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Analysis of improved Nernst–Planck–Poisson models of isothermal compressible electrolytes subject to chemical reactions: The case of a degenerate mobility matrix

Pierre-Etienne Druet

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Weierstrass Institute
Mohrenstr. 39
10117 Berlin
Germany
E-Mail: pierre-etienne.druet@wias-berlin.de

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Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS)
Leibniz-Institut im Forschungsverbund Berlin e. V.
Mohrenstraße 39
10117 Berlin
Germany

Fax: +49 30 20372-303
E-Mail: preprint@wias-berlin.de
World Wide Web: http://www.wias-berlin.de/

Abstract

We continue our investigations of the improved Nernst–Planck–Poisson model introduced in [DGM13]. In the paper [DDGG16] the analysis relies on the hypothesis that the mobility matrix has maximal rank under the constraint of mass conservation (rank $N-1$ for a mixture of N species). In this paper we allow for the case that the positive eigenvalues of the mobility matrix tend to zero along with the partial mass densities of certain species. In this approach the mobility matrix has a variable rank between zero and $N-1$ according to the number of locally available species. We set up a concept of weak solution able to deal with this scenario, showing in particular how to extend the fundamental notion of *differences of chemical potentials* that supports the modelling and the analysis in [DDGG16]. We prove the global-in-time existence in this solution class.

1 Introduction

We consider a bounded domain $\Omega \subset \mathbb{R}^3$ representing an electrolytic solution. The boundary of Ω possesses a disjoint decomposition $\partial\Omega = \Gamma \cup \Sigma$: The surface Γ represents an *active surface*, an interface between the electrolyte and an external material. In the context of batteries this external material is often a metallic 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 specific volume $V_i \in \mathbb{R}_+$. We assume that the system is isothermal. In $]0, T[\times\Omega$ the mixture obeys the following system of partial differential equations

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

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

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

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. We assume that its density $\varrho\psi$ is given in the form $\varrho\psi = h(\theta,\, \rho)$, where the function h is defined via

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

Here h_i^{ref} ($i = 1, \ldots, N$) are constants related to certain reference states of the pure constituents. The *number densities* $n_1, \ldots, n_N$ 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 $\mu_i = \partial_{\rho_i} h(\theta,\, \rho_1, \ldots, \rho_N)$ for $i = 1, \ldots, N$. Thus, under the particular constitutive assumption (4)

$$\mu_i = c_i + K\, \tfrac{V_i}{m_i}\, F'(n \cdot V) + \tfrac{k_B\, \theta}{m_i}\, \ln y_i \; \text{ for } i = 1, \ldots, N\,, \tag{5}$$

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

$$J^i = -\sum_{j=1}^{N} M_{i,j}\, D^j \quad \text{for } i = 1, \ldots, N\,, \tag{6a}$$

$$D^j := \nabla \left(\frac{\mu_j}{\theta}\right) + \frac{1}{\theta}\, \frac{z_j}{m_j}\, \nabla\phi \quad \text{for } j = 1, \ldots, N \tag{6b}$$

$$r_i = -\sum_{k=1}^{s} \partial_{D_k^{\text{R}}} \Psi(D_1^{\text{R}}, \ldots, D_s^{\text{R}})\, \gamma_i^k, \qquad D_k^{\text{R}} := \gamma^k \cdot \mu \tag{6c}$$

$$\mathbb{S}^{\text{visc}}(\nabla v) = \eta\, D(v) + \lambda\, \operatorname{div} v\, \text{Id} \tag{6d}$$

$$p = -h(\theta,\, \rho) + \sum_{i=1}^{N} \mu_i\, \rho_i \tag{6e}$$

$$n^F = \sum_{i=1}^{N} \tfrac{z_i}{m_i}\, \rho_i \tag{6f}$$

In (6a), 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 (6c), $s \in \mathbb{N} \cup \{0\}$ 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

$\gamma^k := \gamma_i^{\text{stoi},k} m_i$ for $i = 1, \ldots, N$ and $k = 1, \ldots, s$. The reaction potential Ψ is defined on $\mathbb{R}^s$ and assumed convex. The entries of the vector $D^{\text{R}} \in \mathbb{R}^s$ are called reaction driving forces. The assumption (6d) 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 (6e) for the pressure is called the Gibbs-Duhem equation, while (6f) is actually the definition of the free charge density.

The equations (1), (2), (3) with the constitutive equations (6) 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

$$\begin{gathered} v = 0 \text{ on }]0,T[\times\partial\Omega \\ \phi = \phi_0 \text{ on }]0,T[\times\Gamma, \quad \nabla\phi\cdot\nu = 0 \text{ on }]0,T[\times\Sigma \end{gathered} \tag{7}$$

At second, for the diffusion-reaction equation we assume that

$$J^i \cdot \nu = 0 \text{ on }]0,T[\times\partial\Omega \text{ for } i = 1,\ldots,N$$

In connection to (7), this condition means that no adsorption of species is taking place on $]0,T[\times\partial\Omega$. Let us add that due to the preliminary work in the section 5.3 of [DDGG16], we know that surface chemical reactions and surface adsorption can to a certain extend be modelled by the condition $J^i\cdot\nu = -\hat{r}_i^{\Gamma} + J_i^0$. Here $\hat{r}^{\Gamma}$ has the structure of a reaction term and J^0 can be understood as an external source. Our methods fully allow to consider also this more general condition, but as it leads to additional technical work, we will not do it here.

The mobility matrix In [DDGG16], the existence of weak solutions was proved for the case that the *mobility matrix* M is of the form $M = \overline{M}(\rho_1,\ldots,\rho_N)$ with a matrix-valued mapping $\overline{M}$ satisfying the following conditions:

(a) Continuity: $\overline{M}$ is a continuous map from $\mathbb{R}^N_+$ into the set of $\mathbb{R}^{N\times N}$ symmetric, positive semi definite matrices (Notation: $\mathbb{R}^{N\times N}_{\text{sym},+}$);

(b) 'Mass conservation': $\overline{M}(\rho)\,1^N = 0$ for all $\rho\in\mathbb{R}^N_+$ ($1^N := (1,\,1,\ldots,1)\in\mathbb{R}^N$);

(c) Linear growth: There is a constant $\bar{\lambda} > 0$ such that $|\overline{M}(\rho)| \leq \bar{\lambda}\,(1+|\rho|)$ for all $\rho\in\mathbb{R}^N$;

(d) rank $\overline{M} = N-1$: Denoting $\lambda_1(\rho)\geq\lambda_2(\rho)\geq\ldots\geq\lambda_N(\rho) = 0$ the ordered eigenvalues of $\overline{M}(\rho)$, there is $\underline{\lambda} > 0$ such that the second smallest eigenvalue satisfies $\lambda_{N-1}(\rho)\geq\underline{\lambda}$ for all $\rho\in\mathbb{R}^N_+$.

The main result of [DDGG16] shows that, except for the possible occurrence of a complete vacuum (which would be non-physical under the assumptions of the model), the weak solution satisfies $\rho_i > 0$ almost everywhere in $]0,T[\times\Omega$ for $i = 1,\ldots,N$. This means that all N components of the mixture are (almost) everywhere available. In particular, the choices of the mobility matrix allowed in [DDGG16] are suited to describe mixtures that do not exhibit species vanishing.

On the other hand, local species vanishing is certainly a phenomenon of interest. If the mass density ρ_i of a species tends to zero, then also the corresponding diffusion flux J^i must tend to zero. This is a necessary consequence of the physical definition $J^i = \rho_i\,(v^i - v)$ of the diffusion flux. Here v^i is the (partial) velocity of constituent i and v is the barycentric velocity. In the regime of finite velocities, we must expect the asymptotical behaviour

$$\frac{|J^i|}{\rho_i} \leq C\,. \tag{8}$$

In this paper we investigate choices of the matrix M, and we set up a concept of weak solution, that allow for the local emergence of *sub-mixtures* of size strictly smaller than N. More precisely, we assume that the model specifies species that may vanish locally, for which the corresponding fluxes have the property (8). In order to fix ideas, we shall call these species the *critical species*. Thus, from the viewpoint of notation, there is an index set $I_{\overline{M}} \subseteq \{1,\ldots,N\}$ specified by the model, such that for all $i \in I_{\overline{M}}$, the diffusion flux J^i of the species $\mathrm{A_i}$ vanishes if its mass density ρ_i tends to zero. For the map $\overline{M}$ it is therefore natural to assume, instead of (d), that

$$\text{rank}\,\overline{M}(\rho) = |\{1,\ldots,N\}\setminus I_{\overline{M}}| + |\{i \in I_{\overline{M}} \,:\, \rho_i > 0\}| - 1 \tag{9}$$

Here $|\cdot|$ applied to a discrete set denotes the cardinality. The assumption (9) means that the rank of the mobility matrix is $N-1$ minus the number of vanishing species with index in the set $I_{\overline{M}}$. In this paper, we will focus on the assumption that $\overline{M}$ degenerates at linear rate, meaning that there is a constant $C_1 > 0$ such that

$$|\overline{M}_{i,j}(\rho)| \leq C_1\,\rho_i \text{ for all } i,\, j \in I_{\overline{M}}, \quad \rho \in \mathbb{R}^N_{0,+}\,. \tag{10}$$

This is motivated by (8). At second, we require that $\overline{M}$ does not degenerate faster than linearly. Denoting $\lambda_1(\rho) \geq \ldots \geq \lambda_{N-1}(\rho) \geq \lambda_N(\rho)$ the ordered eigenvalues of $\overline{M}(\rho)$, we choose a permutation $\{i_1(\rho),\ldots,i_N(\rho)\}$ of the index set $\{1,\ldots,N\}$ such that the p first indices $\{i_1,\ldots,i_p\}$ correspond to the non-critical species, that is, $\{i_1,\ldots,i_p\} = I^{\mathsf{c}}_{\overline{M}} := \{1,\ldots,N\}\setminus I_{\overline{M}}$ and such that the indices $i_{p+1},\ldots,i_N$ correspond to the ordering $\rho_{i_{p+1}} \geq \ldots, \geq \rho_{i_N}$ of the mass densities. The mapping $\overline{M}$ degenerates at linear rate if there is some $c > 0$ such that

$$\lambda_{k-1}(\rho) \geq c\,\rho_{i_k} \text{ for } k = p+1,\ldots,N\,. \tag{11}$$

It might appear non trivial to verify the condition (11) for concrete choices of $\overline{M}$. In the case of a mapping $\overline{M}$ of class C^1, we can show that the handy criterion

$$\partial_{\rho_k}\overline{M}_{k,k}(\rho) \geq c_0 > 0 \text{ on the hypersurface } \{\rho \in \mathbb{R}_{0,+} \,:\, \rho_k = 0\} \text{ for all } k \in I_{\overline{M}} \tag{12}$$

suffices for (11). Typical examples of a map $\overline{M}$ satisfying (a), (b), (c) and (10), (12) are

$$\overline{M}_{i,j}(\rho) = d\,\rho_i\,\left(\delta_{i,j} - \frac{\rho_j}{\sum_{k=1}^N \rho_k}\right) \text{ for } i,j = 1,\ldots,N\,.$$

Here, $d > 0$ is some diffusion constant. In this case $I_{\overline{M}} = \{1, \dots, N\}$, and making use of (6e), (6f) and $\varrho := \sum_{i=1}^N \rho_i$, the diffusion fluxes are

$$J^i = d\, \rho_i \, \Big(\nabla \mu_i - \tfrac{1}{\varrho} \nabla p + (\tfrac{z_i}{m_i} - \tfrac{n^F}{\varrho}) \nabla \phi \Big) \text{ for } i = 1, \dots, N\,.$$

Every diffusion flux is proportional to the corresponding mass density. A more subtle example is the ansatz of the paper [DGM13], where

$$\overline{M}(\rho) = \mathcal{P}^T \, \mathrm{diag}(d_1 \, \rho_1, \dots, d_{N-1}\, \rho_{N-1}, \, 1)\, \mathcal{P}, \;\; \mathcal{P} := \begin{pmatrix} 1 & 0 & \dots & 0 & -1 \\ 0 & 1 & \dots & 0 & -1 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & -1 \\ 0 & 0 & \dots & 0 & 0 \end{pmatrix} \in \mathbb{R}^{N\times N}\,.$$

In this case, the assumption (10) holds true for $I_{\overline{M}} = \{1, \dots, N-1\}$, and the diffusion fluxes are

$$J^i = \begin{cases} d_i \, \rho_i \, \Big(\nabla (\mu_i - \mu_N) + (\frac{z_i}{m_i} - \frac{z_N}{m_N}) \nabla \phi \Big) & \text{if } i < N \\ - \sum_{k=1}^{N-1} J^k & \text{for } i = N \end{cases}.$$

Thus the species $\mathrm{A_N}$ (the solvent in electrochemical applications) enjoys a singular status.

The assumption $M = \overline{M}(\rho)$ in connection to (10) leads to difficulties in mathematical analysis in connection to two possible extreme behaviours of the total mass density ϱ: emergence of a vacuum ($\varrho = 0$) or blow-up ($\varrho = +\infty$). We are not able to overcome them directly. Though the principal modelling principles based on (4) and (6) in fact completely fail if the total mass density is lower/larger than some critical positive values, the analysis has to require an extension of the constitutive relations (6a) also in extreme cases. Instead of $M = \overline{M}(\rho)$, we will therefore investigate a model where the mobility matrix depends on a regularised mass density

$$M = f_0(\varrho) \, \overline{M}(\tilde{\rho}^{\delta_0})\,. \tag{13}$$

Here, $f_0 \in C^{0,1}(\mathbb{R}^+)$ is a globally Lipschitz continuous function bounded away from zero by some positive constant $\underline{f}_0$. The parameter $\delta_0 > 0$ is an arbitrarily small, but fixed number, and the *modified mass density vector* $\tilde{\rho}^{\delta_0} \in \mathbb{R}^N_+$ associated with $\rho \in \mathbb{R}^N_+$ is chosen to satisfy

$$\tilde{\rho}^{\delta_0} = \rho \qquad\qquad \text{for } \delta_0 \le \sum_{i=1}^N \rho_i \le \delta_0^{-1} \tag{14}$$

$$c_0(\varrho)\, \tilde{\rho}_i^{\delta_0} \le \rho_i \le c_1(\varrho)\, \tilde{\rho}_i^{\delta_0} \text{ for } i = 1, \dots, N\,. \tag{15}$$

The functions $c_0, \, c_1$ in (15) are positive, continuous functions defined on $]0, +\infty[$. The model (13) possesses the following properties:

- It is, due to (14), identical with the original model $M = \overline{M}(\rho)$ in the range of admissible total mass densities $\delta_0 \le \varrho \le \delta_0^{-1}$ (for appropriate choices of f_0);
- It provides, in view of (15), the correct asymptotic of species vanishing for all $0 < \varrho < +\infty$;
- Allows to overcome the analytical difficulties associated with the possible emergence of a vacuum, or the blow-up of the mass density.

Assumptions on the remaining data For the analysis we assume $F \in C(\mathbb{R}_{0,+}) \cap C^2(\mathbb{R}^+)$ is convex. Moreover, we assume that there are $\frac{3}{2} < \alpha < +\infty$ and constants $0 < c_0,\ c_1$ such that

$$F(s) \geq c_0\, s^{\alpha} - c_1 \quad \text{for all } s > 0\,. \tag{16}$$

In the neighbourhood of zero, we assume that $F(s)$ behaves like $s \ln s$, more precisely we assume that there is $s_0 > 0$ and constants $k_0,\ k_1 > 0$ such that

$$\frac{k_0}{s} \leq F''(s) \leq \frac{k_1}{s} \text{ for all } s \in [0,\ s_0]\,. \tag{17}$$

It was show in the paper [DDGG16] that these assumptions are favourable. For the reaction potential Ψ, we assume that it is of class $C^2(\mathbb{R}^s)$, non-negative, that $\nabla\Psi(0) = 0$ and moreover that

$$\frac{\Psi(D^{\mathsf{R}})}{|D^{\mathsf{R}}|} \to \infty \text{ for } |D^{\mathsf{R}}| \to \infty\,. \tag{18}$$

The domain $\Omega \subset \mathbb{R}^3$ possesses a boundary of class $\mathcal{C}^{0,1}$. In connection to 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

$$\begin{aligned} -\triangle u = f \text{ in } [W^{1,\beta'}_{\Gamma}(\Omega)]^* \text{ implies } u \in W^{1,\beta}_{\Gamma}(\Omega) \\ \text{for all } f \in [W^{1,\beta'}_{\Gamma}(\Omega)]^* \text{ and all } \beta \in]r',\ r[\,. \end{aligned} \tag{19}$$

We require that (see [DDGG16] for details)

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

whit α from (16). This of course might be a restriction only if $\alpha < 2$. For the boundary data, we assume that

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

2 Sub-mixtures

In this section we show that the assumption (4) on the free energy function h and the assumption (10) for the mapping $\overline{M}$ allow at the formal level for a model consistent local reduction of the number of constituents of the mixture. We define for $(t,\ x) \in Q$ the local dimension number

$$N_1(\rho(t,\ x)) := |\{i \in \{1, \ldots, N\}\ :\ \rho_i(t,\ x) > 0\}|\,.$$

If $N_1 < N$, a sub-mixture occurs locally in Q. We then expect that the equations (1) and the constitutive equations (6) possess natural extensions so that the sub-mixture is described by the same modelling principles. In the remainder of the paper $I \subset \{1, \ldots, N\}$ always denote an ordered index set, and $I^{\mathsf{c}} := \{1, \ldots, N\} \setminus I$.

Proposition 2.1. *Assume* (10) *for a given index set* $I_{\overline{M}}$. *Then, the model for a mixture of* N *species based on the equations* (1) *and the constitutive relations* (6) *allows (formally) for the consistent occurrence of every sub-mixture associated with an index set* $I = \{i_1, \ldots, i_{N_1}\} \supseteq I^c_{\overline{M}}$. *Then, by definition* $\rho_i > 0$ *for* $i \in I$ *and* $\rho_i = 0$ *for* $i \in I^c$. *We define* $\rho^I := (\rho_{i_1}, \ldots, \rho_{i_{N_1}})$ *and further*

$$h^I(\theta,\, \rho^I) := \sum_{i\in I} h_i^{\mathit{ref}}\, \rho_i + K\, F(\sum_{i\in I} V_i\, n_i) + k_B\, \theta \sum_{i\in I} n_i \sum_{i\in I} y_i\, \ln y_i\,, \tag{21}$$

and $\mu^I := \nabla_{\rho^I} h^I(\theta,\, \rho^I)$. *Then there are:*

(1) A continuous mapping $\overline{M}^I$ *from* $\mathbb{R}^{N_1}_+$ *into* $\mathbb{R}^{N_1\times N_1}_{\mathit{sym},+}$ *such that* $\overline{M}^I\, 1^{N_1} = 0$ *on* $\mathbb{R}^{N_1}_+$;

(2) A number $s^I \in \mathbb{N} \cup \{0\}$, $s^I \leq s$;

(3) Vectors $\gamma^{I,1}, \ldots, \gamma^{I,s^I} \in \mathbb{R}^N$ *satisfying* $\gamma_i^{I,k} = 0$ *for* $i \in I^c$ *and the conditions*

$$\sum_{i\in I} \gamma_i^{I,k} = 0, \quad \sum_{i\in I} \gamma_i^{I,k}\, \frac{z_i}{m_i} = 0 \text{ for } k = 1, \ldots, s^I\,;$$

(4) A convex, non negative potential Ψ^I *defined on* $\mathbb{R}^{s^I}$ *such that* $\nabla\Psi^I(0) = 0$

such that the constitutive relations (6) *allow for the following natural extensions:*

$$J^i = -\sum_{j\in I} \overline{M}^I_{i,j}(\rho^I)\, D^j \quad \text{for } i \in I\,,\ D^j := \nabla\left(\frac{\mu^I_j}{\theta}\right) + \frac{1}{\theta}\, \frac{z_j}{m_j}\, \nabla\phi \quad \text{for } j \in I$$

$$r_i = -\sum_{k=1}^{s^I} \partial_k \Psi^I(D_1^{I,R}, \ldots, D_{s^I}^{I,R})\, \gamma_i^{I,k} \quad \text{for } i \in I \qquad D_k^{I,R} = \gamma^{I,k}\cdot\mu \text{ for } k = 1, \ldots, s^I$$

$$p = -h^I(\theta,\, \rho^I) + \sum_{i\in I} \mu_i\, \rho_i, \quad n^F = \sum_{i\in I} \frac{z_i}{m_i}\, \rho_i$$

The remainder of the section is devoted to the formal proof of this result. At first it is obvious that if ρ_i tends to zero for $i \in I^{\mathrm{c}}$, then $h(\theta,\, \rho)$ converges to $h^I(\theta,\, \rho^I)$, and μ_{i_k} tends to $\nabla_{\rho^I_{i_k}} h^I(\rho^I)$ for $k = 1, \ldots, N_1$. Since we can verify that $\rho_i\, \mu_i$ tends to zero for $i \in I^{\mathrm{c}}$, the pressure p tends to $p^I := -h^I + \sum_{i\in I} \rho_i\, \mu_i$.

Second, the theory of mixtures in [DGM13] requires the existence of a mobility matrix $M^I \in \mathbb{R}^{N_1\times N_1}_{\mathrm{sym},+}$ subject to the constraint $M^I\, 1^{N_1} = 0$ such that the diffusion fluxes obey

$$J^i = \begin{cases} -\sum_{j\in I} M^I_{i,j}\, \left(\nabla\mu_j + \frac{z_j}{m_j}\, \nabla\phi\right) & \text{for } i \in I \\ 0 & \text{for } i \in I^{\mathrm{c}} \end{cases}$$

Under (10), we simply call $\overline{M}^I(\rho) \in \mathbb{R}^{N_1\times N_1}_{\mathrm{sym},+}$ the sub-block associated with cancelling in $\overline{M}(\rho)$ the raws and columns of indices in I^c. Then, we can verify that

$$\operatorname{rank} \overline{M}^I = N_1 - 1, \quad \overline{M}^I\, 1^{N_1} = 0\,.$$

For the chemical reactions, the situation is more complex. We start with some elementary algebraic considerations. If $I = \{i_1, \ldots, i_{N_1}\} \subset \{1, \ldots, N\}$ is an ordered index set of cardinality N_1, we introduce for $X \in \mathbb{R}^N$ the vector $P_I(X) \in \mathbb{R}^N$ such that $(P_I(X))_j = X_j$ for $j \in I$ and $(P_I(X))_j = 0$ for $j \in I^{\mathrm{c}}$.

Let $\gamma^1, \ldots, \gamma^s$ be the vectors associated with the reactions. We introduce

$$\mathcal{V} = \mathcal{V}^I := \operatorname{span}\{P_{I^{\mathrm{c}}}(\gamma^1), \ldots, P_{I^{\mathrm{c}}}(\gamma^s)\}$$
$$d = d^I := \dim \mathcal{V} \leq \min\{|I^{\mathrm{c}}|,\, s\}\,.$$

For notational simplicity, we will assume that the d first vectors $P_{I^{\mathrm{c}}}(\gamma^1),\,\ldots,\,P_{I^{\mathrm{c}}}(\gamma^d)$ are linearly independent. If the number of reactions s is strictly larger than d, then we can moreover introduce coefficients $\{A^j_\ell\}_{j=1\ldots,s-d,\;\ell=1,\ldots,d}$ such that

$$P_{I^{\mathrm{c}}}(\gamma^{d+j}) = \sum_{\ell=1}^{d} A^j_\ell P_{I^{\mathrm{c}}}(\gamma^\ell)\,. \tag{22}$$

For $k = 1, \ldots, s-d$ we now define a reduced vector

$$\gamma^{I,k} := \gamma^{d+k} - \sum_{\ell=1}^{d} A^k_\ell\, \gamma^\ell\,.$$

We verify easily that $P_{I^{\mathrm{c}}}(\gamma^{I,k}) = 0$. Since moreover $\gamma^{I,k}$ belongs to the span of $\gamma^1, \ldots, \gamma^s$, the properties of these vectors imply that

$$\gamma^{I,k} \cdot 1^N = 0, \quad \gamma^{I,k} \cdot \frac{z}{m} = 0 \text{ for } k = 1, \ldots, s-d\,.$$

so that the vectors $\gamma^{I,1}, \ldots, \gamma^{I,s-d}$ vectors can be identified again as describing admissible reactions for the mixture associated with the indices in I. In order to finish the proof of Proposition 2.1 concerning the reactions, we now need to quote an auxiliary Lemma. The proof is entirely algebraic and we give it in the Appendix.

Lemma 2.2. *Let $I = \{i_1, \ldots, i_{N_1}\} \subset \{1, \ldots, N\}$ be an ordered index set of cardinality $1 \leq N_1 \leq N$. Denote $d^I = \dim \mathcal{V}^I$, and $s^I := s - d^I$.*

Then, there are:

- *A function $\hat{\Psi}^I \in C^1(\mathbb{R}^{s^I} \times \mathbb{R}^{d^I})$, $(Y,\, w) \mapsto \hat{\Psi}^I(Y,\, w)$ such that for all $w \in \mathbb{R}^{d^I}$ the mapping $Y \mapsto \hat{\Psi}^I(Y,\, w)$ is of class $C^2(\mathbb{R}^{s^I})$, strictly convex, and achieves its minimum at zero;*
- *A mapping $r^0 : \mathbb{R}^{d^I} \to \operatorname{span}\{\gamma^{I,k}\}_{k=1,\ldots,s^I}$ of class $C^1(\mathbb{R}^{d^I})$ with $r^0(0) = 0$;*

such that the algebraic equations $-\sum_{k=1}^{s} \partial_k \Psi(\gamma^1 \cdot \mu, \ldots, \gamma^s \cdot \mu)\, \gamma^k = r$ are valid for $\mu \in \mathbb{R}^N$ and $r \in \operatorname{span}\{\gamma^1, \ldots, \gamma^s\}$ if and only if

$$r = -\sum_{k=1}^{s^I} \partial_{Y_k} \hat{\Psi}^I(\gamma^{I,1} \cdot \mu, \ldots, \gamma^{I,s^I} \cdot \mu;\, \tilde{r})\, \gamma^{I,k} + \sum_{j=1}^{d^I} \tilde{r}_j\, \gamma^j + r^0(\tilde{r})\,,$$

where $\tilde{r}_1, \ldots, \tilde{r}_{d^I}$ are the coordinates of $P_{I^{\mathrm{c}}}(r)$ in $\mathcal{V}^I$ (in the basis $\{P_{I^{\mathrm{c}}}(\gamma^k)\}_{k=1,\ldots,d^I}$).

Assuming for now the validity of Lemma 2.2, we consider the sub-mixture such that $\rho_i = 0$ for $i \in I^{\mathrm{c}}$ in a point of Q. Then, the function ρ_i has a global minimum in this point such that also the derivatives satisfy $\partial_t \rho_i = 0 = \partial_x \rho_i$. Then, the Pdes (1) formally yield

$$\begin{aligned} r_i &= \partial_t \rho_i + \rho_i \operatorname{div} W^i + W^i \cdot \nabla \rho_i = 0 \text{ for } i \in I^{\mathrm{c}} \\ W^i &:= v + J^i/\rho_i \text{ for } i = 1, \ldots, N\,. \end{aligned} \tag{23}$$

Thus the coordinates $\tilde{r}_1, \ldots, \tilde{r}_{d^I}$ of r in $\mathcal{V}^I$ are trivial. For $Y \in \mathbb{R}^{s^I}$, we define $\Psi^I(Y) := \hat{\Psi}^I(Y, 0)$, and the Lemma 2.2 yields (at the formal level) $r = -\sum_{k=1}^{s^I} \partial_k \Psi^I(\gamma^{I,1} \cdot \mu, \ldots, \gamma^{I,s^I} \cdot \mu)\, \gamma^{I,k}$. This finishes the proof of the Proposition 2.1.

3 The concept of solution

As in the paper [DDGG16], the analytical apparatus requires a relaxation of the concept of solution in order to deal with 1) the fact that the mobility matrix has not full rank and 2) the possible occurrence of vacuum. In this paper we must in addition relax the formal model set up in the section 2 concerning sub-mixtures, because the non-linearity of the reaction rates introduces effects that are not captured by the formal reduction of section 2.

We at first introduce a notation. Let $I = \{i_1, \ldots, i_{|I|}\} \subseteq \{1, \ldots, N\}$ be an ordered index set of cardinality $|I|$. Then we define

$$Q^I := \{(t,\, x) \in Q \,:\, \rho_i(t,\, x) > 0 \,\forall\, i \in I, \quad \rho_i(t,\, x) = 0 \,\forall\, i \in I^c\} \tag{24}$$

For two different index sets $I_1,\, I_2$ we have $\lambda_4(Q^{I_1} \cap Q^{I_2}) = 0$. Due to the problem of occurrence of a possible vacuum described in [DDGG16], we can expect to meaningfully introduce the variable q only on the set

$$Q^+(\varrho) := \{(t,\, x) \in Q \,:\, \varrho(t,\, x) > 0\}\,.$$

We next introduce the main concepts needed to describe the solution class: relative chemical potentials, representation of diffusion and reaction phenomena.

3.1 Relative chemical potentials

For a mixture of N constituents, we used in the paper [DDGG16] the variables $\Pi\mu \in \mathbb{R}^{N-1}$ and called the components of this vector 'relative chemical potentials'. Here $\Pi : \mathbb{R}^N \to \mathbb{R}^{N-1}$ is a linear reduction operator defined by means of an arbitrary, but fixed basis $\{\eta^1, \ldots, \eta^{N-1}\}$ of the plane

$$(1^N)^\perp := \{X \in \mathbb{R}^N \,:\, 1^N \cdot X = \sum_{i=1}^N X_i = 0\}$$

via $\Pi\mu := (\mu \cdot \eta^1, \ldots, \mu \cdot \eta^{N-1})$. In the case that the mixture is allowed to reduce locally its index N, this procedure has no natural extension. Nevertheless there is a way to meaningfully introduce relative chemical potentials: We define for $\mu \in \mathbb{R}^N$

$$q = \mu - \max_{j=1,\ldots,N} \mu_j \, 1^N \,. \tag{25}$$

We immediately see that $q_i \leq 0$ for $i = 1, \ldots, N$. Moreover there is i such that $q_i = 0$. Thus the natural domain of the variable q is the $N-1$ dimensional hypersurface $\partial \mathbb{R}^N_-$.

If only $N_1 < N$ species, corresponding to an index set I of indices, are available on a subset Q^I, then $\mu_k = -\infty$ for all $k \in I^c$. Thus, $q_i = \mu_i - \max_{j=1,\ldots,N} \mu_j = \mu_i - \max_{j \in I} \mu_j$ for $i \in I$. In this way, the finite relative chemical potentials are nothing else but the relative chemical potentials of the smaller mixture, and we see that this concept is robust under the reduction of the number of species. Now, a solution to the system of diffusion–reaction equations (1) by given barycentric velocity and electric fields consists of

- A scalar function $\varrho : \; Q \to \mathbb{R}_{0,+}$ (total mass density);
- A vector field $q : \; Q \to \overline{\partial \mathbb{R}^N_-}$ (relative chemical potentials).

The state-variables $\rho_1, \ldots, \rho_N$ are recovered from the total mass density and the (relative) chemical potentials using a similar strategy as in the paper [DDGG16].

Proposition 3.1. *Assume the free energy function h satisfies the ansatz* (4)*, and that the function F belongs to $C^2(\mathbb{R}_+) \cap C(\mathbb{R}_{0,+})$, is convex and possesses a surjective first derivative F'. Then there are mappings:*

- $\mathscr{R} \in C(\mathbb{R}_{0,+} \times \partial \mathbb{R}^N_-; \, \mathbb{R}^N) \cap C^1_{pw}(\mathbb{R}_+ \times \partial \mathbb{R}^N_-; \, \mathbb{R}^N)$*;*
- $\mathscr{M} \in C(\mathbb{R}_+ \times \partial \mathbb{R}^N_-) \cap C^1_{pw}(\mathbb{R}_+ \times \partial \mathbb{R}^N_-)$

such that the non-linear algebraic equations $\mu = \nabla_\rho h(\rho)$ are valid for $\mu \in \mathbb{R}^N$ and $\rho \in \mathbb{R}^N_+$ if and only if there are $\varrho \in \mathbb{R}_+$ and $q \in \partial \mathbb{R}^N_-$ such that

$$\rho = \mathscr{R}(\varrho, \, q), \quad \rho \cdot 1^N = \varrho \text{ and } \mu - \max_{i=1,\ldots,N} \mu_i \, 1^N = q, \quad \max_{i=1,\ldots,N} \mu_i = \mathscr{M}(\varrho, \, q) \,.$$

We prove Proposition 3.1 in the section 4 devoted to preliminary results below. As a fundamental peculiarity of the present problem, the chemical potentials might assume infinite values. Indeed it is obvious to verify that $q_i = -\infty$ for all i such that $\rho_i = 0$. We will therefore need the following complement to Proposition 3.1:

Lemma 3.2. *The mappings $\mathscr{R}$, $\mathscr{M}$ possess natural extensions*

- $\mathscr{R} \in C(\mathbb{R}_+ \times \overline{\partial \mathbb{R}^N_-}; \, \mathbb{R}^N) \cap C^1_{pw}(\mathbb{R}_+ \times \overline{\partial \mathbb{R}^N_-}; \, \mathbb{R}^N)$*;*
- $\mathscr{M} \in C(\mathbb{R}_+ \times \overline{\partial \mathbb{R}^N_-}) \cap C^1_{pw}(\mathbb{R}_+ \times \overline{\partial \mathbb{R}^N_-})$.

This means that for every ordered index set $I = \{i_1, \ldots, i_{N_1}\} \subset \{1, \ldots, N\}$ of cardinality $1 \leq N_1 < N$, there are

- $\mathscr{R}^I \in C(\mathbb{R}_{+,0} \times \partial\mathbb{R}^{N_1}_-;\, \mathbb{R}^{N_1}) \cap C^1_{pw}(\mathbb{R}_+ \times \partial\mathbb{R}^{N_1}_-;\, \mathbb{R}^{N_1})$;
- $\mathscr{M}^I \in C(\mathbb{R}_+ \times \partial\mathbb{R}^{N_1}_-) \cap C^1_{pw}(\mathbb{R}_+ \times \partial\mathbb{R}^{N_1}_-)$

such that if $\{q^n\}_{n\in\mathbb{N}} \subset \partial\mathbb{R}^N_-$ *is a sequence satisfying*

$$\exists\, q_i = \lim_{n\to\infty} q^n_i \text{ for } i \in I, \quad \limsup_{n\to\infty} q^n_i = -\infty \text{ for } i \in I^c\,,$$

then $\mathscr{R}(\varrho,\, q^n) \to \mathscr{R}^I(\varrho,\, q^I)$ *and* $\mathscr{M}(\varrho,\, q^n) \to \mathscr{M}^I(\varrho,\, q^I)$*, with* $q^I := (q_{i_1}, \ldots, q_{i_{N_1}})$*. Moreover for the function* h^I *from* (21) *the non-linear algebraic equations* $\mu^I = \nabla_{\rho^I} h^I(\rho^I)$ *are valid for* $\mu^I \in \mathbb{R}^{N_1}$ *and* $\rho^I \in \mathbb{R}^{N_1}_+$ *if and only if there are* $\varrho \in \mathbb{R}_+$ *and* $q^I \in \partial\mathbb{R}^{N_1}_-$ *such that*

$$\rho^I = \mathscr{R}^I(\varrho,\, q), \quad \rho^I \cdot 1^{N_1} = \varrho$$
$$\mu^I - \max_{i=1,\ldots,N_1} \mu^I_i\, 1^{N_1} = q^I, \quad \max_{i=1,\ldots,N_1} \mu^I_i = \mathscr{M}^I(\varrho,\, q^I)\,.$$

This statement is proved in the algebraic section 4 as well.

3.2 Diffusion fluxes and diffusion entropy production

Due to the fact that the chemical potentials are allowed to assume infinite values, we must in comparison to [DDGG16] change our approach on diffusion phenomena. Basically the vector J of diffusion fluxes is incorporated to the solution vector.

In order to obtain a global representation of the fluxes J that is making the connection to the chemical potentials, we exploit a new (weighted) estimate that shows that the so-called *normalised mass densities* $\rho^{\text{norm}} := \mathscr{R}(1,\, q)$ are bounded in the class $W^{1,0}_2(Q;\, \mathbb{R}^N)$. Here $\mathscr{R}$ denotes the mapping mentioned in the Proposition 3.1 and the Lemma 3.2. Making use of the identity $q = \nabla h(\rho^{\text{norm}}) - \max_{i=1,\ldots,N} \nabla_i h(\rho^{\text{norm}})\, 1^N$, we obtain the equivalent representation

$$\sum_{j=1}^N M_{i,j}\, \nabla q_j = \sum_{k=1}^N \Bigg(\underbrace{\sum_{j=1}^N M_{i,j}\, D^2_{j,k} h(\rho^{\text{norm}})}_{=\mathcal{D}_{i,k}} \Bigg)\, \nabla \mathscr{R}_k(1,\, q)\,. \tag{26}$$

We call the newly introduced matrix $\mathcal{D} := M\, D^2 h(\rho^{\text{norm}})$ a diffusion matrix.

The natural energy identity for the problem (1), (2), (3) has been derived in [DDGG16], Definition 4.2. In comparison to this paper, we also use another representation of the entropy production due to diffusion. In the case that the rank of the mobility matrix M is $N-1$ we have

$$\xi_D := \sum_{i=1}^N J^i \cdot D^i = M\, D \cdot D = M^{-1}\, J \cdot J$$
$$M^{-1}\, J \cdot J := \sum_{i=1}^{N-1} \frac{1}{\lambda_i(M)}\, (e^i(M) \cdot J)^2\,. \tag{27}$$

Here, $\lambda_1(M), \ldots, \lambda_{N-1}(M)$ denote the positive eigenvalues of M. The corresponding eigenvectors are denoted $e^1(M), \ldots, e^{N-1}(M)$. Assume now that the mixture can locally reduce its index. If the eigenvalues of M are ordered in such a way that $\lambda_1(M) \geq \ldots \geq \lambda_{N-1}(M)$, then we obtain a natural representation of the entropy production due to diffusion via

$$\xi_D = \sum_{i=1}^{N_2(t,x)-1} \frac{1}{\lambda_i(M)} \, (e^i(M) \cdot J)^2 =: M^{-1} \, J \cdot J \, .$$

Here N_2 is the number defined via $N_2(t, \, x) := |I^{\mathsf{c}}_{\overline{M}}| + |\{i \in I_{\overline{M}} \, : \, \rho_i > 0\}|$.

3.3 Representation of the reactions

The representation of the reaction term for weak solutions is affected by the fact that in approximating schemes, we do not obtain the strong, or pointwise convergence of the components of relative chemical potentials that tend to $-\infty$. Thus, the reaction driving forces $\gamma^k \cdot q$ might oscillate. On the other hand, the relationship between production rate and driving forces is given by $-R = \nabla\Psi(D^{\mathsf{R}})$ and is in general non-linear. Thus we see that, in general, weak limits of production rates and driving forces do not satisfy the latter identity. In fact, a weak limit of the vector D^{R} cannot even be called a driving force for the reactions, since its vanishing does not imply $R = 0$ any more.

We introduce the vector field R of the reaction rates, assuming values in $\mathbb{R}^s$, as a new variable in the solution vector. In this way, the reaction term associated with the weak solution has globally a representation $r_i = \sum_{k=1}^s R_k \, \gamma_i^k$ for $i = 1, \ldots, N$.

The weak limit of the reaction driving force still contributes to entropy. On a set Q^I of the structure (24), we can split the driving force D^{R}_k as

$$D^{\mathsf{R}}_k = \gamma^k \cdot q = \gamma^k \cdot P_I(q) + \gamma^k \cdot P_{I^{\mathsf{c}}}(q) \, .$$

Since $P_I(q)$ is finite on Q^I and since D^{R} satisfies a bound in the Orlicz class L_Ψ due to the energy identity, the component $\gamma^k \cdot P_{I^{\mathsf{c}}}(q)$ remains finite even if $q_i \to -\infty$ for $i \in I^{\mathsf{c}}$. Introduce a linear space $\mathcal{V}^I := \operatorname{span}\{P_{I^{\mathsf{c}}}(\gamma^1), \ldots, P_{I^{\mathsf{c}}}(\gamma^s)\}$. Due to the latter consideration, we obtain that the projection of $P_{I^{\mathsf{c}}}(q)$ in $\mathcal{V}^I$ is bounded in $L^1(Q^I)$. Thus, a weak limit of $\gamma^k \cdot q$ can be described as

$$\gamma^k \cdot (P_I(q) + X^I) \text{ for a certain } X^I \in \mathcal{V}^I \, .$$

Recall that for the reaction entropy production ξ_{R} we have the representation

$$\xi_{\mathsf{R}} = -R \cdot D^{\mathsf{R}} = \Psi(D^{\mathsf{R}}) + \Psi^*(-R) \, .$$

For the weak solution, we obtain due to the previous considerations

$$\xi_{\mathsf{R}} \geq \Psi^*(-R) + \sum_{I \subset \{1,\ldots,N\}} \chi_{Q^I} \, \Psi(\gamma^1 \cdot (P_I(q) + X^I), \ldots, \gamma^s \cdot (P_I(q) + X^I)) \, .$$

Thus, if we define

$$\widetilde{\Psi}^I(q^I) := \inf_{X\in\mathcal{V}^I} \Psi(\gamma^1\cdot(P_I(q)+X^I),\ldots,\gamma^s\cdot(P_I(q)+X^I))\,, \tag{28}$$

we see that $\xi_{\mathsf{R}} \geq \Psi^*(-R) + \sum_I \chi_{Q^I}\,\widetilde{\Psi}^I(q^I) =: \Psi^*(-R) + \widetilde{\Psi}(q)$.

We will make use the latter inequality as a relaxation of the entropy concept concerning the reactions. Only in the case that R depends linearly on D^{R} we also recover the representation of Proposition 2.1 of the reaction density. In this case

$$r_i(t,\,x) = \begin{cases} -\sum_{k=1}^{s^I} \nabla_k \Psi^I(\gamma^{I,1}\cdot q,\ldots,\gamma^{I,s^I}\cdot q)\,\gamma_i^{I,k} & \text{for } i\in I\\ 0 & \text{for } i \in I^c\end{cases}$$

3.4 Weak solution

An essential property of solutions is the energy identity. In the context of weak solutions, it is relaxed to a dissipation inequality.

Definition 3.3. *We say that* $(\varrho,\,q,\,v,\,\phi,\,J,\,R)$ *satisfies the* (global) energy (in)equality *with free energy function* h *and mobility matrix* M *if and only if the associated fields and variables* (6) *satisfy for almost all* $t\in]0,T[$

$$\begin{aligned}
&\int_\Omega \left\{\frac{1}{2}\,\varrho\,v^2 + \frac{1}{2}\,\epsilon_0\,(1+\chi)\,|\nabla\phi|^2 + h(\rho)\right\}(t)\\
&\quad + \int_{Q_t}\left\{\mathbb{S}(\nabla v)\,:\,\nabla v + M^{-1}\,J\cdot J + (\widetilde{\Psi}(q) + \Psi^*(-R))\right\}\\
&\overset{(\leq)}{=} \int_\Omega \left\{\frac{1}{2}\,\varrho_0\,|v^0|^2 + \frac{1}{2}\,\epsilon_0\,(1+\chi)\,|\nabla\phi_0(0)|^2 + h(\rho^0)\right\}\\
&- \int_\Omega \left\{n^F\,\phi_0 - \epsilon_0\,(1+\chi)\,\nabla\phi\cdot\nabla\phi_0\right\}\Big|_0^t + \int_{Q_t}\left\{n^F\,\phi_{0,t} - \epsilon_0\,(1+\chi)\,\nabla\phi\cdot\nabla\phi_{0,t}\right\}\,.
\end{aligned}$$

Here $\tilde{\Psi}$ *is defined via* (28).

The estimates resulting from the energy identity and the assumptions on the data yield the natural solution class for the problem. For the variables ϱ, ϕ and v we introduce the conditions

$$\varrho \in L^{\infty,\alpha}(Q_T;\,\mathbb{R}_{0,+}) \tag{29}$$

$$v \in W^{1,0}_{2,S}(Q_T;\,\mathbb{R}^3) \tag{30}$$

$$\sqrt{\varrho}\,v \in L^{\infty,2}(Q_T;\,\mathbb{R}^3) \tag{31}$$

$$\phi \in L^\infty(Q_T),\quad \nabla\phi \in L^{\infty,\beta}(Q_T;\,\mathbb{R}^3)\,, \tag{32}$$

with the exponents $\alpha > 3/2$ and $r(\Omega,\Gamma) > 2$ of the conditions (16) and (19), and with

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

Due to weighted regularity, the natural class for the variable q is intricate. The relative chemical potentials are a Lebesque measurable mapping $q\,:\,Q^+(\varrho) \to \overline{\partial\mathbb{R}^N_-} = \{q \in [-\infty,\, 0]^N\,:\, q_i = 0$ for at least one $i\}$ such that

$$\mathscr{R}(1,\, q) \in \widetilde{L}^\infty_\varrho(Q;\, \mathbb{R}^N) \cap \widetilde{W}^{1,0}_{\varrho,2}(Q;\, \mathbb{R}^N)\,. \tag{33}$$

Here, we define $f \in \widetilde{X}_\varrho$ ($X = L^\infty(Q)$ or $X = W^{1,0}_2(Q)$) via the condition

$$\exists\, g \in X\,:\, g = f \text{ almost everywhere in } Q^+(\varrho) \tag{34}$$

$$\|f\|_{\widetilde{X}_\varrho} := \inf_{g\in X \text{ with (34)}} \|g\|_X\,.$$

For the variables J, we have the regularity

$$J \in L^{2,\frac{2\alpha}{1+\alpha}}(Q;\, \mathbb{R}^{N\times 3}), \quad 1^N \cdot J = 0 \text{ almost everywhere in } Q\,, \tag{35}$$

and the weighted regularity

$$M^{-1}\, J \cdot J \in L^1(Q)\,, \tag{36}$$

with the definition (27). For the variable R we consider the conditions

$$-R \in L_{\Psi^*}(Q;\, \mathbb{R}^s)\ . \tag{37}$$

The natural class $\mathcal{B}$ also encodes an information concerning the conservation of global mass. We additionally introduce the auxiliary variable

$$\bar{\rho} := \int_\Omega \rho = \int_\Omega \mathscr{R}(\varrho,\, q)\,, \tag{38}$$

and a function $\Phi^* \in C(\mathbb{R}_+ \times \mathbb{R}_+)$ constructed from the function Ψ as in the paper [DDGG16]. We are now in the position to introduce the solution class.

Definition 3.4. *Let* $(\varrho,\, q,\, v,\, \phi,\, J,\, R)$ *such that* ϱ *satisfies* (29)*,* v *satisfies* (30)*,* (31)*,* ϕ *satisfies* (32)*, and* q *satisfies* (33)*. We define a number*

$$\begin{aligned}
&[(\varrho,\, q,\, v,\, \phi,\, J,\, R)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,\overline{M},\,\Psi)} := \\
&\quad \|\varrho\|_{L^{\infty,\alpha}(Q)} + \|v\|_{W^{1,0}_2(Q)} + \|\sqrt{\varrho}\, v\|_{L^{\infty,2}(Q_T)} + \|\phi\|_{L^\infty(Q)} + \|\nabla\phi\|_{L^{\infty,\beta}(Q)} \\
&\quad + \|J\|_{L^{2,\frac{2\alpha}{1+\alpha}}(Q)} + [-R]_{L_{\Psi^*}(Q)} + \|p\|_{L^{\min\{1+\frac{1}{\alpha},\,\frac{5}{3}-\frac{1}{\alpha}\}}(Q)} \\
&\quad + [\bar{\rho}]_{C_{\Phi^*}([0,T])} + \|\mathscr{R}(1,\, q)\|_{\widetilde{W}^{1,0}_{\varrho,2}(Q)}\,.
\end{aligned}$$

We say that $(\varrho,\, q,\, v,\, \phi,\, J,\, R)$ *belongs to the class* $\mathcal{B} = \mathcal{B}(T,\, \Omega,\, \alpha,\, \overline{M},\, \Psi)$ *if and only if* $[(\varrho,\, q,\, v,\, \phi\, J,\, R)]_{\mathcal{B}(T,\,\Omega,\,\alpha,\,\overline{M},\,\Psi)}$ *is finite.*

We now give the definition of a weak solution.

Definition 3.5. *We call* weak solution *to the Problem* (P) *a vector* $(\varrho,\, q,\, v,\, \phi,\, J,\, R) \in \mathcal{B}(T,\, \Omega,\, \alpha,\, \overline{M},\, \Psi)$ *such that the energy inequality and the global mass identity of Definition 3.3 are valid and such that the quantities* $\rho := \mathscr{R}(\varrho,\, q)\, \chi_{Q^+(\varrho)}$, *and* r, p *and* n^F *obeying the definitions* (6)*, satisfy the relations*

$$- \int_Q \rho \cdot \psi_t - \int_Q (\rho_i\, v + J^i) \cdot \nabla\psi_i = \int_\Omega \rho^0 \cdot \psi(0) + \int_Q r \cdot \psi \tag{39}$$

$$- \int_Q \varrho\, v \cdot \eta_t - \int_Q \varrho\, v \otimes v \,:\, \nabla\eta - \int_Q p \, \operatorname{div}\eta + \int_Q \mathbb{S}(\nabla v) \,:\, \nabla\eta \tag{40}$$

$$= \int_\Omega \varrho_0\, v^0 \cdot \eta(0) - \int_Q n^F\, \nabla\phi \cdot \eta$$

$$\epsilon_0\, (1+\chi) \int_Q \nabla\phi \cdot \nabla\zeta = \int_Q n^F\, \zeta\,, \qquad \phi = \phi_0 \text{ as traces on }]0,T[\times\Gamma\,. \tag{41}$$

for all $\psi \in C^1_c([0,T[;\, C^1(\overline{\Omega};\, \mathbb{R}^N))$, $\eta \in C^1_c([0,T[;\, C^1_c(\Omega;\, \mathbb{R}^3))$ *and* $\zeta \in L^1(0,T;\, W^{1,2}_\Gamma(\Omega))$. *Moreover, the following identities are valid: If* $I \subseteq \{1,\ldots,N\}$ *is an ordered set of indices with cardinality larger than one, then*

$$J^i = \begin{cases} \sum_{k=1}^N \mathcal{D}_{i,k}\, \nabla\mathscr{R}_k(1,\, q) + \sum_{j=1}^N M_{i,j}\, \frac{z_j}{m_j}\, \nabla\phi & \text{for } i \in I \\ 0 & \text{for } i \in I^c \end{cases} \quad \text{a. e. in } Q^I\,,$$

with the matrix $\mathcal{D}$ *defined in* (26) *and* Q^I *as in* (24).

3.5 Main result

Theorem 3.6. *Let* $\Omega \in C^{0,1}$. *Assume that the free energy function* F *satisfies* (16) *and* (17) *and that the mobility matrix* M *is given by* (13) *with* $\overline{M}$ *satisfying* (a), (b), (c) *and the conditions* (10), (12) *for a fixed index set* $I_{\overline{M}} \subseteq \{1,\ldots,N\}$ *arbitrary. Let* $\Psi \in C^2(\mathbb{R}^s)$ *be convex, and satisfy* $\nabla\Psi(0) = 0$ *and* (18). *Assume that the initial data* ρ^0 *and* v^0, *and the boundary datum* ϕ_0 *satisfies* (20). *Assume moreover that one of the following conditions is valid:*

(1) $\alpha \geq 2$;

(2) $\frac{9}{5} \leq \alpha < 2$ *and* $r(\Omega,\, \Gamma) > \alpha'$;

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

Then, the problem (P) *possesses a weak solution in class* $\mathcal{B}(T,\, \Omega,\, \alpha,\, \overline{M},\, \Psi)$.

For the case that the index set $I_{\overline{M}}$ is a strict subset of $\{1,\ldots,N\}$, we have an additional information for the species corresponding to the indices in $I^{\mathsf{c}}_{\overline{M}} = \{1,\ldots,N\} \setminus I_{\overline{M}}$.

Proposition 3.7. *Assumptions of Theorem 3.6 with* $I^{\mathsf{c}}_{\overline{M}} \neq \emptyset$. *For all* $i \in I^{\mathsf{c}}_{\overline{M}}$ *and all compact sets* $K \subset\subset \{t \in]0,T[:\ \bar{\rho}_i(t) > 0\}$

$$\|q_i\|_{L^2(Q^+(\varrho)\cap[K\times\Omega])} < +\infty\,.$$

In words, this statement means that at every time for which the total mass $\bar{\rho}_i = \int_\Omega \rho_i \, dx$ of constituent $i \in I^{\mathsf{c}}_M$ does not vanish, the domain Ω is decomposed into a set in which this constituent is almost everywhere available and a set occupied by a complete vacuum. Thus, in the physical regime (no vacuum), the constituents with index in I^{c}_M (for instance the solvent $\mathrm{A_N}$ in the original model of [DGM13]) do not locally vanish as long as they are not entirely consumed.

The remainder of the paper is devoted to the proof of these results. In the next section we set up the preliminaries that allow to deal with the new condition (10).

4 Preliminaries

4.1 Relative chemical potentials, normalised mass densities

At first we introduce the mappings $\mathscr{R}$ and $\mathscr{M}$ associated with the equations $\mu = \nabla_\rho h(\rho)$.

It turns out convenient to introduce the relative chemical potentials in the following way: For $i = 1, \ldots, N$, and $\mu \in \mathbb{R}^N$, we define $q_i = \mu_i - \sup_{j=1,\ldots,N} \mu_j$. Then the variable q takes values in the $\partial \mathbb{R}^N_-$. Throughout the paper we employ the notations $\mathbb{R}_{0,+} = \mathbb{R}_+ \cup \partial \mathbb{R}_+$ and $\mathbb{R}^N_{0,+} = \mathbb{R}^N_+ \cup \partial \mathbb{R}^N_+$. Moreover we abbreviate $\mathbb{1} := 1^N$, and we denote $\mathbb{1}^\perp := \{X \in \mathbb{R}^N : X \cdot \mathbb{1} = 0\}$.

Lemma 4.1. *There are a function $\mathscr{M} \in C(\mathbb{R}_+ \times \partial \mathbb{R}^N_-)$ and a vector field $\mathscr{R} \in C(\mathbb{R}_{0,+} \times \partial \mathbb{R}^N_-; \, \mathbb{R}^N_{0,+})$ such that the equations (cp.* (5)*)*

$$\mu = \nabla h(\rho) \tag{42}$$

are valid for $\mu \in \mathbb{R}^N$ and $\rho \in \mathbb{R}^N_+$ if and only if there are $\varrho \in \mathbb{R}_+$ and $q \in \partial \mathbb{R}^N_-$ such that

$$\rho = \mathscr{R}(\varrho, \, q), \;\; \rho \cdot \mathbb{1} = \varrho, \qquad \mu - \sup_{i=1,\ldots,N} \mu_i \, \mathbb{1} = q, \qquad \sup_{i=1,\ldots,N} \mu_i = \mathscr{M}(\varrho, \, q) \, .$$

Moreover $\mathscr{R}$ establishes a bijection between $\mathbb{R}_+ \times \partial \mathbb{R}^N_-$ and $\mathbb{R}^N_+$.

Proof. Assume that $\mu = \nabla h(\rho)$ for some $\mu \in \mathbb{R}^N$ and $\rho \in \mathbb{R}^N_+$. Let $i_0 \in \{1, \ldots, N\}$ be arbitrary. We consider the basis $\{\xi^1, \ldots, \xi^N\}$ of $\mathbb{R}^N$ given by $\{e^1, \ldots, e^{i_0-1}, \, e^{i_0+1}, \ldots, e^N, \, \mathbb{1}\}$. Then the associated basis vectors $\eta^1, \ldots, \eta^N$ such that $\eta^i \cdot \xi^j = \delta_{i,j}$ for $i, j = 1, \, \ldots, N$ are

$$\eta^k = \begin{cases} e^k - e^{i_0} & \text{for } k = 1, \ldots, i_0 - 1 \\ e^{k+1} - e^{i_0} & \text{for } k = i_0, \ldots, N-1 \\ e^{i_0} & \text{for } k = N \end{cases} .$$

We apply the Corollaries 5.2, 5.3 of [DDGG16] and obtain that there are mappings $\mathscr{R} = \mathscr{R}^{i_0}$ and $\mathscr{M} = \mathscr{M}^{i_0} \in C^1(\mathbb{R}_+, \, \mathbb{R}^{N-1})$ such that the validity of (42) is equivalent with the existence of a pair $(r, \, p) \in \mathbb{R}_+, \, \mathbb{R}^{N-1}$ depending on i_0 such that

$$\begin{aligned} &\rho = \mathscr{R}^{i_0}(r, \, p), \quad r = \rho \cdot \mathbb{1} \\ &p = (\mu \cdot \eta^1, \ldots, \mu \cdot \eta^{N-1}), \quad \mu_{i_0} = \mathscr{M}^{i_0}(r, \, p) \, . \end{aligned}$$

For the proof we must recall from the proof of Corollary 5.2 of [DDGG16] that the number $\mathscr{M}^{i_0}(r,\,p)$ is defined as the unique solution to the implicitly equation

$$r = \mathbb{1}\cdot\nabla h^*\left(\sum_{k=1}^{N-1} p_k\,\xi^k + \mathscr{M}^{i_0}(r,\,p)\,\mathbb{1}\right)\,. \tag{43}$$

Here, h^* is the Legendre-transform of the free energy function h which is a convex function of class C^2 defined on the entire $\mathbb{R}^N$. Moreover, the vector field $\mathscr{R}^{i_0}$ is defined via $\mathscr{R}^{i_0}(r,\,p) := \nabla h^*(\sum_{k=1}^{N-1} p_k\,\eta^k + \mathscr{M}^{i_0}(r,\,p)\,\mathbb{1})$.

We now introduce the maps $\mathscr{R}$ and $\mathscr{M}$. At first we define these mappings on $\mathbb{R}_+\times(\partial\mathbb{R}^N_-)_o$. The surface $(\partial\mathbb{R}^N_-)_o$ consists of the relative interiors of the planar faces of $\partial\mathbb{R}^N_-$. If $q\in(\partial\mathbb{R}^N_-)_o$, there is a unique $i_0\in\{1,\ldots,N\}$ such that $q_{i_0}=0$. For $s>0$ we then define

$$\begin{aligned} p = p(i_0) &:= (q_1,\ldots,q_{i_0-1},\,q_{i_0+1},\ldots,q_N)\\ \mathscr{M}(s,\,q) &:= \mathscr{M}^{i_0}(s,\,p),\quad \mathscr{R}(s,\,q) := \mathscr{R}^{i_0}(s,\,p)\,. \end{aligned}$$

We easily see that these definitions at once yield continuous extensions of $\mathscr{M}$, $\mathscr{R}$ to $\partial\mathbb{R}^N_-$. Indeed, if $q\in\partial\mathbb{R}^N_-$ is such that there are $i_0\neq i_1$, $q_{i_0}=0=q_{i_1}$, then

$$\sum_{k=1}^{N-1} p_k(i_0)\,\xi^k(i_0) = \sum_{i\neq i_0} q_i\,e^i = \sum_{i=1}^{N} q_i\,e^i = \sum_{i\neq i_1} q_i\,e^i = \sum_{k=1}^{N-1} p_k(i_1)\,\xi^k(i_1)\,.$$

Call $\Pi := \sum_{k=1}^{N-1} p_k(i_0)\,\xi^k(i_0)$. Then, using the construction (43), we see that

$$\mathbb{1}\cdot\nabla h^*(\Pi + \mathscr{M}^{i_0}(r,\,p(i_0))\,\mathbb{1}) = r = \mathbb{1}\cdot\nabla h^*(\Pi + \mathscr{M}^{i_1}(r,\,p(i_1))\,\mathbb{1})\,,$$

and it follows first that $\mathscr{M}^{i_0}(r,\,p(i_0)) = \mathscr{M}^{i_1}(r,\,p(i_1))$, and second, making use of the definition of $\mathscr{R}^{i_0}$ that $\mathscr{R}^{i_0}(r,\,p(i_0)) = \mathscr{R}^{i_1}(r,\,p(i_1))$. This shows that $\mathscr{M}$ is of class $C(\mathbb{R}_+\times\partial\mathbb{R}^N_-)$. Moreover, $\mathscr{R}$ is of class $C(\mathbb{R}_+\times\partial\mathbb{R}^N_-;\,\mathbb{R}^N)$. Making use of the additional information $\mathscr{R}_i(s,\,q)\leq\sum_{i=1}^N\rho_i = s$, we obtain even via trivial extension that $\mathscr{R}\in C(\mathbb{R}_{0,+}\times\partial\mathbb{R}^N_-;\,\mathbb{R}^N)$.

At last, it remains to prove the bijective character of $\mathscr{R}$. Let $\rho\in\mathbb{R}^N_+$ arbitrary. Then, we can choose i_0 such that $\nabla_{i_0}h(\rho) = \max_{i=1,\ldots,N}\nabla_i h(\rho)$, and since we know that $\mathscr{R}^{i_0}$ is a bijection (see the Corollary 5.3 in [DDGG16]), there is $p\in\mathbb{R}^{N-1}$ such that $\rho = \mathscr{R}^{i_0}(\rho\cdot\mathbb{1},\,p)$. We then define

$$q = (p_1,\ldots,p_{i_0-1},\,0,\,p_{i_0},\ldots,\,p_N)\,,$$

and by definition we obtain that $\rho = \mathscr{R}(\rho\cdot\mathbb{1},\,q)$. This proves the surjectivity. In order to prove the injectivity, assume that $\mathscr{R}(s_1,\,q^1) = \mathscr{R}(s_2,\,q^2) =:\rho$. Then $s_1 = \sum_{i=1}^N\mathscr{R}_i(s_1,\,q^1) = \sum_{i=1}^N\mathscr{R}_i(s_2,\,q^2) = s_2$. We call $s_1 = s = s_2$. Further

$$\nabla h^*(q^1 + \mathscr{M}(s,\,q^1)\,\mathbb{1}) = \mathscr{R}(s,\,q^1) = \mathscr{R}(s,\,q^2) = \nabla h^*(q^2 + \mathscr{M}(s,\,q^2)\,\mathbb{1})\,,$$

and since ∇h^* is invertible, it follows that

$$q^1 + \mathscr{M}(s,\,q^1)\,\mathbb{1} = q^2 + \mathscr{M}(s,\,q^2)\,\mathbb{1}\,.$$

On the other hand, since $\mathscr{M}(s^1,\,q^1) = \max_{i=1,\ldots,N}\nabla_i h(\rho) = \mathscr{M}(s^2,\,q^2)$ by construction, it follows that $\mathscr{M}(s,\,q^1) = \mathscr{M}(s,\,q^2)$ and finally that $q^1 = q^2$. □

Lemma 4.2. *Define $\mathscr{M}$ and $\mathscr{R}$ as in the Lemma 4.1. Then there is a positive constant C such that for all $q \in \partial\mathbb{R}^N_-$*

$$|\mathscr{M}(s,\, q)| \leq C\,(1 + \max\{s^{\alpha-1},\, s^{-1}\})\,. \tag{44}$$

The function $\mathscr{M}$ is of class $C^1_{pw}(\mathbb{R}_+ \times \partial\mathbb{R}^N_-)$ and its derivatives satisfy the inequalities

$$\frac{1}{C_1\, s} \leq |\partial_s \mathscr{M}(s,\, q)| \leq \frac{K\, F''(s)}{C_0}\,, \quad |\nabla^\tau_q \mathscr{M}(s,\, q)| \leq \left(\frac{C_1}{C_0}\, K\, s\, F''(s)\right)^{1/2}$$

The vector field $\mathscr{R}$ is of class $C^1_{pw}(\mathbb{R}_+ \times \partial\mathbb{R}^N_-;\, \mathbb{R}^N)$ and its derivatives satisfy the inequalities

$$|\partial_s \mathscr{R}(s,\, q)| \leq \left(\frac{C_1}{C_0}\, K\, s\, F''(s)\right)^{1/2}\,, \quad |\nabla^\tau_q \mathscr{R}(s,\, q)| \leq C_1\, s\,.$$

Here $C_0,\, C_1$ are positive constants, and ∇^τ_q is the tangential gradient on $\partial\mathbb{R}^N_-$. Moreover, for $i, j = 1, \ldots, N$

$$|\partial^\tau_{q_j} \mathscr{R}_i(s,\, q)| \leq C\, \min\{\rho_i,\, \rho_j\} \text{ if } e^j \text{ is tangential to } \partial\mathbb{R}^N_-\,.$$

Proof. Let $(s,\, q) \in \mathbb{R}_+ \times \partial\mathbb{R}^N_-$. We define $\rho := \mathscr{R}(s,\, q)$ and $\mu := q + \mathscr{M}(s,\, q)\, \mathbb{1}$. Since $\mathscr{M}(s,\, q) = \max_{i=1,\ldots,N} \mu_i$, we can resort to the representation (4) of the free energy function to see for a certain i_0 that

$$\mathscr{M}(s,\, q) \leq c_{i_0} + \frac{V_{i_0}}{m_{i_0}}\, K\, F'(\tfrac{V}{m} \cdot \rho) + \frac{k_B\, \theta}{m_{i_0}}\, \ln y_{i_0}\,.$$

Thus, as $y_{i_0} \leq 1$,

$$\mathscr{M}(s,\, q) \leq c_{i_0} + \frac{V_{i_0}}{m_{i_0}}\, K\, [F']^+(\tfrac{V}{m} \cdot \rho) \leq \tilde{c}_1\, (1 + |\rho|^{\alpha-1}) \leq c_1\, (1 + s^{\alpha-1})\,.$$

Choose an index i_1 such that $n_{i_1} = \max_{i=1,\ldots,N} n_i$. Then $y_{i_1} \geq 1/N$ and it follows that

$$\begin{aligned}\mathscr{M}(s,\, q) \geq \mu_{i_1} &\geq c_{i_1} - \frac{V_{i_1}}{m_{i_1}}\, K\, |[F']^-(\tfrac{V}{m} \cdot \rho)| - \frac{k_B\, \theta}{m_{i_1}}\, \ln N \\ &\geq -\, c_0\, (1 + s^{-1})\,.\end{aligned}$$

Thus, we can conclude that (44) is valid. Next we investigate the derivatives. The Corollaries 5.2 and 5.3 of [DDGG16] yield the representation

$$\partial_s \mathscr{M}(s,\, q) = \frac{1}{D^2 h^* \mathbb{1} \cdot \mathbb{1}}, \quad \partial_s \mathscr{R}_i(s,\, q) = \frac{D^2 h^* e^i \cdot \mathbb{1}}{D^2 h^* \mathbb{1} \cdot \mathbb{1}} \text{ for } i = 1, \ldots, N\,. \tag{45}$$

Here, h^* is the Legendre-transform of the free energy function h. In (45), it is evaluated at the point $\mu = \nabla h(\rho)$.

Owing to the Lemma 5.7 of [DDGG16], we can rely uniformly on $\mathbb{R}^N_+$ on the estimates

$$|D^2_{i,j}h^*(\nabla h(\rho))| \leq C_1\, \min\{\rho_i,\, \rho_j\} \leq C_1\, s$$
$$D^2h^*(\nabla h(\rho))\, \mathbb{1}\cdot\mathbb{1} \geq C_0\, \frac{1}{K\, F''(s)}$$

Therefore it follows that

$$\frac{1}{C_1\, s} \leq \partial_s \mathscr{M}(s,\, q) \leq \frac{K\, F''(s)}{C_0}$$
$$|\partial_s \mathscr{R}_i(s,\, q)| \leq \left(\frac{D^2h^*_{i,i}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\right)^{1/2} \leq \left(\frac{C_1}{C_0}\, K\, s\, F''(s)\right)^{1/2}\, .$$

Next we compute from (43) that the tangential derivatives on the planar face $\mathcal{F}_{i_0}$ are given by

$$\partial_{q_j}\mathscr{M}(s,\, q) = -\frac{D^2h^*e^j\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}} \text{ for } j\in\{1,\ldots,N\}\setminus\{i_0\}$$
$$\partial_{q_j}\mathscr{R}_i(s,\, q) = D^2h^*e^j\cdot e^i - \frac{D^2h^*e^j\cdot\mathbb{1}\; D^2h^*e^i\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}} \text{ for } j\in\{1,\ldots,N\}\setminus\{i_0\} \qquad (46)$$

We obtain the estimates

$$|\nabla^\tau_q \mathscr{M}(s,\, q)| \leq \left(\frac{C_1}{C_0}\, K\, s\, F''(s)\right)^{1/2}, \quad |\nabla^\tau_q \mathscr{R}(s,\, q)| \leq C_1\, s\, .$$

Here ∇^τ_q is the tangential gradient on $(\partial\mathbb{R}^N_-)_o$. We also obtain that

$$|\partial^\tau_{q_j}\mathscr{R}_i(s,\, q)| \leq C\, \min\{\rho_i,\, \rho_j\} \text{ for } e^j \text{ tangential to } \partial\mathbb{R}^N_-\, .$$

□

Next we show a compactification property of the functions $\mathscr{R}$ and $\mathscr{M}$ which is necessary to deal with chemical potentials of infinite value. We introduce the following way of speaking:

Remark 4.3. *We say that a sequence $\{q^n\}_{n\in\mathbb{N}} \subset \partial\mathbb{R}^N_-$ converges in $\overline{\partial\mathbb{R}^N_-}$ if there exist $k\in\{1,\ldots,N\}$ and an ordered set $I=\{i_1,\ldots,i_k\}\subseteq\{1,\ldots,N\}$ such that*

$$\exists \lim_{n\to\infty} q_i^n \in \mathbb{R}_{0,-} \text{ for all } i\in I$$
$$\limsup_{n\to\infty} q_i^n = -\infty \text{ for all } i\in\{1,\ldots,N\}\setminus I\, .$$

We call $q^I := (\lim_{n\to\infty} q^n_{i_1},\ldots,\lim_{n\to\infty} q^n_{i_k}) \in \mathbb{R}^k$ the 'limit element' of $\{q^n\}_{n\in\mathbb{N}}$.

Lemma 4.4. *Let $1\leq k\leq N$ and $I=\{i_1,\ldots,i_k\}\subset\{1,\ldots,N\}$ be an ordered index set. Then, there are a function $\mathscr{M}^I \in C(\mathbb{R}_+\times\partial\mathbb{R}^k_-)\cap C^1_{pw}(\mathbb{R}_+\times\partial\mathbb{R}^k_-)$ as well as a functions $\mathscr{R}^I_1\ldots,\mathscr{R}^I_k \in C(\mathbb{R}_{0,+}\times\partial\mathbb{R}^k_-)\cap C^1_{pw}(\mathbb{R}_+\times\partial\mathbb{R}^k_-)$ with values in $\mathbb{R}_{0,+}$ with the following property: If $q^n\to q^I$ in $\overline{\partial\mathbb{R}^N_-}$ (sense of Remark 4.3), then for $s>0$ arbitrary*

$$\mathscr{M}(s,\, q^n)\to\mathscr{M}^I(s,\, q^I), \quad \mathscr{R}(s,\, q^n)\to\mathscr{R}^I(s,\, q^I)\, ,$$

and moreover

$$\begin{aligned}\partial_s\mathscr{M}(s,\,q^n) &\to \partial_s\mathscr{M}^I(s,\,q^I)\\ \partial_s\mathscr{R}(s,\,q^n) &\to \partial_s\mathscr{R}^I(s,\,q^I)\\ \partial_{q_{i_j}}\mathscr{M}(s,\,q^n) &\to \partial_{q^I_j}\mathscr{M}^I(s,\,q^I) \text{ for } j=1,\ldots,k\\ \partial_{q_{i_j}}\mathscr{R}(s,\,q^n) &\to \partial_{q^I_j}\mathscr{R}^I(s,\,q^I) \text{ for } j=1,\ldots,k\end{aligned}$$

Proof. Preliminary consideration: We consider a sequence $\{(\rho^n,\,\mu^n)\}_{n\in\mathbb{N}} \subset \mathbb{R}^N_+ \times \mathbb{R}^N$ connected via $\mu_n = \nabla h(\rho^n)$. We assume that there exists $\lim_{n\to\infty}\rho^n \in \mathbb{R}^N_{0,+}$ and that $\rho^n\cdot\mathbb{1} \to s > 0$. For $i\in\{1,\ldots,N\}$ arbitrary, it then obviously follows that $\rho^n_i \to 0$ if and only if $\mu^n_i \to -\infty$. We define

$$J := \{j\in\{1,\ldots,N\} \,:\, \lim_{n\to\infty}\rho^n_j > 0\} \quad |J| := \text{ cardinality of } J\,.$$

Then, there is an ordered representation $J=\{j_1,\ldots,j_{|J|}\}$, and we easily show that $h(\rho^n)\to h^J(\rho_{j_1},\ldots,\rho_{j_{|J|}})$, with h^J given by the formula (21) (with $I := J$). Thus the conjugate function satisfies

$$\begin{aligned}h^*(\mu^n) = \sum_{i=1}^N \mu^n_i\,\rho^n_i - h(\rho^n) &\to \sum_{j\in J}\mu_j\,\rho_j - h^J(\rho_{j_1},\ldots,\rho_{j_{|J|}})\\ &= (h^J)^*(\mu_{j_1},\ldots,\mu_{j_{|J|}}))\\ \nabla_{j_\ell}h^*(\mu^n) = \rho^n_{j_\ell} &\to \rho_{j_\ell} = \nabla_\ell(h^J)^*(\mu_{j_1},\ldots,\mu_{j_{|J|}}) \text{ for } \ell=1,\ldots,|J|\,.\end{aligned} \tag{47}$$

Here $(h^J)^*$ is the Legendre transform of the function h^J in $\mathbb{R}^{|J|}$.

Consider a sequence $\{q^n\}\in\partial\mathbb{R}^N_-$ converging to q^I in the sense of Remark 4.3. We define corresponding $\mu^n := q^n + \mathscr{M}(s,\,q^n)$, and $\rho^n := \nabla h^*(\mu^n) = \mathscr{R}(s,\,q^n)$.

At first we have to show that there is a function $\mathscr{M}^I$ defined in $\mathbb{R}_+\times\partial\mathbb{R}^k_-$ such that $\mathscr{M}(s,\,q^n)\to\mathscr{M}^I(s,\,q^I)$. We define $\mathscr{M}^I := x$ as the unique solution to the implicit equation

$$s = \sum_{\ell=1}^k \nabla_\ell(h^I)^*(q^I + x\,\mathbb{1})\,.$$

Indeed, from the construction of the implicit function $\mathscr{M}$ in (43), we know that

$$s = \mathbb{1}\cdot\nabla h^*(q^n + \mathscr{M}(s,\,q^n)\,\mathbb{1})\,.$$

Since $|\mathscr{M}(s,\,q^n)| \le C(s)$ (see the inequality (44)), we can extract from every subsequence a sub-subsequence, say n_j, such that $\mathscr{M}(s,\,q^{n_j})\to\tilde{x}\in\mathbb{R}$ as $j\to\infty$. For this sequence, the criterion (47) yields

$$s = \sum_{\ell=1}^k \nabla_\ell(h^I)^*(q^I + \tilde{x}\,\mathbb{1})\,.$$

Thus, it follows that $\lim_{n\to\infty} \mathscr{M}(s,\, q^n)$ exists and is equal to the implicit function $\mathscr{M}^I(s,\, q^I)$. Next we observe that $\mathscr{R}(s,\, q^n) = \nabla h^*(q^n + \mathscr{M}(s,\, q^n)\, \mathbb{1})$ satisfies

$$\mathscr{R}_{i_j}(s,\, q^n) \to \mathscr{R}^I_j(s,\, q^I) := \nabla_j (h^I)^*(q^I + \mathscr{M}^I(s,\, q^I)\, 1^k) \text{ for } j = 1, \ldots, k\,,$$

With the convergence of $\mathscr{R}$ at hand, the convergence of the derivatives follows from the representation formula (45), (46). ☐

Remark 4.5. *Making use of the Lemma 4.2, we see that $\mathscr{R}$ and its derivatives admit a continuous extension on $\overline{\partial\mathbb{R}^N_-}$ in a very precise sense. We from now on write shortly*

$$\mathscr{R} \in (C \cap C^1_{pw})(\mathbb{R}_+ \times \overline{\partial\mathbb{R}^N_-};\, \mathbb{R}^N_+)$$

as an abbreviation for the convergence properties stated in Lemma 4.4.

Next we investigate the curves $s \mapsto \mathscr{R}(s,\, q)$. We introduce to this aim the mass fraction mapping $X(s,\, q) := \frac{\mathscr{R}(s,q)}{s}$ which is obviously well-defined from $\mathbb{R}_+ \times \partial\mathbb{R}^N_-$ into the set $\mathbb{R}^N_{1,+} = \{X \in \mathbb{R}^N_+\,;\, \sum_{i=1}^N X_i = 1\}$.

Lemma 4.6. *There is a constant $C = C(\theta,\, K,\, V,\, m) > 0$ such that for all $q \in \partial\mathbb{R}^N_-$ and all $0 < s_1 < s_2 < +\infty$*

$$\mathscr{R}(s_2,\, q) \leq \mathscr{R}(s_1,\, q)\, (\max\{1,\, \frac{1}{s_1}\})^{1+C}\, \bar{k}(s_1,\, s_2),$$
$$\bar{k}(s_1,\, s_2) := \begin{cases} s_2^{1+C} & \textit{if } s_2 < 1 \\ e^{\frac{1+C}{\alpha-1}\,(s_2^{\alpha-1} - \max\{s_1,1\}^{\alpha-1})} & \textit{otherwise} \end{cases}$$

and moreover

$$\mathscr{R}(s_2,\, q) \geq \mathscr{R}(s_1,\, q)\, (\min\{1,\, s_1\})^C\, \underline{k}(s_1,\, s_2)$$
$$\underline{k}(s_1,\, s_2) := \begin{cases} s_2^{-C} & \textit{if } s_2 < 1 \\ e^{-\frac{C}{\alpha-1}\,(s_2^{\alpha-1} - \max\{s_1,1\}^{\alpha-1})} & \textit{otherwise} \end{cases}$$

Proof. We fix $q \in \partial(\mathbb{R}^N_-)_0$. Throughout the proof $\mathscr{R}(s) := \mathscr{R}(s,\, q)$. Due to Lemma 4.1, there holds

$$\partial_s \mathscr{R}_i(s) = \frac{D^2 h^* e^i\, \mathbb{1}}{D^2 h^* \mathbb{1}\, \mathbb{1}} (\nabla h(\mathscr{R}(s)) = \frac{\mathscr{R}_i(s)}{s}\, (1 + c_i(s))$$

$$c_i(s) := \frac{1}{k_B\, \theta}\, \frac{m_i - \frac{\mathscr{R}(s)\cdot \mathbb{1}}{\mathscr{R}(s)\cdot \frac{V}{m}}\, V_i - (m \cdot \mathscr{R}(s) - \frac{\mathscr{R}(s)\cdot V}{\mathscr{R}(s)\cdot \frac{V}{m}})}{\frac{s}{K\, F''(\mathscr{R}(s)\cdot \frac{V}{m})\, (\mathscr{R}(s)\cdot \frac{V}{m})^2} + \frac{1}{k_B\, \theta}\, \left(m \cdot \mathscr{R}(s) + \frac{s\, \frac{V^2}{m}\cdot \mathscr{R}(s)}{(\mathscr{R}(s)\cdot \frac{V}{m})^2} - 2\, \frac{\mathscr{R}(s)\cdot V}{\mathscr{R}(s)\cdot \frac{V}{m}}\right)}$$

For $s \in \mathbb{R}_+$, $X \in \mathbb{R}^N_{1,+}$ and $i = 1, \ldots, N$, we define

$$\begin{aligned}\gamma_i(s,\, X) &:= \gamma(s,\, X;\, \theta,\, K,\, V,\, m)\\ &= \frac{1}{k_B\,\theta}\,\frac{m_i - \frac{V_i}{X\cdot\frac{V}{m}} - (m\cdot X - \frac{X\cdot V}{X\cdot\frac{V}{m}})}{\frac{1}{K\,F''(s\,X\cdot\frac{V}{m})\,s\,X\cdot\frac{V}{m}\,(X\cdot\frac{V}{m})} + \frac{1}{k_B\,\theta}\,\left(m\cdot X + \frac{\frac{V^2}{m}\cdot X}{(\frac{V}{m}\cdot X)^2} - 2\,\frac{X\cdot V}{X\cdot\frac{V}{m}}\right)}\end{aligned}$$

Making use of the latter abbreviation, we equivalently express the latter relation via

$$\partial_s \mathscr{R}_i(s) = X_i(s)\,(1 + \gamma_i(s,\, X(s))))\,. \tag{48}$$

We recall that $c_0 \leq F''(t)\,t \leq c_1\,\max\{1,\, t\}^{\alpha-1}$ for all $t \in \mathbb{R}_+$. Moreover, for $i = 1, \ldots, N$ we can introduce $A_i = (m_i\,X_i)^{1/2}$ and $B_i := (\frac{V}{m}\cdot X)^{-1}\,V_i\,(\frac{X_i}{m_i})^{1/2}$ and see that

$$m\cdot X + \frac{\frac{V^2}{m}\cdot X}{(\frac{V}{m}\cdot X)^2} - 2\,\frac{X\cdot V}{X\cdot\frac{V}{m}} = |A-B|^2 \geq 0\,.$$

Thus, we easily show that $|\gamma_i(s,\, X)| \leq C(\theta,\, K,\, V,\, m)\,\max\{1,\, s^{\alpha-1}\}$. Owing to (48), it now follows that

$$\begin{aligned}\partial_s \ln \mathscr{R}_i(s) &\leq (1+C)\,\frac{\max\{1,\, s^{\alpha-1}\}}{s}\\ \partial_s \ln \mathscr{R}_i(s) &\geq -C\,\frac{\max\{1,\, s^{\alpha-1}\}}{s}\,.\end{aligned}$$

The claim follows easily. □

For $\rho \in \mathbb{R}^N_+$, there is $q \in \partial\mathbb{R}^N_-$ such that $\rho = \mathscr{R}(\rho\cdot\mathbb{1},\, q)$ (Lemma 4.1). We define the normalisation ρ^{norm} of ρ via

$$\rho^{\text{norm}} := \mathscr{R}(1,\, q)\,.$$

Making use of the properties of $\mathscr{R}$, we show that $\sum_{i=1}^N \rho_i^{\text{norm}} = 1$. Moreover, applying the Lemma 4.6 we find that

$$\begin{cases}(\rho\cdot\mathbb{1})^C \leq \frac{\rho_i^{\text{norm}}}{\rho_i} \leq \left(\frac{1}{\rho\cdot\mathbb{1}}\right)^{1+C} & \text{if } \rho\cdot\mathbb{1} \leq 1\\ e^{-\frac{1+C}{\alpha-1}\,(\rho\cdot\mathbb{1})^{\alpha-1}} \leq \frac{\rho_i^{\text{norm}}}{\rho_i} \leq e^{\frac{C}{\alpha-1}\,(\rho\cdot\mathbb{1})^{\alpha-1}} & \text{otherwise}\end{cases}$$

4.2 Preliminary properties associated with the mobility matrix

In this section, we consider a mapping $\overline{M} \in C^1(\mathbb{R}^N_{0,+};\mathbb{R}^{N\times N}_{\text{sym},+})$ such that the properties

$$\overline{M}(\rho)\,\mathbb{1} = 0 \tag{49}$$

$$\overline{M}_{i,j}(\rho) \leq C\,\rho_i \text{ for } i,j \in I_{\overline{M}} \subseteq \{1,\ldots,N\} \tag{50}$$

$$\text{rank}\,\overline{M}(\rho) = |I^{\text{c}}_{\overline{M}}| + |\{i \in I_{\overline{M}}\,:\,\rho_i > 0\}| - 1\,. \tag{51}$$

are satisfied uniformly. Here $I_{\overline{M}}$ is an ordered index set fixed by the model. We moreover assume linear growth of $\overline{M}$ so that the norm $\|M\|_{C^1}$ is in fact a global Lipschitz constant. We commence with two technical lemmas.

Lemma 4.7. *Let $\overline{M} \in C^1(\mathbb{R}^N_{0,+}; \mathbb{R}^{N\times N}_{sym,+})$ satisfies the conditions* (49), (50) *and* (51). *Assume moreover that there is a constant $c_0 > 0$ such that for all $\rho \in \mathbb{R}^N_{0,+} \setminus \{0\}$*

$$\partial_{\rho_k} \overline{M}_{k,k}(\rho) \geq c_0 \text{ for all } k \in I_{\overline{M}}\,. \tag{52}$$

Denote $\lambda_1(\rho) \geq \ldots, \geq \lambda_N(\rho) = 0$ the ordered eigenvalues of $\overline{M}(\rho)$. For $\rho \in \mathbb{R}^N_+$, let $\{i_1, \ldots, i_N\}$ be a permutation depending on ρ of the index set $\{1, \ldots, N\}$ such that $\{i_1, \ldots, i_p\} = I^{\mathsf{c}}_{\overline{M}}$ and such that $\rho_{i_{p+1}} \geq \rho_{i_{p+2}} \geq \ldots \geq \rho_{i_N}$. Then there are $\underline{\lambda} > 0$ and a constant $c_1 > 0$ depending on c_0, $\|\overline{M}\|_{C^1}$ and on N such that for all $\rho \in \mathbb{R}^N_+$

$$\begin{aligned}
&\lambda_j(\rho) \geq \underline{\lambda} \text{ for } j = 1, \ldots, p-1\\
&\lambda_j(\rho) \geq c_1 \min\{1,\, \rho_{i_{j+1}}\} \text{ for } j = p, \ldots, N-1\,.
\end{aligned}$$

Proof. We abbreviate $p := |I^{\mathsf{c}}_{\overline{M}}| \geq 0$. Due to (51), the rank of $\overline{M}(\rho)$ is at least $p-1$ on $\mathbb{R}^N_{0,+}$, so that the eigenvalues $\lambda_1(\rho), \ldots, \lambda_{p-1}(\rho)$ are strictly positive on $\mathbb{R}^N_{0,+}$. Thus, since $\overline{M}$ is continuous, λ_{p-1} achieves a strictly positive minimum on $\mathbb{R}^N_{0,+}$, which we denote $\underline{\lambda}$.

The remainder of the proof is devoted to the second inequality. We introduce the planar faces of $\partial\mathbb{R}^N_+$ via $\mathcal{F}_i := \{\rho \in \mathbb{R}^N_{0,+} \,:\, \rho_i = 0\}$ for $i = 1, \ldots, N$. Consider a vector $\bar{\rho}$ in the relative interior $\mathcal{F}_{j_0,o}$ of $\mathcal{F}_{j_0}$, $j_0 \in I_{\overline{M}}$. This means that j_0 is exactly the one index such that $\bar{\rho}_{j_0} = 0$. Then, owing to (50), the matrix $\overline{M}(\bar{\rho})$ has a trivial eigenvalue associated with the eigenvector e^{j_0}.

Consider next $\rho \in \mathbb{R}^N_+$, and let $\xi^1(\rho), \ldots, \xi^{N-1}(\rho)$, $\mathbb{1}/\sqrt{N}$ be any system of orthonormal eigenvectors of $\overline{M}(\rho)$. If ρ approaches some element $\bar{\rho}$ in $\mathcal{F}_{j_0,o}$ the second smallest eigenvalue $\lambda_{N-1}(\rho)$ tends to zero. The limiting eigenvector $\xi^{N-1}(\bar{\rho})$ satisfies $\xi^{N-1}(\bar{\rho}) \in \operatorname{span}\{e^{j_0},\, \mathbb{1}\}$, and since $\xi^{N-1} \cdot \mathbb{1} = 0$ it follows that

$$\xi^{N-1}(\bar{\rho}) = \frac{1}{\sqrt{2\,(1 - 1/\sqrt{N})}}\,(e^{j_0} - \frac{\mathbb{1}}{\sqrt{N}}) =: \alpha\, e^{j_0} + \beta\, \mathbb{1}\,.$$

Thus as $\rho \to \bar{\rho}$ we have the convergence

$$\lambda_{N-1}(\rho) \to 0, \quad \xi^{N-1}(\rho) \to \alpha\, e^{i_0} + \beta\, \mathbb{1}\,. \tag{53}$$

On the other hand, exploiting the orthonormalty of $\{\xi^i\}_{i=1,\ldots,N}$ we obtain for all $i,\ j = 1, \ldots, N$ and $\rho \in \mathbb{R}^N_+$ the formula

$$\partial_{\rho_i}\lambda_j(\rho) = (\partial_{\rho_i}\overline{M})(\rho)\, \xi^j(\rho) \cdot \xi^j(\rho)\,.$$

For $\rho \to \bar{\rho} \in \mathcal{F}_{j_0,o}$ and $j = N-1$, we obtain from (53) and (49), (52) that

$$\partial_{\rho_{j_0}}\lambda_{N-1}(\bar{\rho}) = \alpha^2\,(\partial_{\rho_{j_0}}\overline{M}_{j_0,j_0})(\bar{\rho}) \geq c_0\,.$$

Thus, since $\overline{M}$ is of class C^1, there is a neighbourhood U of the hyper-surface $\bigcup_{i\in I_{\overline{M}}} \mathcal{F}_i$ in $\mathbb{R}^N_+$ such that $\lambda_{N-1}(\rho) \geq \tilde{c}_0 \min_{i\in I_{\overline{M}}} \rho_i = \tilde{c}_0\, \rho_{i_N}$ therein. Recall that in $\mathbb{R}^N_+ \setminus U$ we must have rank $\overline{M}(\rho) = N-1$. Thus

$$\begin{aligned}\lambda_{N-1}(\rho) &\geq \min\{\inf_{\mathbb{R}^N_+\setminus U} \lambda_{N-1},\, \inf_{\overline{U}} \lambda_{N-1}\}\\ &\geq c_1\, \min\{1,\, \rho_{i_N}\}\,.\end{aligned}$$

The procedure can be iterated. In the next step we consider the matrix $\overline{M}(\rho)$ on a planar face of $\partial\mathbb{R}^N_-$, say $\mathcal{F}_{j_0}$, $j_0 \in I_{\overline{M}}$. Denote $\overline{M}^{j_0}(\rho)$ the $(N-1)\times(N-1)$ matrix associated with cancelling the row and column with index j_0 in $\overline{M}(\rho)$. The relative boundary of $\mathcal{F}_{j_0}$ is composed of the $(N-2)-$dimensional manifolds $\mathcal{C}_i = \{\rho \in \mathcal{F}_{j_0} \,:\, \rho_i = 0\}$, $i \in \{1,\ldots,N\}\setminus\{j_0\}$. The relative interior $\mathcal{C}_{i,o}$ is the subset of $\mathcal{C}_i$ such that $\rho_i = 0$ for exactly the index i.

Just as before, we can show for each part $\mathcal{C}_{j_1,o}$ of $\partial\mathcal{F}_{j_0}$ such that $j_1 \in I_{\overline{M}}$ that

$$\partial_{j_1}\lambda_{\inf}(\overline{M}^{j_0}(\rho)) = (\partial_{\rho_{j_1}} \overline{M}_{j_1,j_1})(\rho) \geq c_0 \text{ on } \mathcal{C}_{j_1,o}\,.$$

Thus, $\partial_{j_1}\lambda_{N-2}(\rho) \geq c_0$ on $\mathcal{C}_{j_1,o}$, and there is a neighbourhood of the set $\bigcup_{j_1\in I_{\overline{M}},\, j_1\neq j_0} \mathcal{C}_{j_1}$ in the face $\mathcal{F}_{j_0}$ such that $\lambda_{N-2}(\rho) \geq \tilde{c}_0\, \rho_{j_1} = \tilde{c}_0\, \rho_{i_{N-1}}$. Thus for all $j_0 \in I_{\overline{M}}$

$$\lambda_{N-2}(\rho) \geq c_1\, \min\{1,\, \rho_{i_{N-1}}\} \text{ on } \mathcal{F}_{j_0}$$

For $\rho \in \mathbb{R}^N_+$, it follows that

$$\begin{aligned}\lambda_{N-2}(\rho) &\geq \lambda_{N-2}(\rho_1,\ldots,\rho_{i_N-1},\, 0,\, \rho_{i_N+1},\ldots,\rho_N) - \|\overline{M}\|_{C^1}\, \rho_{i_N}\\ &\geq c_1\, \min\{1,\, \rho_{i_{N-1}}\} - \|\overline{M}\|_{C^1}\, \rho_{i_N}\,.\end{aligned}$$

Thus, for the case that $\rho_{i_N} \leq c_1/(2\,\|\overline{M}\|_{C^1})\, \min\{1,\, \rho_{i_{N-1}}\}$, we obtain that

$$\lambda_{N-2}(\rho) \geq \frac{c_1}{2}\, \min\{1,\, \rho_{i_{N-1}}\}\ .$$

Otherwise $\rho_{i_N} \geq c_1/(2\,\|\overline{M}\|_{C^1})\, \min\{1,\, \rho_{i_{N-1}}\}$ and it follows that

$$\lambda_{N-2}(\rho) \geq \lambda_{N-1}(\rho) \geq c_1\, \min\{1,\, \rho_{i_N}\} \geq \tilde{c_1}\, \min\{1,\, \rho_{i_{N-1}}\}\,.$$

Overall $\lambda_{N-2}(\rho) \geq c\, \min\{1,\, \rho_{i_{N-1}}\}$. We spare the reader with the details of the continuation of this rather tedious procedure. □

Lemma 4.8. *Let $\overline{M} \in C^1(\mathbb{R}^N_{0,+};\mathbb{R}^{N\times N}_{sym,+})$ satisfy the conditions* (49) *and* (50)*. For $\rho \in \mathbb{R}^N_+$, let $\{i_1,\ldots,i_N\}$ be a permutation of the index set $\{1,\ldots,N\}$ such that $\{i_1,\ldots,i_p\} = I^c_{\overline{M}}$ and such that $\rho_{i_{p+1}} \geq \rho_{i_{p+2}} \geq \ldots \geq \rho_{i_N}$. Then there is a constant $c > 0$ depending on $\|\overline{M}\|_{C^1}$ such that for any system of orthonormal eigenvectors $\xi^1,\ldots,\xi^N$ of $\overline{M}(\rho)$ associated with the ordered eigenvalues $\lambda_1 \geq \ldots, \geq \lambda_N$ and for every $k \in \{p+2,\ldots,N\}$*

$$\operatorname{dist}(\xi^{k-1},\, \operatorname{span}\{e^{i_k},\ldots,e^{i_N},\, \mathbb{1}\} \cap B_1) \leq c\, \rho_{i_k}\,.$$

Proof. Let $k \in \{p+2, \ldots, N\}$. Suppose that $\rho_{i_k} = \ldots = \rho_{i_N} = 0$, while $\rho_{i_{p+1}}, \ldots, \rho_{i_{k-1}} > 0$. Then, the assumption (50) implies that $e^{i_k}, \ldots, e^{i_N},\, \mathbb{1}$ are eigenvectors of $\overline{M}(\rho)$ associated with a trivial eigenvalue. These eigenvalues are precisely $\lambda_N, \ldots, \lambda_{k-1}$. Thus, the corresponding eigenvectors $\xi^N, \ldots, \xi^{k-1}$ have to span the linear space $\operatorname{span}\{e^{i_k}, \ldots, e^{i_N},\, \mathbb{1}\}$.

For $\rho \in \mathbb{R}^N_+$ we can use the Lipschitz property of $\overline{M}$ to see that

$$|\xi^j(\rho) - \xi^j(\rho_1, \ldots, \underbrace{0, \ldots, 0}_{i_k,\ldots,i_N \text{th} components}, \ldots, \rho_N)| \le C_{\overline{M}}\, \rho_{i_k} \text{ for all } j\,.$$

Thus, as $\xi^{k-1} \in \operatorname{span}\{e^{i_k}, \ldots, e^{i_N},\, \mathbb{1}\} \cap B_1$ whenever $\rho_{i_k} = 0$, we obtain that

$$\operatorname{dist}(\xi^{k-1}(\rho),\, \operatorname{span}\{e^{i_k}, \ldots, e^{i_N},\, \mathbb{1}\} \cap B_1) \le C_{\overline{M}}\, \rho_{i_k}\,.$$

□

After establishing these two technical points we now turn to the properties actually of interest to us in order to obtain estimates on the chemical potentials.

Lemma 4.9. *Let $b \in L^\infty(\mathbb{R}^N_{0,+};\, \mathbb{1}^\perp)$ be a vector field such that $b_i(\rho) \le c_b\, \rho_i$ for $i = 1, \ldots, N$ and all ρ in $\mathbb{R}^N_{0,+}$. For $r \in \mathbb{R}^N_+$, denote $\{i_1(r), \ldots, i_N(r)\}$ a permutation of the index set $\{1, \ldots, N\}$ as in Lemma 4.7. For all $r,\, \rho \in \mathbb{R}^N_+$, the system of equations $\overline{M}(r)\, X = b(\rho)$ possesses a unique solution $X = X(r, \rho) \in \mathbb{1}^\perp$ such that*

$$|X| \le C(N,\, \overline{M})\, c_b \left(\sum_{i \in I_{\overline{M}}} \frac{\rho_i}{r_i} + |\rho| \right)\,.$$

Proof. Consider the system of equations $\overline{M}(r)\, X = b(\rho)$. Then, the unique solution $X \in \mathbb{1}^\perp$ is given by $X = \sum_{i=1}^{N-1} \frac{b(\rho)\cdot\xi^i(r)}{\lambda_i(r)}\, \xi^i(r)$. We now apply the Lemma 4.8, and we obtain for $k = p+2, \ldots, N$ the existence of vectors $a^k,\, c^k \in \mathbb{R}^N$ such that

$$\xi^{k-1}(r) = a^k + c^k, \quad a^k \in \operatorname{span}\{e^{i_k}, \ldots, e^{i_N},\, \mathbb{1}\} \cap B_1, \quad |c^k| \le c\, r_{i_k}\,.$$

Note that since $c^k = \xi^{k-1}(r) - a^k$, it follows that $|c^k| \le 2$, and therefore $|c^k| \le c\, \min\{1, r_{i_k}\}$.

Clearly, since $b \cdot \mathbb{1} = 0$, it follows that

$$|b(\rho)\cdot a^k| \le |a^k| \left| \sum_{j=k}^N b(\rho)\cdot e^{i_j} \right| \le c_b \sum_{j=k}^N \rho_{i_j}$$

$$|b(\rho) \le c^k| \le c\, c_b\, |\rho|\, \min\{1,\, r_{i_k}\}\,.$$

Thus $|b(\rho)\cdot\xi^{k-1}(r)| \le c_b\, \left(\sum_{j=k}^N \rho_{i_j} + c\, |\rho|\, \min\{1,\, r_{i_k}\}\right)$. Making use of the Lemma 4.7, $\lambda_{k-1}(r) \ge c_1\, \min\{1,\, r_{i_k}\}$. Thus

$$|X| \le \sum_{k=2}^{p+1} \frac{|b(\rho)\cdot\xi^{k-1}(r)|}{\lambda_{k-1}(r)} + \sum_{k=p+2}^N \frac{|b(\rho)\cdot\xi^{k-1}(r)|}{\lambda_{k-1}(r)}$$

$$\le c_b\, \underline{\lambda}^{-1}\, |\rho| + c_b \sum_{k=p+2}^N \frac{1}{\min\{r_{i_k},\, 1\}} \sum_{j=k}^N \rho_{i_j}\,.$$

Next we observe by the definition of $i_{p+1}, \dots, i_N$ that

$$\sum_{k=p+2}^{N} \frac{1}{\min\{r_{i_k},\, 1\}} \sum_{j=k}^{N} \rho_{i_j} \le \sum_{k=p+2}^{N} \sum_{j=k}^{N} \frac{\rho_{i_j}}{\min\{r_{i_j},\, 1\}} \le C \left(|\rho| + \sum_{i \in I_{\overline{M}}} \frac{\rho_i}{r_i} \right) .$$

The claim follows. □

Corollary 4.10. *Let $b \in L^\infty(\mathbb{R}^N_{0,+};\, \mathbb{1}^\perp)$ be a vector field such that $b_i(\rho) \le c_b\, \rho_i$ for $i = 1, \dots, N$ and all ρ in $\mathbb{R}^N_{0,+}$. Let $q \in \partial\mathbb{R}^N_-$ and $0 < s,\, t < +\infty$. Then, the system of equations $\overline{M}(\mathscr{R}(s,\, q))\, X = b(\mathscr{R}(t,\, q))$ possesses a unique solution $X \in \mathbb{1}^\perp$ such that*

$$|X| \le \begin{cases} C\, c_b\, \left(\max\{1,\, s^{-1}\}^{1+C}\, \bar{k}(s,\, t) + t\right) & \text{if } s < t \\ C\, c_b\, \left(\frac{1}{\min\{1,\, t\}^C\, \underline{k}(t,\, s)} + t\right) & \text{if } s \ge t \end{cases}$$

where $\bar{k}(\cdot,\, \cdot)$, $\underline{k}(\cdot,\, \cdot)$ are the functions defined in the Lemma 4.6.

Proof. In the statement of Lemma 4.9, we choose $r = \mathscr{R}(s,\, q)$ and $\rho = \mathscr{R}(t,\, q)$. We apply the estimates of Lemma 4.6 and the claim follows. □

Corollary 4.11. *Let $\rho \in \mathbb{R}^N_+$ such that $\sum_{i=1}^N \rho_i \ge \delta_0 > 0$. Let $k_0 \in \{1, \dots, N\}$ be an index such that $\rho_{k_0} = \max_{i=1,\dots,N} \rho_i$. Then, for all $i \in I^{\mathsf{c}}_{\overline{M}}$ the equations $\overline{M}(\rho)\, X = e^i - e^{k_0}$ possess a unique solution $X^i \in (1^N)^\perp$ such that $|X^i| \le c(\delta_0)$.*

Proof. The unique solution to $\overline{M}(\rho)\, X = e^i - e^{k_0}$ is given by

$$X = \sum_{j=1}^{N-1} \frac{(e^i - e^{k_0}) \cdot \xi^j(\rho)}{\lambda_j(\rho)}\, \xi^j(\rho) .$$

Due to the Lemma 4.8, there are for $j = p+2, \dots, N$ vectors $a^j,\, c^j \in \mathbb{R}^N$ such that

$$\xi^{j-1}(\rho) = a^j + c^j, \quad a^j \in \operatorname{span}\{e^{i_j}, \dots, e^{i_N},\, \mathbb{1}\} \cap B_1, \quad |c^j| \le c\, \rho_{i_j} .$$

From the choice of $i \in I^{\mathsf{c}}_{\overline{M}}$ and of $i_{p+1}, \dots, i_N \in I_{\overline{M}}$, we obtain that $e^i \cdot e^{i_j} = 0$ for $j = p+1, \dots, N$. Moreover

$$|(e^i - e^{k_0}) \cdot a^j| = \left| \sum_{\ell=j}^{N} e^{k_0} \cdot e^{i_\ell} \right| = \begin{cases} 1 & \text{if } k_0 \in I_{\overline{M}} \text{ and } \rho_{k_0} \le \rho_{i_j} \\ 0 & \text{otherwise} \end{cases}$$

Moreover, note that $|c^j| = |\xi^{j-1}(\rho) - a^j| \le 2$, and therefore $|c^j| \le c\, \min\{1,\, \rho_{i_j}\}$, and $|(e^i - e^{k_0}) \le c^j| \le c\, \min\{1,\, \rho_{i_j}\}$. Therefore

$$\begin{aligned} |X| &\le \sum_{j=2}^{p+1} \frac{|(e^i - e^{k_0}) \cdot \xi^{j-1}(\rho)|}{\lambda_{j-1}(\rho)} + \sum_{j=p+2}^{N} \frac{|(e^i - e^{k_0}) \cdot \xi^{j-1}(\rho)|}{\lambda_{j-1}(\rho)} \\ &\le c\, \underline{\lambda}^{-1} + c \sum_{j=p+2}^{N} \frac{\min\{1,\, \rho_{i_j}\}}{\lambda_{j-1}(\rho)} + \chi_{I_{\overline{M}}}(k_0) \sum_{j \in \{p+2,\dots,N\},\, \rho_{i_j} \ge \rho_{k_0}} \frac{1}{\lambda_{j-1}(\rho)} \\ &\le C\, (1 + \chi_{I_{\overline{M}}}(k_0)\, \min\{1,\, \rho_{k_0}\}^{-1}) . \end{aligned}$$

It remains to observe that the definition of k_0 implies that $\rho_{k_0} \ge N^{-1} \sum_{i=1}^N \rho_i \ge N^{-1}\, \delta_0$. □

5 The existence procedure

At first using the main existence Theorem 4.4 for the case of positive mobilities (cp. [DDGG16]), we construct approximate solutions. We will prove existence for the model where the mobility matrix is given by

$$M = f_0(\varrho)\,\overline{M}(\mathscr{R}(T_{\delta_0}(\varrho),\, q))\,.$$

Here $T_{\delta_0}(\varrho) := \min\{\max\{\delta_0,\, \varrho\},\, \delta_0^{-1}\}$ is a cut-off operator from below and above, while f_0 is a globally Lipschitz continuous, strictly positive function on $\mathbb{R}_{0,+}$. Moreover, we choose a convex non-decreasing weight function $\omega \in C^2(\mathbb{R})$ via the formula (148)-(150) of [DDGG16] in order to regularise the free energy. Further specification is not necessary here.

Proposition 5.1. *For $n \in \mathbb{N}$, and $\mu \in \mathbb{R}^N$ define*

$$q := \mu - \sup_{i=1,\ldots,N} \mu_i\, 1^N, \quad \varrho := \sum_{i=1}^{N} (\partial_i h^*(\mu) + \frac{1}{n}\,\omega'(\mu_i))$$

$$M^n = M^n(\mu) := f_0(\varrho)\,\overline{M}(\mathscr{R}(T_{\delta_0}(\varrho),\, q)) + \frac{1}{n}\,\mathit{Id}\,.$$

Assume that $\alpha > 3$. Then, there is a vector $(\mu^n,\, v^n,\, \phi^n) \in \mathcal{B}(T,\, \Omega,\, \alpha,\, N,\, \Psi)$ (see [DDGG16], Definition 4.1) solving $(P) = (P_n)$ in the sense of Definition 4.3 in [DDGG16].

Proof. We can apply the approximation/existence procedure of the section 11 in [DDGG16] based on a Galerkin 'discretisation'. Note that M^n is a function of μ instead of ρ as in fact required in this paper. But on the one hand, we easily show that the correct growth condition

$$f_0(\varrho)\,|\overline{M}(T_{\delta_0}(\varrho),\, q))| \leq C(\delta_0,\, f_0)\,(1 + |\rho|), \quad \rho := \mathscr{R}(\varrho,\, q)$$

is satisfied. On the other hand, since M^n has full rank $= N$ for all $n \in \mathbb{N}$, the estimate of Lemma 8.19 in [DDGG16] guaranties that vacuum does not occur. Thus, pointwise convergence of the chemical potentials μ is equivalent with pointwise convergence of the partial mass densities ρ, and the strategy of section 11 of [DDGG16] can be applied one to one. □

5.1 A priori estimates

Since the Definition 3.5 implies that an energy inequality is satisfied, we automatically obtain the natural *a priori* estimates. We define (see [DDGG16] for details)

$$\begin{aligned}
\rho_i^n &:= \partial_i h^*(\mu^n) + \tau\,\omega'(\mu_i^n) \text{ for } i = 1, \ldots, N\,,\\
D_k^{\mathsf{R},n} &:= \gamma^k \cdot \mu^n \text{ for } k = 1, \ldots, s\,,\\
J^{i,n} &:= M_{i,j}^n\,\left(\nabla \mu_j^n + \tfrac{z_j}{m_j}\,\nabla \phi_n\right)\\
p_n &:= h^*(\mu^n) + \frac{1}{n}\,\sum_{i=1}^{N} \omega(\mu_i^n), \quad n_n^F := \sum_{i=1}^{n} \rho_i^n\,\tfrac{z_i}{m_i}\,.
\end{aligned}$$

Proposition 5.2. *Let* $\beta := \min\{r(\Omega,\, \Gamma),\, \frac{3\alpha}{(3-\alpha)^+}\} \geq \alpha'$*. Then*

$$\begin{aligned}
\|\rho^n\|_{L^{\infty,\alpha}(Q)} + \|\sqrt{\varrho_n}\, v^n\|_{L^{\infty,2}(Q;\,\mathbb{R}^3)} &\leq C_0\,,\\
\|v^n\|_{W^{1,0}_2(Q;\,\mathbb{R}^3)} &\leq C_0\,,\\
\|\phi_n\|_{L^\infty(Q)} + \|\phi_n\|_{L^\infty(0,T;\,W^{1,\beta}(\Omega))} &\leq C_0\\
\|D^{R,n}\|_{L_\Psi(Q;\,\mathbb{R}^s)} &\leq C_0\\
\sum_{i=1}^N \|J^{i,n}\|_{L^{2,\frac{2\alpha}{1+\alpha}}(Q)} + [-R^n]_{L_{\Psi^*}(Q;\,\mathbb{R}^s)} &\leq C_0\\
\|p_n\|_{L^{1+\min\{\frac{1}{\alpha},\frac{2}{3}-\frac{1}{\alpha}\}}(Q)} &\leq C_0\\
\|n^F_n\, \nabla\phi_n\|_{L^{\infty,\frac{\beta\alpha}{\beta+\alpha}}(Q;\,\mathbb{R}^3)} &\leq C_0\,.
\end{aligned}$$

Proof. These are direct consequences of the energy inequality and of the Navier-Stokes equations (pressure bound). Compare to the Propositions 8.1, 8.2 and the Lemma 8.5 in [DDGG16]. □

The main difference to the paper [DDGG16]is that we do not possess a global control on ∇q, but only weighted estimates. Thus, the procedure described in the section 8.2 of [DDGG16] to control the chemical potentials must be adapted.

Lemma 5.3. *Let* $u \in C^1(\overline{Q},\, \mathbb{R}_+)$*. Then the shifted mass density vector* $\tilde{\rho}^n := \mathscr{R}(u,\, q^n)$ *satisfies* $\|\nabla\tilde{\rho}^n\|_{L^2(Q;\,\mathbb{R}^{N\times 3})} \leq C_0(\|u\|_{C^1(\overline{Q})})$.

Proof. Throughout this proof we forget about the indices n. We compute

$$\nabla\tilde{\rho}_i = \nabla\mathscr{R}_i(u,\, q) = \mathscr{R}_{i,s}(u,\, q)\, \nabla u + \sum_{j=1}^N \mathscr{R}_{i,q_j}\, \nabla q_j\,.$$

Making use of (46), we can resort to the representation

$$\begin{aligned}
\nabla\tilde{\rho}_i - \mathscr{R}_{i,s}(u,\, q)\, \nabla u &= \sum_{j=1}^{N-1} \left(D^2h^*e^i\cdot e^j - \frac{D^2h^*e^i\cdot \mathbb{1}\, D^2h^*e^j\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\right)\, \nabla q_j\\
&= \sum_{j=1}^{N} \left(D^2h^*e^i\cdot e^j - \frac{D^2h^*e^i\cdot \mathbb{1}\, D^2h^*e^j\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\right)\, \nabla q_j
\end{aligned}$$

We now call $b_j(\tilde{\rho}) := D^2h^*e^i\cdot e^j - \frac{D^2h^*e^i\cdot\mathbb{1}\, D^2h^*e^j\cdot\mathbb{1}}{D^2h^*\mathbb{1}\cdot\mathbb{1}}$ at $\mu := \nabla h(\tilde{\rho})$. We obtain owing to Lemma 4.2 that $b_j(\tilde{\rho}) \leq c_b\, \tilde{\rho}_j$ for $j = 1, \ldots, N$. Moreover we obviously have $b\cdot\mathbb{1} = 0$. Let $s_1 := T_{\delta_0}(\varrho)$. Invoking the Corollary 4.10, the system of equations

$$\overline{M}(\mathscr{R}(s_1,\, q))\, X = b(\tilde{\rho}) = b(\mathscr{R}(u,\, q))\,,$$

possesses a unique solution $X \in \mathbb{1}^{\perp}$ such that $|X| \leq \bar{C}(\|u\|_{L^\infty},\, \delta_0)$. Thus

$$
\begin{aligned}
\nabla \tilde{\rho}_i - \mathscr{R}_{i,s}(u,\, q)\, \nabla u &= \sum_{j=1}^{N} \overline{M}(\mathscr{R}(s_1,\, q))_j\, \nabla q_j \cdot X \\
&= \sum_{j=1}^{N} \overline{M}(\mathscr{R}(s_1,\, q))_j\, \left(\nabla \mu_j + \frac{z_j}{m_j}\, \nabla \phi\right) \cdot X - \nabla \phi \sum_{j=1}^{N} \overline{M}(\mathscr{R}(s_1,\, q))_j\, \frac{z_j}{m_j} \cdot X \\
&= \overline{M}(\mathscr{R}(s_1,\, q))\, D \cdot X - \nabla \phi\, \frac{z}{m} \cdot b\,.
\end{aligned}
$$

Further, it follows that

$$
\begin{aligned}
|\nabla \tilde{\rho}_i - \mathscr{R}_{i,s}(u,\, q)\, \nabla u| \leq & \sqrt{\overline{M}(\mathscr{R}(s_1,\, q))\, D \cdot D}\, \sqrt{\overline{M}(\mathscr{R}(s_1,\, q))\, X \cdot X} \\
& + |\tfrac{z}{m}|\, |\nabla \phi|\, c_b\, |\mathscr{R}(u,\, q)|\,.
\end{aligned}
$$

The choice of our approximation mappings M^n guaranties that $\overline{M}(\mathscr{R}(s,\, q)) \leq \underline{f}_0^{-1}\, M^n$ in the sense of positive semi definite matrices. It follows that

$$
\begin{aligned}
|\nabla \tilde{\rho}_i - \mathscr{R}_{i,s}(u,\, q)\, \nabla u| &\leq \underline{f}_0^{-1} \sqrt{M\, D \cdot D}\, \sqrt{\overline{M}(\mathscr{R}(s_1,\, q))\, X \cdot X} + C\, |\nabla \phi|\, |u| \\
&\leq C(\|u\|_{L^\infty(Q)})\, (\sqrt{M\, D \cdot D} + |\nabla \phi|)\,.
\end{aligned}
$$

We note that $M\, D \cdot D$ is the dissipation due to diffusion which is bounded in $L^1(Q)$. Finally we observe that $|\mathscr{R}_{i,s}(u,\, q)\, \nabla u| \leq C\, |u|^{\frac{\alpha-1}{2}}\, |\nabla u|$, and the claim follows from the bounds of Proposition 5.2. ☐

We also note a special estimate for associated with the index set $I^{\mathsf{c}}_{\overline{M}}$.

Lemma 5.4. *For $i \in I^{\mathsf{c}}_{\overline{M}}$ and parameters $\epsilon,\, \delta > 0$, define*

$$
\mathcal{J}^{i,n}_{\epsilon,\delta} := \{t \in]0, T[\,:\, |\{x \,:\, \rho_i^n(t,\, x) \geq \epsilon\}| \geq \delta\}\,, \quad |\cdot| := \lambda_3
$$

Then the sequence of functions $q_i^n(t,\, x)\, \chi_{\mathcal{J}^{i,n}_{\epsilon,\delta}}(t)$ satisfies a uniform bound in $L^2(Q)$.

Proof. Define $k_0 = k_0(t, x)$ as an index such that $\mathscr{R}_{k_0}(s_1,\, q) = \sup_{k=1,\ldots,N} \mathscr{R}_k(s_1,\, q)$. Here and throughout this proof, we omit the n indices and we abbreviate $s_1 := T_{\delta_0}(\varrho)$. Due to the Corollary 4.10, we can solve for all $i \in I^{\mathsf{c}}_{\overline{M}}$ the equations $\overline{M}(\mathscr{R}(s_1,\, q^n))\, X = e^i - e^{k_0}$, and the solutions satisfy $|X^i| \leq c(\delta_0)$. Thus

$$
\overline{M}(\mathscr{R}(s_1,\, q^n))\, X \cdot D = \nabla(q_i - q_{k_0}) + (\tfrac{z_i}{m_i} - \tfrac{z_{k_0}}{m_{k_0}})\, \nabla \phi\,.
$$

It follows that

$$
\begin{aligned}
|\nabla(q_i - q_{k_0})| &\leq 2\, |\tfrac{z}{m}|\, |\nabla \phi| + \sqrt{\overline{M}(\mathscr{R}(s_1,\, q^n))\, D \cdot D}\, \sqrt{\overline{M}(\mathscr{R}(s_1,\, q^n))\, X \cdot X} \\
&= 2\, |\tfrac{z}{m}|\, |\nabla \phi| + \sqrt{\overline{M}(\mathscr{R}(s_1,\, q^n))\, D \cdot D}\, \sqrt{(e^i - e^{k_0}) \cdot X} \\
&\leq c\, (|\nabla \phi| + \sqrt{M\, D \cdot D})\,.
\end{aligned}
$$

Thus, $\|\nabla(q_i - q_{k_0})\|_{L^2(Q)} \leq C_0$. Next recall that $q_{k_0} = \nabla_{k_0} h(\mathscr{R}(s_1, q)) - \mathscr{M}(s_1, q)$. Since $\mathscr{M}(s_1, q) \leq c_1 (1 + s_1^{\alpha-1})$ (Proof of Lemma 4.2), and since the choice of k_0 ensures $\mathscr{R}_{k_0}(s_1, q)/s_1 \geq N^{-1}$

$$\begin{aligned} q_{k_0} &= c_{k_0} + K \, \tfrac{V_{k_0}}{m_{k_0}} \, F'(\tfrac{V}{m} \cdot \mathscr{R}(s_1, q)) + \frac{k_B \, \theta}{m_0} \, \ln y_{k_0} - \mathscr{M}(s_1, q) \\ &\geq -\tilde{c}_1(\delta_0) \, (1 + s_1^{\alpha-1}) \, . \end{aligned}$$

Since moreover $q_{k_0} \leq 0$, it follows that $|q_{k_0}| \leq \tilde{c}_1(\delta_0) \, (1 + s_1^{\alpha-1}) \leq c_1(\delta_0)$ and we conclude that $\|q_{k_0}\|_{L^\infty(Q)} \leq C_0$. Next we make use of an inequality in the paper [DDGG16] (Lemma 8.7, (191)). For $\epsilon, \, \delta > 0$ arbitrary and $t \in]0, T[$ we obtain the alternative

$$\begin{cases} \|q_i(t) - q_{k_0}(t)\|_{L^1(\Omega)} \leq C^*(\delta) \, (\|\nabla(q_i(t) - q_{k_0}(t))\|_{L^1(\Omega)} + \epsilon^{-1}) \\ \text{or} \\ |\{x \, : \, q_i(t,x) - q_{k_0}(t,x) < \epsilon^{-1}\}| \leq \delta \text{ or } |\{x \, : \, q_i(t,x) - q_{k_0}(t,x) > -\epsilon^{-1}\}| \leq \delta \, . \end{cases}$$

We are going to precise this alternative. First, making use of the Sobolev embedding theorem

$$\|q_i(t) - q_{k_0}(t)\|_{L^2(\Omega)} \leq C \, \|\nabla(q_i(t) - q_{k_0}(t))\|_{L^2(\Omega)} + \|q_i(t) - q_{k_0}(t)\|_{L^1(\Omega)} \, .$$

Thus, we obtain for $t \in]0, T[$ the new alternative

$$\begin{cases} \|q_i(t)\|_{L^2(\Omega)} \leq (C^*(\delta) + 1) \, (\|\nabla(q_i(t) - q_{k_0}(t))\|_{L^2(\Omega)} + \epsilon^{-1}) + \|q_{k_0}\|_{L^\infty(Q)} \\ \text{or} \\ |\{x \, : \, q_i(t,x) - q_{k_0}(t,x) < \epsilon^{-1}\}| \leq \delta \text{ or } |\{x \, : \, q_i(t,x) - q_{k_0}(t,x) > -\epsilon^{-1}\}| \leq \delta \, . \end{cases}$$

Second, for ϵ appropriate, we have $|\{x \, : \, |q_{k_0}(t)| \geq \epsilon^{-1}\}| = 0$, therefore

$$|\{x \, : \, q_i(t,x) - q_{k_0}(t,x) > -\epsilon^{-1}\}| \leq \delta \Rightarrow |\{x \, : \, q_i(t,x) > -2\,\epsilon^{-1}\}| \leq \delta \, .$$

Moreover, recalling the Lemma 8.8 of [DDGG16]

$$|\{x \, : \, q_i(t,x) > -2\,\epsilon^{-1}\}| \leq \delta \Longrightarrow |\{x \, : \, \rho_i(t, \, x) > \epsilon/2\}| \leq \delta + C_0 \, \epsilon^\alpha \, .$$

Thus we attain for $t \in]0, T[$ the new alternative

$$\begin{cases} \|q_i(t)\|_{L^2(\Omega)} \leq (C^*(\delta) + 1) \, (\|\nabla(q_i(t) - q_{k_0}(t))\|_{L^2(\Omega)} + \epsilon^{-1}) + \|q_{k_0}\|_{L^\infty(Q)} \\ \text{or} \\ |\{x \, : \, \rho_i(t, \, x) > \epsilon/2\}| \leq \delta + C_0 \, \epsilon^\alpha \, . \end{cases}$$

□

5.2 Extraction of weakly convergent subsequences

The extraction of weakly convergent subsequences has been extensively described in the section 9 of [DDGG16]. Exploiting informations on distributional time-derivatives of ρ, $\varrho \, v$ and ϕ, it is possible to identify the weak limits of the products $\varrho \, v$ and $\varrho \, v \otimes v$ and to obtain the compactness of $\nabla\phi$. Since we have no new conceptual input, we quote without further comments the following Lemma.

Lemma 5.5. *It is possible to extract a subsequence such that*

$$\rho^n \to \rho \text{ weakly in } L^\alpha(Q;\,\mathbb{R}^N), \quad \rho^n(t) \to \rho(t) \text{ weakly in } L^\alpha(\Omega;\,\mathbb{R}^N) \text{ for a. a. } t \in [0,T]$$
$$J^n \to J \text{ weakly in } L^{2,\frac{2\alpha}{1+\alpha}}(Q;\,\mathbb{R}^{N\times 3})$$
$$R^n \to R \text{ weakly in } L^1(Q;\,\mathbb{R}^s)$$
$$v^n \to v \text{ weakly in } W^{1,0}_2(Q;\,\mathbb{R}^3)$$
$$p_n \to p \text{ weakly in } L^{1+\min\{\frac{1}{\alpha},\,\frac{2}{3}-\frac{1}{\alpha}\}}(Q)$$
$$\phi_n \to \phi \text{ strongly in } W^{1,0}_2(Q)$$
$$\tfrac{z}{m}\cdot\rho^n\,\nabla\phi_n \to \tfrac{z}{m}\cdot\rho\,\nabla\phi \text{ weakly in } L^1(Q;\,\mathbb{R}^3)$$
$$\varrho_n\,v^n\otimes v^n \to \varrho\,v\otimes v \text{ weakly in } L^{\frac{5\alpha-3}{3\,\alpha}}(Q;\,\mathbb{R}^{3\times 3})$$
$$\varrho_n\,(v^n - v) \to 0 \text{ strongly in } L^1(Q;\,\mathbb{R}^3)\,.$$

Note that Lemma 5.5 guaranties the passage to the limit in the distributional relations (39), (40), (41). All the problem is to prove the connection relation between p and ρ and to introduce limit chemical potentials in order to connect J and R with the driving forces.

6 Compactness

6.1 Compactness of the total mass density

The first task is to prove the compactness of the sequence of total mass densities $\{\varrho^n\}_{n\in\mathbb{N}}$. The core of the method is the Lions-technique described extensively in the section 10 of [DDGG16], which relies on the estimates of Proposition 5.2, the (weak) compactness statements of Lemma 5.5 and the structural properties of the Navier-Stokes system. In fact, we need only to derive one single property of the *pressure function* which will turn out sufficient in order that the Lions machinery of section 10 the paper [DDGG16] applies. The pressure function $P\,:\,\mathbb{R}_+\times\partial\mathbb{R}^N_-$ is defined via $P(s,\,q) := h^*(q+\mathscr{M}(s,\,q)\,\mathbb{1})$. It is elementary to show using (6e) that

$$P(s,\,q) = (-F + \text{id}\,F')(\tfrac{V}{m}\cdot\mathscr{R}(s,\,q)) \text{ for all } (s,\,q)\in\mathbb{R}_+\times\partial\mathbb{R}^N_-\,. \tag{54}$$

The derivatives of the pressure function are given by the expressions

$$\partial_s P(s,\,q) = \frac{s}{D^2h^*\mathbb{1}\cdot\mathbb{1}}\,,$$
$$\partial_{q_j} P(s,\,q) = \mathscr{R}_j(s,\,q) - s\,\frac{D^2h^*\mathbb{1}\cdot e^j}{D^2h^*\mathbb{1}\cdot\mathbb{1}} \text{ if } e^j \text{ is tangent to } \partial\mathbb{R}^N_-\,.$$

where h^* is evaluated at $\mu = q+\mathscr{M}(s,\,q)\,\mathbb{1} = \nabla h(\mathscr{R}(s,\,q))$. Owing to the Lemma 4.2, this implies the inequalities

$$\frac{1}{C_1} \leq \partial_s P(s,\,q) \leq \frac{K}{C_0}\,F''(s)\,s \tag{55}$$
$$|\partial_{q_j} P(s,\,q)| \leq C\,\mathscr{R}_j(s,\,q)\,(1+K\,F''(s)\,s)\,.$$

From our approximation scheme of Proposition 5.1, we obtain that

$$p_n = P(\varrho_n,\, q^n)\,.$$

We shall make use of the Lemma 4.9 in order to obtain a control on *modified pressure gradients*.

Lemma 6.1. *Let P be the pressure function of* (54). *Let $u \in C^1(\overline{Q};\, \mathbb{R}_{0,+})$. Then $\|\nabla P(u,\, q^n)\|_{L^2(Q)} \leq C_0(u)$.*

Proof. We make use of the representation $P(u,\, q^n) = (-F + \mathsf{Id}\, F')(\frac{V}{m} \cdot \mathscr{R}(u,\, q^n))$. Thus

$$\nabla P(u,\, q^n) = (\mathsf{Id}\, F'')(\tfrac{V}{m} \cdot \mathscr{R}(u,\, q^n))\, \frac{V}{m} \cdot \nabla \mathscr{R}(u,\, q^n)\,.$$

On the one hand $(\mathsf{Id}\, F'')(\frac{V}{m} \cdot \mathscr{R}(u,\, q^n)) \leq (\mathsf{Id}\, F'')(|\frac{V}{m}|\, |\mathscr{R}(u,\, q^n)|) \leq C\, \|u\|_{L^\infty(Q)}^{\alpha-1}$. On the other hand, we apply the Lemma 5.3 in order to control $\nabla \mathscr{R}(u,\, q^n)$. □

With this statement we can establish the uniform-in-time compactness of the sequence $\{\varrho^n\}$ as long as $\alpha > 3$. We follow the lines of section 10 in [DDGG16]. For $k \in \mathbb{N}$, and $s \in \mathbb{R}_+$ we denote $T_k(s) := \min\{s,\, k\}$, and we extract a diagonal subsequence such that

$$T_k(\varrho_n) \to a_k \text{ weakly in } L^p(Q) \text{ for some } p > 1\,.$$

It turns out that everything is reduced to the conclusion of the following Lemma.

Lemma 6.2. *For all $t \in [0, T]$ there holds:*

$$\limsup_{n\to\infty} \int_{Q_t} (p_n\, T_k(\varrho_n) - p\, a_k) \geq c_0\, \limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_n) - a_k)^2\,.$$

If P is moreover a convex function of ϱ, then

$$\limsup_{n\to\infty} \int_{Q_t} p_n\, T_k(\varrho_n) \geq \int_{Q_t} p\, T_k(\varrho) + c_0\, \limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_n) - T_k(\varrho))^2\,.$$

Proof. We can represent $p_n = P(\varrho_n,\, q^n)$. Due to (55), $\partial_s P \geq c_0$. For arbitrary non-negative $u \in C^1(\overline{Q})$, we have

$$(P(\varrho_n,\, q^n) - P(u,\, q^n))\, (T_k(\varrho_n) - T_k(u)) \geq c_0\, (T_k(\varrho_n) - T_k(u))^2\,.$$

In particular, we choose $u = u_{n,\delta} := (\phi_\delta \star T_k(\varrho_n))$, where ϕ_δ is a smooth time-space convolution kernel and $\delta > 0$ is fixed. We note that $|P(u_{n,\delta},\, q^n)| \leq c\, |u_{n,\delta}|^\alpha \leq C_\delta$. Moreover, the Lemma 6.1 yields $\|\nabla P(u_{n,\delta},\, q^n)\|_{L^2(Q)} \leq C(\|u_{n,\delta}\|_{W^{1,\infty}(Q)}) \leq C_{0,\delta}$. Thus, we can find $b \in L^\infty_+(Q)$, $\nabla b \in L^2(Q)$ and a subsequence in n such that $P(u_{n,\delta},\, q^n) \to b$ weakly in $L^p(Q)$ for all $1 \leq p < +\infty$ and $\nabla P(u_{n,\delta},\, q^n) \to \nabla b$ in $L^2(Q)$. Exploiting the weak convergence $p_n \rightharpoonup p$ and $T_k(\varrho_n) \rightharpoonup a_k$, we then show that

$$\begin{aligned}
&\limsup_{n\to\infty} \int_{Q_t} p_n\, T_k(\varrho_n) - \int_{Q_t} p\, T_k(\phi_\delta \star a_k) \\
&\quad \geq \int_{Q_t} b\, (a_k - T_k(\phi_\delta \star a_k)) + c_0\, \limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_n) - T_k(\phi_\delta \star a_k))^2\,.
\end{aligned}$$

Letting δ tend to zero $\limsup_{n\to\infty} \int_{Q_t} (p_n\, T_k(\varrho_n) - p\, a_k) \geq c_0\, \limsup_{n\to\infty} \int_{Q_t} (T_k(\varrho_n) - a_k)^2$. □

We can conclude this subsection with the following statement (see [DDGG16], Lemma 10.6 and Lemma 10.10):

Proposition 6.3. *Let $\alpha > 3$. Then, the family $\bigcup_{t\in]0,T[}\bigcup_{n\in\mathbb{N}}\{\varrho_n(t)\}$ is compact in $L^1(\Omega)$.*

6.2 Compactness of the partial mass densities

We prove a preliminary inequality.

Lemma 6.4. *Consider the mapping $\mathscr{R}$ of Corollary 4.1. Let $K \subset L^1(\Omega;\, \mathbb{R}^N)$ be a weakly sequentially compact set, and $K^* \subset L^1_+(\Omega)$ a sequentially compact set. Let $\phi^1,\, \phi^2, \ldots \in C^\infty(\overline{\Omega},\, \mathbb{R}^N)$ be a countable, dense subset of $C^\infty_c(\Omega,\, \mathbb{R}^N)$.*

For all $\delta > 0$, there are $C(\delta) > 0$ and $k(\delta) \in \mathbb{N}$ such that

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

for all $w^i = (w^i_1,\, \bar{w}^i) \in L^1(\Omega;\, \mathbb{R}_{0,+} \times \partial\mathbb{R}^N_-)$ ($i = 1, 2$) such that $\mathscr{R}(1,\, \bar{w}^i) \in W^{1,1}(\Omega;\, \mathbb{R}^N)$ and such that

$$\mathscr{R}(w^i) \in K, \quad w^i_1 \in K^* \text{ for } i = 1, 2, \quad \|\mathscr{R}(w^1) - \mathscr{R}(w^2)\|_{L^1(\Omega)} \geq \delta\,.$$

Proof. If the claim is not true, there is $\delta_0 > 0$ such that for all $n \in \mathbb{N}$, we can find for $i = 1, 2$ a $w^{i,n} \in L^1(\Omega;\, \mathbb{R}_{0,+} \times \partial\mathbb{R}^N_-)$ such that $\mathscr{R}(w^{i,n}) \in K$, $w^{i,n}_1 \in K^*$ and such that $\|\mathscr{R}(w^{1,n}) - \mathscr{R}(w^{2,n})\|_{L^1(\Omega)} \geq \delta_0$ satisfying moreover the property

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

As the set K is bounded, we obtain first that $\|\nabla\mathscr{R}(1,\, \bar{w}^{i,n})\|_{L^1(\Omega)} \leq C\, \delta_0^{-1}$ for all $n \in \mathbb{N}$. Therefore, we can extract a subsequence such that

$$\exists \lim_{n\to\infty} \mathscr{R}(1,\, \bar{w}^{i,n}) \text{ almost everywhere in } \Omega\,.$$

Thus, using the bijective character of $\mathscr{R}$, we easily show that $\bar{w}^{i,n}$ converges pointwise almost everywhere in the sense of the compactification 4.3.

We further note that $w^{i,n}_1 \in K^*$ implies for a subsequence that $w^i_1(x) := \lim_{n\to\infty} w^{i,n}_1(x)$ exists in $\mathbb{R}_{0,+}$ for almost all $x \in \Omega$. Thus, the limit of $\mathscr{R}(w^{i,n}_1,\, \bar{w}^{i,n})$ exists almost everywhere in Ω and the claim follows, since the condition $\|\mathscr{R}(w^{1,n}) - \mathscr{R}(w^{2,n})\|_{L^1(\Omega)} \geq \delta_0$ is violated for large values of n. □

Corollary 6.5. *There is a subsequence for which there exists* $\lim_{n\to\infty} \rho^n(t,\, x)$ *for almost all* $(t,\, x) \in Q$. *Moreover, in the set* $Q^+(\varrho)$ *there exists* $\lim_{n\to\infty} q^n(t,\, x)$ *in the sense of the Remark 4.3.*

Proof. We apply the inequality of the previous Lemma with $w^1 := (\varrho_n(t),\, q^n(t))$ and $w^2 := (\varrho_{n+p}(t),\, q^{n+p}(t))$. We choose $K := \bigcup_{n\in\mathbb{N},\, t\in]0,T[}\{\rho^n(t)\}$ and $K^* := \bigcup_{n\in\mathbb{N},\, t\in]0,T[}\{\varrho^n(t)\}$. Thus, we obtain that either $\|\rho^n(t) - \rho^{n+p}(t)\|_{L^1(\Omega)} \leq \delta$, or that

$$\begin{aligned}\|\rho^n(t) - \rho^{n+p}(t)\|_{L^1(\Omega)} \leq & \delta\left(\|\nabla\mathscr{R}(1,\, q^n(t))\|_{L^1(\Omega)} + \|\nabla\mathscr{R}(1,\, q^{n+p}(t))\|_{L^1(\Omega)}\right) \\ & + C(\delta) \sum_{i=1}^{k(\delta)} \left| \int_\Omega (\rho^n(t) - \rho^{n+p}(t)) \cdot \phi^i \right| .\end{aligned}$$

Thus it easily follows after integration on $[0,T]$ that

$$\begin{aligned}\|\rho^n - \rho^{n+p}\|_{L^1(Q)} \leq & \;\delta\,(1 + 2\sup_{n\in\mathbb{N}} \|\nabla\mathscr{R}(1,\, q^n)\|_{L^1(Q)}) \\ & + C(\delta) \sum_{i=1}^{k(\delta)} \int_0^T \left| \int_\Omega (\rho^n(t) - \rho^{n+p}(t)) \cdot \phi^i \right| \\ \leq & \; C_1\,\delta + 2\,C(\delta) \sum_{i=1}^{k(\delta)} \sup_{j\geq n} \int_0^T \left| \int_\Omega (\rho^j(t) - \rho(t))) \cdot \phi^i \right|\end{aligned}$$

Therefore

$$\begin{aligned}&\limsup_{n\to\infty} \sup_{p\geq 0} \|\rho^n - \rho^{n+p}\|_{L^1(Q)} \\ &\quad\leq C_1\,\delta + 2\,C(\delta) \sum_{i=1}^{k(\delta)} \limsup_{n\to\infty} \sup_{j\geq n} \int_0^T \left| \int_\Omega (\rho^j(t) - \rho(t))) \cdot \phi^i \right| \\ &\quad= C_1\,\delta + 2\,C(\delta) \sum_{i=1}^{k(\delta)} \limsup_{n\to\infty} \int_0^T \left| \int_\Omega (\rho^n(t) - \rho(t))) \cdot \phi^i \right|\end{aligned}$$

The integrand $|\int_\Omega (\rho^n(t) - \rho(t)))\cdot\phi^i|$ is majorated by $c_{\phi^i}\, \|\rho^n\|_{L^{\infty,1}(Q)}$ and converges pointwise to zero. Thus, $\limsup_{n\to\infty} \sup_{p\geq 0} \|\rho^n - \rho^{n+p}\|_{L^1(Q)} = 0$, and this establishes the strong convergence in $L^1(Q;\, \mathbb{R}^N)$.

It also follows that $\mathscr{R}(\varrho,\, q^n)$ converges almost everywhere, and we use the properties of $\mathscr{R}$ to show that q^n converges in the sense of the Remark 4.3 in $Q^+(\varrho)$. This means that for every index set $I \subset \{1, \ldots, N\}$ with cardinatlity $|I| \geq 1$, there exists a vector field $q^I \,:\, Q^I \to \mathbb{R}^{|I|}$ such that

$$q^n_{i_k} \to q^I_k \text{ almost everywhere in } Q^I \text{ for } I = \{i_1, \ldots, i_{|I|}\}$$
$$\limsup_{n\to\infty} q^n_i = -\infty \text{ almost everywhere in } Q^I \text{ for all } i \in I^{\mathsf{c}}$$

□

6.3 Limit identification

Consider an index set $I \subseteq \{1, \ldots, N\}$ with $|I| \geq 1$. It is obvious by definition that $Q^I \subseteq Q^+(\varrho)$. On the other hand, $\varrho > 0$ implies that there is at least one index such that $\rho^{i_0} > 0$. Therefore, up to a set of measure zero

$$Q^+(\varrho) = \bigcup_{I \subseteq \{1,\ldots,N\},\, I \neq \emptyset} Q^I \,,$$

Thus, $q^n \to q$ almost everywhere in $\bigcup_{I \subseteq \{1,\ldots,N\},\, I \neq \emptyset} Q^I$, and this implies that

$$\exists \lim_{n\to\infty} \rho^{n,\text{norm}} = \mathscr{R}^I(1,\, q^I) \text{ almost everywhere in } Q^I \,.$$

Moreover, since $\rho = \mathscr{R}(\varrho,\, q)$ in $Q^+(\varrho)$ due to the same reasons, we obtain that

$$\lim_{n\to\infty} \rho^{n,\text{norm}} = \mathscr{R}(1,\, q) = \rho^{\text{norm}} \text{ almost everywhere in } Q^+(\varrho) \,. \tag{56}$$

On the other hand, the sequence $\{\rho^{n,\text{norm}}\}$ is uniformly bounded in the class $L^\infty(Q;\, \mathbb{R}^N) \cap L^2(0,T;\, W^{1,2}(\Omega;\, \mathbb{R}^N))$. Thus, there is $u \in L^\infty(Q;\, \mathbb{R}^N) \cap L^2(0,T;\, W^{1,2}(\Omega;\, \mathbb{R}^N))$ such that

$$\rho^{n,\text{norm}} \to u \text{ weakly in } L^2(Q) \quad \nabla\rho^{n,\text{norm}} \to \nabla u \text{ weakly in } L^2(Q) \,.$$

Combining with (56), we clearly obtain that $\rho^{\text{norm}} = u$ in $Q^+(\varrho)$. This shows that the normalisation of the limit mass densities in $Q^+(\varrho)$ belongs to the restriction of elements of $L^\infty(Q;\, \mathbb{R}^N) \cap L^2(0,T;\, W^{1,2}(\Omega;\, \mathbb{R}^N))$ to this set.

Consider next the sequence of total mass densities $\{\bar{\rho}_n\}_{n\in\mathbb{N}}$. Due to the estimate in the class $C_{\Phi^*}([0,T])$, we obtain that $\bar{\rho}^n \to \bar{\rho} = \int_\Omega \rho$ uniformly on $[0,T]$. Let $K \subset\subset \{t \,:\, \bar{\rho}_i(t) > 0\}$. Then $\inf_{n\geq n_0,\, t\in K} \bar{\rho}^n(t) > 0$ for n_0 appropriate. Thus, we can find parameters $\epsilon,\, \delta > 0$ such that

$$K \subseteq \mathcal{J}^{i,n}_{\epsilon,\delta} := \{t \in]0,T[\,:\, |\{x \,:\, \rho^n_i(t,\, x) \geq \epsilon\}| \geq \delta\} \;.$$

Recall now the statement of Lemma 5.4. For $i \in I^{\mathsf{c}}_{\overline{M}}$, we obtain that

$$\|q^n_i\|_{L^2(K\times\Omega)} \leq \|q^n_i\, \chi_{\mathcal{J}^{i,n}_{\epsilon,\delta}}(t)\|_{L^2(K\times\Omega)} \leq C_0(K) \,.$$

Thus, by Fatou's Lemma $\|q_i\|_{L^2(Q^+\cap[K\times\Omega])} \leq \liminf_{n\to\infty} \|q^n_i\|_{L^2(K\times\Omega)} < +\infty$. This proves the statement 3.7.

We next investigate the limit diffusion fluxes J. We start from the equivalent representation

$$J^{n,i} = \sum_{k=1}^N \mathcal{D}^n_{i,k}\, \nabla\rho^{n,\text{norm}}_k + \nabla\phi_n\, M^n \tfrac{z}{m} \cdot e^i + \frac{1}{n}\, \nabla\rho^{n,\text{norm}}_i$$

$$\mathcal{D}^n_{i,k} := f_0(\varrho_n)\, \sum_{j=1}^n \overline{M}(\mathscr{R}(T_{\delta_0}(\varrho_n),\, q^n))_{i,j}\, D^2h_{j,k}(\rho^{n,\text{norm}}) \,.$$

We make use of (differentiate in (5))

$$D^2 h_{j,k}(\rho^{n,\text{norm}}) = \frac{V_j}{m_j}\,\frac{V_k}{m_k}\, K\, F''(\tfrac{V}{m}\cdot \rho^{n,\text{norm}}) - \frac{k_B\,\theta}{m_j\,m_k}\,\frac{1}{\frac{1}{m}\cdot\rho^{n,\text{norm}}} + \frac{k_B\,\theta}{m_j}\,\frac{\delta_{j,k}}{\rho_j^{n,\text{norm}}}\,.$$

Since $\sum_{i=1}^N \rho_i^{n,\text{norm}} = 1$ it follows that $|D^2 h_{j,k}(\rho^{n,\text{norm}})| \leq c\,(1 + \frac{\delta_{j,k}}{\rho_j^{n,\text{norm}}})$. We recall also that $|\overline{M}(\rho)_{i,j}| \leq C\, \min\{\rho_i,\,\rho_j\}$, and we obtain that

$$|\mathcal{D}^n_{i,k}| \leq c\, f_0(\varrho_n) \left(|\mathscr{R}(T_{\delta_0}(\varrho_n),\, q^n)| + \sum_{i=1}^N \frac{\mathscr{R}_i(T_{\delta_0}(\varrho_n),\, q^n)}{\mathscr{R}_i(1,\, q^n)}\right) \leq c(\delta_0,\, f_0)\,(1+\varrho_n)$$

We make use of the pointwise convergence of $\rho^{n,\text{norm}}$ in the set Q^+, and we obtain that $\mathcal{D}^n \to \mathcal{D} = M_{i,j}\, D^2 h_{j,k}(\rho^{\text{norm}})$ pointwise almost everywhere in $Q^+(\varrho)$. Moreover, we can choose for every $\epsilon > 0$ a set $Q^+_\epsilon \subset Q^+$, $\lambda_4(Q^+ \setminus Q^+_\epsilon) \leq \epsilon$ such that ϱ_n converges uniformly on Q^+_ϵ (Egoroff theorem). It clearly follows that

$$J^{n,i} \to \sum_{k=1}^N \mathcal{D}_{i,k}\,\nabla\rho_k^{\text{norm}} + \nabla\phi\, M\,\tfrac{z}{m}\cdot e^i \text{ weakly in } L^1(Q^+_\epsilon)\,.$$

This shows that $J = \mathcal{D}\,\nabla\rho^{\text{norm}} + \nabla\phi\, M\,\frac{z}{m}$ first in Q^+_ϵ, and then letting ϵ tend to zero also almost everywhere in Q^+.

6.4 Passage to the limit in the energy identity

Passage to the limit with the entropy production due to diffusion $M^n\, D^n \cdot D^n$ Here we use the equivalent representation

$$M^n\, D^n \cdot D^n = [M^n]^{-1}\, J^n \cdot J^n = \sum_{i=1}^{N-1} \frac{1}{\lambda_i(M^n)}\, |J^{i,n} \cdot \xi^i(M^n)|^2\,.$$

At first we note that for $i = 1, \ldots, N-1$, the sequence $[\lambda_i(M^n)]^{-1/2}\, J^n \cdot \xi^i(M^n))$ is bounded in $L^2(Q;\, \mathbb{R}^3)$. Thus, there is a limiting element $a^i \in L^2(Q;\, \mathbb{R}^3)$ such that $[\lambda_i(M^n)]^{-1/2}\, J^n \cdot \xi^i(M^n)) \to a^i$ weakly in L^2 and $\|a^i\|_{L^2} \leq \liminf_{n\to\infty} \int_Q M^n\, D^n \cdot D^n$.

Next we consider the set $Q^{I,\epsilon} := \{(t,\,x) \in Q^I \,:\, \rho^i(t,\,x) \geq \epsilon \text{ for all } i \in I\}$. Due to the Egoroff Theorem, we can find $\tilde{Q}^{I,\epsilon} \subset Q^{I,\epsilon}$ with $\lambda_4(Q^{I,\epsilon} \setminus \tilde{Q}^{I,\epsilon}) \leq \epsilon$ and $\rho^{i,n} \to \rho^i$ uniformly on $\tilde{Q}^{I,\epsilon}$.

Assume now that the cardinality of I satisfies $|I| \geq 2$. Then by assumption, the $|I|-1$ first eigenvalues $\lambda_1(M^n), \ldots, \lambda_{|I|-1}(M^n)$ form sequences uniformly bounded away from zero on $\tilde{Q}^{I,\epsilon}$.

$$[\lambda_i(M^n)]^{-1/2} \to [\lambda_i(M)]^{-1/2} \text{ strongly in } L^p(\tilde{Q}^{I,\epsilon})\,.$$

Since on the other hand $J^n \cdot \xi^i(M^n) \to J \cdot \xi^i(M)$ weakly in $L^{2\alpha/(1+\alpha)}(Q^+)$, it follows that

$$a^i = [\lambda_i(M)]^{-1/2}\, J \cdot \xi^i(M) \text{ a. e. in } \tilde{Q}^{I,\epsilon} \text{ for } i = 1, \ldots, |I| - 1\,,$$

and letting ϵ tend to zero, we obtain the latter representation almost everywhere in Q^I. Thus

$$\int_{Q^I} \sum_{i=1}^{|I|-1} \frac{1}{\lambda_i(M)}\, |J^n \cdot \xi^i(M)|^2 \leq \liminf_{n\to\infty} \int_{Q^I} M^n\, D^n \cdot D^n\,.$$

Passage to the limit with the entropy production due to reaction $\int_Q(\Psi(D^{\mathsf{R},n})+\Psi^*(-R^n))$
Let I be an index set. Recall that $q_i^n \to q_i$ pointwise almost everywhere in Q^I for all $i \in I$. Due to the Egoroff theorem, there is for all $\ell \in \mathbb{N}$ a set $A^\ell \subset Q^I$ such that $\lambda_4(Q^I \setminus A^\ell) \leq \ell^{-1}$ and the convergence is uniform on A^ℓ. Consider now for $\ell \in \mathbb{N}$ a set

$$Q^{I,\ell} := \{(t,\, x) \in Q^I \,:\, |q^I| \leq \ell\} \cap A^\ell\,.$$

We split the reaction driving forces $\gamma^k \cdot q^n = \gamma^k \cdot P_I(q^n) + \gamma^k \cdot P_{I^c}(q^n)$, and we obtain for n an estimate

$$\int_{Q^I_\ell} \Psi(\gamma^1 \cdot P_{I^c}(q^n), \ldots, \gamma^s \cdot P_{I^c}(q^n)) \leq [D^{\mathsf{R},n}]_{L_\Psi(Q)} + C(\ell)\,. \tag{57}$$

We define X^n to be the orthogonal projection of q^n on the space $\mathcal{V}^I = \mathrm{span}\{P_{I^c}(\gamma^k)\}_{k=1,\ldots,s}$. Due to (57), we can extract a subsequence such that X^n converges weakly in $L^1(Q^I_\ell;\, \mathbb{R}^s)$ to a limit element X, and this yields

$$\lim_{n\to\infty} \int_{Q^{I,\ell}} \Psi(D^{\mathsf{R},n}) \geq \int_{Q^{I,\ell}} \Psi(\gamma^1 \cdot (P_I(q) + X), \ldots, \gamma^s \cdot (P_I(q) + X)) \geq \int_{Q^{I,\ell}} \widetilde{\Psi}^I(q^I)\,,$$

where we make use of the definition

$$\widetilde{\Psi}^I(q^I) := \inf_{X \in \mathcal{V}^I} \Psi(\gamma^1 \cdot (P_I(q) + X), \ldots, \gamma^s \cdot (P_I(q) + X))\,.$$

Thus, if we make use of the fact that $R^n \to R$ in $L^1(Q;\, \mathbb{R}^s)$, it follows that

$$\liminf_{n\to\infty} \int_Q (\Psi(D^{\mathsf{R},n}) + \Psi^*(-R^n)) \geq \int_Q (\Psi^*(-R) + \sum_{I\subset\{1,\ldots,N\}} \chi_{Q^I}\, \widetilde{\Psi}^I(q^I))\,.$$

This finishes the proof of Theorem 3.6 in case that $\alpha > 3$.

6.5 The case $\alpha \leq 3$

The matrices M^n have full rank and generate a perturbation in the equation of conservation of total mass. It was a technical requirement of the Lions method that the pressure growth satisfies $\alpha > 3$ to pass to the limit $n \to \infty$. If the growth exponent of the mechanical free energy (via the function F) is in the range $\frac{3}{2} < \alpha \leq 3$, we assume first that we have replaced F by

F_δ, with $F_\delta(s) = F(s) + \delta\, s^4$. Using the approximation method of Proposition 5.1, we then establish existence for the regularised problem and we obtain a solution family indexed by δ. In this subsection we briefly indicate how to pass to the limit $\delta \to 0$ in order to complete the proof of the Theorem 3.6.

In fact, it turns out that the compactness of the family of mass densities $\{\rho_\delta\}_{\delta>0}$ is sufficient to derive the result. In order to prove the compactness, we will use the following information (the validity of which follows from the definition of the class $\mathcal{B}$): For all $u \in C^1(\overline{Q};\, \mathbb{R}_+)$ there is an extension function $f = f_{\delta,u} \in L^\infty(Q;\, \mathbb{R}^N_+)$, $\nabla f \in L^2(Q;\, \mathbb{R}^{N\times 3})$ such that

$$\begin{aligned} &\|f\|_{L^\infty(Q;\mathbb{R}^N)} + \|\nabla f\|_{L^2(Q;\mathbb{R}^{N\times 3})} \leq C_0(\|u\|_{C^1}) \\ &\qquad\qquad\qquad \mathscr{R}(u,\, q^\delta) = f \text{ almost everywhere in } Q^+(\varrho_\delta)\,. \end{aligned} \tag{58}$$

Recall that $\mathscr{R}(u,\, q^\delta)$ is well defined in $Q^+(\varrho_\delta)$ for q^δ in the class $\mathcal{B}$.

Let us now show how we derive the validity of the Lemma 6.2. We express

$$\begin{aligned} &\int_{Q^+(\varrho_\delta)} (P(\varrho_\delta,\, q^\delta)\, T_k(\varrho_\delta) - P(\varrho_\delta,\, q^\delta)\, u) \\ &\quad = \int_{Q^+(\varrho_\delta)} (P(\varrho_\delta,\, q^\delta) - P(u,\, q^\delta))\, (T_k(\varrho_\delta) - u) + \int_{Q^+(\varrho_\delta)} P(u,\, q^\delta))\, (T_k(\varrho_\delta) - u) \\ &\quad \geq c_0 \int_{Q^+(\varrho_\delta)} (T_k(\varrho_\delta) - u)^2 + \int_{Q^+(\varrho_\delta)} P(u,\, q^\delta)\, (T_k(\varrho_\delta) - u) \end{aligned}$$

We now call $\tilde{p}_\delta := (-F + \mathrm{Id}\, F')(\frac{V}{m} \cdot f)$. Then, $\tilde{p}_\delta = P(u,\, q^\delta))$ on Q^+. Moreover, on $Q \setminus Q^+$, we have $\tilde{p}_\delta\, (T_k(\varrho_\delta) - u) = -\tilde{p}_\delta\, u \leq 0$. It follows that

$$\begin{aligned} \int_Q (P(\varrho_\delta,\, q^\delta)\, T_k(\varrho_\delta) - P(\varrho_\delta,\, q^\delta)\, u) &= \int_{Q^+(\varrho_\delta)} (P(\varrho_\delta,\, q^\delta)\, T_k(\varrho_\delta) - P(\varrho_\delta,\, q^\delta)\, u) \\ &\geq c_0 \int_{(Q^+(\varrho_\delta)} (T_k(\varrho_\delta) - u)^2 + \int_Q \tilde{p}_\delta\, (T_k(\varrho_\delta) - u)\,. \end{aligned}$$

Thus, denoting p the weak limit of $\{p_\delta\}$ we then obtain as in the proof of Lemma 6.2

$$\liminf_{\delta\to 0} \int_Q p_\delta\, T_k(\varrho_\delta) - \int_Q p\, u \geq c_0\, \liminf_{\delta\to 0} \int_{(Q^+(\varrho_\delta)} (T_k(\varrho_\delta) - u)^2\,.$$

Thus, as $u \to a_k$

$$\liminf_{\delta\to 0} \int_Q p_\delta\, T_k(\varrho_\delta) - \int_Q p\, a_k \geq c_0\, \liminf_{\delta\to 0} \int_{(Q^+(\varrho_\delta)} (T_k(\varrho_\delta) - a_k)^2\,.$$

This is sufficient to obtain the uniform in time compactness of the family of total mass densities $\{\varrho_\delta\}_{\delta>0}$.

We obtain the compactness of the partial mass densities with an inequality similar to Lemma 6.4, 6.5, Here we have to replace $\mathscr{R}(1,\, q^i)$ which are not defined in vacuum by the extension functions given in the definition of the class $\widetilde{W}^{1,0}_{\varrho,2}(Q)$. We spare the reader with the technical details.

A Appendix

Proof of Lemma 2.2 Let $r \in \mathrm{span}\{\gamma^1, \ldots, \gamma^s\}$ and $\mu \in \mathbb{R}^N$ be given.

We denote $D^{\mathsf{R}} = (\gamma^1 \cdot \mu, \ldots, \gamma^s \cdot \mu) \in \mathbb{R}^s$. Let $I \subset \{1, \ldots, N\}$ be an ordered index set. We are going to construct the solution operator of the algebraic equations

$$-\sum_{k=1}^{s} \underbrace{\partial_k \Psi(D^{\mathsf{R}})}_{=:R_k} \gamma_i^k = r_i \text{ for } i \in I^{\mathsf{c}}\,. \tag{59}$$

By assumption, $P_{I^{\mathsf{c}}}(r) \in \mathcal{V}$. Therefore, there is a representation $r_i = \sum_{k=1}^d \tilde{r}_k\, \gamma_i^k$ for all $i \in I^{\mathsf{c}}$, with the coordinates $\tilde{r}_1, \ldots, \tilde{r}_d$ of $P_{I^{\mathsf{c}}}(r)$ in $\mathcal{V}$. Making use of the matrix A from (22), we see that the conditions (59) are then equivalent for $i \in I^{\mathsf{c}}$ to

$$\sum_{k=1}^{d} R_k\, \gamma_i^k + \sum_{k=d+1}^{s} R_k\, (\sum_{\ell=1}^{d} A_\ell^{k-d}\, \gamma_i^\ell) = \sum_{\ell=1}^{d} \tilde{r}_\ell\, \gamma_i^\ell\,.$$

Obviously, making use of the fact that $\{P_{I^{\mathsf{c}}}(\gamma^k)\}_{k=1,\ldots,d}$ is a basis of $\mathcal{V}$, the latter is valid if and only if

$$R_\ell + \sum_{k=d+1}^{s} A_\ell^{k-d}\, R_k = \tilde{r}_\ell \quad \text{for } \ell = 1, \ldots, d\,. \tag{60}$$

We next interpret (60) as implicit equation as follows: For $X \in \mathbb{R}^d$ and $Y \in \mathbb{R}^{s-d}$ we define

$$\mathcal{L}(X,\, Y) := (X,\, Y + A\, X) \in \mathbb{R}^d \times \mathbb{R}^{s-d}$$
$$\tilde{\Psi}(X,\, Y) := \Psi(\mathcal{L}(X,\, Y))\,.$$

Consider now the points Y and X defined via

$$Y_\ell := \gamma^{I,\ell} \cdot \mu \text{ for } \ell = 1, \ldots, s-d, \quad X_\ell := \gamma^\ell \cdot \mu \text{ for } \ell = 1, \ldots, d\,.$$

Then, we have the identities

$$\gamma^j \cdot \mu = \begin{cases} X_j & \text{for } j = 1, \ldots, d \\ Y_{j-d} + \sum_{k=1}^d A_k^{j-d}\, X_k & \text{for } j = d+1, \ldots, s\,. \end{cases}$$

Straightforward calculations now show that the equations (60) are equivalent to $-\partial_{X_\ell} \tilde{\Psi}(X,\, Y) = \tilde{r}_\ell$ for $\ell = 1, \ldots, d$, or more precisely

$$\partial_X \tilde{\Psi} \left(\underbrace{\gamma^1 \cdot \mu, \ldots,\, \gamma^d \cdot \mu}_{=X},\, \underbrace{\gamma^{I,1} \cdot \mu, \ldots,\, \gamma^{I,s-d} \cdot \mu}_{=Y} \right) = -\tilde{r}\,. \tag{61}$$

Next we want to compute the functional matrix of the system (60), (61). To this aim, we make use of the potential Ψ and we split its variable $D^{\mathsf{R}} \in \mathbb{R}^s$ as $(D,\, \bar{D}) \in \mathbb{R}^d \times \mathbb{R}^{s-d}$. Then for $k,\, \ell = 1, \ldots, d$

$$\partial^2_{X_k, X_\ell} \tilde{\Psi}(X,\, Y) = \partial^2_{D_k, D_l} \Psi + A_\ell^T \partial^2_{D_k, \bar{D}} \Psi + A_k^T \partial^2_{D_\ell, \bar{D}} \Psi + A_\ell^T\, A_k^T \partial^2_{\bar{D}, \bar{D}} \Psi\,, \tag{62}$$

where Ψ is evaluated at $\mathcal{L}(X,\, Y)$. For $\eta \in \mathbb{R}^d$ arbitrary, it follows that

$$\begin{aligned}\partial^2_{X,\,X}\tilde{\Psi}(X,\,Y)\,\eta\cdot\eta &= \partial^2\Psi(\eta,\,A\,\eta)\cdot(\eta,\,A\,\eta)\\ &\geq \lambda_{\inf}(\partial^2\Psi)\,(\eta^2+|A\eta|^2) \geq c_0\,|\eta|^2\,.\end{aligned}$$

Thus, it turns out that $\tilde{\Psi}$ is strictly convex in the first variable, and the equations $-\partial_X\tilde{\Psi}(X,\,Y) = \tilde{r}$ define implicitly the variable X as a function of $\tilde{r} \in \mathbb{R}^d$ and $Y \in \mathbb{R}^{s-d}$. We denote G, $(Y,\,\tilde{r}) \mapsto X$ the solution mapping. Clearly, $G(Y,\,\tilde{r})$ is nothing else but $\nabla\tilde{\Psi}^*(-\tilde{r},\,Y)$ of the convex conjugate in the first variable X of the function $\tilde{\Psi}$. For the derivatives of the solution mapping G, we obtain that

$$\begin{aligned}G_{i,Y_j}(Y,\,\tilde{r}) &= -\sum_{\ell=1}^{d}(\partial^2\tilde{\Psi}_{X,X})^{-1}_{i,\ell}\,\partial^2\tilde{\Psi}_{X_\ell,Y_j}\\ &= -\sum_{\ell=1}^{d}(\partial^2\tilde{\Psi}_{X,X})^{-1}_{i,\ell}\,\left(\partial^2_{D_l,\bar{D}_j}\Psi + A^T_\ell\,\partial^2_{\bar{D}_j,\bar{D}}\Psi\right)\\ G_{\tilde{r}}(Y,\,\tilde{r}) &= -(\partial^2\tilde{\Psi}_{X,X})^{-1}\,.\end{aligned}$$

Due to (61) we obtain for $\ell = 1,\ldots,d$ that

$$\gamma^\ell\cdot\mu = G_\ell(\gamma^{I,1}\cdot\mu,\ldots,\,\gamma^{I,s-d}\cdot\mu,\,\tilde{r})\,.$$

We define $s^I := s-d$ the *reduced number of reactions*. For $(Y,\,\tilde{r}) \in \mathbb{R}^{s^I}\times\mathbb{R}^d$, introduce the reduced potential

$$\begin{aligned}\hat{\Psi}(Y,\,\tilde{r}) :=&\Psi(\mathcal{L}(G(Y,\,\tilde{r}),\,Y)) + \tilde{r}\cdot G(Y,\,\tilde{r})\\ &- Y\cdot\nabla_{\bar{D}}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0)) - (\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0)) + \tilde{r}\cdot G(0,\,\tilde{r}))\,. \qquad (63)\end{aligned}$$

Next we shall prove that $\hat{\Psi} \in C^1(\mathbb{R}^{s^I}\times\mathbb{R}^d)$ is non-negative, and the function $Y \mapsto \hat{\Psi}(Y,\,\tilde{r})$ is C^2 and convex for all $\tilde{r} \in \mathbb{R}^d$.

Making use of the definition (63), we compute for $k = 1,\ldots,s^I$

$$\begin{aligned}\partial_{Y_k}\hat{\Psi}(Y,\,\tilde{r}) &= (\partial_X\tilde{\Psi}(G(Y,\,\tilde{r}),\,Y)+\tilde{r})\cdot G_{Y_k}(Y,\,\tilde{r}) + \tilde{\Psi}_{Y_k}(G(Y,\,\tilde{r}),\,Y)\\ &\qquad - \nabla_{\bar{D}_k}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\\ &= \tilde{\Psi}_{Y_k}(G(Y,\,\tilde{r}),\,Y) - \nabla_{\bar{D}_k}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\\ &= \partial_{k+d}\Psi(\mathcal{L}(G(Y,\,\tilde{r}),\,Y)) - \partial_{k+d}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\,. \qquad (64)\end{aligned}$$

Here we use that G is the solution mapping to $-\partial_X\tilde{\Psi}(X,\,Y) = \tilde{r}$. Since $\nabla\Psi$ is of class $\mathcal{C}^1$, we obtain from (64) that $\partial_Y\hat{\Psi}$ is of class $\mathcal{C}^1$ as well. Moreover it is obvious that $\partial_Y\hat{\Psi}(0,\,\tilde{r}) = 0$.

For $k,\,\ell = 1,\ldots,s^I$, we further compute

$$\partial_{Y_k,Y_\ell}\hat{\Psi}(Y,\,\tilde{r}) = \tilde{\Psi}_{Y_k,X}(G(Y,\,\tilde{r}),\,Y)\cdot G_{Y_\ell}(Y,\,\tilde{r}) + \tilde{\Psi}_{Y_k,Y_\ell}(G(Y,\,\tilde{r}),\,Y)\,.$$

Due to (60) that we can differentiate in Y, we have for $m = 1,\ldots,d$ and $k = 1,\ldots,s^I$ that $\partial^2_{X_m,X}\tilde{\Psi}\,\partial_{Y_k}G + \partial^2_{X_m,Y_k}\tilde{\Psi} = 0$. Thus

$$\partial^2_{Y_k,Y_\ell}\hat{\Psi}(Y,\,\tilde{r}) = \tilde{\Psi}_{Y_k,Y_\ell} - (\tilde{\Psi}_{X,X})^{-1}\,\tilde{\Psi}_{Y_k,X}\,\tilde{\Psi}_{Y_\ell,X}\,,$$

where $D^2\tilde{\Psi}$ is evaluated at $(G(Y,\,\tilde{r}),\,Y)$. Thus, $\partial^2_{Y,Y}\hat{\Psi}$ is the Schur complement of the block $\partial^2_{X,X}\tilde{\Psi}$ of the Hessian $D^2\tilde{\Psi}$. Since $\tilde{\Psi}$ is a strictly convex function (see (62)), this proves that $D^2\hat{\Psi}$ is strictly positive definite, which is sufficient for the strict convexity. Further, making use the identity (60),

$$\begin{aligned} r &= \sum_{\ell=1}^{s} R_\ell\,\gamma^\ell = \sum_{\ell=1}^{d} R_\ell\,\gamma^\ell + \sum_{\ell=d+1}^{s} R_\ell\,\gamma^\ell \\ &= \sum_{\ell=1}^{d}(\tilde{r}_\ell - \sum_{k=d+1}^{s} A_\ell^{k-d}\,R_k)\,\gamma^\ell + \sum_{k=d+1}^{s} R_k\,\gamma^k \\ &= \sum_{\ell=1}^{d}\tilde{r}_\ell\,\gamma^\ell + \sum_{k=d+1}^{s} R_k\,(\gamma^{k-d} - \sum_{\ell=1}^{d} A_\ell^{k-d}\,\gamma^\ell) \\ &= \sum_{\ell=1}^{d}\tilde{r}_\ell\,\gamma^\ell + \sum_{k=d+1}^{s} R_k\,\gamma^{I,k-d}\,. \end{aligned}$$

Using now (64), we see for $k = 1,\ldots,s^I$

$$-R_{k+d} = \partial_{Y_k}\hat{\Psi}(Y,\,\tilde{r}) + \partial_{k+d}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\,, \quad Y = (\gamma^{I,1}\cdot\mu,\ldots,\gamma^{I,s^I}\cdot\mu)$$

It follows that

$$\begin{aligned} r = &-\sum_{k=1}^{s^I}\partial_{Y_k}\hat{\Psi}(\gamma^{I,1}\cdot\mu,\ldots,\gamma^{I,s^I}\cdot\mu,\,\tilde{r})\,\gamma^{I,k} \\ &-\sum_{k=1}^{s^I}\partial_{k+d}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\,\gamma^{I,k} + \sum_{\ell=1}^{d}\tilde{r}_\ell\,\gamma^\ell\,. \end{aligned}$$

We set $r^0 := -\sum_{k=1}^{s^I}\partial_{k+d}\Psi(\mathcal{L}(G(0,\,\tilde{r}),\,0))\,\gamma^{I,k}$ and the claim follows.

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