ANALYSIS OF MAXWELL–STEFAN SYSTEMS FOR HEAT CONDUCTING FLUID MIXTURES

CHRISTOPH HELMER AND ANSGAR JÜNGEL

Abstract. The global-in-time existence of bounded weak solutions to the Maxwell–Stefan–Fourier equations in Fick–Onsager form is proved. The model consists of the mass balance equations for the partial mass densities and and the energy balance equation for the total energy. The diffusion and heat fluxes depend linearly on the gradients of the thermo-chemical potentials and the gradient of the temperature and include the Soret and Dufour effects. The cross-diffusion system exhibits an entropy structure, which originates from the thermodynamic modeling. The lack of positive definiteness of the diffusion matrix is compensated by the fact that the total mass density is constant in time. The entropy estimate yields the a.e. positivity of the partial mass densities and temperature. Also diffusion matrices are considered that degenerate for vanishing partial mass densities.

1. Introduction

Maxwell–Stefan equations describe the dynamics of multicomponent fluids by accounting for the gradients of the chemical potentials as driving forces. The global existence analysis is usually based on the so-called entropy or formal gradient-flow structure. Up to our knowledge, almost all existence results are concerned with the isothermal setting. Exceptions are the local-in-time existence result of [22] and the coupled Maxwell–Stefan and compressible Navier–Stokes–Fourier systems analyzed in [19, 27], where no temperature gradients in the diffusion fluxes (Soret effect) have been taken into account. In this paper, we suggest and analyze for the first time Maxwell–Stefan–Fourier systems in Fick–Onsager form, including Soret and Dufour effects.

1.1. **Model equations.** We consider the evolution of the partial mass densities $\rho_i(x,t)$ and temperature $\theta(x,t)$ in a fluid mixture, governed by the equations

$$\partial_t \rho_i + \operatorname{div} J_i = r_i, \quad J_i = -\sum_{j=1}^n M_{ij}(\boldsymbol{\rho},\theta)\nabla q_j - M_i(\boldsymbol{\rho},\theta)\nabla\frac{1}{\theta}, \tag{1}$$

Date: October 30, 2020.

2000 *Mathematics Subject Classification.* 35K51, 35K55, 82B35.

Key words and phrases. Fick–Onsager cross-diffusion equations, Maxwell–Stefan systems, fluid mixtures, existence of solutions, positivity.

The authors thank the anonymous reviewers for helping us to improve significantly the initial version of the paper. The authors have been partially supported by the Austrian Science Fund (FWF), grants P30000, P33010, F65, and W1245.

$$\partial_t(\rho\theta) + \operatorname{div} J_e = 0, \quad J_e = -\kappa(\theta)\nabla\theta - \sum_{j=1}^n M_j(\boldsymbol{\rho},\theta)\nabla q_j \quad \text{in } \Omega,\ i=1,\ldots,n, \tag{2}$$

where $\Omega \subset \mathbb{R}^3$ is a bounded domain, $\boldsymbol{\rho} = (\rho_1,\ldots,\rho_n)$ is the vector of mass densities, $\rho = \sum_{i=1}^n \rho_i$ is the total mass density, and $q_i = \log(\rho_i/\theta)$ is the thermo-chemical potential of the ith species. The diffusion fluxes are denoted by J_i, the reaction rates by r_i, the energy flux by J_e, and the heat conductivity by $\kappa(\theta)$. The functions M_{ij} are the diffusion coefficients, and the terms $M_i\nabla(1/\theta)$ and $\sum_{j=1}^n M_j\nabla q_j$ describe the Soret and Dufour effect, respectively.

We prescribe the boundary and initial conditions

$$J_i\cdot\nu = 0, \quad J_e\cdot\nu + \lambda(\theta_0-\theta) = 0 \quad \text{on } \partial\Omega,\ t>0, \tag{3}$$

$$\rho_i(\cdot,0) = \rho_i^0, \quad (\rho_i\theta)(\cdot,0) = \rho_i^0\theta^0 \quad \text{in } \Omega,\ i=1,\ldots,n, \tag{4}$$

where ν is the exterior unit normal vector to $\partial\Omega$, $\theta_0 > 0$ is the constant background temperature, and $\lambda \geq 0$ is a relaxation parameter. Equations (3) mean that the fluid cannot leave the domain Ω, while heat transfer through the boundary is possible (if $\lambda \neq 0$).

In Maxwell–Stefan systems, the driving forces d_i are usually given by linear combinations of the diffusion fluxes [6, Sec. 14]:

$$\partial_t\rho_i + \operatorname{div} J_i = r_i, \quad d_i = -\sum_{j=1}^n b_{ij}\rho_i\rho_j\left(\frac{J_i}{\rho_i} - \frac{J_j}{\rho_j}\right), \quad i=1,\ldots,n, \tag{5}$$

where $b_{ij} = b_{ji} \geq 0$ for $i,j=1,\ldots,n$. It is shown in [7] that the Fick–Onsager and Maxwell–Stefan formulations are equivalent, at least in the isothermal case. We show in Section 2 that (5) can be written as (1) for a special choice of d_i, M_{ij}, and M_i in the non-isothermal situation.

We say that the diffusion fluxes in (1) are in *Fick–Onsager form*. As the heat flux is given by Fourier's law, we call system (1)–(2) the *Maxwell–Stefan–Fourier* equations in Fick–Onsager form. We refer to Section 2 for details of the modeling.

To fulfill mass conservation, the sum of the diffusion fluxes and the sum of the reaction terms should vanish, i.e. $\sum_{i=1}^n J_i = 0$ and $\sum_{i=1}^n r_i = 0$ (see Section 2). Then, summing (1) over $i=1,\ldots,n$, we see that the total mass density $\rho(\cdot,t) = \sum_{i=1}^n \rho_i(\cdot,t) = \rho^0$ is constant in time (but generally not in space). Another consequence of the identity $\sum_{i=1}^n J_i = 0$ is that the diffusion matrix has a nontrivial kernel, and we assume that

$$\sum_{i=1}^n M_{ij} = 0 \quad \text{for } j=1,\ldots,n, \quad \sum_{i=1}^n M_i = 0. \tag{6}$$

For our first existence result, we suppose that the matrix (M_{ij}) is symmetric and positive semidefinite in the sense that there exists $c_M > 0$ such that

$$\sum_{i,j=1}^n M_{ij}(\boldsymbol{\rho},\theta)z_iz_j \geq c_M|\Pi\boldsymbol{z}|^2 \quad \text{for } \boldsymbol{z}\in\mathbb{R}^n,\ \boldsymbol{\rho}\in\mathbb{R}_+^n,\ \theta\in\mathbb{R}_+, \tag{7}$$

where $\Pi = I - \mathbf{1}\otimes\mathbf{1}/n$ is the orthogonal projection on $\operatorname{span}\{\mathbf{1}\}^\perp$. This condition holds for non-dilute fluids; we refer to Section 1.4 for a weaker condition.

Notation. We write $\boldsymbol{z}$ for a vector of $\mathbb{R}^n$ with components $z_1,\ldots,z_n$ and $\boldsymbol{z}'$ for a vector of $\mathbb{R}^{n-1}$ with components $z_1,\ldots,z_{n-1}$. In particular, $\mathbf{1}=(1,\ldots,1)\in\mathbb{R}^n$. Furthermore, we set $\mathbb{R}_+=[0,\infty)$ and $\Omega_T=\Omega\times(0,T)$.

1.2. **Mathematical ideas.** The mathematical difficulties of system (1)–(2) are the cross-diffusion structure, the lack of coerciveness of the diffusion operator, and the temperature terms. In particular, it is not trivial to verify the positivity of the temperature. These difficulties are overcome by exploiting the entropy structure of the equations. We describe the main ideas for the first existence result. More precisely, we use the mathematical entropy

$$h = \sum_{i=1}^n \rho_i(\log\rho_i - 1) - \rho\log\theta.$$

Introducing the relative thermo-chemical potentials $v_i = \partial h/\partial\rho_i - \partial h/\partial\rho_n = q_i - q_n$ for $i=1,\ldots,n$ and interpreting h as a function of $(\boldsymbol{\rho}',\theta)$, a formal computation (which is made precise for an approximate scheme; see (26)) shows that

$$\begin{aligned}\frac{d}{dt}\int_\Omega h(\boldsymbol{\rho}',\theta)dx &+ \frac{c_M}{2}\int_\Omega\left(\frac{1}{n}|\nabla\boldsymbol{v}|^2 + |\nabla\Pi\boldsymbol{q}|^2\right)dx \\ &+ \int_\Omega \kappa(\theta)|\nabla\log\theta|^2dx + \lambda\int_{\partial\Omega}\left(\frac{\theta_0}{\theta}-1\right)ds \le \sum_{i=1}^{n-1}\int_\Omega r_iv_idx. \end{aligned} \tag{8}$$

The bound for $\nabla\boldsymbol{v}$ comes from the positive definiteness of the *reduced* diffusion matrix $(M_{ij})_{i,j=1}^{n-1}$; see Lemma 4. Under suitable conditions on the heat conductivity and the reaction rates, this so-called entropy inequality provides gradient estimates for $\boldsymbol{v}$, $\log\theta$, θ, and $\Pi\boldsymbol{q}$, but not for the full vector $\boldsymbol{q}$. This problem was overcome in [10] for a more general (but stationary) multicomponent Navier–Stokes–Fourier system by using tools from mathematical fluid dynamics (effective viscous flux identity and Feireisl's oscillations defect measure). In our model, the situation is much simpler. Indeed, the relation $v_i = \log\rho_i - \log\rho_n$ can be inverted yielding

$$\rho_i = \frac{\rho^0\exp(v_i)}{\sum_{j=1}^n\exp(v_j)}, \quad i=1,\ldots,n-1, \quad \rho_n = \rho^0 - \sum_{j=1}^{n-1}\rho_j, \tag{9}$$

which suggests to work with the *reduced* vector $\boldsymbol{\rho}'=(\rho_1,\ldots,\rho_{n-1})$. Moreover, this shows that ρ_i stays bounded in some interval $(0,\rho^*)$ and, in view of the bound for $\nabla\boldsymbol{v}$, that $\nabla\boldsymbol{\rho}$ is bounded in $L^2(\Omega)$. Together with a bound for the (discrete) time derivative of ρ_i, we deduce the strong convergence of ρ_i from the Aubin–Lions compactness lemma.

Still, there remains a difficulty. The estimate for $\kappa(\theta)^{1/2}\nabla\log\theta$ in $L^2(\Omega)$ from (8) is not sufficient to define $\kappa(\theta)\nabla\theta$ in the weak formulation. In the Navier–Stokes–Fourier equations, this difficulty is handled by replacing the local energy balance by the local entropy inequality and the global energy balance [17]. We choose another approach. The idea is to derive better estimates for the temperature by using θ as a test function in the weak formulation of (2). If $\kappa(\theta) \geq c_\kappa \theta^2$ for some $c_\kappa > 0$ and M_j/θ is assumed to be bounded, then a formal computation, which is made precise in Lemma 5, gives

$$\begin{aligned} \frac{1}{2}\frac{d}{dt}\int_\Omega \rho^0\theta^2 dx + c_\kappa \int_\Omega \theta^2|\nabla\theta|^2 dx - \lambda\int_{\partial\Omega}(\theta_0-\theta)\theta ds \\ = \sum_{j=1}^{n-1}\int_\Omega \frac{M_j}{\theta}\theta\nabla v_j\cdot\nabla\theta dx \leq \frac{c_\kappa}{2}\int_\Omega \theta^2|\nabla\theta|^2 dx + C\sum_{j=1}^{n-1}\int_\Omega |\nabla v_j|^2 dx. \end{aligned} \tag{10}$$

Since ∇v_j is bounded in L^2, this yields uniform bounds for θ^2 in $L^\infty(0,T;L^1(\Omega))$ and $L^2(0,T;H^1(\Omega))$. These estimates are sufficient to treat the term $\kappa(\theta)\nabla\theta$. The delicate point is to choose the approximate scheme in such a way that estimates (8) and (10) can be made rigorous; we refer to Section 3 for details.

1.3. **State of the art.** Before we state our main result, we review the state of the art of Maxwell–Stefan and related models. The isothermal equations were derived from the multi-species Boltzmann equations in the diffusive approximation in [3, 9]. The Fick–Onsager form of the Maxwell–Stefan equations was rigorously derived in Sobolev spaces from the multi-species Boltzmann system in [4]. The Maxwell–Stefan equations in the Fick–Onsager form, coupled with the momentum balance equation, can be identified as a rigorous second-order Chapman–Enskog approximation of the Euler (–Korteweg) equations for multicomponent fluids; see [21] for the Euler–Korteweg case and [26] for the Euler case. The work [8] is concerned with the friction limit in the isothermal Euler equations using the hyperbolic formalism developed by Chen, Levermore, and Liu. A formal Chapman–Enskog expansion of the stationary non-isothermal model was presented in [28]. Another non-isothermal Maxwell–Stefan system was derived in [2], but the energy flux is different from the expression in (2).

The existence analysis of (isothermal) Maxwell–Stefan equations started with the paper [18], where the existence of global-in-time weak solutions near the constant equilibrium was proved. A proof of local-in-time classical solutions to Maxwell–Stefan systems was given in [5], and regularity and instantaneous positivity for the Maxwell–Stefan system were shown in [20]. In [25], the entropy or formal gradient-flow structure was revealed, which allowed for the proof of global-in-time weak solutions with general initial data. Maxwell–Stefan systems, coupled to the Poisson equation for the electric potential, were analyzed in [24].

Alt and Luckhaus [1] proved a global existence result for parabolic systems related to the Fick–Onsager formulation. However, their result cannot be directly applied to system (1) because of the lack of coerciveness. Moreover, this theory does not yield L^∞ bounds. They are obtained from the technique of [23], but the treatment of Soret and Dufour terms requires some care and is not contained in that work.

All the mentioned results hold if the barycentric velocity vanishes. For non-vanishing fluid velocities, the Maxwell–Stefan equations need to be coupled to the momentum balance. The Maxwell–Stefan equations were coupled to the incompressible Navier–Stokes equations in [11], and the global existence of weak solutions was shown. A similar result can be found in [12], where the incompressibility condition was replaced by an artificial time derivative of the pressure and the limit of vanishing approximation parameters was performed. Coupled Maxwell–Stefan and compressible Navier–Stokes equations were analyzed in [7], and the local-in-time existence analysis was performed. A global existence analysis for a general isothermal Maxwell–Stefan–Navier–Stokes system was performed in [14]. For the existence analysis of coupled stationary Maxwell–Stefan and compressible Navier–Stokes–Fourier systems, we refer to [10, 19, 27]. In [10], temperature gradients were included in the partial mass fluxes, but only the stationary model was investigated. The global-in-time existence of weak solutions to the transient Maxwell–Stefan–Fourier equations is missing in the literature and proved in this paper for the first time.

1.4. **Main results.** We impose the following assumptions:

(H1) *Domain:* $\Omega\subset\mathbb{R}^3$ is a bounded domain with a Lipschitz continuous boundary.

(H2) *Data:* $\theta^0\in L^\infty(\Omega)$, $\inf_\Omega\theta^0>0$, $\theta_0>0$, $\lambda\ge 0$; $\rho_i^0\in H^1(\Omega)\cap L^\infty(\Omega)$ satisfies $0<\rho_*\le\rho_i^0\le\rho^*$ in Ω for some ρ_*, $\rho^*>0$.

(H3) *Diffusion coefficients:* For $i,j=1,\ldots,n$, the coefficients M_{ij}, $M_j\in C^0(\mathbb{R}^n_+\times\mathbb{R}_+)$ satisfy (6) and M_{ij}, M_i/θ are bounded functions.

(H4) *Heat conductivity:* $\kappa\in C^0(\mathbb{R}_+)$ and there exist c_κ, $C_\kappa>0$ such that for all $\theta\ge 0$,

$$c_\kappa(1+\theta^2)\le\kappa(\theta)\le C_\kappa(1+\theta^2).$$

(H5) *Reaction rates:* $r_1,\ldots,r_n\in C^0(\mathbb{R}^n\times\mathbb{R}_+)\cap L^\infty(\mathbb{R}^n\times\mathbb{R}_+)$ satisfies $\sum_{i=1}^n r_i=0$ and there exists $c_r>0$ such that for all $\boldsymbol{q}\in\mathbb{R}^n$ and $\theta>0$,

$$\sum_{i=1}^n r_i(\Pi\boldsymbol{q},\theta)q_i\le -c_r|\Pi\boldsymbol{q}|^2.$$

The bounds on ρ^0 in Hypothesis (H2) are needed to derive the positivity and boundedness of the partial mass densities. In the example presented in Section 2, the coefficients M_{ij} and M_i/θ depend on ρ_i; since we prove the existence of L^∞ solutions ρ_i, the functions M_{ij} and M_i are indeed bounded, as required in Hypothesis (H3). The growth condition for the heat conductivity in Hypothesis (H4) is used to derive higher integrability of the temperature, see (10), which allows us to treat the heat flux term. If $\lambda=0$, we can impose the weaker condition $\kappa(\theta)\ge c_\kappa\theta^2$. Hypothesis (H5) is satisfied for the reaction terms used in [14]. The bound for $\sum_{i=1}^n r_iq_i$ gives a control on the $L^2(\Omega)$ norm of $\Pi\boldsymbol{q}$. Together with the estimates for $\nabla(\Pi\boldsymbol{q})$ from (8), we are able to infer an $H^1(\Omega)$ estimate for $\Pi\boldsymbol{q}$. A more natural $L^2(\Omega)$ bound for $\boldsymbol{q}$ may be derived under the assumption that the total initial density does not lie on a critical manifold associated to the reaction rates; we refer to [14, Theorem 11.3] for details. Vanishing reaction rates are allowed in Theorem 2 below.

Our first main result is as follows.

Theorem 1 (Existence)**.** *Let Hypotheses (H1)–(H5) hold, let* (M_{ij}) *satisfy* (7)*, and let* $T>0$*. Then there exists a weak solution* $(\boldsymbol{\rho},\theta)$ *to* (1)–(4) *satisfying* $\rho_i>0$*,* $\theta>0$ *a.e. in* Ω_T*,*

$$\rho_i\in L^\infty(\Omega_T)\cap L^2(0,T;H^1(\Omega))\cap H^1(0,T;H^2(\Omega)'),\tag{11}$$

$$v_i \in L^2(0,T;H^1(\Omega)), \quad (\Pi \boldsymbol{q})_i \in L^2(0,T;H^1(\Omega)), \tag{12}$$

$$\theta \in L^2(0,T;H^1(\Omega)) \cap W^{1,16/15}(0,T;W^{1,16}(\Omega)'), \quad \log\theta \in L^2(0,T;H^1(\Omega)); \tag{13}$$

where $v_i = \log(\rho_i/\rho_n)$ *and* $(\Pi\boldsymbol{q})_i = v_i - \sum_{j=1}^n v_j/n$ *for* $i = 1,\ldots,n$*; it holds that*

$$\int_0^T \langle \partial_t \rho_i, \phi_i \rangle dt + \int_0^T \int_\Omega \bigg(\sum_{j=1}^{n-1} M_{ij} \nabla v_j - \frac{M_i}{\theta} \nabla \log\theta \bigg) \cdot \nabla \phi_i dxdt = \int_0^T \int_\Omega r_i \phi_i dxdt, \tag{14}$$

$$\begin{aligned} &\int_0^T \langle \partial_t(\rho\theta), \phi_0 \rangle dt + \int_0^T \int_\Omega \kappa(\theta) \nabla\theta \cdot \nabla\phi_0 dxdt + \int_0^T \int_\Omega \sum_{j=1}^{n-1} M_j \nabla v_j \cdot \nabla \phi_0 dxdt \\ &\quad = \lambda \int_0^T \int_{\partial\Omega} (\theta_0 - \theta)\phi_0 dxds \end{aligned} \tag{15}$$

for all $\phi_1,\ldots,\phi_n \in L^2(0,T;H^1(\Omega))$, $\phi_0 \in L^\infty(0,T;W^{1,\infty}(\Omega))$ *with* $\nabla\phi_0 \cdot \nu = 0$ *on* $\partial\Omega$, *and* $i = 1,\ldots,n$*; and the initial conditions* (4) *are satisfied in the sense of* $H^2(\Omega)'$ *and* $W^{1,16}(\Omega)'$*, respectively.*

The weak formulation can be written in various variable sets since

$$\begin{aligned} \sum_{j=1}^{n-1} M_{ij} \nabla v_j &= \sum_{j=1}^{n} M_{ij} \nabla (\Pi\boldsymbol{q})_j = \sum_{j=1}^{n} M_{ij} \nabla q_j, \\ \sum_{j=1}^{n-1} M_{j} \nabla v_j &= \sum_{j=1}^{n} M_{j} \nabla (\Pi\boldsymbol{q})_j = \sum_{j=1}^{n} M_{j} \nabla q_j, \end{aligned}$$

whenever the corresponding variables are defined. Thus, our definition of a weak solution is compatible with (1)–(2). The proof is based on a suitable approximate scheme, uniform bounds coming from entropy estimates, and $H^1(\Omega)$ estimates for the partial mass densities. More precisely, we use two levels of approximations. First, we replace the time derivative by an implicit Euler discretization to overcome issues with the time regularity. Second, we add higher-order regularizations for the thermo-chemical potentials and the logarithm of the temperature $w = \log\theta$ to achieve $H^2(\Omega)$ regularity for these variables. Since we are working in three space dimensions, we conclude $L^\infty(\Omega)$ solutions, which are needed to define properly $\rho_i = \exp(w + q_i)$.

A priori estimates are deduced from a discrete version of the entropy inequality (8). They are derived from the weak formulation by using v_i and $e^{-w_0} - e^{-w}$ as test functions, where $w_0 = \log\theta_0$. The entropy structure is only preserved if we add additionally a $W^{1,4}(\Omega)$ regularization and some lower-order regularization in w. The properties for the heat conductivity allow us to obtain estimates for θ in $H^1(\Omega)$ and for $\nabla\log\theta$ in $L^2(\Omega)$. Property (7) provides gradient estimates for $\boldsymbol{v}$ and, in view of (9), also for $\boldsymbol{\rho}$.

Condition (7) provides a control on the relative thermo-chemical potentials v_i, but it excludes the dilute limit, i.e. situations when the mass densities vanish. This situation is included in the recent work [16], which deals with the isothermal case. We are able to replace condition (7) by a degenerate one, which allows for dilute mixtures:

$$\sum_{i,j=1}^n M_{ij}(\boldsymbol{\rho},\theta)z_iz_j \geq c_M\sum_{i=1}^n \rho_i(\Pi\boldsymbol{z})_i^2 \quad \text{for } \boldsymbol{z}\in\mathbb{R}^n,\ \boldsymbol{\rho}\in\mathbb{R}^n_+,\ \theta\in\mathbb{R}_+. \tag{16}$$

This corresponds to "degenerate" diffusion coefficients M_{ij}; see Section 2 for a motivation. Although this hypothesis seems to complicate the problem, there are two advantages. First, it allows us to derive a gradient bound for $\rho_i^{1/2}$, and second, it helps us to avoid the bound from r_i in Hypothesis (H5). In fact, we may assume that $r_i = 0$.

Theorem 2 (Existence, "degenerate" case)**.** *Let condition* (16) *be satisfied. Moreover, let Hypotheses (H1)–(H4) hold for $T>0$ and additionally, $(\rho_i^0)^{1/2}\in H^1(\Omega)\cap L^\infty(\Omega)$, M_{ij}/ρ_j and M_j/ρ_j are bounded, $r_i=0$ for all $i,j=1,\ldots,n$. Then there exists a weak solution $(\boldsymbol{\rho},\theta)$ to* (1)–(4) *satisfying $\rho_i\geq 0$, $\theta>0$ a.e. in Ω_T,* (11), (13), *and the weak formulation* (14)–(15) *with, respectively,*

$$\sum_{i=1}^n \frac{M_{ij}}{\rho_j}\nabla\rho_j,\quad \sum_{i=1}^n\frac{M_i}{\rho_i}\nabla\rho_i \quad \textit{instead of}\quad \sum_{i=1}^{n-1}M_{ij}\nabla v_j,\quad \sum_{i=1}^{n-1}M_i\nabla v_i.$$

The paper is organized as follows. We explain the thermodynamical modeling of (1)–(2) in Section 2 and show that the Maxwell–Stefan formulation (5) for specific d_i can be written as (1) for certain coefficients M_{ij} and M_i. Theorems 1 and 2 are proved in Sections 3 and 4, respectively.

2. Modeling

We consider an ideal fluid mixture consisting of n components with the same molar masses in a fixed container $\Omega\subset\mathbb{R}^3$. The balance equations for the partial mass densities ρ_i are given by

$$\partial_t\rho_i + \operatorname{div}(\rho_i v_i) = r_i,\quad i=1,\ldots,n,$$

where v_i are the partial velocities and r_i the reaction rates. Introducing the total mass density $\rho=\sum_{i=1}^n\rho_i$, the barycentric velocity $v=\rho^{-1}\sum_{i=1}^n\rho_iv_i$, and the diffusion fluxes $J_i=\rho_i(v_i-v)$, we can reformulate the mass balances as

$$\partial_t\rho_i + \operatorname{div}(\rho_i v + J_i) = r_i,\quad i=1,\ldots,n. \tag{17}$$

By definition, we have $\sum_{i=1}^n J_i = 0$, which means that the total mass density satisfies $\partial_t\rho+\operatorname{div}(\rho v)=0$. We assume that the barycentric velocity vanishes, $v=0$, i.e., the barycenter of the fluid is not moving. Consequently, the total mass density is constant in time.

The non-isothermal dynamics of the mixture is assumed to be given by the balance equations

$$\partial_t\rho_i+\operatorname{div}J_i=r_i,\quad \partial_tE+\operatorname{div}J_e=0,\quad i=1,\ldots,n,$$

where J_e is the energy flux and E the total energy. We suppose that the diffusion fluxes are proportional to the gradients of the thermo-chemical potentials q_j and the temperature gradient (Soret effect) and that the energy flux is linear in the temperature gradient and the gradients of q_j (Dufour effect):

$$J_i = -\sum_{j=1}^n M_{ij}\nabla q_j - M_i\nabla\frac{1}{\theta}, \quad i=1,\ldots,n, \quad J_e = -\kappa(\theta)\nabla\theta - \sum_{j=1}^n M_j\nabla q_j.$$

The proportionality factor $\kappa(\theta)$ between the heat flux and the temperature gradient is the heat (or thermal) conductivity.

The thermo-chemical potentials and the total energy are determined in a thermodynamically consistent way from the free energy

$$\psi(\boldsymbol{\rho},\theta) = \theta\sum_{i=1}^n \rho_i(\log\rho_i - 1) - \rho\theta(\log\theta - 1).$$

For simplicity, we have set the heat capacity equal to one. The physical entropy s, the chemical potentials μ_i, and the total energy E are defined by the free energy according to

$$\begin{aligned} s &= -\frac{\partial\psi}{\partial\theta} = -\sum_{i=1}^n \rho_i(\log\rho_i - 1) + \rho\log\theta, \\ \mu_i &= \frac{\partial\psi}{\partial\rho_i} = \theta(\log(\rho_i/\theta) + 1), \quad i=1,\ldots,n, \\ E &= \psi + \theta s = \rho\theta. \end{aligned}$$

We introduce the mathematical entropy $h := -s$ and the thermo-chemical potentials $q_j = \mu_j/\theta = \log(\rho_j/\theta)+1$ for $j=1,\ldots,n$. These definitions lead to system (1)–(2). The Gibbs–Duhem relation yields the pressure $p = -\psi + \sum_{i=1}^n \rho_i\mu_i = \rho\theta$ of an ideal gas mixture. Note that we do not need a pressure blow-up at $\rho = 0$ to exclude vacuum or a superlinear growth in θ to control the temperature. Note also that, because of the nonvanishing pressure, one may criticize the choice of vanishing barycentric velocity. In the general case, the mass and energy balances need to be coupled to the momentum balance for v. Such systems, but only for isothermal or stationary systems, have been analyzed in, e.g., [10, 11, 14, 15]. The choice $v = 0$ is a mathematical simplification.

If the molar masses m_i of the components are not the same, we need to modify the free energy according to [10, Remark 1.2]

$$\psi = \theta\sum_{i=1}^n \frac{\rho_i}{m_i}\left(\log\frac{\rho_i}{m_i} - 1\right) - c_W\rho\theta(\log\theta - 1),$$

where $c_W > 0$ is the heat capacity. For simplicity, we have set $m_i = 1$ and $c_W = 1$.

We show that the Maxwell–Stefan equations

$$\partial_t\rho_i + \operatorname{div} J_i = r_i, \quad d_i = -\sum_{j=1}^n b_{ij}\rho_i\rho_j\left(\frac{J_i}{\rho_i} - \frac{J_j}{\rho_j}\right), \quad i=1,\ldots,n, \tag{18}$$

with $b_{ij} = b_{ji} > 0$ can be formulated as (1) for a specific choice of d_i, M_{ij}, and M_i. The coefficients b_{ij} may be interpreted as friction coefficients and can depend on $(\boldsymbol{\rho},\theta)$; see [7, Section 4]. The equivalence between the Fick–Onsager and Maxwell-Stefan formulations was thoroughly investigated in [7], and we adapt their proof to our non-isothermal framework. For this, we introduce the matrix $B = (B_{ij})$ satisfying $B_{ii} = \sum_{j=1,\, j\neq i}^n b_{ij}\rho_j$ and $B_{ij} = -b_{ij}\rho_i$ for $j \neq i$. It is not invertible since $\boldsymbol{\rho} \in \ker(B)$, but its group inverse $B^{\#}$ exists uniquely, satisfying $BB^{\#} = B^{\#}B = I - (\boldsymbol{\rho}/\rho) \otimes \mathbf{1}$ and

$$\sum_{j=1}^n B_{ij}^{\#}\rho_j = 0, \quad \sum_{j=1}^n B_{ji}^{\#} = 0 \quad \text{for } i = 1, \dots, n. \tag{19}$$

Furthermore, we introduce the projection $P = (P_{ij}) = I - \mathbf{1} \otimes (\boldsymbol{\rho}/\rho)$ on $\operatorname{span}\{\boldsymbol{\rho}\}^\perp$.

Proposition 3. *Define the driving forces*

$$d_i = \rho_i \nabla \frac{\mu_i}{\theta} - \frac{\rho_i}{\rho\theta}\nabla(\rho\theta) - 2\rho_i\theta\nabla\frac{1}{\theta} + q_i\rho_i\nabla\log\theta \quad \textit{for } i = 1, \dots, n, \tag{20}$$

where the numbers $q_i \in \mathbb{R}$ satisfy $\sum_{i=1}^n q_i\rho_i = 0$. Then (5) can be written as (1) with

$$M_{ij} = \sum_{k=1}^n B_{ik}^{\#}\rho_k P_{kj}, \quad M_i = -\theta\sum_{k=1}^n B_{ik}^{\#}\rho_k q_k \quad \textit{for } i, j = 1, \dots, n, \tag{21}$$

where (M_{ij}) is symmetric and M_{ij} and M_i satisfy (6).

The first three terms in the driving forces (20) are the same as [7, (4.18)] and [6, (2.11)], while the last term is motivated from [28, (A5)]. A computation shows that $\sum_{i=1}^n d_i = 0$ which is consistent with (18). It is argued in [7] that M_{ij} is of the form $\rho_i(a_i(\boldsymbol{\rho},\theta)\delta_{ij} + \rho_j S_{ij}(\boldsymbol{\rho},\theta))$ for some functions a_i and S_{ij}, and in the nondegenerate case, one may assume that $a_i(\boldsymbol{\rho},\theta)$ stays positive when $\boldsymbol{\rho} \to \widetilde{\boldsymbol{\rho}}$ with $\widetilde{\rho}_i = 0$ [7, (6.6)]. This formulation motivates condition (16).

Proof. The proof is based on the equivalence between the Fick–Onsager and Maxwell–Stefan formulations elaborated in [7, Section 4] for the isothermal case. First, the driving forces can be formulated as

$$d_i = \rho_i\nabla\frac{\mu_i}{\theta} - \rho_i\nabla\log\frac{\rho}{\theta} + q_i\rho_i\nabla\log\theta,$$

which shows that

$$\sum_{j=1}^n \rho_j\nabla\frac{\mu_j}{\theta} = \sum_{j=1}^n\left(d_j + \rho_j\nabla\log\frac{\rho}{\theta} - q_j\rho_j\nabla\log\theta\right) = \rho\nabla\log\frac{\rho}{\theta}.$$

Consequently, another formulation is

$$d_i = \rho_i\nabla\frac{\mu_i}{\theta} - \frac{\rho_i}{\rho}\sum_{j=1}^n\rho_j\nabla\frac{\mu_j}{\theta} + q_i\rho_i\nabla\log\theta = \sum_{j=1}^n\rho_i P_{ij}\nabla\frac{\mu_j}{\theta} + q_i\rho_i\nabla\log\theta.$$

Setting $R = \operatorname{diag}(\rho_1, \ldots, \rho_n)$ and $\boldsymbol{q}^* = \operatorname{diag}(q_1\rho_1, \ldots, q_n\rho_n)$, we obtain $\boldsymbol{d} = RP\nabla(\boldsymbol{\mu}/\theta) + \boldsymbol{q}^*\nabla \log\theta$. On the other hand, by (18),

$$d_i = -\bigg(\sum_{j=1,\, j\neq i}^n b_{ij}\rho_j\bigg)J_i + \sum_{j=1,\, j\neq i}^n b_{ij}\rho_i J_j = -\sum_{j=1}^n B_{ij}J_j.$$

This shows that $\boldsymbol{d} = -B\boldsymbol{J}$ and hence $\boldsymbol{J} = -B^\#\boldsymbol{d} = -B^\# RP\nabla(\boldsymbol{\mu}/\theta) - B^\#\boldsymbol{q}^*\nabla\log\theta$. Thus, defining M_{ij} and M_i as in (21), it follows that

$$J_i = -\sum_{j=1}^n M_{ij}\nabla\frac{\mu_j}{\theta} - M_i\nabla\frac{1}{\theta}.$$

The matrix $\tau = BR$ is symmetric and so does $\tau^\#$. Moreover, by [7, (4.26)], $B^\# = P^\top R\tau^\# P^\top$. Therefore, $M = B^\# RP = P^\top R\tau^\# RP$ is symmetric. We deduce from the properties (19) that

$$\sum_{j=1}^n M_{ij} = \sum_{j,k=1}^n B^\#_{ik}\rho_k\bigg(\delta_{kj} - \frac{\rho_j}{\rho}\bigg) = 0, \quad \sum_{i=1}^n M_i = -\theta\sum_{j=1}^n\bigg(\sum_{i=1}^n B^\#_{ij}\bigg)\rho_j q_j = 0.$$

This finishes the proof. □

3. Proof of Theorem 1

The idea of the proof is to reformulate equations (1)–(2) in terms of the relative potentials v_i, to approximate the resulting equations by an implicit Euler scheme, and to add some higher-order regularizations in space for the variables v_i and $w = \log\theta$. The de-regularization limit is based on the compactness coming from the entropy estimates and an estimate for the temperature.

Set $w_0 = \log\theta_0$, $\varepsilon > 0$, $N \in \mathbb{N}$, and $\tau = T/N > 0$. To simplify the notation, we set $\boldsymbol{v} = (\boldsymbol{v}', 0) = (v_1, \ldots, v_{n-1}, 0)$ and $\bar{\boldsymbol{v}} = (\bar v_1, \ldots, \bar v_{n-1}, 0)$. Let $(\bar{\boldsymbol{v}}, \bar w) \in L^\infty(\Omega; \mathbb{R}^{n+1})$ be given, and set $\rho_i(\boldsymbol{v}) = \rho^0 e^{v_i}/\sum_{j=1}^n e^{v_j}$ for $i = 1, \ldots, n-1$, $\rho_n = \rho^0 - \sum_{i=1}^{n-1}\rho_i$, and $q_i = \log\rho_i - w$ for $i = 1, \ldots, n$. We define the approximate scheme

(22)
$$0 = \frac{1}{\tau}\int_\Omega(\rho_i(\boldsymbol{v}) - \bar\rho_i(\bar{\boldsymbol{v}}))\phi_i dx + \int_\Omega\bigg(\sum_{j=1}^{n-1}M_{ij}(\boldsymbol{\rho}, e^w)\nabla v_j - M_i(\boldsymbol{\rho}, e^w)e^{-w}\nabla w\bigg)\cdot\nabla\phi_i dx$$
$$+ \varepsilon\int_\Omega\big(D^2 v_i : D^2\phi_i + v_i\phi_i\big)dx - \int_\Omega r_i(\Pi\boldsymbol{q}, e^w)\phi_i dx,$$

(23)
$$0 = \frac{1}{\tau}\int_\Omega(E - \bar E)\phi_0 dx + \int_\Omega\bigg(\kappa(\theta)\nabla\theta + \sum_{j=1}^{n-1}M_j(\boldsymbol{\rho}, e^w)\nabla v_j\bigg)\cdot\nabla\phi_0 dx$$
$$- \lambda\int_{\partial\Omega}(\theta_0 - \theta)\phi_0 ds + \varepsilon\int_\Omega e^w\big(D^2 w : D^2\phi_0 + |\nabla w|^2\nabla w\cdot\nabla\phi_0\big)dx$$

$$+ \varepsilon \int_\Omega (e^{w_0} + e^w)(w - w_0)\phi_0 dx$$

for test functions $\phi_i \in H^2(\Omega)$, $i = 0, \ldots, n-1$. Here, $D^2 u$ is the Hessian matrix of the function u, ":" denotes the Frobenius matrix product, and $E = \rho^0\theta$, $\bar{E} = \rho^0\bar{\theta}$. The lower-order regularization $\varepsilon(e^{w_0} + e^w)(w - w_0)$ yields an $L^2(\Omega)$ estimate for w. Furthermore, the higher-order regularization guarantees that v_i, $w \in H^2(\Omega) \hookrightarrow L^\infty(\Omega)$, while the $W^{1,4}(\Omega)$ regularization term for w allows us to estimate the higher-order terms when using the test function $e^{-w_0} - e^{-w}$.

Step 1: solution of the linearized approximate problem. In order to define the fixed-point operator, we need to solve a linearized problem. To this end, let $y^* = (\boldsymbol{v}^*, w^*) \in W^{1,4}(\Omega;\mathbb{R}^n)$ and $\sigma \in [0,1]$ be given. We want to find the unique solution $y = (\boldsymbol{v}', w) \in H^2(\Omega;\mathbb{R}^n)$ to the linear problem

$$a(y,\phi) = \sigma F(\phi) \quad \text{for all } \phi = (\phi_0, \ldots, \phi_{n-1}) \in H^2(\Omega;\mathbb{R}^n), \tag{24}$$

where

$$\begin{aligned} a(y,\phi) &= \int_\Omega \sum_{i,j=1}^{n-1} M_{ij}(\boldsymbol{\rho}^*, e^{w^*})\nabla v_j \cdot \nabla \phi_i dx + \int_\Omega \kappa(e^{w^*})e^{w^*}\nabla w \cdot \nabla \phi_0 dx \\ &\quad + \varepsilon \int_\Omega \sum_{i=1}^{n-1} \big(D^2 v_i : D^2\phi_i + v_i\phi_i\big) \\ &\quad + \varepsilon \int_\Omega e^{w^*}\big(D^2 w : D^2\phi_0 + |\nabla w^*|^2 \nabla w \cdot \nabla \phi_0\big) + \varepsilon \int_\Omega (e^{w_0} + e^{w^*}) w\phi_0 dx, \\ F(\phi) &= -\frac{1}{\tau}\int_\Omega \sum_{i=1}^{n-1} (\rho_i^* - \bar{\rho}_i)\phi_i dx - \frac{1}{\tau}\int_\Omega (E^* - \bar{E})\phi_0 dx + \lambda \int_{\partial\Omega} (e^{w_0} - e^{w^*})\phi_0 dx \\ &\quad + \int_\Omega \sum_{i=1}^{n-1} M_i(\boldsymbol{\rho}^*, e^{w^*})e^{-w^*}\nabla w^* \cdot \nabla \phi_i dx - \int_\Omega \sum_{j=1}^{n-1} M_j(\boldsymbol{\rho}^*, e^{w^*})\nabla v_j^* \cdot \nabla \phi_0 dx \\ &\quad + \int_\Omega \sum_{i=1}^{n} r_i(\Pi \boldsymbol{q}^*, e^{w^*})\phi_i dx + \varepsilon \int_\Omega (e^{w_0} + e^{w^*}) w_0 \phi_0 dx \end{aligned}$$

and $\rho_i^* = \rho_i(\boldsymbol{v}^*)$, $\rho^* = \sum_{i=1}^n \rho_i^*$, $E^* = \rho^0 e^{w^*}$. By Hypothesis (H3) and the generalized Poincaré inequality [29, Chap. 2, Sec. 1.4], we have

$$a(y,y) \geq \varepsilon \int_\Omega \big(|D^2\boldsymbol{v}|^2 + |\boldsymbol{v}|^2\big)dx + \varepsilon \int_\Omega e^{w^*}(|D^2 w|^2 + w^2)dx \geq \varepsilon C(\|\boldsymbol{v}\|_{H^2(\Omega)}^2 + \|w\|_{H^2(\Omega)}^2).$$

Thus, a is coercive. Moreover, a and F are continuous on $H^2(\Omega;\mathbb{R}^n)$. The Lax–Milgram lemma shows that (24) possesses a unique solution $(\boldsymbol{v}', w) \in H^2(\Omega;\mathbb{R}^n)$.

Step 2: solution of the approximate problem. The previous step shows that the fixed-point operator $S : W^{1,4}(\Omega;\mathbb{R}^n) \times [0,1] \to W^{1,4}(\Omega;\mathbb{R}^n)$, $S(y^*,\sigma) = y$, where $y = (\boldsymbol{v}', w)$ solves (24), is well defined. It holds that $S(y,0) = 0$, S is continuous, and since S maps to $H^2(\Omega;\mathbb{R}^n)$, which is compactly embedded into $W^{1,4}(\Omega;\mathbb{R}^n)$, it is also compact. It remains to determine a uniform bound for all fixed points y of $S(\cdot,\sigma)$, where $\sigma\in(0,1]$. Let y be such a fixed point. Then $y\in H^2(\Omega;\mathbb{R}^n)$ solves (24) with $(\boldsymbol{v}^*,w^*)$ replaced by $y=(\boldsymbol{v}',w)$. With the test functions $\phi_i=v_i$ for $i=1,\ldots,n-1$ and $\phi_0=e^{-w_0}-e^{-w}$ (we need this test function since $\phi_0=-e^{-w}$ does not allow us to control the lower-order term), we obtain

$$
\begin{aligned}
0 &= \frac{\sigma}{\tau}\int_\Omega\sum_{i=1}^{n-1}(\rho_i(\boldsymbol{v})-\rho_i(\bar{\boldsymbol{v}}))v_i dx + \frac{\sigma}{\tau}\int_\Omega (E-\bar{E})(-e^{-w})dx + \frac{\sigma}{\tau}\int_\Omega(E-\bar{E})e^{-w_0}dx \\
&\quad + \int_\Omega\sum_{i,j=1}^{n-1}M_{ij}\nabla v_i\cdot\nabla v_j dx + \int_\Omega \kappa(e^w)e^w\nabla w\cdot\nabla(-e^{-w})dx - \sigma\int_\Omega\sum_{i=1}^{n-1}r_iv_i dx \\
&\quad - \sigma\int_\Omega\sum_{j=1}^{n-1}M_je^{-w}\nabla w\cdot\nabla v_j dx + \sigma\int_\Omega\sum_{j=1}^{n-1}M_j\nabla v_j\cdot\nabla(-e^{-w})dx \\
&\quad - \sigma\lambda\int_{\partial\Omega}(e^{w_0}-e^w)(e^{-w_0}-e^{-w})dx + \varepsilon\int_\Omega\sum_{i=1}^{n-1}\big(|D^2v_i|^2+v_i^2\big)dx \\
&\quad + \varepsilon\int_\Omega(e^{w_0}+e^w)(w-w_0)(e^{-w_0}-e^{-w})dx \\
&\quad + \varepsilon\int_\Omega\big(|D^2w|^2 - D^2w:\nabla w\otimes\nabla w+|\nabla w|^4\big)dx \\
&=: I_1+\cdots+I_{12}.
\end{aligned}
$$

We see immediately that $I_7+I_8=0$. Furthermore,

$$
I_1+I_2 = \frac{\sigma}{\tau}\int_\Omega\bigg(\sum_{i=1}^{n-1}(\rho_i-\bar{\rho}_i)\frac{\partial h}{\partial\rho_i} + (\theta-\bar{\theta})\frac{\partial h}{\partial\theta}\bigg)dx.
$$

The function $(\boldsymbol{\rho}',\theta)\mapsto h(\boldsymbol{\rho}',\theta)=\sum_{i=1}^n\rho_i(\log\rho_i-1)-\rho^0\log\theta$ with $\rho_n=\rho^0-\sum_{i=1}^{n-1}\rho_i$ is convex, since the second derivatives are given by

$$
\frac{\partial^2 h}{\partial\rho_i^2}=\frac{1}{\rho_i}+\frac{1}{\rho_n},\quad \frac{\partial^2 h}{\partial\theta^2}=\frac{\rho^0}{\theta^2},\quad \frac{\partial^2 h}{\partial\rho_i\partial\theta}=0,\quad \frac{\partial^2 h}{\partial\rho_i\partial\rho_j}=\frac{1}{\rho_n},
$$

hence we can conclude in the same way as in [25] that the Hessian is positive definite by Sylvester's criterion. This shows that

$$
h(\boldsymbol{\rho}',\theta)-h(\bar{\boldsymbol{\rho}}',\bar{\theta}) \le \sum_{i=1}^{n-1}\frac{\partial h}{\partial\rho_i}(\boldsymbol{\rho}',\theta)(\rho_i-\bar{\rho}_i) + \frac{\partial h}{\partial\theta}(\boldsymbol{\rho}',\theta)(\theta-\bar{\theta})
$$

and consequently,

$$
I_1+I_2 \ge \frac{\sigma}{\tau}\int_\Omega\big(h(\boldsymbol{\rho}',\theta)-h(\bar{\boldsymbol{\rho}}',\bar{\theta})\big)dx.
$$

For the estimate of I_4, we need the following lemma.

Lemma 4. *Let the matrix $(M_{ij}) \in \mathbb{R}^{n\times n}$ satisfy* (6) *and* (7)*. Then*

$$\sum_{i,j=1}^{n-1} M_{ij}(z_i - z_n)(z_j - z_n) \geq \frac{c_M}{n}\sum_{i=1}^{n-1}|z_i - z_n|^2.$$

Proof. We use (6) and then (7) to find for any $\boldsymbol{z} \in \mathbb{R}^n$ that

$$\sum_{i,j=1}^{n-1} M_{ij}(z_i - z_n)(z_j - z_n) = \sum_{i,j=1}^{n} M_{ij} z_i z_j \geq c_M|\Pi\boldsymbol{z}|^2. \tag{25}$$

By Jensen's inequality, we have $(n-1)\sum_{i=1}^{n-1} z_i^2 \geq (\sum_{i=1}^{n-1} z_i)^2$, which is equivalent to $n|\Pi\boldsymbol{z}|^2 \geq \sum_{i=1}^{n-1}(z_i - z_n)^2$. Inserting this inequality into (25) finishes the proof. □

By Lemma 4 and Hypothesis (H5),

$$\begin{aligned} I_4 &= \frac{1}{2}\int_\Omega\bigg(\sum_{i,j=1}^{n} M_{ij}\nabla q_i\cdot\nabla q_j + \sum_{i,j=1}^{n-1} M_{ij}\nabla v_i\cdot\nabla v_j\bigg)dx \\ &\geq \frac{c_M}{2}\int_\Omega|\nabla\Pi\boldsymbol{q}|^2dx + \frac{c_M}{2n}\int_\Omega|\nabla\boldsymbol{v}|^2dx, \\ I_6 &= \sigma\int_\Omega\sum_{i=1}^{n} r_i q_i dx \geq \sigma c_r\int_\Omega|\Pi\boldsymbol{q}|^2dx. \end{aligned}$$

Next, we have

$$\begin{aligned} I_5 &= \int_\Omega \kappa(e^w)|\nabla w|^2dx, \quad I_9 = 2\sigma\lambda\int_{\partial\Omega}(\cosh(w_0 - w) - 1)ds \geq 0, \\ I_{11} &= 2\varepsilon\int_\Omega(w - w_0)\sinh(w - w_0)dx \geq \varepsilon\int_\Omega(w - w_0)^2\,dx, \\ I_{12} &= \frac{\varepsilon}{2}\int_\Omega\big(|D^2w|^2 + |D^2w - \nabla w\otimes\nabla w|^2 + |\nabla w|^4\big)dx. \end{aligned}$$

Summarizing these estimates and applying the generalized Poincaré inequality, we arrive at the *discrete entropy inequality*

$$\begin{aligned} &\frac{\sigma}{\tau}\int_\Omega\big(h(\boldsymbol{\rho}',\theta) + e^{-w_0}E\big)dx + \frac{c_M}{2}\int_\Omega\bigg(\frac{1}{n}|\nabla\boldsymbol{v}|^2 + |\nabla\Pi\boldsymbol{q}|^2 + \sigma c_r|\Pi\boldsymbol{q}|^2\bigg)dx \\ &\qquad + \varepsilon C\big(\|\boldsymbol{v}\|^2_{H^2(\Omega)} + \|w\|^2_{H^2(\Omega)} + \|w\|^4_{W^{1,4}(\Omega)}\big) + \int_\Omega\kappa(e^w)|\nabla w|^2dx \\ &\leq \frac{\sigma}{\tau}\int_\Omega\big(h(\bar{\boldsymbol{\rho}}',\bar\theta) + e^{-w_0}\bar{E}\big)dx + 2\varepsilon\|w_0\|^2_{L^2(\Omega)}. \end{aligned} \tag{26}$$

We observe that the left-hand side is bounded from below since $-\rho^0\log\theta + e^{-w_0}E = \rho^0(-\log\theta + \theta/\theta_0)$ is bounded from below. The bound for $\Pi\boldsymbol{q}$ implies an $L^2(\Omega)$ bound for $\boldsymbol{v}$ since $|\boldsymbol{v}|^2 \leq n|\Pi\boldsymbol{q}|^2$; see the proof of Lemma 4.

Estimate (8) gives a uniform bound for $(\boldsymbol{v}', w)$ in $H^2(\Omega;\mathbb{R}^n)$ and consequently also in $W^{1,4}(\Omega;\mathbb{R}^n)$, which proves the claim. We infer from the Leray–Schauder fixed-point theorem that there exists a solution $(\boldsymbol{v}', w)$ to (22)–(23).

Step 3: temperature estimate. We need a better estimate for the temperature.

Lemma 5. *Let $(\boldsymbol{\rho}, w)$ be a solution to (22)–(23) and set $\theta = e^w$. Then there exists a constant $C > 0$ independent of ε and τ such that*

$$\frac{1}{\tau}\int_\Omega \rho^0\theta^2 dx + \frac{1}{2}\int_\Omega \kappa(\theta)|\nabla\theta|^2 dx \le C + \frac{1}{\tau}\int_\Omega \rho^0\bar\theta^2 dx + C\int_\Omega |\nabla \boldsymbol{v}|^2 dx.$$

Proof. We use the test function θ in (23). Observing that $(E-\bar E)\theta = \rho^0(\theta-\bar\theta)\theta \ge (\rho^0/2)(\theta^2-\bar\theta^2)$ and that $\kappa(\theta)\ge c_\kappa(1+\theta^2)$ by Hypothesis (H4), we find that

$$\begin{aligned}
&\frac{1}{2\tau}\int_\Omega \rho^0(\theta^2-\bar\theta^2)dx + \frac{1}{2}\int_\Omega \kappa(\theta)|\nabla\theta|^2 dx + \frac{c_\kappa}{2}\int_\Omega \theta^2|\nabla\theta|^2 dx - \lambda\int_{\partial\Omega}(\theta_0-\theta)\theta dx \\
&\le -\sum_{j=1}^{n-1}\int_\Omega M_j\nabla v_j\cdot\nabla\theta dx - \varepsilon\int_\Omega \theta(D^2\log\theta : D^2\theta + |\nabla\log\theta|^2\nabla\log\theta\cdot\nabla\theta)dx \\
&\quad - \varepsilon\int_\Omega(\theta_0+\theta)(\log\theta-\log\theta_0)\theta dx \\
&=: J_1 + J_2 + J_3. \qquad (27)
\end{aligned}$$

Since M_j/θ is assumed to be bounded,

$$J_1 \le \frac{c_\kappa}{2}\int_\Omega \theta^2|\nabla\theta|^2 dx + C\sum_{j=1}^{n-1}\int_\Omega |\nabla v_j|^2 dx.$$

Furthermore,

$$\begin{aligned}
J_2 &= -\varepsilon\int_\Omega\Big(-\frac{1}{\theta}\nabla\theta\cdot D^2\theta\nabla\theta + |D^2\theta|^2 + \frac{1}{\theta^2}|\nabla\theta|^4\Big)dx \\
&= -\frac{\varepsilon}{2}\int_\Omega\bigg(|D^2\theta|^2 + \frac{1}{\theta^2}|\nabla\theta|^4 + \Big|D^2\theta - \frac{1}{\theta}\nabla\theta\otimes\nabla\theta\Big|^2\bigg)dx \le 0.
\end{aligned}$$

The last integral J_3 is bounded since $-\theta^2\log\theta$ is the dominant term. The last term on the left-hand side of (27) is bounded from below by $-(\lambda/2)\int_{\partial\Omega}\theta_0^2 dx$, which finishes the proof. □

Remark 6. Better estimates can be derived if we assume that $\kappa(\theta)\ge c_\kappa(1+\theta^{\alpha+1})$ for $\alpha\in(1,2)$. Indeed, using θ^α as a test function in (23), we find that

$$\begin{aligned}
&\frac{1}{\tau}\int_\Omega \rho^0(\theta-\bar\theta)\theta^\alpha dx + \alpha c_\kappa\int_\Omega \theta^{2\alpha}|\nabla\theta|^2 dx - \lambda\int_{\partial\Omega}(\theta_0-\theta)\theta^\alpha dx \\
&\le -\alpha\sum_{j=1}^{n-1}\int_\Omega M_j\theta^{\alpha-1}\nabla v_j\cdot\nabla\theta dx - \varepsilon\int_\Omega(\theta_0+\theta)(\log\theta-\log\theta_0)\theta^\alpha dx
\end{aligned}$$

$$
\begin{aligned}
&- \varepsilon \int_\Omega \theta\big(D^2\log\theta : D^2\theta^\alpha + |\nabla\log\theta|^2\nabla\log\theta\cdot\nabla\theta^\alpha\big)dx \\
&=: J_4 + J_5 + J_6. \qquad (28)
\end{aligned}
$$

A tedious but straightforward computation shows that $J_6 \geq 0$ if $\alpha \in (1,2)$. Furthermore, since M_j/θ is bounded,

$$
J_4 \leq \frac{\alpha c_\kappa}{2}\int_\Omega \theta^{2\alpha}|\nabla\theta|^2dx + C\sum_{j=1}^{n-1}\int_\Omega |\nabla v_j|^2dx.
$$

The first integral on the right-hand side is controlled by the left-hand side of (28). This yields a bound for $\theta^{\alpha+1} \in L^\infty(0,T;L^1(\Omega)) \cap L^2(0,T;H^1(\Omega)) \subset L^{8/3}(\Omega_T)$ (see Lemma 8) and consequently $\theta \in L^{8(\alpha+1)/3}(\Omega_T)$, which is better than the result in Lemma 8. ☐

Step 4: uniform estimates. Let $((\boldsymbol{v}')^k, w^k)$ be a solution to (22)–(23) for given $(\boldsymbol{v}')^{k-1} = \bar{\boldsymbol{v}}'$ and $w^{k-1} = \bar{w}$, where $k \in \mathbb{N}$. We set

$$
\theta^k = \exp(w^k), \quad \rho_i^k = \exp(w^k + q_i^k) = \frac{\rho^0 e^{v_i^k}}{\sum_{j=1}^n e^{v_j^k}}
$$

for $i = 1,\ldots,n-1$, and $E^k = \rho^0\theta^k$. We introduce piecewise constant functions in time. For this, let $\rho_i^{(\tau)}(x,t) = \rho_i^k(x)$, $\theta^{(\tau)}(x,t) = \theta^k(x)$, $v_i^{(\tau)}(x,t) = v_i^k(x)$, $q_i^{(\tau)} = \log(\rho_i^{(\tau)}/\theta^{(\tau)})$, and $E^{(\tau)}(x,t) = E^k(x)$ for $x \in \Omega$, $t \in ((k-1)\tau, k\tau]$, $k = 1,\ldots,N$. At time $t = 0$, we set $\rho_i^{(\tau)}(x,0) = \rho_i^0(x)$ and $\theta^{(\tau)}(x,0) = \theta^0(x)$ for $x \in \Omega$. Furthermore, we introduce the shift operator $(\sigma_\tau\rho_i^{(\tau)})(x,t) = \rho_i^{k-1}(x)$ for $x \in \Omega$, $t \in ((k-1)\tau, k\tau]$. Let $(\boldsymbol{\rho}')^{(\tau)} = (\rho_1^{(\tau)},\ldots,\rho_{n-1}^{(\tau)})$. Then $((\boldsymbol{\rho}')^{(\tau)}, \theta^{(\tau)})$ solves (see (22)–(23))

$$
\begin{aligned}
0 &= \frac{1}{\tau}\int_0^T\int_\Omega (\rho_i^{(\tau)} - \sigma_\tau\rho_i^{(\tau)})\phi_i dxdt \qquad (29)\\
&\quad + \int_0^T\int_\Omega \bigg(\sum_{j=1}^{n-1} M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)} + M_i(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla\frac{1}{\theta^{(\tau)}}\bigg)\cdot\nabla\phi_i dxdt \\
&\quad + \varepsilon\int_0^T\int_\Omega \big(D^2 v_i^{(\tau)} : D^2\phi_i + v_i^{(\tau)}\phi_i\big)dxdt - \int_0^T\int_\Omega r_i(\Pi\boldsymbol{q}^{(\tau)},\theta^{(\tau)})\phi_i dxdt, \\
0 &= \frac{1}{\tau}\int_0^T\int_\Omega (E^{(\tau)} - \sigma_\tau E^{(\tau)})\phi_0 dxdt - \lambda\int_0^T\int_{\partial\Omega}(\theta_0 - \theta^{(\tau)})\phi_0 dsdt \qquad (30)\\
&\quad + \int_0^T\int_\Omega \bigg(\kappa(\theta^{(\tau)})\nabla\theta^{(\tau)} + \sum_{j=1}^{n-1} M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)}\bigg)\cdot\nabla\phi_0 dxdt \\
&\quad + \varepsilon\int_0^T\int_\Omega \theta^{(\tau)}\big(D^2\log\theta^{(\tau)} : D^2\phi_0 + |\nabla\log\theta^{(\tau)}|^2\nabla\log\theta^{(\tau)}\cdot\nabla\phi_0\big)dxdt \\
&\quad + \varepsilon\int_0^T\int_\Omega (\theta_0 + \theta^{(\tau)})(\log\theta^{(\tau)} - \log\theta_0)\phi_0 dxdt.
\end{aligned}
$$

The discrete entropy inequality (26) and the L^∞ bound for $\rho_i^{(\tau)}$ imply the following uniform bounds:

$$\begin{aligned}\|\rho_i^{(\tau)}\|_{L^\infty(0,T;L^\infty(\Omega))} + \|\theta^{(\tau)}\|_{L^\infty(0,T;L^1(\Omega))} &\le C,\\ \|v_i^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|\kappa(\theta^{(\tau)})^{1/2}\nabla\log\theta^{(\tau)}\|_{L^2(\Omega_T)} &\le C,\\ \varepsilon^{1/2}\|v_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} + \varepsilon^{1/2}\|\log\theta^{(\tau)}\|_{L^2(0,T;H^2(\Omega))} &\le C,\\ \varepsilon^{1/4}\|\log\theta^{(\tau)}\|_{L^4(0,T;W^{1,4}(\Omega))} &\le C,\end{aligned}$$

for all $i = 1,\ldots,n-1$, where $C > 0$ is independent of ε and τ. Hypothesis (H4) yields

$$\|\nabla\theta^{(\tau)}\|_{L^2(\Omega_T)} + \|\nabla\log\theta^{(\tau)}\|_{L^2(\Omega_T)} \le C. \tag{31}$$

Lemma 7 (Estimates for the temperature)**.** *There exists a constant $C > 0$ which does not depend on ε or τ such that*

$$\|\theta^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} + \|\log\theta^{(\tau)}\|_{L^2(0,T;H^1(\Omega))} \le C. \tag{32}$$

Proof. The entropy inequality shows that $-\log\theta^{(\tau)}+\theta^{(\tau)}$ is uniformly bounded from above, which shows that $|\log\theta^{(\tau)}|$ is uniformly bounded too and hence, $\log\theta^{(\tau)}$ is bounded in $L^\infty(0,T;L^1(\Omega))$. Together with the $L^\infty(0,T;L^1(\Omega))$ bound for $\theta^{(\tau)}$, estimate (31), and the Poincaré–Wirtinger inequality, we find that

$$\begin{aligned}\|\theta^{(\tau)}\|_{L^2(\Omega_T)} &\le C\|\theta^{(\tau)}\|_{L^2(0,T;L^1(\Omega))} + \|\nabla\theta^{(\tau)}\|_{L^2(\Omega_T)} \le C,\\ \|\log\theta^{(\tau)}\|_{L^2(\Omega_T)} &\le C\|\log\theta^{(\tau)}\|_{L^2(0,T;L^1(\Omega))} + \|\nabla\log\theta^{(\tau)}\|_{L^2(\Omega_T)} \le C,\end{aligned}$$

from which we conclude the proof. □

We proceed by proving more uniform estimates. Because of the $L^2(\Omega_T)$ bound of $\nabla v_i^{(\tau)}$ and

$$\begin{aligned}\int_0^T\int_\Omega|\nabla\rho_i^{(\tau)}|^2dxdt &= \int_0^T\int_\Omega|\nabla\rho^0|^2\bigg|\frac{\exp(v_i^{(\tau)})}{\sum_{j=1}^n\exp(v_j^{(\tau)})}\bigg|^2dxdt\\ &\quad+\int_0^T\int_\Omega\bigg|\frac{\exp(v_i^{(\tau)})\nabla v_i^{(\tau)}}{\sum_{j=1}^n\exp(v_j^{(\tau)})} - \frac{\exp(v_i^{(\tau)})\sum_{j=1}^n\exp(v_j^{(\tau)})\nabla v_j^{(\tau)}}{(\sum_{j=1}^n\exp(v_j^{(\tau)}))^2}\bigg|^2dxdt\\ &\le\int_0^T\int_\Omega|\nabla\rho^0|^2dxdt + 2\int_0^T\int_\Omega|\nabla\boldsymbol{v}|^2dxdt \le C,\end{aligned} \tag{33}$$

$(\nabla\rho_i^{(\tau)})$ is bounded in $L^2(\Omega_T)$ and, taking into account the L^∞ bound for $\rho_i^{(\tau)}$, the family $(\rho_i^{(\tau)})$ is bounded in $L^2(0,T;H^1(\Omega))$. By Lemma 5 and Hypothesis (H4), $(\nabla(\theta^{(\tau)})^2)$ is bounded in $L^2(\Omega_T)$. Therefore, since $((\theta^{(\tau)})^2)$ is bounded in $L^1(\Omega_T)$, the Poincaré–Wirtinger inequality gives a uniform bound for $(\theta^{(\tau)})^2$ in $L^2(0,T;H^1(\Omega))$. These bounds yields higher integrability of $\theta^{(\tau)}$, as shown in the following lemma.

Lemma 8. *There exists $C > 0$ independent of ε and τ such that $(\theta^{(\tau)})$ is bounded in $L^{16/3}(\Omega_T)$.*

Proof. We deduce from the bound for $(\theta^{(\tau)})^2$ in $L^2(0,T;H^1(\Omega)) \subset L^2(0,T;L^6(\Omega))$ that $(\theta^{(\tau)})$ is bounded in $L^4(0,T;L^{12}(\Omega))$. By interpolation with $1/r = \alpha/12 + (1-\alpha)/2$ and $r\alpha = 4$,

$$\begin{aligned}\|\theta^{(\tau)}\|_{L^r(\Omega_T)}^r &= \int_0^T \|\theta^{(\tau)}\|_{L^r(\Omega)}^r dt \le \int_0^T \|\theta^{(\tau)}\|_{L^{12}(\Omega)}^{r\alpha} \|\theta^{(\tau)}\|_{L^2(\Omega))}^{r(1-\alpha)} dt \\ &\le \|\theta^{(\tau)}\|_{L^\infty(0,T;L^2(\Omega))}^{r(1-\alpha)} \int_0^T \|\theta^{(\tau)}\|_{L^{12}(\Omega)}^4 dt \le C.\end{aligned}$$

The solution of $1/r = \alpha/12 + (1-\alpha)/2$ and $r\alpha = 4$ is $\alpha = 3/4$ and $r = 16/3$. □

Lemma 9. *There exists $C > 0$ independent of ε and τ such that*

$$\tau^{-1}\|\rho_i^{(\tau)} - \sigma_\tau \rho_i^{(\tau)}\|_{L^2(0,T;H^2(\Omega)')} + \tau^{-1}\|\theta^{(\tau)} - \sigma_\tau\theta^{(\tau)}\|_{L^{16/15}(0,T;W^{1,16}(\Omega)')} \le C. \tag{34}$$

Proof. Let $\phi_0 \in L^{16}(0,T;W^{1,16}(\Omega))$, $\phi_1, \ldots, \phi_{n-1} \in L^2(0,T;H^2(\Omega))$ and set $M_i^{(\tau)} = M_i(\boldsymbol{\rho}^{(\tau)}, \theta^{(\tau)})$, $r_i^{(\tau)} = r_i(\boldsymbol{\rho}^{(\tau)}, \theta^{(\tau)})$ for $i = 1, \ldots, n-1$. It follows from (29)–(30) and Hypotheses (H3)–(H5) that

$$\begin{aligned}\frac{1}{\tau}\bigg|\int_0^T\int_\Omega (\rho_i^{(\tau)} - \sigma_\tau\rho_i^{(\tau)})\phi_i dxdt\bigg| &\le C\|\nabla \boldsymbol{v}^{(\tau)}\|_{L^2(\Omega_T)}\|\nabla\boldsymbol{\phi}\|_{L^2(\Omega_T)} \\ &\quad + \sum_{i=1}^{n-1}\|M_i^{(\tau)}/\theta^{(\tau)}\|_{L^\infty(\Omega_T)}\|\nabla\log\theta^{(\tau)}\|_{L^2(\Omega_T)}\|\nabla\boldsymbol{\phi}\|_{L^2(\Omega_T)} \\ &\quad + \varepsilon\|\boldsymbol{v}^{(\tau)}\|_{L^2(0,T;H^2(\Omega))}\|\boldsymbol{\phi}\|_{L^2(0,T;H^2(\Omega))} + \|\boldsymbol{r}^{(\tau)}\|_{L^2(\Omega_T)}\|\boldsymbol{\phi}\|_{L^2(\Omega_T)} \\ &\le C\|\boldsymbol{\phi}\|_{L^2(0,T;H^2(\Omega))},\end{aligned}$$

and

$$\begin{aligned}&\frac{1}{\tau}\bigg|\int_0^T\int_\Omega (E^{(\tau)} - \sigma_\tau E^{(\tau)})\phi_0 dxdt\bigg| \\ &\le C + C\|\theta^{(\tau)}\|_{L^{8/3}(\Omega_T)}\|\nabla(\theta^{(\tau)})^2\|_{L^2(\Omega_T)}\|\nabla\phi_0\|_{L^8(\Omega_T)} \\ &\quad + \sum_{j=1}^{n-1}\|M_j^{(\tau)}/\theta^{(\tau)}\|_{L^\infty(\Omega_T)}\|\theta^{(\tau)}\|_{L^{8/3}(\Omega_T)}\|\nabla v_j^{(\tau)}\|_{L^2(\Omega_T)}\|\nabla\phi_0\|_{L^8(\Omega_T)} \\ &\quad + \lambda\|\theta_0 - \theta^{(\tau)}\|_{L^{8/7}(0,T;L^{8/7}(\partial\Omega))}\|\phi_0\|_{L^8(0,T;L^8(\partial\Omega))} \\ &\quad + \varepsilon\|\theta^{(\tau)}\|_{L^3(\Omega_T)}\|\log\theta^{(\tau)}\|_{L^2(0,T;H^2(\Omega))}\|\nabla\phi_0\|_{L^6(\Omega_T)} \\ &\quad + \varepsilon\|\theta^{(\tau)}\|_{L^{16/3}(\Omega_T)}\|\nabla\log\theta^{(\tau)}\|_{L^4(\Omega_T)}^3\|\nabla\phi_0\|_{L^{16}(\Omega_T)} \\ &\quad + \varepsilon C\big(1 + \|\theta^{(\tau)}\log\theta^{(\tau)}\|_{L^2(\Omega_T)}\big)\|\phi_0\|_{L^2(\Omega_T)} \le C\|\phi_0\|_{L^{16}(0,T;W^{1,16}(\Omega))}.\end{aligned}$$

Since $|E^{(\tau)} - \sigma_\tau E^{(\tau)}| = \rho^0|\theta^{(\tau)} - \sigma_\tau\theta^{(\tau)}| \ge \rho_*|\theta^{(\tau)} - \sigma_\tau\theta^{(\tau)}|$, this concludes the proof. □

Step 5: limit $(\varepsilon,\tau) \to 0$. Estimates (33)–(34) allow us to apply the Aubin–Lions lemma in the version of [13]. Thus, there exist subsequences that are not relabeled such that as

$(\varepsilon,\tau)\to 0$,

$$\rho_i^{(\tau)}\to\rho_i,\quad \theta^{(\tau)}\to\theta\quad\text{strongly in } L^2(\Omega_T),\ i=1,\ldots,n-1. \tag{35}$$

The $L^\infty(\Omega_T)$ bound for $(\rho_i^{(\tau)})$ and the $L^{16/3}(\Omega_T)$ bound for $(\theta^{(\tau)})$ imply the stronger convergences

$$\begin{aligned} \rho_i^{(\tau)}\to\rho_i &\quad\text{strongly in } L^r(\Omega_T) \text{ for all } r<\infty, \\ \theta^{(\tau)}\to\theta &\quad\text{strongly in } L^\eta(\Omega_T) \text{ for all } \eta<16/3. \end{aligned}$$

The uniform bounds also imply that, up to subsequences,

$$\begin{aligned} \rho_i^{(\tau)}\rightharpoonup\rho_i &\quad\text{weakly in } L^2(0,T;H^1(\Omega)), \\ \theta^{(\tau)}\rightharpoonup\theta &\quad\text{weakly in } L^2(0,T;H^1(\Omega)), \\ \nabla v_i^{(\tau)}\rightharpoonup\nabla v_i &\quad\text{weakly in } L^2(0,T;L^2(\Omega)), \\ \tau^{-1}(\rho_i^{(\tau)}-\sigma_\tau\rho_i^{(\tau)})\rightharpoonup\partial_t\rho_i &\quad\text{weakly in } L^2(0,T;H^2(\Omega)'), \\ \tau^{-1}(\theta^{(\tau)}-\sigma_\tau\theta^{(\tau)})\rightharpoonup\partial_t\theta &\quad\text{weakly in } L^{16/15}(0,T;W^{2,16}(\Omega)'), \end{aligned}$$

where $i=1,\ldots,n-1$ and $j=1,\ldots,n$. Moreover, as $(\varepsilon,\tau)\to 0$,

$$\varepsilon\log\theta^{(\tau)}\to 0,\quad \varepsilon v_i^{(\tau)}\to 0\quad\text{strongly in } L^2(0,T;H^2(\Omega)).$$

At this point, v_i is any limit function; we prove below that $v_i=\log(\rho_i/\rho_n)$.

We deduce from the linearity and boundedness of the trace operator $H^1(\Omega)\hookrightarrow H^{1/2}(\partial\Omega)$ that

$$\theta^{(\tau)}\rightharpoonup\theta\quad\text{weakly in } L^2(0,T;H^{1/2}(\partial\Omega)).$$

Using the compact embedding $H^{1/2}(\partial\Omega)\hookrightarrow L^2(\partial\Omega)$, this gives

$$\theta^{(\tau)}\to\theta\quad\text{strongly in } L^2(0,T;L^2(\partial\Omega)).$$

The a.e. convergence of ρ_i for $i=1,\ldots,n-1$ implies that, up to a subsequence,

$$\rho_n^{(\tau)}=\rho^0-\sum_{i=1}^{n-1}\rho_i^{(\tau)}\to\rho^0-\sum_{i=1}^{n-1}\rho_i=:\rho_n\quad\text{a.e. in } \Omega_T.$$

Next, we prove that θ and ρ_i are positive a.e. We know already that $\theta^{(\tau)}$ and $\rho_i^{(\tau)}$ are positive in Ω_T. It follows from the $L^\infty(0,T;L^1(\Omega))$ bound for $\log\theta^{(\tau)}$ and the a.e. pointwise convergence $\theta^{(\tau)}\to\theta$ that $\log\theta$ is finite a.e. and therefore $\theta>0$ a.e. in Ω_T. For the positivity of ρ_i, we observe first that there exists a constant $C(n)>0$ such that for all $z_1,\ldots,z_{n-1}\in\mathbb{R}$,

$$\log\bigg(1+\sum_{i=1}^{n-1}e^{z_i}\bigg)\le C(n)\bigg(1+\sum_{i=1}^{n-1}|z_i|\bigg).$$

Since $\rho_i^{(\tau)} = \rho^0 \exp(v_i^{(\tau)})/\sum_{j=1}^n \exp(v_j^{(\tau)})$, $\rho^0 \geq \rho_*$, and $v_i^{(\tau)}$ is bounded in $L^1(\Omega)$, this implies for sufficiently small $\delta > 0$ that

$$\begin{aligned}\operatorname{meas}\big\{(x,t) : \rho_i^{(\tau)}(x,t) \leq \delta\big\} &= \operatorname{meas}\left\{(x,t) : -\log \frac{\rho^0(x)\exp(v_i^{(\tau)}(x,t))}{\sum_{j=1}^n \exp(v_j^{(\tau)}(x,t))} \geq -\log\delta\right\} \\ &\leq \operatorname{meas}\left\{(x,t) : \sum_{j=1}^n |v_j^{(\tau)}(x,t)| \geq C(1-\log\delta+\log\rho_*)\right\} \\ &\leq \frac{C}{-\log\delta}\int_0^T\int_\Omega\sum_{i=1}^n |v_i^{(\tau)}(x,t)|dxdt \leq \frac{C}{-\log\delta}, \quad i=1,\ldots,n-1.\end{aligned}$$

We infer from

$$\begin{aligned}\operatorname{meas}\big\{\liminf_{(\varepsilon,\tau)\to 0}\{(x,t) : \rho_i^{(\tau)}(x,t)\leq\delta\}\big\} &\leq \liminf_{(\varepsilon,\tau)\to 0}\operatorname{meas}\{(x,t) : \rho_i^{(\tau)}(x,t)\leq\delta\} \\ &\leq \limsup_{(\varepsilon,\tau)\to 0}\operatorname{meas}\{(x,t) : \rho_i^{(\tau)}(x,t)\leq\delta\} \leq \operatorname{meas}\big\{\limsup_{(\varepsilon,\tau)\to 0}\{(x,t) : \rho_i^{(\tau)}(x,t)\leq\delta\}\big\},\end{aligned}$$

and the pointwise convergence $\rho_i^{(\tau)} \to \rho_i$ that in fact equality holds in the previous chain of inequalities, which means that

$$\operatorname{meas}\{(x,t) : \rho_i(x,t)\leq\delta\} = \lim_{(\varepsilon,\tau)\to 0}\operatorname{meas}\{(x,t) : \rho_i^{(\tau)}(x,t)\leq\delta\} \leq \frac{C}{-\log\delta}$$

and $\rho_i > 0$ a.e. in the limit $\delta \to 0$, where $i = 1,\ldots,n-1$. We prove in a similar way for $\rho_n^{(\tau)} = \rho^0/(\sum_{j=1}^n \exp(v_i^{(\tau)})) > 0$ that $\rho_n > 0$ a.e.

As $\rho_i^{(\tau)}$ converges a.e. to an a.e. positive limit, we have

$$v_i^{(\tau)} = \log\rho_i^{(\tau)} - \log\rho_n^{(\tau)} \to \log\rho_i - \log\rho_n \quad \text{a.e. in } \Omega_T.$$

Thus $v_i = \log\rho_i - \log\rho_n$. Furthermore, $q_i^{(\tau)} = \log\rho_i^{(\tau)} - \log\theta^{(\tau)} \to \log\rho_i - \log\theta =: q_i$ and

$$(\Pi\boldsymbol{q}^{(\tau)})_i = v_i^{(\tau)} - \frac{1}{n}\sum_{j=1}^n v_j^{(\tau)} \to v_i - \frac{1}{n}\sum_{j=1}^n v_j =: U_i \quad \text{a.e. in } \Omega_T.$$

This shows that $v_i = q_i - q_n$ and $U_i = (q_i - q_n) - \sum_{j=1}^n (q_j - q_n)/n = (\Pi\boldsymbol{q})_i$. The a.e. convergence of $(\Pi\boldsymbol{q}^{(\tau)})$ and the boundedness of r_i by Hypothesis (H5) lead to

$$r_i(\Pi\boldsymbol{q}^{(\tau)},\theta^{(\tau)}) \to r_i(\Pi\boldsymbol{q},\theta) \quad \text{strongly in } L^\eta(\Omega_T),\ \eta < \infty.$$

By assumption, $M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})$ and $M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})/\theta^{(\tau)}$ are bounded. Then the strong convergences imply that these sequences are converging in $L^q(\Omega_T)$ for $q < \infty$, and the limits can be identified. Thus,

$$\begin{aligned}M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)}) &\to M_{ij}(\boldsymbol{\rho},\theta) \quad \text{strongly in } L^q(\Omega_T), \\ M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})/\theta^{(\tau)} &\to M_j(\boldsymbol{\rho},\theta)/\theta \quad \text{strongly in } L^q(\Omega_T) \text{ for all } q<\infty.\end{aligned}$$

This shows that

$$M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)}) = \frac{1}{\theta^{(\tau)}}M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\theta^{(\tau)} \to \frac{1}{\theta}M_j(\boldsymbol{\rho},\theta)\theta = M_j(\boldsymbol{\rho},\theta)$$

strongly in $L^\eta(\Omega_T)$ for $\eta < 16/3$. Moreover, taking into account (32), we have

$$M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla\frac{1}{\theta^{(\tau)}} = -\frac{M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})}{\theta^{(\tau)}}\nabla\log\theta^{(\tau)} \rightharpoonup \frac{M_j(\boldsymbol{\rho},\theta)}{\theta}\nabla\log\theta$$

weakly in $L^\eta(\Omega_T)$ for $\eta < 8/3$. Finally, by the weak convergence of $(\nabla\boldsymbol{v}^{(\tau)})$ in $L^2(\Omega_T)$,

$$\begin{aligned}
M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)} &\rightharpoonup M_{ij}(\boldsymbol{\rho},\theta)\nabla v_j \quad \text{weakly in } L^\eta(\Omega_T),\ \eta < 2, \\
M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)} &\rightharpoonup M_j(\boldsymbol{\rho},\theta)\nabla v_j \quad \text{weakly in } L^\eta(\Omega_T),\ \eta < 16/11, \\
M_j(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla\frac{1}{\theta^{(\tau)}} &\rightharpoonup -\frac{1}{\theta^2}M_j(\boldsymbol{\rho},\theta)\nabla\theta \quad \text{weakly in } L^\eta(\Omega_T),\ \eta < 8/7.
\end{aligned}$$

These convergences allow us to perform the limit $(\varepsilon,\tau)\to 0$. Finally, we can show as in [23, p. 1980f] that the linear interpolant $\widetilde{\rho}_i^{(\tau)}$ of $\rho_i^{(\tau)}$ and the piecewise constant function $\rho_i^{(\tau)}$ converge to the same limit, which leads to $\rho_i^0 = \widetilde{\rho}_i^{(\tau)}(0) \rightharpoonup \rho_i(0)$ weakly in $H^2(\Omega)'$. Thus, the initial datum $\rho_i(0) = \rho_i^0$ is satisfied in the sense of $H^2(\Omega)'$. Similarly, $(\rho\theta)(0) = \rho^0\theta^0$ in the sense of $W^{1,16}(\Omega)'$. This finishes the proof.

4. Proof of Theorem 2

The proof of Theorem 2 is very similar to that one from Section 3, therefore we present only the changes in the proof. Steps 1–3 are the same as in the previous section. Only the estimate of I_4 is different:

$$I_4 = \int_\Omega\sum_{i,j=1}^{n-1}M_{ij}\nabla v_i\cdot\nabla v_j dx = \int_\Omega\sum_{i,j=1}^{n}M_{ij}\nabla q_i\cdot\nabla q_j dx \geq \frac{c_M}{n}\int_\Omega\sum_{i=1}^n\rho_i|\nabla(\Pi\boldsymbol{q})_i|^2dx.$$

This gives a uniform estimate for $\int_\Omega\rho_i^{(\tau)}|\nabla(\Pi\boldsymbol{q}^{(\tau)})_i|^2dx$. We claim that it yields a bound for $\nabla(\rho_i^{(\tau)})^{1/2}$ in $L^2(\Omega_T)$. Indeed, we insert the definitions $q_i^{(\tau)} = \log(\rho_i^{(\tau)}/\theta^{(\tau)})$ and $(\Pi\boldsymbol{q}^{(\tau)})_i = q_i^{(\tau)} - \sum_{j=1}^n q_j^{(\tau)}/n = \log\rho_i^{(\tau)} - \sum_{j=1}^n(\log\rho_j^{(\tau)})/n$ to find that

$$\begin{aligned}
\sum_{i=1}^n\rho_i|\nabla(\Pi\boldsymbol{q}^{(\tau)})_i|^2 &= \sum_{i=1}^n\rho_i^{(\tau)}\bigg|\nabla\log\rho_i^{(\tau)} - \frac{1}{n}\sum_{j=1}^n\nabla\log\rho_j^{(\tau)}\bigg|^2 \\
&= \sum_{i=1}^n\rho_i^{(\tau)}|\nabla\log\rho_i^{(\tau)}|^2 - \frac{2}{n}\nabla\rho^0\cdot\sum_{j=1}^n\nabla\log\rho_j^{(\tau)} + \frac{\rho^0}{n^2}\bigg|\sum_{j=1}^n\nabla\log\rho_j^{(\tau)}\bigg|^2 \\
&\geq 4\sum_{i=1}^n|\nabla(\rho_i^{(\tau)})^{1/2}|^2 - 4|\nabla(\rho^0)^{1/2}|^2.
\end{aligned}$$

This shows the claim.

In contrast to Step 4 in Section 3, we do not have a uniform bound for $v_i^{(\tau)}$ in $L^2(0,T;H^1(\Omega))$ but a bound for $(\rho_i^{(\tau)})^{1/2}$. We deduce from the L^∞ bound for $\rho_i^{(\tau)}$ a bound for $\rho_i^{(\tau)}$ in $L^2(0,T;H^1(\Omega))$, using $\nabla\rho_i^{(\tau)} = (\rho_i^{(\tau)})^{1/2}\nabla(\rho_i^{(\tau)})^{1/2}$. This bound changes the proof of estimate (34) for the time translates. In fact, we just have to replace the estimations involving $\nabla v_j^{(\tau)}$:

$$\int_0^T\int_\Omega\bigg|\sum_{j=1}^{n-1}M_{ij}^{(\tau)}\nabla v_j^{(\tau)}\cdot\nabla\phi_j dxdt\bigg|dxdt = \int_0^T\int_\Omega\bigg|\sum_{j=1}^{n}M_{ij}^{(\tau)}\nabla\log\rho_j^{(\tau)}\cdot\nabla\phi_i\bigg|dxdt$$
$$\le\sum_{j=1}^n\|M_{ij}^{(\tau)}/\rho_j^{(\tau)}\|_{L^\infty(\Omega_T)}\|\nabla\rho_j^{(\tau)}\|_{L^2(\Omega_T)}\|\nabla\phi_i\|_{L^2(\Omega_T)},$$
$$\int_0^T\int_\Omega\bigg|\sum_{j=1}^{n-1}M_{j}^{(\tau)}\nabla v_j^{(\tau)}\cdot\nabla\phi_0\bigg|dxdt = \int_0^T\int_\Omega\bigg|\sum_{j=1}^{n}M_{j}^{(\tau)}\nabla\log\rho_j^{(\tau)}\cdot\nabla\phi_0\bigg|dxdt$$
$$\le\sum_{j=1}^n\|M_{ij}^{(\tau)}/\rho_j^{(\tau)}\|_{L^\infty(\Omega_T)}\|\nabla\rho_j^{(\tau)}\|_{L^2(\Omega_T)}\|\nabla\phi_0\|_{L^2(\Omega_T)}.$$

This yields (34).

The $L^2(0,T;H^1(\Omega))$ estimate for $\rho_i^{(\tau)}$ and (34) allow us to apply the Aubin–Lions lemma in the version of [13] yielding, up to a subsequence, the strong convergence $\rho_i^{(\tau)}\to\rho_i$ in $L^2(\Omega_T)$ as $(\varepsilon,\tau)\to 0$ and, because of the boundedness of $\rho_i^{(\tau)}$, in $L^r(\Omega_T)$ for any $r<\infty$.

It remains to perform the limit $(\varepsilon,\tau)\to 0$ in the terms involving $\boldsymbol{v}^{(\tau)}$,

$$\sum_{j=1}^n M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)},\quad \sum_{i=1}^n M_{i}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_i^{(\tau)},\quad \varepsilon\theta^{(\tau)}(D^2v_j^{(\tau)}+v_j^{(\tau)}).$$

The last term is easy to treat: The bound for $\sqrt{\varepsilon}v_j^{(\tau)}$ in $L^2(0,T;H^2(\Omega))$ and the strong convergence of $\theta^{(\tau)}$ imply that $\varepsilon\theta^{(\tau)}(D^2v_j^{(\tau)}+v_j^{(\tau)})\to 0$ strongly in $L^2(\Omega_T)$. Since $M_{ij}/\rho_j^{(\tau)}$ is bounded by assumption, we have $M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})/\rho_j^{(\tau)}\to M_{ij}(\boldsymbol{\rho},\theta)/\rho_j$ strongly in $L^r(\Omega_T)$ for $r<\infty$. Hence, using (6) and the weak convergence of $(\nabla\rho_j^{(\tau)})$ in $L^2(\Omega_T)$,

$$\sum_{j=1}^{n-1} M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_j^{(\tau)} = \sum_{j=1}^n\frac{M_{ij}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})}{\rho_j^{(\tau)}}\nabla\rho_j^{(\tau)}\rightharpoonup\sum_{j=1}^n\frac{M_{ij}(\boldsymbol{\rho},\theta)}{\rho_j}\nabla\rho_j$$

weakly in $L^\eta(\Omega_T)$ for $\eta<2$. Since $(M_{ij}/\rho_j^{(\tau)})\nabla\rho_j^{(\tau)}$ is bounded in $L^2(\Omega_T)$, this convergence also holds in $L^2(\Omega_T)$. The limit in the second term $\sum_{i=1}^n M_i(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_i^{(\tau)}$ is performed in an analogous way, leading to

$$\sum_{i=1}^n M_{i}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})\nabla v_i^{(\tau)} = \sum_{i=1}^n\frac{M_{i}(\boldsymbol{\rho}^{(\tau)},\theta^{(\tau)})}{\rho_i^{(\tau)}}\nabla\rho_i^{(\tau)}\rightharpoonup\sum_{i=1}^n\frac{M_{i}(\boldsymbol{\rho},\theta)}{\rho_i}\nabla\rho_i$$

weakly in $L^2(\Omega_T)$. This finishes the proof.

References

[1] H. W. Alt and S. Luckhaus. Quasilinear elliptic-parabolic differential equations. *Math. Z.* 183 (1983), 311–341.

[2] B. Anwasia, M. Bisi, F. Salvarani, and A. J. Soares. On the Maxwell–Stefan diffusion limit for a reactive mixture of polyatomic gases in non-isothermal setting. *Kinetic Related Models* 13 (2020), 63–95.

[3] A. Bondesan and M. Briant. Stability of the Maxwell–Stefan system in the diffusion asymptotics of the Boltzmann multi-species equation. Submitted for publication, 2019. arXiv:1910.08357.

[4] M. Briant and B. Grec. Rigorous derivation of the Fick cross-diffusion system from the multi-species Boltzmann equation in the diffusive scaling. Submitted for publication, 2020. arXiv:2003.07891.

[5] D. Bothe. On the Maxwell–Stefan equations to multicomponent diffusion. In: J. Escher et al. (eds). *Parabolic Problems. Progress in Nonlinear Differential Equations and their Applications*, pp. 81–93. Springer, Basel, 2011.

[6] D. Bothe and W. Dreyer. Continuum thermodynamics of chemically reacting fluid mixtures. *Acta Mech.* 226 (2015), 1757–1805.

[7] D. Bothe and P.-E. Druet. Mass transport in multicomponent compressible fluids: Local and global well-posedness in classes of strong solutions for general class-one models. Submitted for publication, 2020. arXiv:2001.08970.

[8] L. Boudin, B. Grec, and V. Pavan. Diffusion models for mixtures using a stiff dissipative hyperbolic formalism. *J. Hyperbol. Eqs.* 16 (2019), 293–312.

[9] L. Boudin, B. Grec, M. Pavić, and F. Salvarani. Diffusion asymptotics of a kinetic model for gaseous mixtures. *Kinetic Related Models* 6 (2013), 137–157.

[10] M. Buliček, A. Jüngel, M. Pokorný, and N. Zamponi. Existence analysis of a stationary compressible fuid model for heat-conducting and chemically reacting mixtures. Submitted for publication, 2020. arXiv:2001.06082.

[11] X. Chen and A. Jüngel. Analysis of an incompressible Navier–Stokes–Maxwell–Stefan system. *Commun. Math. Phys.* 340 (2015), 471–497.

[12] M. Dolce and D. Donatelli. Artificial compressibility method for the Navier–Stokes–Maxwell–Stefan system. *J. Dyn. Diff. Eqs.*, 2019. https://doi.org/10.1007/s10884-019-09808-4.

[13] M. Dreher and A. Jüngel. Compact families of piecewise constant functions in $L^p(0,T;B)$. *Nonlin. Anal.* 75 (2012), 3072–3077.

[14] W. Dreyer, P.-E. Druet, P. Gajewski, and C. Guhlke. Analysis of improved Nernst–Planck–Poisson models of compressible isothermal electrolytes. *Z. Angew. Math. Phys.* 71 (2020), no. 119, 68 pages.

[15] P.-E. Druet. Analysis of improved Nernst–Planck–Poisson models of isothermal compressible electrolytes subject to chemical reactions: The case of a degenerate mobility matrix. WIAS Preprint no. 2321, WIAS Berlin, Germany, 2016.

[16] P.-E. Druet. A theory of generalised solutions for ideal gas mixtures with Maxwell–Stefan diffusion. Submitted for publication, 2020. WIAS Preprint no. 2700, WIAS Berlin, Germany.

[17] E. Feireisl and A. Novotný. *Singular Limits in Thermodynamics of Viscous Flows.* Birkhäuser, Basel, 2009.

[18] V. Giovangigli and M. Massot. The local Cauchy problem for multicomponent flows in full vibrational non-equilibrium. *Math. Meth. Appl. Sci.* 21 (1998), 1415–1439.

[19] V. Giovangigli, M. Pokorný, and E. Zatorska. On the steady flow of reactive gaseous mixture. *Analysis (Berlin)* 35 (2015), 319–341.

[20] M. Herberg, M. Meyries, J. Prüss, and M. Wilke. Reaction-diffusion systems of Maxwell–Stefan type with reversible mass-action kinetics. *Nonlin. Anal.* 159 (2017), 264–284.

[21] X. Huo, A. Jüngel, and A. Tzavaras. High-friction limits of Euler flows for multicomponent systems. *Nonlinearity* 32 (2019), 2875–2913.

[22] H. Hutridurga and F. Salvarani. Existence and uniqueness analysis of a non-isothermal cross-diffusion system of Maxwell–Stefan type. *Appl. Math. Lett.* 75 (2018), 108–113.

[23] A. Jüngel. The boundedness-by-entropy method for cross-diffusion systems. *Nonlinearity* 28 (2015), 1963–2001.

[24] A. Jüngel and O. Leingang. Convergence of an implicit Euler Galerkin scheme for Poisson–Maxwell–Stefan systems. *Adv. Comput. Math.* 45 (2019), 1469–1498.

[25] A. Jüngel and I. V. Stelzer. Existence analysis of Maxwell–Stefan systems for multicomponent mixtures. *SIAM J. Math. Anal.* 45 (2013), 2421–2440.

[26] L. Ostrowski and C. Rohde. Compressible multi-component flow in porous media with Maxwell–Stefan diffusion. To appear in *Math. Meth. Appl. Sci.*, 2020. arXiv:1905.08496.

[27] T. Piasecki and M. Pokorný. Weak and variational entropy solutions to the system describing steady flow of a compressible reactive mixture. *Nonlin. Anal.* 159 (2017), 365–392.

[28] S. Takata and K. Aoki. Two-surface problems of a multicomponent mixture of vapors and noncondensable gases in the continuum limit in the light of kinetic theory. *Phys. Fluids* 11 (1999), 2743–2756.

[29] R. Temam. *Infinite-Dimensional Dynamical Systems in Mechanics and Physics*, 2nd edn. Springer, New York, 1997.

Institute for Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstrasse 8–10, 1040 Wien, Austria
E-mail address: christoph.helmer@tuwien.ac.at

Institute for Analysis and Scientific Computing, Vienna University of Technology, Wiedner Hauptstrasse 8–10, 1040 Wien, Austria
E-mail address: juengel@tuwien.ac.at