

Nečas Center for Mathematical Modeling

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Incompressible mixtures with thermal diffusion cross effects

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Abstract

The model for ionized mixtures featuring chemical reactions and thermal diffusion cross effects is presented. The thermodynamic consistency of the model is used as the main ingredient for the proof of the existence its solution, which is done by combining regularization, time discretization and the Galerkin method.

1 Introduction

The main purpose of this article is to prove existence of a model for fluid mixtures. The diffusion is governed by gradient of chemical potentials and temperature. The main purpose of this article is to begin mathematical exploitation of the duality between chemical potentials and species concentrations. The entropy in the model is the simplified version of the entropy for the ideal gas. The model is compatible with the GENERIC framework. The main improvement in comparison to previous works [3, 25, 27, 28] is using the chemical potentials directly in the model and apriori estimates in view of the thermodynamics of the model. The main purpose of this article is not to derive new classes of models for fluid mixtures but to present a new view of rather standard models. The compressible case have been analyzed in [1, 8]. For alternative models see articles [4, 17].

Modelling of ionized mixtures is very important for designing of devices, such as fuel cells (see eg. [22, 30]), or in biology (see eg. [6, 15, 16]). This subject has been studied from thermodynamical point of view for a long period. The basic of the approach used here is the barycentric velocity and has been invented by Eckart and Prigogine, see [5, 23]. We use the linear treatment of the chemical reactions, as used in the book [14], which is a good summary of the theory of linear irreversible thermodynamics. A similar treatment of chemical reactions appears already in [21]. The gradient structure of chemical reactions is emphasised in [19]. The diffusion matrix have been studied in [10]. The theory

implicitly assumes that we can find every component of the mixture in every macroscopic point of the domain. This assumption was used in its full strength in rational thermodynamics, see for example [20, 24, 29]. The assumption might be relaxed in the phenomenological thermodynamics framework to the assumption that chemical potential of each constituent is defined almost everywhere in the domain. Another relaxation of the assumption was done in [18]. A different approach was used to obtain results for mono-atomic gases. In this case macroscopic, equations are obtained as a limit from the system of Boltzmann's equations. This approach was used in [9] on gases without ionization or chemical reactions. Chemical reactions were added in [11]. The thermodynamical treatment is based on the article [32], which presents the mixture model in light of the GENERIC framework. For more information see [31] or [12].

In section 3 we formulate the model both in terms of partial differential equations and the GENERIC framework. In section 4 we formulate assumptions on constitutive functions and formulate the main theorem of the article. The section 7 is devoted to the proof of existence of weak solution. The proof is organized as follows: First we discretize the system in time and partly in space. The discretization is done in a way such that the mass densities of all constituents are positive almost everywhere. Second we prove the existence of the discretized solution by the degree argument. Third we derive a priori estimates on the solution and converge from the discretization. Important consequence of a priori estimates is that the temperature is positive almost everywhere. In the section 6 we give an example of choice of the data which satisfy assumptions of the main theorem.

2 Nomenclature

Equation variables:

e	internal energy,
q	electric charge, $q = \sum z_i \rho_i$,
v	velocity,
χ	coldness, $\chi = \frac{1}{\theta}$,
μ	vector of chemical potentials,
ϕ	electric potential,
ρ	vector of species densities,
θ	temperature,
ζ	vector of rescaled chemical potentials, $\zeta = -\chi\mu$,

Equation data:

a_{ki}	stoichiometric coefficient for k -th reaction and i -th species,
M	matrix of diffusion coefficients,
\mathbf{m}	vector of thermodiffusion coefficients,
r	vector of reaction rates,
s	entropy density,
z	specific charges vector,
\mathfrak{D}	boundary diffusion matrix,
α	boundary permeability,
χ_Σ	coldness of the exterior, $\chi_\Sigma = \frac{1}{\theta_\Sigma}$,
ϵ	permittivity,
η	viscosity,
κ_Σ	heat transfer coefficient of the boundary,
ϱ	bulk density — given material parameter,
ζ_Σ	vector of rescaled exterior chemical potentials, $\zeta_\Sigma = -\chi_\Sigma \mu_\Sigma$,
ν	outward normal to the boundary,

GENERIC building blocks:

E	energy functional,
S	entropy functional,
$\{\cdot, \cdot\}$	Poisson bracket,
$[\cdot, \cdot]$	dissipative bracket.

3 Formulation of the model

The presented model is a combination of the model derived in [32] with model studied in [28]. It consists from the momentum balance and the incompressibility constraint.

$$\varrho \frac{\partial v}{\partial t} + \operatorname{div}(\varrho v \otimes v) + \nabla \pi - \operatorname{div}(2\eta^\theta(\rho, \theta, Dv)Dv) = -q\nabla\phi, \quad (1)$$

$$\operatorname{div}v = 0, \quad (2)$$

the mass balances for each constituent

$$\frac{\partial \rho_i}{\partial t} + \operatorname{div}\left(\rho_i v + \sum_{j=1}^L M_{ij}^\theta(\rho, \theta) \left(-\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi\right)\right) = r_i^\theta(\rho, \frac{\mu}{\theta}, \theta), \quad (3)$$

the internal energy balance

$$\begin{aligned}
& \frac{\partial e}{\partial t} + \operatorname{div} (ev - \kappa^\theta(\rho, \theta) \nabla \theta) \\
& + \operatorname{div} \left(\sum_{i,j=1}^L \mathbf{m}_i M_{ij}^\theta(\rho, \theta) \left(-\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi \right) \right) \\
& = - \sum_{i,j=1}^L z_i M_{ij}^\theta(\rho, \theta) \left(-\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi \right) \cdot \nabla \phi \\
& \quad + \eta^\theta(\rho, \theta, Dv) |Dv|^2, \tag{4}
\end{aligned}$$

and the Poisson equation

$$-\operatorname{div} \epsilon \nabla \phi = q, \tag{5}$$

where the vector of chemical potentials μ , temperature θ and the electric charge q are defined by means of the entropy density s and specific charges z_i :

$$\frac{\mu_i}{\theta} = -\frac{\partial s(\rho, e)}{\partial \rho_i}, \quad \frac{1}{\theta} = \frac{\partial s(\rho, e)}{\partial e}, \quad q = \sum_{i=1}^L z_i \rho_i. \tag{6}$$

The constraint (2) is justified by the constant density ϱ and in fact represents the continuity equation for the total mass density. The stress tensor in (1) represents the non-Newtonian p -power law. This makes the model applicable on shear-thinning and shear-thickening fluids. The force $q \nabla \phi$ in (1) is the Lorenz force due to Coulomb electrostatic interactions. The equation (3) is a convection–reaction–diffusion equation with a more general form of diffusion flux. The term $\sum_{j=1}^L M_{ij}^\theta(\rho, \theta) \nabla - \frac{\mu_j}{\theta}$ is a generalized and thermodynamically correct form of the Fick’s law. The term $\frac{z_j}{\theta} \nabla \phi$ represents the diffusion caused by the electric field – the tendency of the mixture to get into the electro-neutral state. The equation (4) represents the heat transfer. There are two heat sources. The source term $\eta^\theta(\rho, \theta, Dv) |Dv|^2$ represents the heat created by friction. The term $\sum_{i,j=1}^L M_{ij}^\theta(\rho, \theta) \left(-\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi \right) \cdot z_i \nabla \phi$ represents both the Joule heat and the Peltier effect. The heat transfer is due to convection, Fourier law and diffusion fluxes. The equation (5) is the quasi-static approximation of Maxwell equations.

Equations (1 – 6) are assumed to be satisfied in a bounded domain $\Omega \subset \mathbb{R}^3$.

We assume the following boundary conditions on $\partial\Omega$:

$$v = 0, \quad (7)$$

$$\begin{aligned} & \sum_{j=1}^L M_{ij}^\theta(\rho, \theta) \left(-\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi \right) \cdot \nu \\ & = -\sum_{j=1}^L \mathfrak{D}_{ij} \left(-\frac{\mu_j}{\theta} + \frac{(\mu_\Sigma)_j}{\theta_\Sigma} - z_j(\phi - \phi_\Sigma) \right), \end{aligned} \quad (8)$$

$$\begin{aligned} & \left(\kappa^\theta(\rho, \theta) \nabla \theta + \sum_{i,j=1}^L \mathbf{m}_i M_{ij}^\theta(\rho, \theta) \left(\nabla \frac{\mu_j}{\theta} + \mathbf{m}_j \nabla \frac{1}{\theta} - \frac{z_j}{\theta} \nabla \phi \right) \right) \cdot \nu \\ & = -\kappa_\Sigma \left(\frac{1}{\theta} - \frac{1}{\theta_\Sigma} \right), \end{aligned} \quad (9)$$

$$\epsilon \nabla \phi \cdot \nu = -\alpha(\phi - \phi_\Sigma). \quad (10)$$

Boundary conditions used here represent a container with permeable walls — membranes. The boundary condition (7) is the well known no-slip boundary condition. The condition (8) represents the diffusion of constituents through boundary. The diffusion is driven by differences of chemical potential and electric field over the membrane. The boundary condition (9) says that the heat transport through the boundary is driven by differences in temperature. The particular form of fluxes is inspired by (85). The boundary condition (10) represents the action of the external electric field. The form of the boundary condition (10) violates our definition of the electrostatic energy on the boundary. However it is not so surprising in spite of the fact that the formula was derived by analogy with the case of finitely many point charges and we do not have any explicit formula for the energy in the complete Maxwell system. Let us also note that the description of interactions on the boundary helps us to facilitate the mathematical theory.

Inspired by (6) we introduce new variables:

$$\begin{aligned} \text{the coldness} & \quad \chi := \frac{1}{\theta}, \quad \chi_\Sigma := \frac{1}{\theta_\Sigma}, \\ \text{and the vector of rescaled chemical potentials} & \quad \zeta := \frac{1}{\theta} \mu, \quad \zeta_\Sigma := \frac{1}{\theta_\Sigma} \mu_\Sigma. \end{aligned}$$

For the function $f^\theta = f^\theta(\rho, \theta)$ we define a function $f = f(\rho, \chi) = f^\theta \left(\rho, \frac{1}{\chi} \right)$.

4 The weak formulation and the main theorem

Equations will be solved on the domain Ω and time interval $I = [0, T]$. We denote by G the Gibb's simplex

$$G = \left\{ x \in \mathbb{R}^L : \sum_{i=1}^L x_i = \varrho \ \& \ \forall i : x_i \geq 0 \right\}.$$

We will use the vector $\ell = (1, \dots, 1)$ and the space $G' = \ell^\perp$. Symbols P and P_z will denote orthogonal projections

$$P : \mathbb{R}^L \rightarrow G'$$

and

$$P_z : \mathbb{R}^L \rightarrow G' \cap z^\perp$$

It is easy to check that $P\nabla f = \nabla Pf$ and $P_z\nabla f = \nabla P_z f$. For functions with values in \mathbb{R}^n we use the standard notation $C^k(\bar{\Omega}; \mathbb{R}^n)$ for the space of k times continuously differentiable functions, $C^\infty(\bar{\Omega}; \mathbb{R}^n)$ for the intersection $\bigcap_{k=1}^\infty C^k(\bar{\Omega}; \mathbb{R}^n)$, $L^p(\Omega; \mathbb{R}^n)$ for the Lebesgue spaces and $W^{k,p}(\Omega; \mathbb{R}^n)$ for the Sobolev spaces. For function depending on space and time we will denote corresponding spaces by $C^\infty(I \times \Omega; \mathbb{R}^n)$ and $L^p(I \times \Omega; \mathbb{R}^n)$. By $C_{0,\text{div}}^\infty(\Omega; \mathbb{R}^3)$, respectively $W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3)$, we will denote corresponding spaces of functions with zero trace and divergence. For X a Banach space we will denote by $C^1(\Omega; X)$ the space of continuous functions with values in X , $L^p(\Omega; X)$ will denote the standard Bochner space and $\mathcal{M}(\Omega; X)$ will denote the space of X valued measures. By the symbol $a \otimes b$ we will denote matrix with entries $(a \otimes b)_{ij} := a_i b_j$. For a function f we denote by f' its derivative.

We make several assumptions on the data: We need a smoothness of the boundary of Ω to have compact embedding of Sobolev functions into $C^k(\bar{\Omega})$.

$$\Omega \text{ is a } C^1 \text{ domain.} \quad (11)$$

We assume that chemical reactions conserve mass and electric charge to get mass balance and energy balance:

$$\sum_{i=1}^L r_i = 0, \quad \sum_{i=1}^L z_i r_i = 0. \quad (12)$$

We have a technically important assumption concerning the relation between chemical reactions and thermodiffusion coefficients. This assumption is needed to get estimates on the coldness in (42–45).

$$\exists A \in \mathbb{R}^L \ A \cdot \mathbf{m} \neq 0 : \forall \zeta \in \mathbb{R}^L : r(\zeta) \cdot \zeta \geq |A \cdot \zeta|^2. \quad (13)$$

We have stronger assumptions on the diffusion matrix M than just positive semi-definiteness needed for the second law (88). To read the estimate (40) we need positive definiteness on the subspace G' :

$$M \in C((\mathbb{R}^+)^{L+1}; \mathbb{R}^{L \times L}), \quad M(\rho, \chi) \leq C, \quad (14)$$

$$\exists \alpha \forall \rho \forall \chi \forall x : M(\rho, \chi) x \cdot x \geq \alpha |Px|^2. \quad (15)$$

The boundary diffusion matrix has to satisfy the same positive definiteness property to guarantee (38):

$$\exists \alpha_\Sigma \forall x \in \mathbb{R}^L : \mathfrak{D}x \cdot x \geq \alpha_\Sigma |Px|^2. \quad (16)$$

We also require diffusion fluxes to sum up to zero to get the total mass conservation:

$$\forall \rho \in G \ \forall \chi \in \mathbb{R} \ \forall j = 1, \dots, L : \sum_{i=1}^L M_{ij}(\rho, \chi) = 0, \quad \sum_{i=1}^L \mathfrak{D}_{ij} = 0. \quad (17)$$

The growth estimates on the viscosity η allow us to test the Navier–Stokes equation by solution and obtain strong convergence the velocity gradient.

$$\eta \in C((\mathbb{R}^+)^{L+1} \times \mathbb{R}^{3 \times 3}), \quad (18)$$

$$\bar{\eta}|Dv|^{p-2} \geq \eta(\rho, \chi, Dv) \geq \underline{\eta}|Dv|^{p-2} > 0, \quad p > \frac{11}{5}, \quad (19)$$

The growth assumption on the heat conduction coefficient κ is motivated by estimates (44) and (49). The limit of the value of r is to keep the term $\kappa \nabla \theta$ equi-integrable. For computation of the limit see (82).

$$\kappa \in C((\mathbb{R}^+)^{L+1}), \quad (20)$$

$$\underline{\kappa}_1 + \underline{\kappa}_2 \chi^{4(r-1)/r} \leq \kappa(\rho, \chi) \leq \bar{\kappa}_1 + \bar{\kappa}_2 \chi^{4(r-1)/r}, \quad r < 10 - \sqrt{80}. \quad (21)$$

The entropy density is assumed to be a differentiable strictly concave function with logarithmic growth in internal energy:

$$s \in C^2((\mathbb{R}^+)^{L+1}), \quad (22)$$

$$s(\rho, e) = s_\rho(\rho) + s_e(e), \quad \bar{s}_1 \ln e + \bar{s}_2 \geq s_e(e), \quad \bar{s}_3 \geq s_\rho(\rho) \quad (23)$$

We need the entropy to be strictly concave to transfer the information from chemical potential to species densities in (47).

$$\forall \rho \in G, \forall e, \forall x \in \mathbb{R}^L : -s''_\rho(\rho)x \cdot x \geq \underline{\mu}|x|^2. \quad (24)$$

The heat capacity is assumed to be bounded from below to transfer the information from the temperature to the internal energy in (56).

$$-\frac{1}{(s'_e)^2} s''_e \geq \underline{\theta} > 0. \quad (25)$$

We also assume that composition of the mixture is uniquely determined by chemical potentials and that internal energy is uniquely determined by the temperature, so we can construct the approximate solution in terms of chemical potentials and logarithm of temperature.

$$\text{The mapping } \rho \rightarrow s'_\rho(\rho) \text{ has an inverse } \rho = \rho(s'_\rho), \quad (26)$$

$$\text{the mapping } \rho \rightarrow s'_e(e) \text{ has an inverse } e = e(s'_e).$$

We also assume some characterisation of the manifold G to set properly the fix-point theorem in the lemma 7.4,

$$\exists \hat{\mu} : G' \rightarrow \mathbb{R}^L \text{ such that } \forall \tilde{\mu} \in G' \quad \rho(\tilde{\mu} + \hat{\mu}(\tilde{\mu})) \in G. \quad (27)$$

Due to assumption (12) and (17), the only effective part of chemical potential is Ps'_ρ . We assume that in the case of constant density we can control whole chemical potential by its effective part, as we need in (46):

$$\forall \rho \in G : |s'_\rho(\rho)| \leq C(|Ps'_\rho(\rho)| + 1). \quad (28)$$

Initial conditions will be qualified as follows:

$$v_0 \in L^2(\Omega; \mathbb{R}^3), \quad (29)$$

$$\rho_0(x) \in G \quad \forall x, \quad (30)$$

$$e_0 \in L^1(\Omega), \quad (31)$$

$$s(\rho_0, e_0) \in L^1(\Omega). \quad (32)$$

Definition 4.1. As a weak solution to the problem (1–6) with boundary conditions (7–10) we will call the six-couple $(v, \rho, \zeta, e, \chi, \phi)$ such that

$$\begin{aligned} v &\in L^\infty(I; L^2(\Omega; \mathbb{R}^3)) \cap L^p\left(I; W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3)\right), \\ \rho &\in L^\infty(I \times \Omega; \mathbb{R}^L), \\ \zeta &\in L^r(I; L^{3r/(3-r)}(\Omega; \mathbb{R}^L)), \\ P\zeta &\in L^r(I; W^{1,r}(\Omega; \mathbb{R}^L)), \\ e &\in L^\infty(I; L^1(\Omega)) \cap L^{5/4-\delta}(I; W^{1,5/4-\delta}(\Omega)), \\ \chi &\in L^r(I; W^{1,r}(\Omega)), \\ \frac{1}{\chi} &\in L^{5/4-\delta}(I; W^{1,5/4-\delta}(\Omega)), \\ \phi &\in L^\infty(I; W^{1,2}(\Omega)), \end{aligned}$$

with r from (21), and which satisfy

$$\begin{aligned} \int_{I \times \Omega} -\varrho v \cdot \frac{\partial \varphi}{\partial t} + (-\varrho v \otimes v + \eta(\rho, \chi, Dv)Dv) : \nabla \varphi \, dxdt \\ = \int_{I \times \Omega} -q \nabla \phi \cdot \varphi \, dxdt + \int_{\Omega} v_0 \cdot \varphi(0) \, dx \end{aligned} \quad (33)$$

with every $\varphi \in C^1\left(I; C_{0,\text{div}}^\infty(\overline{\Omega}; \mathbb{R}^3)\right)$ such that $\varphi(T) = 0$ and

$$\begin{aligned} \int_{I \times \Omega} -\rho \cdot \frac{\partial \varphi}{\partial t} - (\rho \otimes v + M(\rho, \chi)(\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi)) : \nabla \varphi \, dxdt \\ = \int_{I \times \partial \Omega} \mathfrak{D}(\zeta - \zeta_\Sigma - z(\phi - \phi_\Sigma)) \cdot \varphi \, dSdt + \int_{I \times \Omega} r(\zeta) \cdot \varphi \, dxdt \\ + \int_{\Omega} \rho_0 \cdot \varphi(0) \, dx \end{aligned}$$

with every $\varphi \in C^1(I \times \overline{\Omega})$ such that $\varphi(T) = 0$ and also

$$\begin{aligned} \int_{I \times \Omega} -e \frac{\partial \varphi}{\partial t} + \left(-ev + \kappa(\rho, \chi) \nabla \frac{1}{\chi}\right) \cdot \nabla \varphi \, dxdt \\ - \int_{I \times \Omega} M(\rho, \chi)(\nabla \zeta + \mathbf{m} \nabla \chi - \chi z \otimes \nabla \phi) : (\mathbf{m} \nabla \varphi - z \otimes \nabla \phi \varphi) \, dxdt \\ - \int_{I \times \partial \Omega} \kappa_\Sigma(\chi - \chi_\Sigma) \varphi \, dS = \int_{I \times \Omega} \eta(\rho, \chi, Dv) |Dv|^2 \varphi \, dxdt + \int_{\Omega} e_0 \varphi(0) \, dS \end{aligned} \quad (34)$$

with every $\varphi \in C^1(I \times \overline{\Omega})$ such that $\varphi(T) = 0$ and eventually also

$$\int_{I \times \Omega} \epsilon \nabla \phi \cdot \nabla \varphi \, dxdt + \int_{I \times \partial \Omega} \alpha(\phi - \phi_\Sigma) \varphi \, dSdt = \int_{I \times \Omega} q \varphi \, dxdt \quad (35)$$

with every $\varphi \in C^1(I \times \bar{\Omega})$, where q , ζ and χ are given by (6).

We will prove the following theorem:

Theorem 4.2. *Let assumptions (11–32) hold. Then there exists at least one weak solution to the problem (1–6) with boundary conditions (7–10).*

The proof is based on ideas from the article [1]. The treatment of the energy equation is a simplified version of [2]. Some advanced techniques concerning the time discretization are taken from [26]. Apriori estimates are based on the first and second laws of thermodynamics stated in [32].

5 Formal apriori estimates

The conclusion $\rho_i > 0$ is a consequence of (26). As $\sum_{i=1}^L \rho_i = \varrho$ and $\rho_i \geq 0$ we have the estimate $\|\rho\|_{L^\infty(I \times \Omega; \mathbb{R}^L)} \leq \varrho$. Testing (35) by $\Delta\phi$ we obtain that $\|\phi\|_{W^{2,2}(\Omega)} \leq C$.

Now we use the thermodynamical estimates motivated by (87) and (88). The main motivation is a proper choice of test-functions. First we establish the first law (see (87)). We test (33) by v , (34) by $z\phi$ and (34) by 1. Using the time derivative of (35), namely

$$\int_{\Omega} \phi z \cdot \frac{\partial \rho}{\partial t} dx = \int_{\Omega} \epsilon \nabla \phi \cdot \nabla \frac{\partial \phi}{\partial t} dx + \int_{\partial \Omega} \alpha \frac{\partial \phi}{\partial t} \cdot \phi dS$$

we arrive at the equation

$$\begin{aligned} & \frac{\partial}{\partial t} \int_{\Omega} \frac{1}{2} |v|^2 + \frac{\epsilon}{2} |\nabla \phi|^2 + e dx \\ &= - \int_{\partial \Omega} \mathfrak{D}(\zeta - \zeta_{\Sigma} - z(\phi - \phi_{\Sigma})) \cdot z\phi + \kappa_{\Sigma}(\chi - \chi_{\Sigma}) dS \\ &\leq C(\|P\zeta\|_{L^2(\partial \Omega; \mathbb{R}^L)} + \|\zeta_{\Sigma}\|_{L^2(\partial \Omega; \mathbb{R}^L)} + \|\chi\|_{L^2(\partial \Omega)} + \|\chi_{\Sigma}\|_{L^2(\partial \Omega)}), \end{aligned} \quad (36)$$

which corresponds to (87). Next we use (84) as test-functions. Next we test the equation (58) by $-\zeta$ and the equation (59) by $-\chi$ and use (24). The result is:

$$\begin{aligned} & \frac{\partial}{\partial t} \int_{\Omega} -s(\rho, e) dx + \int_{\Omega} \kappa(\rho, \chi) \nabla_{\chi}^{\perp} \cdot \nabla \chi + r(\zeta) \cdot \zeta dx \\ &+ \int_{\Omega} M(\rho, \chi) (\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi) : (\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi) dx \\ &+ \int_{\partial \Omega} \mathfrak{D} \zeta \cdot \zeta + \alpha \frac{1}{\theta^2} dS = \int_{\partial \Omega} \mathfrak{D}(\zeta_{\Sigma} + z(\phi - \phi_{\Sigma})) \cdot \zeta + \kappa_{\Sigma} \chi_{\Sigma} \chi dS \\ &\leq \|P\zeta\|_{L^2(\partial \Omega; \mathbb{R}^L)} (\|\zeta_{\Sigma}\|_{L^2(\partial \Omega; \mathbb{R}^L)} + \|\phi\|_{L^2(\partial \Omega)} + \|\phi_{\Sigma}\|_{L^2(\partial \Omega)}) \\ &\quad + \|\chi\|_{L^2(\partial \Omega)} \|\chi_{\Sigma}\|_{L^2(\partial \Omega)} \end{aligned} \quad (37)$$

and corresponds to (88). By the assumption (16) we have

$$\int_{I \times \partial \Omega} \mathfrak{D} \zeta \cdot \zeta dS dt \geq \alpha_{\Sigma} \|\zeta\|_{L^2(I \times \Omega; \mathbb{R}^L)}^2. \quad (38)$$

Application of assumptions (15), (86), (21), (29), (29) and (32) together with the Young and the discrete Gronwall inequalities gives us

$$\int_{\Omega} -s(\rho, e) dx \leq C. \quad (39)$$

The estimate (39) together with the assumption (23) and (26) allows us to conclude that $e > 0$ and $\chi > 0$ almost everywhere.

Now we use the Gronwall lemma on the sum (37) + $(K + 1)$ (36). We thus get estimates on $\|v\|_{L^2(\Omega; \mathbb{R}^3)}$ and $\|e\|_{L^1(\Omega)}$.

By the assumption (15) we have

$$\begin{aligned} \int_{I \times \Omega} M(\rho, \chi) (\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi) : (\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi) dx dt \\ \geq \alpha \|P(\nabla \zeta + \mathbf{m} \otimes \nabla \chi - \chi z \otimes \nabla \phi)\|_{L^2(I \times \Omega; \mathbb{R}^{L \times 3})}^2. \end{aligned} \quad (40)$$

By estimates (40) and (38) we have

$$\|P_z(\zeta + \mathbf{m}\chi)\|_{L^2(\Omega; W^{1,2}(\Omega; \mathbb{R}^L))} \leq C. \quad (41)$$

Next we use the assumption (86) to get

$$\int_{I \times \Omega} r(\zeta) \cdot \zeta dx dt \geq \|A \cdot \zeta\|_{L^2(I \times \Omega)}^2. \quad (42)$$

Using assumption (13) together with estimates (41) and (42) we get

$$\|A \cdot \mathbf{m}\| \|\chi\|_{L^2(I \times \Omega)} \leq \|A \cdot \zeta\|_{L^3(\Omega)} + |A| \|P_z(\zeta + \mathbf{m}\chi)\|_{L^2(I \times \Omega; \mathbb{R}^L)} \leq C. \quad (43)$$

Next we use the assumption (21) to get

$$\begin{aligned} \int_{I \times \Omega} \kappa(\rho, \chi) \nabla \frac{1}{\chi} \cdot \nabla \chi dx dt \geq \int_{I \times \Omega} (\chi)^{2(r-2)/r} |\nabla \chi|^2 dx dt \\ \geq \left\| (\chi)^{(r-2)/r} \nabla \chi \right\|_{L^2(I \times \Omega; \mathbb{R}^d)}. \end{aligned} \quad (44)$$

Now we may estimate using estimates (43) and (44)

$$\begin{aligned} \|\nabla \chi\|_{L^r(I \times \Omega; \mathbb{R}^3)} &\leq \left\| (\chi)^{(r-2)/r} \nabla \chi \right\|_{L^2(I \times \Omega; \mathbb{R}^3)} \left\| (\chi)^{(2-r)/r} \right\|_{L^{2r/(2-r)}(I \times \Omega)} \\ &\leq \left\| (\chi)^{(r-2)/r} \nabla \chi \right\|_{L^2(I \times \Omega; \mathbb{R}^3)} \|\chi\|_{L^2(I \times \Omega)}^{(2-r)/2r} \leq C. \end{aligned} \quad (45)$$

Finally we have the estimate on ζ

$$\begin{aligned} \|P\zeta\|_{L^r(I; W^{1,r}(\Omega; \mathbb{R}^L))} &\leq \|P(\nabla \zeta + \mathbf{m}\nabla \chi - \chi z \otimes \nabla \phi)\|_{L^2(I \times \Omega; \mathbb{R}^{L \times 3})} \\ &\quad + C \|\nabla \chi\|_{L^2(I \times \Omega; \mathbb{R}^3)} + C \|\chi\|_{L^r(I; W^{1,r}(\Omega))} \|\phi\|_{L^\infty(I; W^{2,2}(\Omega))} \leq C \end{aligned}$$

and

$$\|\zeta\|_{L^r(I; L^{3r/(3-r)}(\Omega; \mathbb{R}^L))} \leq C(\|P\zeta + 1\|_{L^r(I; W^{1,r}(\Omega; \mathbb{R}^L))} + 1) \leq C. \quad (46)$$

Using the chain rule and (24) gives us

$$|P\nabla\zeta| = |Ps''_{\rho\rho}\nabla\rho| = |Ps''_{\rho\rho}P^T\nabla\rho| \geq \underline{\mu}|\nabla\rho| \quad (47)$$

and as a consequence we get

$$\|\rho\|_{L^r(I;W^{1,r}(\Omega;\mathbb{R}^L))} \leq C.$$

The bound on ∇v is standard consequence of the assumption (19) obtained by testing the equation (57) by v .

We test the equation (34) by

$$\varphi(e) := \frac{1}{1 + \left(1 + \frac{1}{s'_e(e)}\right)^{-\beta}}. \quad (48)$$

We note that

$$\varphi'(e) = \frac{-\beta}{\left(1 + \left(1 + \frac{1}{s'_e(e)}\right)^{-\beta}\right)^2} \left(1 + \frac{1}{s'_e(e)}\right)^{-\beta-1} (\chi_k^n)^{-2} s''_{ee}(e) > 0.$$

Using the assumption (25) and (21) we obtain

$$\begin{aligned} & \frac{\partial}{\partial t} \int_{\Omega} \hat{\varphi}(e) dx + \beta \theta \int_{\Omega} \left(1 + \frac{1}{\chi}\right)^{-1-\beta} \left|\nabla \frac{1}{\chi}\right|^2 dx \\ & \leq \int_{\Omega} M(\rho, \chi) (\nabla\zeta + \mathbf{m} \otimes \nabla\chi - \chi z \otimes \nabla\phi) : (\mathbf{m} \otimes \nabla\varphi(e) - \varphi(e)z \otimes \nabla\phi) dx \\ & \quad + \int_{\partial\Omega} \kappa_{\Sigma} (\chi - \chi_{\Sigma}) \varphi(e) dS. \end{aligned} \quad (49)$$

The function $\hat{\varphi}$ is the primitive function to the function φ from (48). We estimate the right hand side:

$$\int_{I\partial\Omega} \kappa_{\Sigma} (\chi - \chi_{\Sigma}) \varphi(e) dx dt \leq \kappa_{\Sigma} \|\chi - \chi_{\Sigma}\|_{L^r(I;W^{1,r}(\Omega;))} \quad (50)$$

and

$$\begin{aligned} & \int_{I \times \Omega} M(\rho, \chi) (\nabla\zeta + \mathbf{m} \otimes \nabla\chi - \chi z \otimes \nabla\phi) : (\mathbf{m} \otimes \nabla\varphi(e) - z \otimes \nabla\phi\varphi(e)) dx dt \\ & \leq \|\nabla\zeta + \mathbf{m} \otimes \nabla\chi - \chi z \otimes \nabla\phi\|_{L^2(I \times \Omega; \mathbb{R}^{L \times 3})} \\ & \quad \cdot \left(\left(\int_{I \times \Omega} \left(1 + \frac{1}{\chi}\right)^{-\beta-1} \left|\nabla \frac{1}{\chi}\right|^2 dx dt \right)^{1/2} + \|\phi\|_{L^\infty(I;W^{2,2}(\Omega))} \right). \end{aligned} \quad (51)$$

Using the discrete Gronwall lemma on (49) together with (50) and (51) we get the estimate

$$\int_{I \times \Omega} \left(1 + \frac{1}{\chi}\right)^{-1-\beta} \left|\nabla \frac{1}{\chi}\right|^2 dx dt \leq C. \quad (52)$$

We use the estimate (52) to estimate the temperature gradient

$$\begin{aligned}
\left\| \nabla \frac{1}{\chi} \right\|_{L^r(I \times \Omega; \mathbb{R}^3)}^\gamma &\leq \left(\int_{I \times \Omega} \left(1 + \frac{1}{\chi} \right)^{-1-\beta} \nabla \frac{1}{\chi} dx dt \right)^{\gamma/2} \\
&\quad \cdot \left(\int_{I \times \Omega} \left(1 + \frac{1}{\chi} \right)^{(1+\beta)\gamma/(2-\gamma)} dx dt \right)^{(2-\gamma)/2} \\
&\leq C \left(\left\| 1 + \frac{1}{\chi} \right\|_{L^{(1+\beta)\gamma/(2-\gamma)}(I \times \Omega)} \right)^{(2-\gamma)/2}. \tag{53}
\end{aligned}$$

Now we interpolate

$$\left\| 1 + \frac{1}{\chi} \right\|_{L^{(1+\beta)\gamma/(2-\gamma)}(I \times \Omega)} \leq C \left\| \nabla \frac{1}{\chi} \right\|_{L^\gamma(I \times \Omega; \mathbb{R}^3)}^\lambda \left\| 1 + \frac{1}{\chi} \right\|_{L^1(I \times \Omega)}^{1-\lambda} \tag{54}$$

with $\lambda = (2 - \gamma)/(1 + \beta)$. This interpolation holds under the condition

$$\frac{2 - \gamma}{(1 + \beta)\gamma} \geq \frac{2 - \gamma}{1 + \beta} \left(\frac{1}{\gamma} - \frac{1}{3} \right) + 1 - \frac{2 - \gamma}{1 + \beta},$$

which simplifies to

$$\gamma < \frac{5 - 3\beta}{4}.$$

Now we combine (53) and (54) to obtain

$$\left\| \nabla \frac{1}{\chi} \right\|_{L^\gamma(I \times \Omega; \mathbb{R}^3)} \leq C \left\| \nabla \frac{1}{\chi} \right\|_{L^\gamma(I \times \Omega; \mathbb{R}^3)}^{(2-\gamma)/2} \tag{55}$$

and use (55) and Young inequality to obtain the estimate

$$\left\| \nabla \frac{1}{\chi} \right\|_{L^{5/4-\delta}(I \times \Omega; \mathbb{R}^3)} \leq C.$$

Using the chain rule lemma and the assumption (25) gives us

$$\left| \nabla \frac{1}{\chi} \right| = \frac{1}{\chi^2} |\nabla \chi| = \frac{s''_e}{(s'_e)^2} |\nabla e| \geq C |\nabla e|. \tag{56}$$

Testing (33) by v and using (18–19) gives us

$$\frac{\partial}{\partial t} \|v\|_{L^2(\Omega; \mathbb{R}^3)}^2 + \|v\|_{W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3)}^p \leq \|q\|_{L^\infty(\Omega; \mathbb{R}^L)} \|\nabla \phi\|_{L^2(\Omega; \mathbb{R}^3)} \|v\|_{L^p(\Omega; \mathbb{R}^3)}.$$

Using the Gronwall inequality gives us $\|v\|_{L^p(I; W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3))} \leq C$.

6 Examples for entropy and the diffusion matrix

Example 6.1 (the entropy). The entropy given by the formula

$$s(\rho, e) = \ln e - \sum_{i=1}^L \rho_i \ln \rho_i$$

satisfies assumptions (26), (23), (24), (25) and (28)

Proof. First we compute the chemical potentials and coldness

$$\begin{aligned} \zeta_i &:= \frac{\partial s}{\partial \rho_i} = -\ln \rho_i + 1, \\ \chi &:= \frac{\partial s}{\partial e} = \frac{1}{e}. \end{aligned}$$

Thus we see that

$$\begin{aligned} \rho_i &= \exp(-\zeta_i + 1), \\ e &= \frac{1}{\chi} \end{aligned}$$

and that the assumption (26) is satisfied. For the assumption (27) we may pick $\tilde{\zeta} \in G'$ and compute

$$\varrho = \sum_{i=1}^L \rho_i(\tilde{\mu} + \hat{\mu}\ell) = \exp(-\hat{\mu} + 1) \sum_{i=1}^L \exp(\tilde{\mu}_i).$$

Thus we choose

$$\hat{\mu}(\tilde{\mu}) = -1 + \ln \left(\sum_{i=1}^L \exp(\tilde{\mu}_i) / \varrho \right).$$

The assumption (23) is satisfied because

$$\lim_{\rho \rightarrow 0} \rho \ln \rho = 0 \text{ and } \lim_{\rho \rightarrow \infty} \rho \ln \rho = \infty.$$

The assumption (24) is a consequence of positive definiteness of the matrix

$$-\frac{\partial^2 s}{\partial \rho_i \partial \rho_j} = \frac{1}{\rho_i} \delta_{ij}$$

which is uniform for ρ uniformly bounded. As $\sum_{i=1}^L \rho_i = \varrho$ we know that there exists i such that $\rho_i \geq \varrho/L$ and thus $\ln \rho_i \leq C$. The assumption (28) is satisfied because

$$\left| \sum_{i=1}^L \frac{\partial s}{\partial \rho_i} \right| \leq C(\varrho, L) \left(\left| \ln \rho_i - \sum_{i=1}^L \frac{\partial s}{\partial \rho_i} \right| + 1 \right) \leq C(\varrho, L)(|Ps'_\rho| + 1).$$

□

Example 6.2 (Diffusion matrix). The matrix M satisfying (17) and (15) will be generated by the procedure from [32] which is, in fact, identical to the procedure developed in a less general setting in [10]. We choose the matrix in the form $M = M_2^T M_1 M_2$ where

$$(M_1)_{ij} = D_i \max(\rho_i, \delta) \delta_{ij}$$

and

$$(M_2)_{ij} = \delta_{ij} - \frac{D_j \max(\rho_j, \delta)}{\sum_{k=1}^L D_k \max(\rho_k, \delta)}.$$

It is easy to check that M_1 is positive definite and $\ker M_2 = \text{span}\{(1, \dots, 1)\}$. The resulting matrix is

$$M_{ij} = D_i \max(\rho_i, \delta) \left(\delta_{ij} - \frac{D_j \max(\rho_j, \delta)}{\sum_{k=1}^L D_k \max(\rho_k, \delta)} \right).$$

Example 6.3 (Diffusion matrix – other choice). In some cases we might want linear diffusion with no cross effects in $L - 1$ components. For such cases we might want to use the matrix

$$M_{ij}(\rho) := \begin{cases} D_j \max(\rho_j, \delta) \delta_{ij} & \text{for } i < L \text{ \& } j < L, \\ -D_j \max(\rho_j, \delta) & \text{for } i = L \text{ \& } j < L, \\ -D_i \max(\rho_i, \delta) & \text{for } i < L \text{ \& } j = L, \\ \sum_{k=1}^{L-1} D_k \max(\rho_k, \delta) & \text{for } i = L \text{ \& } j = L, \end{cases}$$

which is useful mainly for dilute solutions. It is routine to check that M is positive definite on the space $\{x \in \mathbb{R}^L : x_L = 0\}$. The assumption (15) is then satisfied because the size of the vector with zero sum is determined by size of its first $L - 1$ components.

7 Proof of the main theorem

We regularize the internal energy equation by the term $\Delta^m \ln \chi$ with m from (11). We choose m big enough to have $W^{m,2}(\Omega)$ compactly embedded into $C^2(\bar{\Omega})$, namely $m \geq 4$. Here we need the assumption (11). Moreover we discretize all equations in time by Rothe method and mass and momentum balance and the Poisson equation in space by the Galerkin method.

For this purpose, we introduce the sequence of spaces V_{div}^n as the linear span of the first n eigenvalues of the Stokes operator, V^n as the space of the first n eigenvalues of the Laplace operator. For the Galerkin approximation we choose variable ζ and, by assumption (26), we consider variables ρ and e as functions of ζ and χ . To have the temperature variable ranging the whole \mathbb{R} we use as the variable $\ln \chi$. We put $\tau^n := \frac{T}{n}$ and $\varepsilon^n := \sqrt{\tau^n}$.

Remark 7.1. The time discretization is necessary because the only information we have about chemical potentials is $L^2(\Omega; \mathbb{R}^L)$. If we wanted to get the existence of discretized solution by the theory of ordinary differential equations,

we would have to add additional regularization terms under the time derivative. Such terms would destroy the convergence argument based on the Aubine–Lions lemma. The monotone operators approach fails because of lack of coercivity.

Definition 7.2. As a weak solution to the discretized problem (1–6) we will call sequences $(v_k^n, \rho_k^n, \zeta_k^n, e_k^n, \chi_k^n, \phi_k^n)$ with $k = 1, \dots, n$.

$$\begin{aligned} v_k^n &\in V_{\text{div}}^n, \\ \tilde{\zeta}_k^n &\in (V^n)^L, \quad \sum_{i=1}^L (\tilde{\zeta}_k^n)_i = 0 \\ \zeta_k^n &= \tilde{\zeta}_k^n + \hat{\mu}(\tilde{\zeta}_k^n)\ell \\ \rho_k^n &= (s'_\rho)^{-1}(\zeta_k^n), \\ \ln \chi_k^n &\in W^{m,2}(\Omega), \\ e_k^n &= (s'_e)^{-1}(\chi_k^n), \\ \phi_k^n &\in V^n \end{aligned}$$

satisfying

$$\begin{aligned} \int_{\Omega} \varrho \frac{v_k^n - v_{k-1}^n}{\tau} \varphi - (\varrho v_k^n \otimes v_k^n - 2\eta(\rho_k^n, \chi_k^n, Dv_k^n) Dv_k^n) : \nabla \varphi dx \\ = \int_{\Omega} -q_k^n \nabla \phi_k^n \varphi dx \end{aligned} \quad (57)$$

with $q_k^n := z \cdot \rho_k^n$ and with every $\varphi \in V_{\text{div}}^n$,

$$\begin{aligned} \int_{\Omega} \frac{\rho_k^n - \rho_{k-1}^n}{\tau} \varphi - \rho_k^n \otimes v_k^n : \nabla \varphi dx \\ - \int_{\Omega} M(\rho_k^n, \chi_k^n) (\nabla \zeta_k^n + \mathbf{m} \otimes \nabla \chi_k^n - \chi_k^n z \otimes \nabla \phi_k^n) \cdot \nabla \varphi dx \\ - \int_{\Omega} r(\zeta_k^n) \cdot \varphi dx - \int_{\partial\Omega} \mathfrak{D}(\zeta_k^n - \zeta_{\Sigma} - z(\phi_k^n - \phi_{\Sigma})) \cdot \varphi dS = 0 \end{aligned} \quad (58)$$

with every $\varphi = \tilde{\varphi} + \hat{\varphi}\ell$ such that $\tilde{\varphi} \in (V^n)^L$ and $\hat{\varphi} \in L^2(\Omega; \mathbb{R}^L)$,

$$\begin{aligned} \int_{\Omega} \left(\frac{e_k^n - e_{k-1}^n}{\tau} - \eta(\rho_k^n, \chi_k^n, Dv_k^n) |Dv_k^n|^2 \right) \varphi dx \\ + \int_{\Omega} \left(-e_n^k v_n^k + \kappa(\rho_k^n, \chi_k^n) \nabla \frac{1}{\chi_k^n} \right) \cdot \nabla \varphi dx \\ - \int_{\Omega} M(\rho_k^n, \chi_k^n) (\nabla \zeta_k^n + \mathbf{m} \otimes \nabla \chi_k^n - \chi_k^n z \otimes \nabla \phi_k^n) : (\mathbf{m} \otimes \nabla \varphi - z \otimes \nabla \phi_k^n \varphi) dx \\ - \int_{\Omega} \varepsilon \nabla^m \ln \chi_k^n : \nabla^m \varphi dx - \int_{\partial\Omega} \kappa_{\Sigma}(\chi_k^n - \chi_{\Sigma}) \varphi dS = 0 \end{aligned} \quad (59)$$

with every $\varphi \in W^{m,2}(\Omega)$,

$$\int_{\Omega} \varepsilon \nabla \phi_k^n \cdot \nabla \varphi dx + \int_{\partial\Omega} \alpha(\phi_k^n - \phi_{\Sigma}) \varphi dS = \int_{\Omega} q_k^n \varphi dx \quad (60)$$

with every $\varphi \in V^n$.

We will use the following fix-point theorem (see for example [7])

Lemma 7.3. *Let T be a continuous compact mapping, X a Banach space. Let the set $\{u \in X : \exists \lambda \in [0, 1] \text{ such that } \lambda Tu = u\}$ be bounded. Then T possess at least one fixed point in X .*

Lemma 7.4. *There exists at least one discretized solution.*

Proof. Let us note that by assumptions (17), (12), (27) and (30) the equation (58) is satisfied with every $\varphi = \hat{\varphi}\ell$ with $\hat{\varphi} \in L^2(\Omega)$. We define the mapping \mathfrak{F} as

$$\mathfrak{F} \begin{pmatrix} v \\ \tilde{\zeta} \\ \ln \chi \end{pmatrix} := \begin{pmatrix} -v + \frac{1}{\tau^n}(v - v_{k-1}^n) + \operatorname{div}(v \otimes v + \eta(\rho, \chi)Dv) - q\nabla\phi \\ P(-\tilde{\zeta} + \frac{1}{\tau^n}(\rho - \rho_{k-1}^n) + \operatorname{div}\rho v \\ + \operatorname{div}(M(\chi, \rho)(\nabla\zeta + \mathbf{m} \otimes \nabla\chi + \chi z \otimes \nabla\phi) - r(\zeta)) \\ \frac{1}{\tau^n}(e - e_{k-1}^n) + \operatorname{div}(ev + \kappa(\chi)\nabla\chi^{-1}) \\ + \operatorname{div}(M(\chi, \rho)(\nabla\zeta + \mathbf{m} \otimes \nabla\chi - \chi z \otimes \nabla\phi)\mathbf{m} \\ - \eta(\chi, \rho)|Dv|^2 \\ - M(\chi, \rho(\zeta))(\nabla\zeta + \mathbf{m} \otimes \nabla\chi - \chi z \otimes \nabla\phi) : z \otimes \nabla\phi \end{pmatrix}.$$

Next we define \mathfrak{L} by

$$\mathfrak{L} \begin{pmatrix} v \\ \tilde{\zeta} \\ \ln \chi \end{pmatrix} := \begin{pmatrix} -v \\ -\tilde{\zeta} \\ \Delta^k \ln \chi \end{pmatrix}$$

and put $T = \mathfrak{L}^{-1}\mathfrak{F}$. It is easy to check that $x = (v, \tilde{\zeta}, \ln \chi)$ satisfies (57 – 60) if and only if $x = Tx$. The operator T is a compact mapping

$$T : V_{\operatorname{div}}^n \times (V^n)^{L-1} \times W^{m,2}(\Omega) \rightarrow V_{\operatorname{div}}^n \times (V^n)^{L-1} \times W^{m,2}(\Omega).$$

The set of fix-points of the mapping λT is bounded by the same procedure as in the section 5. Using lemma 7.3 concludes the proof. \square

We define piecewise affine interpolants

$$\begin{aligned} \tilde{v}^n(t) &:= \frac{1}{\tau^n}(t - k\tau^n)v_{k+1}^n + \frac{1}{\tau^n}((k+1)\tau^n - t)v_k^n \\ &\quad \text{for } k\tau^n \leq t \leq (k+1)\tau^n, \\ \tilde{\rho}^n(t) &:= \frac{1}{\tau^n}(t - k\tau^n)\rho_{k+1}^n + \frac{1}{\tau^n}((k+1)\tau^n - t)\rho_k^n \\ &\quad \text{for } k\tau^n \leq t \leq (k+1)\tau^n, \\ \tilde{e}^n(t) &:= \frac{1}{\tau^n}(t - k\tau^n)e_{k+1}^n + \frac{1}{\tau^n}((k+1)\tau^n - t)e_k^k \\ &\quad \text{for } k\tau^n \leq t \leq (k+1)\tau^n, \end{aligned}$$

and the piecewise constant interpolants

$$\begin{aligned}
v^n(t) &:= v_{k+1}^n && \text{for } k\tau^n < t \leq (k+1)\tau^n, \\
\rho^n(t) &:= \rho_{k+1}^n && \text{for } k\tau^n < t \leq (k+1)\tau^n, \\
e^n(t) &:= e_{k+1}^k && \text{for } k\tau^n < t \leq (k+1)\tau^n, \\
\zeta^n(t) &:= \zeta_{k+1}^n && \text{for } k\tau^n < t \leq (k+1)\tau^n, \\
\chi^n(t) &:= \chi_{k+1}^n && \text{for } k\tau^n < t \leq (k+1)\tau^n.
\end{aligned}$$

Testing (57) by $\int_{k\tau}^{(k+1)\tau} \varphi(x, t) dt$, summing and making the integration by parts we get

$$\begin{aligned}
\int_{I \times \Omega} -\tilde{v}^n \frac{\partial \varphi}{\partial t} + (-v^n \otimes v^n + \eta(\rho^n, \chi^n, Dv^n) Dv^n) : \nabla \varphi dx dt \\
= \int_{I \times \Omega} -q^n \nabla \phi^n \varphi dx dt + \int_{\Omega} v_0 \varphi(0) dx.
\end{aligned}$$

Making the same process with the equation (58) gives us

$$\begin{aligned}
&\int_{I \times \Omega} -\tilde{\rho}^n \frac{\partial \varphi}{\partial t} - \rho^n \otimes v^n : \nabla \varphi dx dt \\
&- \int_{I \times \Omega} M(\rho^n, \chi^n) (\nabla \zeta^n + \mathbf{m} \otimes \nabla \chi^n - \chi^n z \otimes \nabla \phi^n) \nabla \varphi dx dt \\
&- \int_{I \times \partial \Omega} \mathfrak{D}(\zeta^n - \zeta_{\Sigma} - z(\phi^n - \phi_{\Sigma})) \cdot \varphi dS dt \\
&= \int_{I \times \Omega} r(\zeta^n) \varphi dx dt + \int_{\Omega} \zeta_0 \varphi(0) dx.
\end{aligned}$$

Testing the equation (59) by $\varphi \in C^\infty(I \times \bar{\Omega})$, such that $\nabla^m \varphi, \dots, \nabla^{2m} \varphi$ vanishes on $\partial \Omega$, gives us

$$\begin{aligned}
&\int_{I \times \Omega} -\tilde{e}^n \frac{\partial \varphi}{\partial t} + \left(-e^n v^n + \kappa(\rho^n, \chi^n) \nabla \frac{1}{\chi^n} \right) \cdot \nabla \varphi + (-1)^{m+1} \ln \chi^k \Delta^m \varphi dx dt \\
&- \int_{I \times \Omega} M(\rho^n, \chi^n) (\nabla \zeta^n + \mathbf{m} \otimes \nabla \chi^n - \chi^n z \otimes \nabla \phi^n) : (\mathbf{m} \otimes \nabla \varphi - z \otimes \nabla \phi^n \varphi) dx dt \\
&- \int_{I \times \partial \Omega} \kappa_{\Sigma} (\chi^n - \chi_{\Sigma}) \varphi dS dt = \int_{I \times \Omega} \eta(\rho^n, \chi^n, Dv^n) |Dv^n|^2 dx dt + \int_{\Omega} e_0 \varphi(0) dx.
\end{aligned}$$

Next we use density argument for all $\varphi \in C^1(I; W^{m,2}(\Omega))$. The equation (60) gives us

$$\int_{I \times \Omega} \epsilon(\rho^n, \chi^n) \nabla \phi^n \cdot \varphi dx dt + \int_{I \times \partial \Omega} \alpha(\phi - \phi_{\Sigma}) \varphi dS dt = \int_{I \times \Omega} q^n \varphi dx dt.$$

Lemma 7.5. *The following apriori estimates hold*

$$\begin{aligned}
& \|\tilde{e}^n\|_{L^\infty(I;L^1(\Omega))\cap L^{5/4-\delta}(I;W^{1,5/4-\delta}(\Omega))} \leq C\delta, \\
& \left\| \frac{1}{\chi^n} \right\|_{L^{5/4-\delta}(I;W^{1,5/4-\delta}(\Omega))} + \|\chi^n\|_{L^r(I;W^{1,r}(\Omega))} \leq C_r, \\
& \|\tilde{\rho}^n\|_{L^\infty(I\times\Omega;\mathbb{R}^L)\cap L^r(I;W^{1,r}(\Omega;\mathbb{R}^L))} + \|P\zeta^n\|_{L^r(I;W^{1,r}(\Omega;\mathbb{R}^L))} \leq C_r, \\
& \|\tilde{v}^n\|_{L^\infty(I;L^2(\Omega;\mathbb{R}^3))\cap L^p(I;W_{0,\text{div}}^{1,p}(\Omega;\mathbb{R}^3))} \leq C, \\
& \left\| \frac{\partial \tilde{e}^n}{\partial t} \right\|_{L^2(I;(C^\infty(\bar{\Omega}))^*)} \leq C, \\
& \sqrt{\tau^n} \left\| \frac{\partial \tilde{\rho}^n}{\partial t} \right\|_{L^2(I\times\Omega;\mathbb{R}^L)} + \left\| \frac{\partial \tilde{\rho}^n}{\partial t} \right\|_{L^2(I;(W^{1,2}(\Omega;\mathbb{R}^L))^*)} \leq C, \\
& \sqrt{\tau^n} \left\| \frac{\partial \tilde{v}^n}{\partial t} \right\|_{L^2(I\times\Omega;\mathbb{R}^3)} + \left\| \frac{\partial \tilde{v}^n}{\partial t} \right\|_{L^p(I;(W_{0,\text{div}}^{1,p}(\Omega;\mathbb{R}^3))^*)} \leq C.
\end{aligned}$$

The estimates for e^n , ρ^n and v^n are analogous. The exponent $r < 10 - \sqrt{80}$ is the same as in the growth assumption (21).

Proof. The proof follows from estimates in section 5. \square

of the theorem 4.2. By apriori estimates from the Lemma 7.5 we may select the following convergent subsequences:

$$v^n \rightharpoonup^* v \text{ in } L^\infty(I;L^2(\Omega;\mathbb{R}^3)) \cap L^p(I;W^{1,p}(\Omega;\mathbb{R}^3)), \quad (61)$$

$$\tilde{v}^n \rightharpoonup^* \tilde{v} \text{ in } L^\infty(I;L^2(\Omega;\mathbb{R}^d)) \cap L^p(I;W_{0,\text{div}}^{1,p}(\Omega;\mathbb{R}^3)), \quad (62)$$

$$\rho^n \rightharpoonup^* \rho \text{ in } L^\infty(I\times\Omega;\mathbb{R}^L) \cap L^r(I;W^{1,r}(\Omega;\mathbb{R}^L)), \quad (63)$$

$$\tilde{\rho}^n \rightharpoonup^* \tilde{\rho} \text{ in } L^\infty(I\times\Omega;\mathbb{R}^L) \cap L^r(I;W^{1,r}(\Omega;\mathbb{R}^L)), \quad (64)$$

$$e^n \rightharpoonup e \text{ in } L^{5/4-\delta}(I;W^{1,5/4-\delta}(\Omega)), \quad (65)$$

$$\phi^n \rightharpoonup \phi \text{ in } L^\infty(I;W^{1,2}(\Omega)). \quad (66)$$

We have identification of limits of interpolants:

$$v^n - \tilde{v}^n \rightarrow 0 \text{ in } L^2(I\times\Omega;\mathbb{R}^3), \quad (67)$$

$$\rho^n - \tilde{\rho}^n \rightarrow 0 \text{ in } L^2(I\times\Omega;\mathbb{R}^L), \quad (68)$$

$$e^n - \tilde{e}^n \rightarrow 0 \text{ in } L^2(I;(C^\infty(\Omega))^*). \quad (69)$$

By the Aubine–Lions lemma with time derivative a measure and (61),(62), (63), (64) and (65) we have

$$v^n \rightarrow v \text{ in } L^2(I\times\Omega;\mathbb{R}^3), \quad (70)$$

$$\rho^n \rightarrow \rho \text{ in } L^2(I\times\Omega;\mathbb{R}^L), \quad (71)$$

$$e^n \rightarrow e \text{ in } L^{5/4-\delta}(I\times\Omega), \quad (72)$$

$$\tilde{e}^n \rightarrow e \text{ in } L^{5/4-\delta}(I\times\Omega). \quad (73)$$

We chose $w^n \in C^1(I; V_{\text{div}}^n)$ such that

$$\begin{aligned} w^n &\rightarrow v \text{ in } L^\infty(I; L^2(\Omega; \mathbb{R}^3)) \cap L^p(I; W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3)), \\ w^n(0) &\rightarrow v(0) \text{ in } L^2(\Omega; \mathbb{R}^3), \\ \frac{\partial w^n}{\partial t} &\rightarrow \frac{\partial v}{\partial t} \text{ in } L^p(I; (W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3))^*). \end{aligned}$$

Next we test the equation (33) by $v^n - w^n$. By the monotonicity of the p -Laplacean and the identity

$$\int_{\Omega} \frac{\partial \tilde{v}^n}{\partial t}(t)(v^n(t) - \tilde{v}^n(t))dx = (T-t) \left\| \frac{\partial \tilde{v}^n}{\partial t}(t) \right\|_{L^2(I \times \Omega; \mathbb{R}^3)}^2 \geq 0$$

we have

$$\begin{aligned} &\frac{\rho}{2} \|\tilde{v}^n(t) - w^n(t)\|_{L^2(\Omega; \mathbb{R}^3)}^2 + \int_0^t (\|\nabla v^n\|_{L^p(\Omega; \mathbb{R}^3 \times 3)}^{p-1} - \|\nabla w^n\|_{L^p(\Omega; \mathbb{R}^3 \times 3)}^{p-1}) \\ &\quad \cdot (\|\nabla v^n\|_{L^p(\Omega; \mathbb{R}^3 \times 3)} - \|\nabla w^n\|_{L^p(\Omega; \mathbb{R}^3 \times 3)}) d\tau \\ &\leq \int_0^t \int_{\Omega} (v^n \otimes v^n - \eta(\rho^n, \chi^n, Dw^n)Dw^n) : \nabla(v^n - w^n) dx dt \\ &+ \int_0^t \int_{\Omega} (q^n \nabla \phi^n + \frac{\partial w^n}{\partial t}) \cdot (v^n - w^n) dx dt + \frac{\rho}{2} \|v^n(0) - w^n(0)\|_{L^2(\Omega; \mathbb{R}^3)}^2 \end{aligned}$$

and thus by assumption (18) and convergences (66), (71), (61) and (70) we obtain the strong convergence

$$v^n \rightarrow v \text{ in } L^p(I; W_{0,\text{div}}^{1,p}(\Omega; \mathbb{R}^3)). \quad (74)$$

Finally testing the equation (35) by $\phi^n - \phi$, using the monotonicity of the Laplace operator and (66) we have

$$\phi^n \rightarrow \phi \text{ in } L^2(I; W^{1,2}(\Omega)). \quad (75)$$

Because we have (72), we have also

$$P\zeta^n \rightharpoonup P\zeta \text{ in } L^r(I; W^{1,r}(\Omega; \mathbb{R}^L)), \quad (76)$$

$$\zeta^n \rightarrow \zeta \text{ in } L^r(I; L^{3r/(3-r)}(\Omega; \mathbb{R}^L)), \quad (77)$$

$$\chi^n \rightharpoonup \chi \text{ in } L^r(I; W^{1,r}(\Omega)), \quad (78)$$

$$\chi^n \rightarrow \chi \text{ in } L^{r-\delta}(I \times \Omega), \quad (79)$$

$$\frac{1}{\chi^n} \rightarrow \frac{1}{\chi} \text{ in } L^{5/4-\delta}(I \times \Omega), \quad (80)$$

$$\frac{1}{\chi^n} \rightharpoonup \frac{1}{\chi} \text{ in } L^{5/4-\delta}(I; W^{1,5/4-\delta}(\Omega)). \quad (81)$$

We need

$$\kappa(\rho^n, \chi^n) \rightarrow \kappa(\rho, \chi) \text{ in } L^s(I \times \Omega) \quad (82)$$

with $s > 5$. By (21) it is equivalent to $\frac{r^2}{4(r-1)} > 5$. After some algebra we arrive on the condition $r < \frac{20-\sqrt{320}}{2} = 10 - 4\sqrt{5}$ or $r > 10 + 4\sqrt{5}$. \square

8 Thermodynamics of the model

Next we express the model in terms of the GENERIC framework [13, 32, 12]. We do this step to motivate thermodynamically estimates done in (36) and (37).

$$\frac{\partial A(x)}{\partial t} = \{A, E\} + [A, S].$$

Here x is the triple $(\rho, \varrho v, e)$, $A = A(\rho, \varrho v, e)$ is an arbitrary functional, E is the energy of the system and S is the entropy of the system.

For simplicity we change boundary conditions to zero flux through boundary.

The starting point is the system derived in [32]. The energy is given by the formula

$$E(\rho, v, e) := \int_{\Omega} \frac{1}{2\varrho} |\varrho v|^2 + e + \frac{\epsilon}{2} |\nabla \phi[\rho]|^2 dx$$

with $\phi[\rho]$ given by (5) with q from (6). The energy variation is given by formula

$$\frac{\delta E}{\delta x} = \begin{pmatrix} z\phi \\ v \\ 1 \end{pmatrix}. \quad (83)$$

Contrary to the result [32] we have $\frac{\delta E}{\delta \rho_i} \neq 0$. The entropy is given by the formula

$$S(\rho, v, e) := \int_{\Omega} s(\rho, e) dx.$$

The entropy variation is given by the formula

$$\frac{\delta S}{\delta x} = \begin{pmatrix} -\frac{1}{\theta} \mu \\ 0 \\ \frac{1}{\theta} \end{pmatrix}. \quad (84)$$

The Poisson bracket are responsible for convective terms, the Lorentz force and the pressure. We use the simplified form of the bracket derived in [32]. The simplification consists in removing the part describing the evolution of the constant bulk density.

$$\begin{aligned} \{A, B\} := & - \int_{\Omega} \sum_{i=1}^L \rho_i \left(\frac{\delta A}{\delta(\varrho v)} \cdot \nabla \frac{\delta B}{\delta \rho_i} - \frac{\delta B}{\delta(\varrho v)} \cdot \nabla \frac{\delta A}{\delta \rho_i} \right) dx \\ & - \int_{\Omega} \varrho v \cdot \left(\frac{\delta A}{\delta(\varrho v)} \nabla \frac{\delta B}{\delta(\varrho v)} - \frac{\delta B}{\delta(\varrho v)} \nabla \frac{\delta A}{\delta(\varrho v)} \right) dx \\ & - \int_{\Omega} e \left(\frac{\delta A}{\delta(\varrho v)} \cdot \nabla \frac{\delta B}{\delta e} - \frac{\delta B}{\delta(\varrho v)} \cdot \nabla \frac{\delta A}{\delta e} \right) dx \\ & - \int_{\Omega} \frac{\delta A}{\delta(\varrho v)} \cdot \nabla \left(\pi_{\text{re}} \frac{\delta B}{\delta e} \right) - \frac{\delta B}{\delta(\varrho v)} \cdot \nabla \left(\pi_{\text{re}} \frac{\delta A}{\delta e} \right) dx. \end{aligned}$$

The pressure π from the Navier–Stokes is decomposed into the sum $\pi = \pi_{\text{re}} + \pi_{\text{ir}}$. The decomposition of the pressure is due to decomposition between reversible and irreversible dynamics. The reversible pressure satisfies

$$\Delta \pi_{\text{re}} = -\text{divdiv}(\varrho v \otimes v) - \text{div} q \nabla \phi.$$

We present a slightly modified dissipative bracket in comparison to [32] to satisfy $[E, S] = 0$. We also choose a different way of introducing the Lagrange multiplier for the constraint $\text{div} v = 0$ to get the usual incompressible equations.

$$\begin{aligned}
[A, B] &:= \int_{\Omega} \eta^{\theta}(\rho, \theta, Dv) \theta \\
&\cdot \left(D \frac{\delta A}{\delta(\rho v)} - Dv \frac{\delta A}{\delta e} - \frac{\pi_{\text{ir}}}{\eta^{\theta}(\rho, \theta, Dv) |Dv|^2} Dv (\text{div} \frac{\delta A}{\delta M}) \right) \\
&\cdot \left(D \frac{\delta B}{\delta(\rho v)} - Dv \frac{\delta B}{\delta e} - \frac{\pi_{\text{ir}}}{\eta^{\theta}(\rho, \theta, Dv) |Dv|^2} Dv (\text{div} \frac{\delta B}{\delta M}) \right) dx \\
&\quad + \int_{\Omega} \kappa^{\theta}(\rho, \theta) \theta^2 (\nabla \frac{\delta A}{\delta e} \cdot \nabla \frac{\delta B}{\delta e}) dx \\
&+ \int_{\Omega} \sum_{i,j=1}^L M_{ij}^{\theta}(\rho, \theta) \left(\nabla \frac{\delta A}{\delta \rho_j} + \mathbf{m}_j \nabla \frac{\delta A}{\delta e} - z_j \nabla \phi \frac{\delta A}{\delta e} \right) \\
&\quad \cdot \left(\nabla \frac{\delta B}{\delta \rho_i} + \mathbf{m}_i \nabla \frac{\delta B}{\delta e} - z_i \nabla \phi \frac{\delta B}{\delta e} \right) dx \\
&+ \int_{\Omega} \sum_{k=1}^{N_r} \left(\sum_{i=1}^L a_{ki}^{\theta}(\rho, \theta) \frac{\delta A}{\delta \rho_i} \right) \left(\sum_{i=1}^L a_{ki}^{\theta}(\rho, \theta) \frac{\delta B}{\delta \rho_i} \right) dx \tag{85}
\end{aligned}$$

with π_{ir} satisfying

$$\Delta \pi_{\text{ir}} = \text{div} \text{div} 2\eta^{\theta}(\rho, \theta, Dv) Dv.$$

Confronting reaction terms in (85) and (3) gives us

$$r_i(\zeta) = \sum_{k=1}^{N_r} a_{ki}^{\theta} \sum_{j=1}^L a_{kj} \zeta_j. \tag{86}$$

To obtain the first law of thermodynamics we compute

$$\begin{aligned}
[A, E] &= \int_{\Omega} \eta^{\theta}(\rho, \theta, Dv) \theta \\
&\cdot \left(D \frac{\delta A}{\delta M} - Dv \frac{\delta A}{\delta e} - \frac{\pi_{\text{ir}}}{\eta^{\theta}(\rho, \theta, Dv) |Dv|^2} Dv (\text{div} \frac{\delta A}{\delta M}) \right) \\
&\cdot \left(Dv - Dv - \frac{\pi_{\text{ir}}}{\eta^{\theta}(\rho, \theta, Dv) |Dv|^2} Dv (\text{div} v) \right) dx \\
&\quad + \int_{\Omega} 2\kappa^{\theta}(\rho, \theta) \theta^2 (\nabla \frac{\delta A}{\delta e} \cdot \nabla 1) dx \\
&+ \int_{\Omega} \sum_{i,j} M_{ij}^{\theta}(\rho, \theta) \left(\nabla \frac{\delta A}{\delta \rho_j} + \mathbf{m}_j \nabla \frac{\delta A}{\delta e} - z_j \nabla \phi \frac{\delta A}{\delta e} \right) \\
&\quad \cdot (z_i \nabla \phi + \mathbf{m}_i \nabla 1 - z_i \nabla \phi) dx \\
&+ \int_{\Omega} \sum_{k=1}^{N_r} \left(\sum_i a_{ki}^{\theta}(\rho, \theta) \frac{\delta A}{\delta \rho_i} \right) \left(\sum_j a_{kj}^{\theta}(\rho, \theta) z_j \phi \right) dx.
\end{aligned}$$

Now we get the first law of thermodynamics, i.e. the energy conservation

$$\frac{\partial E}{\partial t} = \{E, E\} = 0. \tag{87}$$

For the second law we compute

$$\begin{aligned}
\{E, S\} &= - \int_{\Omega} \sum_{i=1}^L \rho_i v \cdot \nabla \frac{\partial s}{\partial \rho_i} dx - \int_{\Omega} e v \cdot \nabla \frac{\partial s}{\partial e} dx - \int_{\Omega} v \cdot \nabla (\pi_{\text{re}} \frac{\partial s}{\partial e}) dx \\
&= \int_{\Omega} v \cdot \nabla s dx
\end{aligned}$$

and thus

$$\frac{\partial S}{\partial t} = [S, S] \geq 0 \quad (88)$$

provided the matrix M is positive semi-definite and κ and η are non-negative. The precise meaning of both laws is stated in equations (36) and (37).

9 Conclusion

In this article we proved the existence of solution to the system of partial differential equations describing fluid mixtures. In the proof we used the thermodynamical consistency of the model, in particular the fact that it can be written in terms of the GENERIC framework. We gave the precise mathematical meaning to the first and the second law of thermodynamics. However, we needed stronger assumptions than assumptions needed for the thermodynamical consistency of the model. The unification of assumptions might be interesting research topic for both mathematical analysis and thermodynamics.

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