))\,. \tag{70}$$

We define $\epsilon_0 := \frac{1}{8\,|c|_\infty}$, $a_0 := \sup_{j,k=1,\dots N} |\frac{V_j}{m_j} - \frac{V_k}{m_k}|$, and for $\epsilon > 0$ and $t \in]0,T[$

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

Due to the inequality (70), the set inclusion

$$\{x \,:\, \hat{q}_i(t,\,x) < -\tfrac{1}{\epsilon}\} \cap A_\epsilon(t) \subseteq \{x \,:\, y_i(t,\,x) \leq e^{-\frac{m_i}{2\,k_B\,\theta\,\epsilon}}\} \tag{71}$$

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

$$\begin{aligned} \Omega \setminus A_\epsilon(t) &= C^+_\epsilon(t) \cup C^-_\epsilon(t)\\ C^-_\epsilon(t) &:= \{x \,:\, F'(\tfrac{V}{m}\cdot\rho(t,x)) \leq -\tfrac{1}{4a_0\epsilon}\}\\ C^+_\epsilon(t) &:= \{x \,:\, F'(\tfrac{V}{m}\cdot\rho(t,x)) \geq \tfrac{1}{4a_0\epsilon}\} \end{aligned}$$

Due to the asymptotic behaviour of the function F' (see (12)), there are $\epsilon_1 > 0$ and $\bar{k}_1,\,\bar{k}_2 > 0$ depending only on F and a_0 such that

$$\begin{aligned} x \in C^-_\epsilon(t) &\Rightarrow \ln(\tfrac{V}{m}\cdot\rho(t,x)) \leq -\frac{\bar{k}_1}{\epsilon}\\ x \in C^+_\epsilon(t) &\Rightarrow (\tfrac{V}{m}\cdot\rho(t,x))^{\alpha-1} \geq \frac{\bar{k}_2}{\epsilon}\,. \end{aligned}$$

In particular, it follows that

$$C^-_\epsilon \subseteq \{x \,:\, \max_{i=1,\dots,N} \rho_i(t,x) \leq \frac{1}{\min_{i=1,\dots,N}\frac{V_i}{m_i}}\, e^{-\frac{\bar{k}_1}{\epsilon}}\}\,, \tag{72}$$

Thus, invoking (71) and (72) we obtain that

$$\begin{aligned} &\{x \,:\, \hat{q}_i(t,\,x) < -\tfrac{1}{\epsilon}\} \cap (\Omega \setminus C^+_\epsilon(t))\\ &\subseteq \{x \,:\, y_i(t,\,x) \leq e^{-\frac{m_i}{2\,k_B\,\theta\,\epsilon}}\} \cup \{x \,:\, \max_{i=1,\dots,N} \rho_i(t,x) \leq \tfrac{\overline{m}}{\underline{V}}\, e^{-\frac{\bar{k}_1}{\epsilon}}\}\,. \end{aligned} \tag{73}$$

Here $\overline{m} := \max_{i=1,\dots,N} m_i$ and $\underline{V} := \min_{i=1,\dots,N} V_i$. On the other hand we readily see that

$$\lambda_3(C^+_\epsilon(t)) \leq \|\varrho\|^\alpha_{L^{\infty,\alpha}(Q)} \sup_{i=1,\dots,N} (\tfrac{V_i}{m_i})^\alpha \left(\frac{\epsilon}{\bar{k}_2}\right)^{\alpha'}\,. \tag{74}$$

Thus, if $\lambda_3(\{x \,:\, \hat{q}_i(t,\,x) \geq -\frac{1}{\epsilon}\}) \leq \delta$, we can invoke (73) and (74) to see that

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

For all $0 < \epsilon < \min\{\epsilon_0,\,\epsilon_1\}$ and $0 < \delta$, we therefore obtain from the latter and (69) that

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

implies

$$\lambda_3(\{x \,:\, y_i(t,x) \leq e^{-\frac{m_i}{2\,k_B\,\theta\,\epsilon}}\} \cup \{x \,:\, \max_{i=1,\dots,N} \rho_i(t,x) \leq \tfrac{\overline{m}}{\underline{V}}\, e^{-\frac{\bar{k}_1}{\epsilon}}\}) \geq \lambda_3(\Omega) - \delta - C_0\,\epsilon^{\alpha'}\,.$$

We further note that

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

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

$$\|\hat{q}_i(t)\|_{L^1(\Omega)} > C^*(\delta)\,(d_0(t) + \epsilon^{-1}\lambda_3(\Omega))$$
$$\text{implies} \tag{75}$$
$$\bar{\rho}_i(t) \leq C_0\,(\delta^{\frac{1}{\alpha'}} + \max\{\epsilon,\, e^{-\frac{C_1}{\epsilon}}\})\,,$$

where $C_0,\, C_1$ are certain constants depending on the data.

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

$$\inf_{j\in J} \|\hat{q}_j(t)\|_{L^1(\Omega)} \geq c_0\,(\|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} - c_1\, r_0(t))\,. \tag{76}$$

We prove this inductively. Suppose that $K \subset \{1, \ldots, N\}$ is any non-critical index set. Then, by definition, there are for all $k \in K$ coefficients $\lambda^k_1, \ldots, \lambda^k_{\tilde{s}}$ such that

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

Thus, elemetarily

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

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

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

Applying this iteratively, we prove the subclaim (76). Now, assume that for parameters $0 < \epsilon < \epsilon_0$ 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. 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 now the first step, (75),

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

Thus, we have proved the new alternative

$$\|\hat{q}_{i_1}(t)\|_{L^1(\Omega)} > \tfrac{1}{c_0}\,(C^*(\delta)\,(d_0(t) + \epsilon^{-1}\,\lambda_3(\Omega)) + c_1\,r_0(t))$$
$$\text{implies that there is } J \supset \{i_1\} \text{ critical such that} \tag{77}$$
$$\max_{j\in J} \bar{\rho}_j(t) \leq C_0\,(\delta^{\frac{1}{\alpha'}} + \max\{\epsilon,\, e^{-\frac{C_1}{\epsilon}}\})$$

Third step: By assumption $\operatorname{dist}(\bar{\rho}_0,\, \mathcal{M}_{\text{crit}}) > 0$. Thus, for every critical selection J, the definition (29) implies that $|P_J(\bar{\rho}(t))| \geq \operatorname{dist}(\bar{\rho}_0,\, M_{\text{crit}}) > 0$. This in turn implies that

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

Thus, there are $\delta_0 > 0$ and $\bar{\epsilon}_0 > 0$ depending only on $\operatorname{dist}(\bar{\rho}_0,\, M_{\text{crit}})$ such that the hypothesis in (77) yields a contradiction for all $\delta \leq \delta_0$ and $0 < \epsilon \leq \min\{\epsilon_0,\, \epsilon_1,\, \bar{\epsilon}_0\}$. For $d_0 := \operatorname{dist}(\bar{\rho}_0,\, M_{\text{crit}})$ one may choose

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

Conclusion: We resize $k := C^*(\frac{\delta_0}{2})\,\epsilon^{-1}\,\lambda_3(\Omega)$. For $k \geq k_0 = C^*(\frac{\delta_0}{2})\,\lambda_3(\Omega)\,[\min\{\epsilon_0,\, \epsilon_1,\, \bar{\epsilon}_0\}]^{-1}$, the set of times such that

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

has measure zero. Thus, standard arguments show that

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

The claim follows easily. □

If the vector of initial total partial masses $\bar{\rho}_0$ is on the critical manifold, we can prove that species do not vanish only locally in time. We will then rely on the following simple observation.

Lemma 8.4. *Assume that* (65) *is valid. Define*

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

Then, there is a time $T_0 > 0$ depending on $\mathcal{B}_0$ (cf. (62)*) and on $\inf_{i=1,\ldots,N} \bar{\rho}_i^0$ such that $T^* \geq T_0$, and $\|q\|_{L^2(Q_t;\mathbb{R}^{N-1})} \leq C_{0,t}$ for all $t < T^*$.*

Proof. We recall Proposition 7.3, and we see that $|\bar{\rho}(t) - \bar{\rho}^0| \leq \tilde{C}_0\,\Phi^*(t,0)$ for all $t \in [0,T]$. Thus, if T_0 is such that $\inf_{i=1,\ldots,N} \bar{\rho}_i^0 - \tilde{C}_0\,\Phi^*(T_0,0) \geq c_0 > 0$, we obtain that $\inf_{i=1,\ldots,N} \bar{\rho}_i(t) > c_0$ for all $t \in [0,T_0]$. Due to the first step of the proof of Theorem 3.1, it then follows that

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

on $[0,\, T_0]$ for all $i = 1,\ldots,N$, δ_0 appropriate, and all $\epsilon \leq \min\{\epsilon_0,\, \epsilon_1\}$. The claim follows. □

A Proofs of some auxiliary statements

We prove the Lemma 7.5.

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

$$\operatorname{div} X = f \text{ in } \Omega, \quad X = 0 \text{ on } \partial\Omega\,, \tag{78}$$

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

$$\|X\|_{W^{1,q}(\Omega)} \leq c_q\,\|f\|_{L^q(\Omega)}, \quad \|X\|_{L^q(\Omega)} \leq c_q\,\|f\|_{[W_0^{1,q'}(\Omega)]^*} \tag{79}$$

are valid. For details about the solution operator, see among others [FNP01], section 3.1.

We begin with the case $\alpha > 3$. Then, for all $\eta \in C^1_c([0,T[;\, C^1_c(\Omega;\, \mathbb{R}^3))$ the function p satisfies

$$\begin{aligned}\int_Q p\,\operatorname{div}\eta = &-\int_Q \varrho\, v\cdot\eta_t - \int_Q \varrho\, v\otimes v\,:\,\nabla\eta + \int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta\\ &- \int_Q (\sum_{i=1}^N J^i\cdot\nabla)\eta\cdot v - \int_\Omega \varrho_0\, v^0\cdot\eta(0) + \int_Q n^F\,\nabla\phi\cdot\eta\,.\end{aligned}$$

We make use of the estimates

$$\begin{aligned}\left|\int_Q \varrho\, v\cdot\eta_t\right| &\leq \|\varrho\, v\|_{L^{2,\frac{6\alpha}{6+\alpha}}(Q)}\,\|\eta_t\|_{L^{2,\frac{6\alpha}{5\alpha-6}}(Q)}\\ \left|\int_Q \varrho\, v\otimes v\,:\,\nabla\eta\right| &\leq \|\varrho\, v^2\|_{L^{1,\frac{3\alpha}{3+\alpha}}(Q)}\,\|\nabla\eta\|_{L^{\infty,\frac{3\alpha}{2\alpha-3}}(Q)}\\ \left|\int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta\right| &\leq c\,\|\nabla v\|_{L^2(Q)}\,\|\nabla\eta\|_{L^2(Q)}\\ \left|\int_Q (\sum_{i=1}^N J^i_\sigma\cdot\nabla)\eta\cdot v\right| &\leq \left\|\sum_{i=1}^N J^i_\sigma\, v\right\|_{L^{1,3/2}(Q)}\,\|\nabla\eta\|_{L^{\infty,3}(Q)}\\ \left|\int_Q n^F\,\nabla\phi\cdot\eta\right| &\leq \|n^F\,\nabla\phi\|_{L^{\infty,1}(Q)}\,\|\eta\|_{L^{1,\infty}(Q)}\\ &\leq c\,\|n^F\,\nabla\phi\|_{L^{\infty,1}(Q)}\|\eta\|_{L^\infty(0,T;\,W^{1,\alpha}(\Omega))}\,.\end{aligned} \tag{80}$$

Let $t \in]0,T[$ and consider according to (78) a solution to the problem

$$\operatorname{div} X = \varrho(t) - \bar{\varrho}(t) \text{ in } \Omega,\ X = 0 \text{ on } \partial\Omega$$

Since $\bar{\varrho}(t) = \|\varrho_0\|_{L^1(\Omega)}$ for all t as a consequence of (25), we obtain the estimate

$$\|X\|_{W^{1,\alpha}(\Omega)} \leq c\,(\|\varrho(t)\|_{L^\alpha(\Omega)} + \|\varrho_0\|_{L^1(\Omega)})\,.$$

The identity (25) also implies that

$$-\int_Q \varrho\,\psi_t = \int_Q \varrho\, v\cdot\nabla\psi + \int_Q \sum_{i=1}^N J^i\cdot\nabla\psi = 0 \text{ for all } \psi \in C^1_c(0,T;\, C^1(\overline{\Omega}))\,,$$

and since we assume $\alpha > 3$, this yields

$$\|\varrho_t\|_{L^2(0,T;\,[W^{1,2}(\Omega)]^*)} \leq \|\varrho\, v\|_{L^2(Q)} + \|\sum_{i=1}^N J^i\|_{L^2(Q)}$$
$$\leq c\,\|\varrho\, v\|_{L^{2,\frac{6\alpha}{6+\alpha}}(Q)} + \|\sum_{i=1}^N J^i\|_{L^2(Q)} \leq C_0\,.$$

Thus the properties (79) imply that

$$\|X_t\|_{L^2(Q)} \leq c\,\|\varrho_t\|_{L^2(0,T;\,[W^{1,2}(\Omega)]^*)} \leq C_0\,.$$

Owing to the inequalities $6\alpha/(5\alpha-6) < 2$ and $3\alpha/(2\alpha-3) < \alpha$, we see that $|\int_Q p\, \operatorname{div} X| \leq C_0$. Thus $\int_Q p\,\varrho \leq C_0$, and since $\varrho \geq c\, p^{1/\alpha}$ the claim follows.

If $\alpha \leq 3$, then we assume that $\mathbb{1}\cdot J = 0$, then p satisfies for all $\eta \in C^1_c([0,T[;\, C^1_c(\Omega;\mathbb{R}^3))$

$$\int_Q p\, \operatorname{div}\eta = -\int_Q \varrho\, v\cdot \eta_t - \int_Q \varrho\, v\otimes v\,:\,\nabla\eta + \int_Q \mathbb{S}(\nabla v)\,:\,\nabla\eta$$
$$- \int_\Omega \varrho_0\, v^0\cdot\eta(0) + \int_Q n^F\,\nabla\phi\cdot\eta\,.$$

We apply the estimates (80) for the right-hand except for the last one. Note further that $3\alpha/(2\alpha-3) \geq 3$, and therefore $\beta \geq \min\{3,\, r(\Omega,\,\Gamma)\} > \alpha'$ by assumption. It follows that $\frac{\beta\alpha}{\beta+\alpha} > 1$, and therefore

$$\left|\int_Q n^F\,\nabla\phi\cdot\eta\right| \leq \|n^F\,\nabla\phi\|_{L^{\frac{\beta\alpha}{\beta+\alpha}}(Q)}\, \|\eta\|_{L^{\frac{\beta\alpha}{\beta\alpha-\beta-\alpha}}(Q)} \leq C_0\,\|\eta\|_{L^\infty(0,T;\,W^{1,\frac{3\alpha}{2\alpha-3}}(\Omega))}\,.$$

It can be shown using (25) that ϱ is a solution to the continuity equation in the sense of *renormalised solutions* (see [Lio98] or [FNP01]) and that it satisfies for all $s > 0$ and $\psi \in C^1_c(0,T;\, C^1(\overline{\Omega}))$

$$-\int_Q \varrho^s\,\psi_t = \int_Q \varrho^s\, v\cdot\nabla\psi + (1-s)\int_Q \rho^s\, \operatorname{div} v\,\psi\,.$$

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 $\|(\varrho^s)'\|_{L^2(0,T;\,[W^{1,\frac{6\alpha}{6+\alpha}}(\Omega)]^*)} \leq C_0$. Now we consider a solution to the problem

$$\operatorname{div} X = \varrho^s(t) - \bar\varrho^s(t) \text{ in } \Omega,\; X = 0 \text{ on } \partial\Omega$$

We obtain that $\|X\|_{L^\infty(0,T;\,W^{1,\frac{3\alpha}{2\alpha-3}}(\Omega))} \leq C_0$ and that $\|X_t\|_{L^{2,\frac{6\alpha}{7\alpha-6}}(Q)} \leq C_0$. We see again that $\int_Q p\, \operatorname{div} X$ is finite, and the claim follows. □

B A special estimate for $\sigma > 0$ and $\tau > 0$

In the case $\sigma > 0$, the dissipation inequality provides $\sqrt{\sigma}\, \|\nabla\mu\|_{L^2(Q)} \leq C_0$ as an additional information. Thus, a gradient bound for *all* coordinates of the vector μ. We recall that we can always express $\rho = \nabla h^*(\mu)$ with the mapping of Lemma 4.7, and therefore

$$\nabla\rho = (\nabla\mu \cdot D^2 h^*(\mu))\,. \tag{81}$$

By means of the inequality (38), this shows that

$$|\nabla\rho| \leq C_1\, \varrho\, |\nabla\mu|\,. \tag{82}$$

Lemma B.1. *Assume* $\sigma > 0$*. Then* $\|\ln\varrho\|_{W^{1,0}_2(Q)} \leq C_0\, \sigma^{-1/2}$*.*

Proof. Let $1 > \gamma > 0$. Due to (81), (82)

$$|\nabla\ln(\varrho+\gamma)| \leq C_1\, \frac{\varrho}{\varrho+\gamma}\, |\nabla\mu| \leq C_1\, |\nabla\mu|\,.$$

Thus, $\sqrt{\sigma}\, \|\nabla\ln(\varrho+\gamma)\|_{L^2(Q)} \leq C$. Let $\epsilon > 0$. For $t \in]0,T[$, we can always show that $|\{x \in \Omega\,:\, \ln(\varrho(t)+\gamma) \leq \epsilon^{-1}\}| \geq |\Omega| - C_0\, e^{-\frac{1}{\epsilon}}$. Applying (68) (see the proof of Lemma 8.2), we find a decomposition $]0,T[= I_1 \cup I_2$ such that

$$\begin{cases} \int_\Omega |\ln(\varrho(t)+\gamma)| \leq C^*(\delta)\, \big((\|\nabla\ln(\varrho(t)+\gamma)\|_{L^1(\Omega)} + \epsilon^{-1}\big) & \text{for } t \in I_1\\ |\{x\in\Omega\,:\, \ln(\varrho(t)+\gamma) \geq -\epsilon^{-1}\}| \leq \delta & \text{for } t \in I_2\,. \end{cases}$$

In particular, choosing $\gamma < 2^{-1}\, e^{-1/\epsilon}$,

$$\begin{cases} \int_\Omega |\ln(\varrho(t)+\gamma)| \leq C^*(\delta)\, (\|\nabla\ln(\varrho(t)+\gamma)\|_{L^1(\Omega)} + \epsilon^{-1}) & \text{for } t \in I_1\\ |\{x\in\Omega\,:\, \varrho(t) \geq 2^{-1}\, e^{-1/\epsilon}\}| \leq \delta & \text{for } t \in I_2\,. \end{cases}$$

Due to the global mass conservation, we find parameter $\epsilon_0 > 0,\ \delta_0 > 0$ depending only on the data such that $I_2 \equiv \emptyset$ for all $\delta \leq \delta_0$ and $\epsilon \leq \epsilon_0$. Thus

$$\int_\Omega |\ln(\varrho(t)+\gamma)| \leq C^*(\delta_0)\, (\|\nabla\ln(\varrho(t)+\gamma)\|_{L^1(\Omega)} + \epsilon_0^{-1}) \text{ for } t \in]0,T[\,.$$

It follows that $\int_Q |\ln(\varrho(t)+\gamma)| \leq C^*(\delta_0)\, (C_0\, \sigma^{-1/2} + \epsilon_0^{-1})$, and letting γ tend to zero, the claim follows. □

The Lemma B.1 allows to show the following statement.

Lemma B.2. *Assume* $\sigma > 0$*. Then*

$$\|((\mathbb{1}\cdot J^\sigma)\cdot\nabla\ln\varrho_\sigma)^+\|_{L^1(Q)} \leq C_0\, \sqrt{\sigma}\,.$$

Proof. Recall that $\varrho_\sigma = \sum_{i=1}^N \partial_i h^*_{\tau,\delta}(\mu^\sigma)$. 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. (42)). Thus

$$D^2_{i,j} h^*_{\tau,\delta}(X) = D^2_{i,j}(h_\delta)^*(X) + \tau\,\omega''(X_i)\,\delta_{i,j}\,.$$

Making use of (38) and of the definition of $h^*_{\delta,\tau}$

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

Moreover, owing to the choice of ω, there is a positive constant c_3 such that $\omega''(X_i) \leq c_3\,\omega'(X_i)$ for all $X \in \mathbb{R}^N$ (cf. (43)), and therefore

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

The two latter inequalities imply for $i, j = 1, \ldots, N$ that

$$\frac{|D^2_{i,j} h^*_{\tau,\delta}(\mu^{\sigma,\delta})|}{\varrho_{\sigma,\delta}} \leq C_1 + c_3 =: C_2 \, . \tag{83}$$

For a while we are now going to forget about the δ indices. We compute that

$$\begin{aligned}\nabla \ln \varrho_\sigma &= \varrho_\sigma^{-1} \sum_{i,j=1}^N D^2_{i,j} h^*_\tau(\mu^\sigma)\,\nabla\mu^\sigma_j \\ &= \frac{D^2 h^*_\tau \mathbb{1}\cdot\mathbb{1}}{\sqrt{N}\,\varrho_\sigma}\,\nabla(\mu^\sigma\cdot\mathbb{1}) + \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot\xi^\ell}{\varrho_\sigma}\,\nabla(\mu^\sigma\cdot\xi^\ell)\,,\end{aligned}$$

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 $D_k := \nabla\mu^\sigma_k + \frac{z_k}{m_k}\nabla\phi_\sigma$, we obtain that

$$\nabla \ln \varrho_\sigma = \frac{D^2 h^*_\tau \mathbb{1}\cdot\mathbb{1}}{\sqrt{N}\,\varrho_\sigma}\,(\mathbb{1}\cdot D) + \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot\xi^\ell}{\varrho_\sigma}\,(\xi^\ell\cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot\frac{z}{m}}{\varrho_\sigma}\,\nabla\phi_\sigma \, .$$

Making use of the identity $-\sum_{i=1}^N J^{i,\sigma} = \sigma\,(\mathbb{1}\cdot D)$

$$\begin{aligned}-\sum_{i=1}^N J^{i,\sigma}\cdot\nabla\ln\varrho_\sigma &= \sigma\,\frac{D^2 h^*_\tau \mathbb{1}\cdot\mathbb{1}}{\sqrt{N}\,\varrho_\sigma}\,(\mathbb{1}\cdot D)^2 \\ &- \sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot\xi^\ell}{\varrho_\sigma}\,(\sum_{i=1}^N J^{i,\sigma})\cdot(\xi^\ell\cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot\frac{z}{m}}{\varrho_\sigma}\,(\sum_{i=1}^N J^{i,\sigma}\cdot\nabla\phi_\sigma) \\ &\geq -\sum_{\ell=1}^{N-1} \frac{D^2 h^*_\tau \mathbb{1}\cdot\xi^\ell}{\varrho_\sigma}\,(\sum_{i=1}^N J^{i,\sigma})\cdot(\xi^\ell\cdot D) - \frac{D^2 h^*_\tau \mathbb{1}\cdot\frac{z}{m}}{\varrho_\sigma}\,(\sum_{i=1}^N J^{i,\sigma}\cdot\nabla\phi_\sigma)\,.\end{aligned} \tag{84}$$

Since $|\xi^\ell\cdot D| \leq c\,|\Pi\,D| \leq c\,\sqrt{MD\cdot D}$ for $\ell = 1, \ldots, N-1$, it follows that

$$\|(\sum_{i=1}^N J^{i,\sigma})\cdot(\xi^\ell\cdot D)\|_{L^1(Q)} \leq \|\sum_{i=1}^N J^{i,\sigma}\|_{L^2(Q)}\,\|\Pi\,D\|_{L^2(Q)} \leq C_0\,\sqrt{\sigma}$$

$$\|(\sum_{i=1}^N J^{i,\sigma})\cdot\nabla\phi_\sigma\|_{L^1(Q)} \leq \|\sum_{i=1}^N J^{i,\sigma}\|_{L^2(Q)}\,\|\nabla\phi_\sigma\|_{L^2(Q)} \leq C_0\,\sqrt{\sigma}\,.$$

Thus, (83) and (84) imply that

$$\|((\mathbb{1}\cdot J^\sigma)\cdot\nabla\ln\varrho_\sigma)^+\|_{L^1(Q)} \leq C_0\,\tilde{C}_1\,\sqrt{\sigma}\,.$$

□

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