Closure conditions for non-equilibrium multi-component models

Siegfried Müller [1]
Maren Hantke [2]
Pascal Richter [3]

[1] Institut für Geometrie und Praktische Mathematik, RWTH Aachen University,
Templergraben 55, D-52056 Aachen, Germany
E-mail address: mueller@igpm.rwth-aachen.de
[2] Institut für Analysis und Numerik, Otto-von-Guericke-Universität Magdeburg, PSF 4120,
D-39016 Magdeburg, Germany
E-mail address: maren.hantke@ovgu.de
[3] Center for Computational Engineering Sciences, RWTH Aachen University, Schinkelstr. 2,
D-52062 Aachen, Germany
E-mail address: richter@mathcces.rwth-aachen.de.

Abstract. A class of non-equilibrium models for compressible multi-component fluids in multi-dimensions is investigated taking into account viscosity and heat conduction. These models are subject to the choice of interfacial pressures and interfacial velocity as well as relaxation terms for velocity, pressure, temperature and chemical potentials. Sufficient conditions are derived for these quantities that ensure meaningful physical properties such as a non-negative entropy production, thermodynamical stability, Galilean invariance as well as mathematical properties such as hyperbolicity, subcharacteristic property and existence of an entropy-entropy flux pair. For the relaxation of chemical potentials a two-component and a three-component model for vapor-water and gas-water-vapor, respectively, is considered.

1. Introduction

Flows of compressible multi-component fluids, where the single components may be in the liquid or the gas phase, respectively, have a wide range of applications. Difficulties in the modeling result from the interaction of the fluids, especially from the exchange of mass and energy across the phase interfaces. So the treatment of the phase interfaces is in the focus of the modeling.

In the literature several models are available that are distinguished in sharp interface and diffuse interface models. A detailed survey of these models can be found in Zein [26]. Here our interest is on multi-component fluids derived from an ensemble averaging procedure of Drew [5]. A comprehensive introduction to these models can be found in the classical book of Drew and Passman [6].

Baer and Nunziato [3] proposed a two-phase model for detonation waves in granular explosives. This model is a full non-equilibrium model, which means, each component has its own pressure, velocity and temperature and is governed by its own set of fluid equations. It was modified and generalized by several authors. For instance, Saurel and Abgrall [24] also included relaxation terms for the pressure and the velocities of the components. By instantaneous relaxation procedures equilibrium values for the pressure and the velocity can be found. Using further relaxation procedures to drive the temperatures and the Gibbs free energies (chemical potentials) into equilibrium mass transfer between the phases can be modeled, see Abgrall et al. [25, 22] or Zein et al. [27].

S. Müller, M. Hantke, & P. Richter

There are simplified models available in the literature that can be derived from the above general model by assuming zero relaxation times, see [15]. Typically these are classified by the number of equations in case of *two* phases in *one* space dimension. For instance, a *six-equation model* with a single velocity is derived by assuming a zero velocity relaxation time. Assuming zero relaxation time for both the velocity and the pressure a *five-equation model* with mechanical equilibrium, i.e., single velocity and single pressure, is deduced in the asymptotic limit. The *four-equation model* has a single velocity, single pressure and also single temperature coinciding with the single-fluid reactive Euler equations. While the *three-equation model* is the system of Euler equations. It has single velocity, pressure, temperature, and also single Gibbs free energy, i.e., it is in full equilibrium. A detailed discussion of these models is beyond the scope of this work. For this purpose the interested reader is referred to [26] and the references cited therein.

Typically reduced models suffer from some short-comings. For instance, conservation of energy might be violated or the system looses its hyperbolicity. Therefore we prefer a full non-equilibrium model taking into account viscosity and heat conduction. For this purpose we consider a general class of non-equilibrium models that is a generalization of the three-phase model investigated by Hèrard, see Remark 7 in [14]. For instance, the Saurel-Abgrall approach [24] fits into this class.

Characteristic for models based on ensemble averaging is the problem to close the set of equations, i.e., find appropriate interfacial pressures and interfacial velocity as well as relaxation terms for velocity, pressure, temperature and chemical potentials. Since the closing procedure is not unique, there is some freedom left for modeling. However, a reasonable model that is acceptable from a physical point of view has to be consistent with the fundamental principles of thermodynamics, e.g., the second law of thermodynamics. Besides this there are also constraints from a mathematical point of view that are related to existence and uniqueness of solutions to the model, e.g., the existence of entropy-entropy flux pairs. When it comes to the numerical solution additional properties are helpful for the design of appropriate schemes, e.g., the hyperbolicity of the transport operator or the sub-characteristic condition. The objective of this paper is to derive constraints for the closing terms such that the aforementioned physical, analytical and numerical properties hold for the non-equilibrium multi-component model. Similar investigations have been performed in case of two-phase models [2, 10, 26, 23] and three-phase models [14]. Here we do not confine ourselves to two and three phases but an arbitrary number of components. Drew and Passmann [6] consider multi-component fluids from a physical point of view but do not investigate analytical and numerical properties of the models.

The paper is organized as follows. In Section 2 we introduce the non-equilibrium multi-component model and derive the model for the mixture as well the model at equilibrium. Then we rewrite these models in terms of primitive quantities in Section 3. Neglecting viscosity and heat conduction some mathematical properties of the models are investigated. In particular, we verify hyperbolicity and the sub-characteristic condition, see Section 4. Furthermore, a physical meaningful model should be Galilean invariant. This is investigated in Section 5. In Section 6 we are concerned with the entropies corresponding to the non-equilibrium model and the mixture model. From the 2nd law of thermodynamics we derive constraints for the definition of the interfacial velocity and pressures. By means of the physical entropy we define in Section 7 a convex entropy function and a compatible entropy flux that form an entropy-entropy flux pair. In particular, the compatibility conditions coincide with constraints for the interfacial pressures and the interfacial velocity derived from thermodynamic principles. In Section 8 we introduce the relaxation terms for mechanical and thermal relaxation as well as relaxation of chemical potentials. In particular, we verify that they are in agreement with the 2nd law of thermodynamics.

2. Mathematical model

First of all, we describe the full non-equilibrium model and then derive from this the mixture model and the equilibrium model.

2.1. Non-equilibrium model

The multi-component flow is described by a non-equilibrium model where all components are present in each point of the space-time continuum. Each component $k = 1, \ldots, K$ has density ρ_k, velocity $\boldsymbol{v}_k$ and pressure p_k, The amount of each component is determined by its volume fraction α_k. The volume fractions are related by the saturation constraint

$$\sum_{k=1}^{K} \alpha_k = 1, \quad \alpha_k \in (0, 1). \tag{2.1}$$

In analogy to the three-phase model of Hèrard [14] the fluid equations for each component can be written as

$$\partial_t \left(\alpha_k \, \rho_k \right) + \nabla \cdot \left(\alpha_k \, \rho_k \, \boldsymbol{v}_k \right) = S_{\alpha\rho,k}, \tag{2.2}$$

$$\partial_t \left(\alpha_k \, \rho_k \, \boldsymbol{v}_k \right) + \nabla \cdot \left(\alpha_k \, \rho_k \, \boldsymbol{v}_k \, \boldsymbol{v}_k^T + \alpha_k \, p_k \, \boldsymbol{I} \right) = \tag{2.3}$$

$$- \sum_{l=1}^{K} P_{k,l} \, \nabla \, \alpha_l + \nabla \cdot \left(\alpha_k \, \boldsymbol{T}_k \right) + \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k},$$

$$\partial_t \left(\alpha_k \, \rho_k \, E_k \right) + \nabla \cdot \left(\alpha_k \, \rho_k \, \boldsymbol{v}_k \left(E_k + p_k/\rho_k \right) \right) = \tag{2.4}$$

$$- \sum_{l=1}^{K} P_{k,l} \, \boldsymbol{V}_I \cdot \nabla \, \alpha_l + \nabla \cdot \left(\alpha_k \, \left(\boldsymbol{v}_k \cdot \boldsymbol{T}_k - \boldsymbol{q}_k \right) \right) + S_{\alpha\rho E,k},$$

taking into account viscosity and heat conduction via the stress tensor $\boldsymbol{T}_k$ and the heat flux $\boldsymbol{q}_k$, but neglecting effects due to surface tension and gravity. In our notation $E_k = e_k + \boldsymbol{v}_k^2/2$ is the total specific energy with e_k the specific internal energy of component k. There may be other contributions to be accounted for, see [6], p. 68 ff and 144 ff. In particular, the term $P_{k,l}$ accounts for different pressures at the phase interface. Without loss of generality we may assume

$$P_{k,k} = 0. \tag{2.5}$$

Otherwise we replace $P_{k,l}$ by $P_{k,l} - P_{k,k}$ due to the saturation condition (2.1). The interfacial velocity is denoted by $\boldsymbol{V}_I$. Obviously, the equations cannot be written in conservative form. Finally, the fluid equations are supplemented by an equation of state

$$p_k = p_k(\rho_k, e_k) \quad \text{resp.} \quad e_k = e_k(\rho_k, p_k) \tag{2.6}$$

for each of the components.

The evolution of the volume fractions is characterized by the non-conservative equation

$$\partial_t \, \alpha_k + \boldsymbol{V}_I \cdot \nabla \, \alpha_k = S_{\alpha,k}, \ k = 1, \ldots, K. \tag{2.7}$$

Due to the saturation condition (2.1) we only need $K - 1$ equations. Without loss of generality we express α_K by the other volume fractions, i.e.,

$$\alpha_K = 1 - \sum_{k=1}^{K-1} \alpha_k, \ \nabla \alpha_K = - \sum_{k=1}^{K-1} \nabla \alpha_k, \ S_{\alpha,K} = - \sum_{k=1}^{K-1} S_{\alpha,k}. \tag{2.8}$$

3

The source terms $S_{\alpha,k}$, $S_{\rho,k}$, $\boldsymbol{S}_{\rho\boldsymbol{v},k}$ and $S_{\rho E,k}$ on the right-hand sides of (2.2), (2.3), (2.4) and (2.7) describe the relaxation process due to mass, momentum, energy transfer and volume fraction between the different components corresponding to the relaxation of velocity, pressure, temperature and chemical potentials, $\xi \in \{v, p, T, \mu\}$, i.e.,

$$S_{\alpha,k} := \sum_\xi S_{\alpha,k}^\xi, \ \ S_{\alpha\rho,k} := \sum_\xi S_{\alpha\rho,k}^\xi, \ \ \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} := \sum_\xi \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}^\xi, \ \ S_{\alpha\rho E,k} := \sum_\xi S_{\alpha\rho E,k}^\xi. \tag{2.9}$$

These depend on the specific components at hand that will be discussed in Section 8.

So far, the model is not yet closed. For this purpose, we have to find closing conditions for the pressures $P_{k,l}$, the interfacial velocity $\boldsymbol{V}_I$ and the relaxation terms $S_{\alpha,k}$, $S_{\alpha\rho,k}$, $\boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}$ and $S_{\alpha\rho E,k}$. In the following sections we will derive appropriate constraints. However, these will not specify a unique model but some options are still remaining for the choice of the interfacial velocity, the relaxation terms, the stress tensor and the heat conduction.

2.2. Mixture model

From the non-equilibrium model we can derive the equations for the mixture. For this purpose we introduce the mixture quantities

$$p := \sum_{k=1}^K \alpha_k\, p_k, \ \ \rho := \sum_{k=1}^K \alpha_k\, \rho_k, \ \ \boldsymbol{v} := \frac{1}{\rho}\sum_{k=1}^K \alpha_k\, \rho_k\, \boldsymbol{v}_k, \tag{2.10}$$

for pressure, density and velocity. Accordingly, we define the specific internal energy, the specific total energy and the specific total enthalpy of the mixture as

$$e := \frac{1}{\rho}\sum_{k=1}^K \alpha_k\, \rho_k\, e_k, \ \ E := \frac{1}{\rho}\sum_{k=1}^K \alpha_k\, \rho_k\, E_k, \ \ H := \frac{1}{\rho}\sum_{k=1}^K \alpha_k\, \rho_k H_k = E + \frac{p}{\rho} \tag{2.11}$$

with $H_k := E_k + p_k/\rho_k$ the total enthalpy of component k. The stress tensor and the heat flux of the mixture are determined by

$$\boldsymbol{T} := \sum_{k=1}^K \alpha_k \boldsymbol{T}_k, \ \ \boldsymbol{q} := \sum_{k=1}^K \alpha_k \boldsymbol{q}_k. \tag{2.12}$$

In order to ensure conservation of mass, momentum and energy of the mixture the relaxation terms (2.9) have to satisfy the conservation constraints

$$\sum_{k=1}^K S_{\alpha,k}^\xi = 0, \ \ \ \sum_{k=1}^K S_{\alpha\rho,k}^\xi = 0, \ \ \ \sum_{k=1}^K \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}^\xi = \boldsymbol{0}, \ \ \ \sum_{k=1}^K S_{\alpha\rho E,k}^\xi = 0 \tag{2.13}$$

for each relaxation type $\xi \in \{v, p, T, \mu\}$. In addition, we need that the interfacial pressures satisfy

$$P_l := \sum_{k=1,k\neq l}^K P_{k,l} \equiv P = const \ \ \ \forall l = 1, \ldots, K. \tag{2.14}$$

Then by summation of the single-component fluid equations (2.2), (2.3), (2.4) and employing the saturation constraint (2.1) as well as the conservation constraints (2.13) and (2.14) we obtain

$$\partial_t\, \rho + \nabla \cdot (\rho\, \boldsymbol{v}) = 0, \tag{2.15}$$

$$\partial_t\, (\rho\, \boldsymbol{v}) + \nabla \cdot (\rho\, \boldsymbol{v}\, \boldsymbol{v}^T + p\, \boldsymbol{I}) = \nabla \cdot \boldsymbol{T} - \tag{2.16}$$

$$\nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \rho_k\, (\boldsymbol{v} - \boldsymbol{v}_k)\, (\boldsymbol{v} - \boldsymbol{v}_k)^T \right),$$

$$\partial_t\, (\rho\, E) + \nabla \cdot (\rho\, \boldsymbol{v}\, (E + p/\rho)) = \nabla \cdot (\boldsymbol{v} \cdot \boldsymbol{T} - \boldsymbol{q}) - \tag{2.17}$$

$$\nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \boldsymbol{T}_k\, (\boldsymbol{v}_k - \boldsymbol{v}) \right) - \nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \rho_k\, (H_k - H)\, (\boldsymbol{v}_k - \boldsymbol{v}) \right).$$

We note that there are contributions corresponding to the slip between the mixture velocity $\boldsymbol{v}$ and the velocities of the components $\boldsymbol{v}_k$. In the multi-component model of Drew and Passman these terms are added to the mixture stress tensor and the mixture heat flux, see [6], p. 82-83. In contrast to the non-equilibrium model, the mixture model is in conservative form if and only if the conditions (2.13) and (2.14) hold.

2.3. Equilibrium model

If the relaxation processes are much faster than the transport and dissipation effects, then the fluid can be considered to be at equilibrium. This state is characterized by vanishing relaxation terms, i.e.,

$$S_{\alpha,k} = 0, \ S_{\alpha\rho,k} = 0, \ \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} = \boldsymbol{0}, \ S_{\alpha\rho E,k} = 0. \tag{2.18}$$

At equilibrium the velocities, pressures and temperatures coincide, i.e.,

$$\boldsymbol{v}_1 = \ldots = \boldsymbol{v}_K = \boldsymbol{v}, \ p_1 = \ldots = p_K = p, \ T_1 = \ldots = T_K = T, \tag{2.19}$$

and the chemical potentials of reacting components are equal. In particular, for the interfacial pressures and interfacial velocity it holds

$$P_{k,l} = p, \ k \neq l, \quad \boldsymbol{V}_I = \boldsymbol{v}. \tag{2.20}$$

Then the mixture model (2.15), (2.16) and (2.17) reduces to the the equilibrium model

$$\partial_t\, \rho + \nabla \cdot (\rho\, \boldsymbol{v}) = 0, \tag{2.21}$$

$$\partial_t\, (\rho\, \boldsymbol{v}) + \nabla \cdot (\rho\, \boldsymbol{v}\, \boldsymbol{v}^T + p\, \boldsymbol{I}) = \nabla \cdot \boldsymbol{T}, \tag{2.22}$$

$$\partial_t\, (\rho\, E) + \nabla \cdot (\rho\, \boldsymbol{v}\, (E + p/\rho)) = \nabla \cdot (\boldsymbol{v} \cdot \boldsymbol{T} - \boldsymbol{q}). \tag{2.23}$$

Note that by definition (2.10) and (2.12) the mixture pressure p, the mixture stress tensor $\boldsymbol{T}$ and the mixture heat flux $\boldsymbol{q}$ depend on the volume fractions α_k. These are determined by the algebraic conditions (2.18) and (2.19).

3. Primitive variables

For the verification of some physical and mathematical properties it will be helpful to rewrite the systems of equations for the non-equilibrium, mixture and the equilibrium model in terms of primitive quantities

3.1. **Non-equilibrium model**

By means of the system (2.2), (2.3), (2.4) and (2.7) we derive evolution equations for the density ρ_k, the velocity $\boldsymbol{v}_k$ and the pressure p_k for each component k. Inserting the evolution equation for the volume fraction (2.7) into the continuity equation (2.2) we obtain

$$\partial_t \, \rho_k + \frac{\rho_k}{\alpha_k} \left(\boldsymbol{v}_k - \boldsymbol{V}_I \right) \cdot \nabla \, \alpha_k + \boldsymbol{v}_k \cdot \nabla \, \rho_k + \rho_k \nabla \cdot \boldsymbol{v}_k = \frac{1}{\alpha_k} \left(S_{\alpha\rho,k} - \rho_k S_{\alpha,k} \right). \tag{3.1}$$

From the momentum equation (2.3) we deduce with (2.2) Cauchy's equation of motion

$$\partial_t \, \boldsymbol{v}_k + \left(\nabla \, \boldsymbol{v}_k \right) \boldsymbol{v}_k + \frac{1}{\rho_k} \nabla \, p_k + \frac{p_k}{\alpha_k \rho_k} \nabla \, \alpha_k \;\; = \;\; \frac{1}{\alpha_k \rho_k} \left(-\sum_{l=1}^{K} P_{k,l} \nabla \, \alpha_l + \nabla \cdot \left(\alpha_k \, \boldsymbol{T}_k \right) \right) +$$
$$\frac{1}{\alpha_k \rho_k} \left(\boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} - S_{\alpha\rho,k} \boldsymbol{v}_k \right). \tag{3.2}$$

Here the gradient of the velocity is defined as $\nabla \, \boldsymbol{v}_k = \left(\nabla \, v_{k,1}, \ldots, \nabla \, v_{k,d} \right)^T$. Then we immediately obtain the evolution equation for the kinetic energy $u_k := \boldsymbol{v}_k^2/2$

$$\partial_t \, u_k + \boldsymbol{v}_k \cdot \left(\nabla \, \boldsymbol{v}_k \, \boldsymbol{v}_k \right) + \frac{1}{\rho_k} \boldsymbol{v}_k \cdot \nabla \, p_k + \frac{p_k}{\alpha_k \rho_k} \boldsymbol{v}_k \cdot \nabla \, \alpha_k = \tag{3.3}$$
$$\frac{1}{\alpha_k \rho_k} \boldsymbol{v}_k \cdot \left(-\sum_{l=1}^{K} P_{k,l} \nabla \, \alpha_l + \nabla \cdot \left(\alpha_k \, \boldsymbol{T}_k \right) \right) + \frac{1}{\alpha_k \rho_k} \boldsymbol{v}_k \cdot \left(\boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} - S_{\alpha\rho,k} \boldsymbol{v}_k \right).$$

Since the total energy is composed of the internal energy and the kinetic energy, we derive the evolution equation for the internal energy $e_k = E_k - u_k$ from the energy equation (2.4), where we employ (2.2) and (3.3). Finally we obtain

$$\partial_t \, e_k + \boldsymbol{v}_k \cdot \left(\nabla \, e_k \right) \;\; = \;\; \frac{1}{\alpha_k \rho_k} \sum_{l=1}^{K} P_{k,l} \left(\boldsymbol{v}_k - \boldsymbol{V}_I \right) \cdot \nabla \, \alpha_l - \frac{p_k}{\rho_k} \nabla \cdot \boldsymbol{v}_k + \tag{3.4}$$
$$\frac{1}{\rho_k} \sum_{i,l=1}^{d} \frac{\partial \, v_{k,l}}{\partial \, x_i} (\boldsymbol{T}_k)_{l,i} - \frac{1}{\alpha_k \rho_k} \nabla \cdot \left(\alpha_k \boldsymbol{q}_k \right) + \frac{1}{\alpha_k \rho_k} S_{e,k}$$

with the relaxation term

$$S_{e,k} := S_{\alpha\rho E,k} - \boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} + S_{\alpha\rho,k}(u_k - e_k). \tag{3.5}$$

Next we derive the evolution equation for the pressure p_k. For this purpose we first note that for any equation of state (2.6) the following relation holds

$$dp_k = \left(\partial p_k / \partial \rho_k \right) d\rho_k + \left(\partial p_k / \partial e_k \right) de_k. \tag{3.6}$$

By means of the continuity equation (3.1) and the energy equation (3.4) we then derive from (3.6)

$$\partial_t \, p_k \;\; + \;\; \sum_{l=1,l \neq k}^{K} \frac{\rho_k}{\alpha_k} C_{k,l}^2 \left(\boldsymbol{v}_k - \boldsymbol{V}_I \right) \cdot \nabla \, \alpha_l + \boldsymbol{v}_k \cdot \nabla \, p_k + \rho_k c_k^2 \nabla \cdot \boldsymbol{v}_k = \tag{3.7}$$
$$\left(\partial p_k / \partial e_k \right) \left(\frac{1}{\rho_k} \sum_{i,l=1}^{d} \frac{\partial \, v_{k,l}}{\partial \, x_i} (\boldsymbol{T}_k)_{l,i} - \frac{1}{\alpha_k \rho_k} \nabla \cdot \left(\alpha_k \boldsymbol{q}_k \right) \right) + \frac{1}{\alpha_k \rho_k} S_{p,k}$$

with the relaxation term

$$S_{p,k} := \rho_k (\partial p_k / \partial \rho_k) \left(S_{\alpha\rho,k} - \rho_k S_{\alpha,k} \right) + \left(\partial p_k / \partial e_k \right) S_{e,k}. \tag{3.8}$$

6

Here the interfacial sound speed and the phase sound speed are defined as

$$C_{k,l}^2 := -\left((\partial p_k/\partial e_k)P_{k,l}/\rho_k^2 + (\partial p_k/\partial \rho_k)\right), \quad c_k^2 := \partial p_k/\partial \rho_k + p_k/\rho_k^2(\partial p_k/\partial e_k). \tag{3.9}$$

3.2. Mixture model

Similar to the non-equilibrium model we derive evolution equations for the mixture quantities ρ, $\boldsymbol{v}$, e and p defined by (2.10) and (2.11) from the evolution equations (2.15), (2.16) and (2.17). First of all, we determine Cauchy's equation of motion from the momentum equation (2.16) where we use the continuity equation (2.15) and the constraint (2.14):

$$\partial_t \boldsymbol{v} + (\nabla \boldsymbol{v})\boldsymbol{v} + \frac{1}{\rho}\nabla p = \frac{1}{\rho}\nabla \cdot \boldsymbol{T} - \frac{1}{\rho}\sum_{l=1}^K P_l \nabla \alpha_l - \frac{1}{\rho}\nabla \cdot \sum_{k=1}^K \alpha_k \rho_k(\boldsymbol{v}_k - \boldsymbol{v})(\boldsymbol{v}_k - \boldsymbol{v})^T. \tag{3.10}$$

Since definition (2.11) of the mixture energy e implies that $\rho e = \sum_{k=1}^K \alpha_k \rho_k e_k$, we obtain by (3.4) and (2.2) the evolution equation for the internal energy

$$\partial_t e + \boldsymbol{v} \cdot \nabla e + \frac{1}{\rho}\sum_{k=1}^K \alpha_k p_k \nabla \cdot \boldsymbol{v}_k = \frac{1}{\rho}\sum_{l,k=1}^K P_{k,l}(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_l - \tag{3.11}$$

$$\frac{1}{\rho}\sum_{k=1}^K \alpha_k \rho_k e_k(\boldsymbol{v}_k - \boldsymbol{v}) + \frac{1}{\rho}\sum_{k=1}^K \sum_{i,l=1}^d \frac{\partial v_{k,l}}{\partial x_i}\alpha_k(\boldsymbol{T}_k)_{l,i} - \frac{1}{\rho}\nabla \cdot \boldsymbol{q} - \frac{1}{\rho}\sum_{k=1}^K(\boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} - S_{\alpha\rho,k}u_k).$$

Finally we determine the evolution equation for the mixture pressure p. Applying the time derivative to the definition (2.10) of p and using (2.7) and (3.7) we obtain

$$\begin{aligned}\partial_t p \quad + \quad &\boldsymbol{v} \cdot \nabla p + \rho c^2 \nabla \cdot \boldsymbol{v} = \tag{3.12}\\ &-\sum_{k=1}^K \rho_k \sum_{l=1,l\neq k}^K C_{k,l}^2(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_l - \sum_{k=1}^K \alpha_k \left(\boldsymbol{v} \cdot \nabla(p_k - p) + (\boldsymbol{v}_k - \boldsymbol{v}) \cdot \nabla p_k\right)\\ &-\sum_{k=1}^K \alpha_k \rho_k c_k^2 \nabla \cdot (\boldsymbol{v}_k - \boldsymbol{v}) + \sum_{k=1}^K \frac{1}{\rho_k}(\partial p_k/\partial e_k)\left(\alpha_k \sum_{i,l=1}^d \frac{\partial v_{k,l}}{\partial x_i}(\boldsymbol{T}_k)_{i,l} - \nabla \cdot (\alpha_k \boldsymbol{q}_k)\right)\\ &+\sum_{k=1}^K \left(p_k S_{\alpha,k} + \frac{1}{\rho_k}S_{p,k}\right).\end{aligned}$$

Here the sound speed of the mixture is defined as

$$c^2 := \frac{1}{\rho}\sum_{k=1}^K \alpha_k \, \rho_k \, c_k^2. \tag{3.13}$$

3.3. Equilibrium model

In case of the equilibrium model the evolution equations for the primitive variables can be directly determined from those of the mixture model where we make use of the equilibrium assumptions (2.18), (2.19) and (2.20) and the saturation condition (2.1). Then Cauchy's equation of motion reads

$$\partial_t \boldsymbol{v} + (\nabla \boldsymbol{v})\boldsymbol{v} + \frac{1}{\rho}\nabla p = \frac{1}{\rho}\nabla \cdot \boldsymbol{T}. \tag{3.14}$$

The energy equation reduces to

$$\partial_t e + \boldsymbol{v} \cdot \nabla e + \frac{p}{\rho} \nabla \cdot \boldsymbol{v} = \frac{1}{\rho} \sum_{i,l=1}^{d} \frac{\partial v_l}{\partial x_i} (\boldsymbol{T})_{l,i} - \frac{1}{\rho} \nabla \cdot \boldsymbol{q}. \tag{3.15}$$

Finally the pressure equation becomes

$$\partial_t p \quad + \quad \boldsymbol{v} \cdot \nabla p + \rho c^2 \nabla \cdot \boldsymbol{v} = \tag{3.16}$$
$$\sum_{k=1}^{K} \frac{1}{\rho_k} (\partial p_k / \partial e_k) \left(\alpha_k \sum_{i,l=1}^{d} \frac{\partial v_l}{\partial x_i} (\boldsymbol{T}_k)_{i,l} - \nabla \cdot (\alpha_k \boldsymbol{q}_k) \right).$$

4. Mathematical properties: hyperbolicity and sub-characteristic condition

Neglecting viscosity and heat conduction as well as relaxation processes in the fluid equations introduced in Section 2 the models reduce to first order systems describing transport effects only. Therefore these systems should be hyperbolic. This ensures that all wave speeds are finite and the system may be locally decoupled. From a mathematical point of view, this property is helpful in the construction of Riemann solvers. Therefore we determine the eigenvalues and eigenvectors corresponding to the non-equilibrium model. From a numerical point of view the relation between the eigenvalues of the non-equilibrium and the equilibrium model are of special interest.

4.1. Non-equilibrium model

Starting point are the evolution equations for the primitive variables (2.7), (3.1) , (3.2) and (3.7). The corresponding first order system then reads

$$\partial_t \alpha_k + \sum_{i=1}^{d} V_{I,i} \frac{\partial \alpha_k}{\partial x_i} = 0 \tag{4.1}$$

$$\partial_t \rho_k + \sum_{i=1}^{d} \left(\frac{\rho_k}{\alpha_k} (v_{k,i} - V_{I,i}) \frac{\partial \alpha_k}{\partial x_i} + v_{k,i} \frac{\partial \rho_k}{\partial x_i} + \rho_k \frac{\partial v_{k,i}}{\partial x_i} \right) = 0, \tag{4.2}$$

$$\partial_t \boldsymbol{v}_k + \sum_{i=1}^{d} \left(v_{k,i} \frac{\partial \boldsymbol{v}_k}{\partial x_i} + \sum_{l=1,l\neq k}^{K} \frac{1}{\alpha_k \rho_k} (P_{k,l} - p_k) \boldsymbol{e}_{i,d} \frac{\partial \alpha_l}{\partial x_i} + \frac{1}{\rho_k} \boldsymbol{e}_{i,d} \frac{\partial p_k}{\partial x_i} \right) = \boldsymbol{0}, \tag{4.3}$$

$$\partial_t p_k + \sum_{i=1}^{d} \left(v_{k,i} \frac{\partial p_k}{\partial x_i} + \sum_{l=1,l\neq k}^{K} \frac{\rho_k}{\alpha_k} C_{k,l}^2 (v_{k,i} - V_{I,i}) \frac{\partial \alpha_l}{\partial x_i} + \rho_k c_k^2 \frac{\partial v_{k,i}}{\partial x_i} \right) = 0, \tag{4.4}$$

where $\boldsymbol{e}_{i,d} \in \mathbb{R}^d$ denotes the unit vector in the ith coordinate direction. In order to characterize hyperbolicity of this system we consider its projection onto normal direction $\xi := \boldsymbol{x} \cdot \boldsymbol{n}$ for arbitrary unit direction $\boldsymbol{n} \in \mathbb{R}^d$. Introducing the vector of primitive variables

$$\boldsymbol{w} = (\alpha_1, \ldots, \alpha_{K-1}, \boldsymbol{w}_1^T, \ldots, \boldsymbol{w}_K^T)^T, \ \boldsymbol{w}_k = (\rho_k, \boldsymbol{v}_k^T, p_k)^T \tag{4.5}$$

the projected system can be written in quasi-conservative form as

$$\partial_t \boldsymbol{w} + \boldsymbol{B}_n(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial \xi} = \boldsymbol{0}. \tag{4.6}$$

The matrix $\boldsymbol{B}_n$ is determined by the block matrix

$$\boldsymbol{B}_n := \sum_{i=1}^{d} \boldsymbol{B}_i \, n_i = \begin{pmatrix} V_{I,n} \, \boldsymbol{I}_{K-1} & & & \\ \boldsymbol{A}_{1,n} & \boldsymbol{B}_{1,n} & & \\ \vdots & & \ddots & \\ \boldsymbol{A}_{K,n} & & & \boldsymbol{B}_{K,n} \end{pmatrix}, \tag{4.7}$$

with the blocks defined as

$$\boldsymbol{A}_{k,n} := \begin{pmatrix} \frac{\rho_k}{\alpha_k} \left(v_{k,n} - V_{I,n}\right) \left(\boldsymbol{e}_{k,K-1}^T - \boldsymbol{1}_{K-1}^T \, \delta_{k,K}\right) \\ -\boldsymbol{n}\boldsymbol{\beta}_k^T \\ \frac{\rho_k}{\alpha_k} \left(v_{k,n} - V_{I,n}\right) \boldsymbol{\gamma}_k^T \end{pmatrix}, \quad \boldsymbol{B}_{k,n} := \begin{pmatrix} v_{k,n} & \rho_k \, \boldsymbol{n}^T & 0 \\ \boldsymbol{0}_d & v_{k,n} \, \boldsymbol{I}_d & \frac{1}{\rho_k} \, \boldsymbol{n} \\ 0 & \rho_k \, c_k^2 \boldsymbol{n}^T & v_{k,n} \end{pmatrix}. \tag{4.8}$$

Here $\boldsymbol{e}_{k,K-1}$ is the kth unit vector in $\mathbb{R}^{K-1}$. In particular, we make the convention $\boldsymbol{e}_{K,K-1} = \boldsymbol{0}$. Furthermore, $\boldsymbol{I}_d$ and $\boldsymbol{I}_{K-1}$ are the unit matrices in $\mathbb{R}^{d \times d}$ and $\mathbb{R}^{(K-1) \times (K-1)}$, respectively, and $\boldsymbol{0}_d$ and $\boldsymbol{1}_{K-1}$ are vectors in $\mathbb{R}^d$ and $\mathbb{R}^{(K-1)}$ with value 0 or 1, respectively. The vectors $\boldsymbol{\beta}_k$ and $\boldsymbol{\gamma}_k$ are defined by its components $l = 1, \dots, K-1$ as

$$\beta_{k,l} := \frac{1}{\alpha_k \rho_k} \left((P_{k,l} - p_k)(1 - \delta_{k,l}) - (P_{k,K} - p_k)(1 - \delta_{k,K})\right), \tag{4.9}$$

$$\gamma_{k,l} := C_{k,l}^2(1 - \delta_{k,l}) - C_{k,K}^2(1 - \delta_{k,K}) \tag{4.10}$$

with $\delta_{k,l}$ the Kronecker symbol. The normal components of the velocities and the interfacial velocity are defined as

$$v_{k,n} := \boldsymbol{v}_k \cdot \boldsymbol{n}, \quad V_{I,n} := \boldsymbol{V} \cdot \boldsymbol{n}. \tag{4.11}$$

Obviously, the eigenvalues of the matrix (4.7) can now be easily computed where we employ the block structure:

$$\det(\boldsymbol{B}_n - \lambda \, \boldsymbol{I}) = \det(V_{n,I} \, \boldsymbol{I}_{K-1} - \lambda \, \boldsymbol{I}_{K-1}) \prod_{k=1}^{K} \det(\boldsymbol{B}_{k,n} - \lambda \, \boldsymbol{I}_{d+2}) = 0 \tag{4.12}$$

Since the matrices $\boldsymbol{B}_{k,n}$ coincide with those in case of a single-phase fluid, we then compute

$$\det(\boldsymbol{B}_{k,n} - \lambda \, \boldsymbol{I}_{d+2}) = (v_{k,n} - \lambda)^d \left((v_{k,n} - \lambda)^2 - c_k^2\right) \tag{4.13}$$

Hence we obtain the following eigenvalues:

$$\begin{aligned} \lambda_{I,k} &= V_{I,n}, \ k = 1, \dots, K-1 \tag{4.14} \\ \lambda_{k,i} &= v_{k,n}, \ k = 1, \dots, K, \ i = 1, \dots, d \tag{4.15} \\ \lambda_{k,\pm} &= v_{k,n} \pm c_k, \ k = 1, \dots, K. \tag{4.16} \end{aligned}$$

Motivated by the block structure of the matrix $\boldsymbol{B}_n$ we make the following ansatz for computing the corresponding left and right eigenvectors

$$\boldsymbol{R}_n := \begin{pmatrix} \boldsymbol{R}_{I,n}^0 & & & \\ \boldsymbol{R}_{I,n}^1 & \boldsymbol{R}_{1,n} & & \\ \vdots & & \ddots & \\ \boldsymbol{R}_{I,n}^K & & & \boldsymbol{R}_{K,n} \end{pmatrix}, \quad \boldsymbol{L}_n := \begin{pmatrix} \boldsymbol{L}_{I,n}^0 & & & \\ \boldsymbol{L}_{I,n}^1 & \boldsymbol{L}_{1,n} & & \\ \vdots & & \ddots & \\ \boldsymbol{L}_{I,n}^K & & & \boldsymbol{L}_{K,n} \end{pmatrix} \tag{4.17}$$

with blocks

$$\boldsymbol{R}_{I,n}^0 := \kappa_0 \boldsymbol{I}_{K-1}, \boldsymbol{L}_{I,n}^0 \in \mathbb{R}^{(K-1) \times (K-1)},$$

$$\boldsymbol{R}_{I,n}^k, \boldsymbol{L}_{I,n}^k \in \mathbb{R}^{(d+2) \times (K-1)}, \quad \boldsymbol{R}_{k,n}, \boldsymbol{L}_{k,n} \in \mathbb{R}^{(d+2) \times (d+2)}, \ k = 1, \dots, K.$$

Here the matrix $\boldsymbol{R}_n$ and $\boldsymbol{L}_n$ are composed of the right and left eigenvectors in its columns and rows, respectively. To determine the blocks $\boldsymbol{R}_{k,n}$ we note that $\lambda_{k,i}$ and $\lambda_{k,\pm}$ are also eigenvalues of the matrix $\boldsymbol{B}_{k,n}$ and the eigenvalue problem for $\boldsymbol{B}_n$ decouples into eigenvalue problems for the matrices $\boldsymbol{B}_{k,n}$ corresponding to a single component. In a first step, we therefore compute the eigenvectors to these sub-problems where we first determine an orthonormal basis $\{\boldsymbol{n}, \boldsymbol{t}_1, \ldots, \boldsymbol{t}_{d-1}\}$ of $\mathbb{R}^d$ such that $\boldsymbol{t}_i \cdot \boldsymbol{t}_j = \delta_{i,j}$ and $\boldsymbol{t}_i \cdot \boldsymbol{n} = 0$. Then the right and left eigenvectors to the eigenvalues (4.15) and (4.16) are

$$\boldsymbol{r}_{k,d} = (1, \boldsymbol{0}_d^T, 0)^T, \ \boldsymbol{r}_{k,i} = (0, \boldsymbol{t}_i^T, 0)^T, \ i = 1, \ldots, d-1, \ \boldsymbol{r}_{k,\pm} = (1, \pm c_k/\rho_k \boldsymbol{n}^T, c_k^2)^T, \tag{4.18}$$

$$\boldsymbol{l}_{k,d} = (1, \boldsymbol{0}_d^T, -c_k^{-2})^T, \ \boldsymbol{l}_{k,i} = (0, \boldsymbol{t}_i^T, 0)^T, \ i = 1, \ldots, d-1, \ \boldsymbol{l}_{k,\pm} = 0.5 c_k^{-2}(1, \pm c_k \rho_k \boldsymbol{n}^T, 1)^T. \tag{4.19}$$

Thus there exists an eigenvalue decomposition of the matrix $\boldsymbol{B}_{k,n}$, i.e.,

$$\boldsymbol{L}_{k,n} \boldsymbol{B}_{k,n} \boldsymbol{R}_{k,n} = \boldsymbol{\Lambda}_{k,n}, \tag{4.20}$$

where $\boldsymbol{L}_{k,n}$ and $\boldsymbol{R}_{k,n}$ are defined by the left and right eigenvectors and $\boldsymbol{\Lambda}_{k,n}$ is a diagonal matrix with eigenvalues on the diagonal

$$\boldsymbol{R}_{k,n} := \begin{pmatrix} 1 & 0 & \ldots & 0 & 1 & 1 \\ -c_k/\rho_k \boldsymbol{n} & \boldsymbol{t}_1 & \ldots & \boldsymbol{t}_{d-1} & \boldsymbol{0}_d & c_k/\rho_k \boldsymbol{n} \\ c_k^2 & 0 & \ldots & 0 & 0 & c_k^2 \end{pmatrix}, \tag{4.21}$$

$$\boldsymbol{L}_{k,n} := \frac{1}{2c_k^2} \begin{pmatrix} 0 & 0 & \ldots & 0 & 2c_k^2 & 0 \\ -c_k \rho_k \boldsymbol{n} & 2c_k^2 \boldsymbol{t}_1 & \ldots & 2c_k^2 \boldsymbol{t}_{d-1} & \boldsymbol{0}_d & c_k \rho_k \boldsymbol{n} \\ 1 & 0 & \ldots & 0 & -2 & 1 \end{pmatrix}^T, \tag{4.22}$$

$$\boldsymbol{\Lambda}_{k,n} := \begin{pmatrix} v_{k,n} - c_k & \boldsymbol{0}_d^T & 0 \\ \boldsymbol{0}_d & v_{k,n} \boldsymbol{I}_d & \boldsymbol{0}_d \\ 0 & \boldsymbol{0}_d^T & v_{k,n} + c_k \end{pmatrix}. \tag{4.23}$$

To calculate the eigenvectors to the multiple eigenvalue $\lambda_{I,i}$ we employ the knowledge of the matrices $\boldsymbol{R}_{k,n}$. According to the block structure of the matrix $\boldsymbol{R}_n$ the matrix of corresponding right eigenvectors needs to satisfy

$$(\boldsymbol{B}_n - \lambda_{I,i} \boldsymbol{I}) \boldsymbol{R}_n = \boldsymbol{0} \Leftrightarrow (\boldsymbol{B}_{k,n} - \lambda_{I,i} \boldsymbol{I}_{d+2}) \boldsymbol{R}_{I,n}^k = -\boldsymbol{A}_{k,n} \boldsymbol{R}_{I,n}^0 = -\kappa_0 \boldsymbol{A}_{k,n}, \ k = 1, \ldots, K.$$

Assuming that the eigenvalue $\lambda_{I,i}$ does not coincide with one of the eigenvalues $\lambda_{k,i}$ and $\lambda_{k,\pm}$, then $\boldsymbol{B}_{k,n} - \lambda_{I,i} \boldsymbol{I}_{d+2}$ is regular and there exists a unique solution for $\boldsymbol{R}_{I,n}^k$. For its representation we introduce

$$\kappa_0 := \prod_{l=1}^K \alpha_l \sigma_k, \ \kappa_k := \prod_{l=1, l \neq k}^K \alpha_l \sigma_k, \ k = 1, \ldots, K$$

with $\delta_k^n := v_{k,n} - V_{I,n}$ and $\sigma_k := (\delta_k^n)^2 - c_k^2$. Then we obtain

$$\boldsymbol{R}_{I,n}^0 := \kappa_0 \boldsymbol{I}_{K-1}, \tag{4.24}$$

$$\boldsymbol{R}_{I,n}^k := \kappa_k \begin{pmatrix} (\delta_k^n)^2 \rho_k \boldsymbol{\gamma}_k^T + \alpha_k \rho_k c_k^2 \boldsymbol{\beta}_k^T \\ -\boldsymbol{n}(\alpha_k \boldsymbol{\beta}_k^T + \boldsymbol{\gamma}_k^T) \delta_k^n \\ -\sigma_k(\boldsymbol{e}_{i,K-1}^T(1 - \delta_{k,K}) - \boldsymbol{1}_{K-1}^T \delta_{k,K}) + \alpha_k \boldsymbol{\beta}_k^T + \boldsymbol{\gamma}_k^T \end{pmatrix} \tag{4.25}$$

Since $\alpha_k \in (0,1)$ according to (2.1), these matrices are regular, i.e., the columns are linearly independent, if and only if

$$\sigma_k \neq 0 \quad \forall\, k = 1, \ldots, K, \tag{4.26}$$

holds. This condition is referred to as the *non-resonance condition*, see [4] in case of a two-velocity-two-pressure model in two-phase flows. Thus the corresponding left eigenvectors are determined by the rows of the inverse of $\boldsymbol{R}_n$. Since $\boldsymbol{L}_n \boldsymbol{R}_n = \boldsymbol{I}$, the blocks turn out to be

$$\boldsymbol{L}_{k,n} = \boldsymbol{R}_{k,n}^{-1}, \; k = 1, \ldots, K, \tag{4.27}$$

$$\boldsymbol{L}_{I,n}^0 = (\boldsymbol{R}_{I,n}^0)^{-1} = \kappa_0^{-1} \boldsymbol{I}_{K-1}, \tag{4.28}$$

$$\boldsymbol{L}_{I,n}^K = -\boldsymbol{L}_{k,n} \boldsymbol{R}_{I,n}^K (\boldsymbol{R}_{I,n}^0)^{-1} = -\kappa_0^{-1} \boldsymbol{L}_{k,n} \boldsymbol{R}_{I,n}^K, \; k = 1, \ldots, K, \tag{4.29}$$

and we obtain for the right eigenvectors

$$\boldsymbol{r}_{I,i} := \kappa_0 \left((\overline{\boldsymbol{r}}_{I,0}^1)^T, (\overline{\boldsymbol{r}}_{I,i}^1)^T, \ldots, (\overline{\boldsymbol{r}}_{I,i}^K)^T \right)^T, \; i = 1, \ldots, K-1. \tag{4.30}$$

with vectors $\overline{\boldsymbol{r}}_{I,i}^k = (\overline{x}_{k,i}, \overline{\boldsymbol{y}}_{k,i}^T, \overline{z}_{k,i})^T$ and their components

$$\overline{z}_{k,i} = \left(\rho_k (\delta_k^n)^2 \gamma_{k,i} + \alpha_k \rho_k c_k^2 \beta_{k,i} \right) / (\alpha_k \sigma_k), \tag{4.31}$$

$$\overline{\boldsymbol{y}}_{k,i} = -\boldsymbol{n} \left(\alpha_k \beta_{k,i} + \gamma_{k,i} \right) \delta_k^n / (\alpha_k \sigma_k), \tag{4.32}$$

$$\overline{x}_{k,i} = \left(-\sigma_k (\delta_{k,i}(1 - \delta_{k,K}) - \delta_{k,K}) + (\alpha_k \beta_{k,i} + \gamma_{k,i}) \right) \rho_k (\alpha_k \sigma_k). \tag{4.33}$$

These are well-defined also in case of $\alpha_k = 0$ or $\sigma_k = 0$. Similar to (4.30) the left eigenvectors are then given by

$$\boldsymbol{l}_{I,i} := \left((\boldsymbol{l}_{I,0}^1)^T, (\boldsymbol{l}_{I,i}^1)^T, \ldots, (\boldsymbol{l}_{I,i}^K)^T \right)^T, \; i = 1, \ldots, K-1. \tag{4.34}$$

with

$$\boldsymbol{l}_{I,i}^0 = \prod_{l=1}^K (\alpha_l \sigma_l)^{-1} \boldsymbol{e}_{i,K-1}, \quad \boldsymbol{l}_{I,i}^k = \frac{1}{2 c_k^2 \alpha_k \sigma_k} (a_k^i, 0, \ldots, 0, b_k^i)^T$$

and

$$a_k^i := c_k \rho_k (\alpha_k \beta_{k,i} + \gamma_{k,i}) \delta_k^n + \sigma_k (\delta_{k,i}(1 - \delta_{k,K}) - \delta_{k,K}) - \alpha_k \beta_{k,i} - \gamma_{k,i},$$

$$b_k^i := -2 c_k^2 \rho_k ((\delta_k^n)^2 \gamma_{k,i} + \alpha_k c_k^2 \beta_{k,i}) - 2\sigma_k (\delta_{k,i}(1 - \delta_{k,K}) - \delta_{k,K}) + 2(\alpha_k \beta_{k,i} + \gamma_{k,i}).$$

After having determined the eigenvalues and the corresponding linearly independent right and left eigenvectors we finally end up with the eigenvalue decomposition of the matrix $\boldsymbol{B}_n$

$$\boldsymbol{L}_n \boldsymbol{B}_n \boldsymbol{R}_n = \boldsymbol{\Lambda}_n \tag{4.35}$$

with the block-diagonal matrix $\boldsymbol{\Lambda}_n = \mathrm{diag}(\boldsymbol{\Lambda}_{0,n}, \boldsymbol{\Lambda}_{1,n}, \ldots, \boldsymbol{\Lambda}_{K,n})$ and $\boldsymbol{\Lambda}_{0,n} := V_{I,n} \boldsymbol{I}_{K-1}$. To verify this decomposition we make use of the identity $\boldsymbol{B}_{k,n} \boldsymbol{R}_{k,n}^k = \boldsymbol{R}_{I,n}^k \boldsymbol{\Lambda}_{0,n} - \boldsymbol{A}_{k,n} \boldsymbol{R}_{I,n}^0$. To conclude the investigation on the hyperbolicity we summarize the findings in the following theorem.

Theorem 4.1. *(Hyperbolicity) Let the interfacial pressures satisfy the conditions (2.5) and (2.14). Let the interfacial velocity $\boldsymbol{V}_I$ not coincide with one of the eigenvalues $\lambda_{k,i}$ and $\lambda_{k,\pm}$ of $\boldsymbol{B}_n$. Then the first order system (4.1), (4.2), (4.3) and (4.4) is hyperbolic, i.e., (i) the eigenvalues of the matrix (4.7) are all real but not necessarily distinct and (ii) there exists a system of linearly independent left and right eigenvectors with (4.35) if and only if the non-resonance condition (4.26) is satisfied.*

This theorem holds true also for the non-equilibrium model (2.2), (2.3), (2.4) and (2.7) neglecting viscosity and heat conduction as well as relaxation processes, because eigenvalues are invariant under a regular, bijective change of variables and the corresponding eigenvectors can be determined by scaling of the original eigenvectors by the Jacobian of the transformation and its inverse, respectively.

Finally we want to remark that the eigenvectors coincide with the one given in [26, 2] in case of a 7-equation model in one space dimension ($K = 2$, $d = 1$).

4.2. Equilibrium model

Similar to the non-equilibrium case we can determine the eigenvalues of the equilibrium model. Starting point are the evolution equations (2.21), (2.22) and (2.23). The corresponding first order system then reads

$$\partial_t \rho + \sum_{i=1}^d \left(v_i \frac{\partial \rho}{\partial x_i} + \rho \frac{\partial v_i}{\partial x_i} \right) = 0, \tag{4.36}$$

$$\partial_t \boldsymbol{v} + \sum_{i=1}^d \left(v_i \frac{\partial \boldsymbol{v}}{\partial x_i} + \frac{1}{\rho} \boldsymbol{e}_i \frac{\partial p}{\partial x_i} \right) = \boldsymbol{0}, \tag{4.37}$$

$$\partial_t p + \sum_{i=1}^d \left(v_i \frac{\partial p}{\partial x_i} + \rho c^2 \frac{\partial v_i}{\partial x_i} \right) = 0, \tag{4.38}$$

Again we consider its projection onto normal direction $\xi := \boldsymbol{x} \cdot \boldsymbol{n}$ for arbitrary unit direction $\boldsymbol{n} \in \mathbb{R}^d$ that can be written in quasi-conservative form

$$\partial_t \boldsymbol{w} + \boldsymbol{B}_n(\boldsymbol{w}) \frac{\partial \boldsymbol{w}}{\partial \xi} = \boldsymbol{0} \tag{4.39}$$

with the vector of primitive variables $\boldsymbol{w} = (\rho, \boldsymbol{v}^T, p)^T$ and matrix

$$\boldsymbol{B}_n := \begin{pmatrix} v_n & \rho \boldsymbol{n}^T & 0 \\ \boldsymbol{0}_d & v_n \boldsymbol{I}_d & \frac{1}{\rho} \boldsymbol{n} \\ 0 & \rho c^2 \boldsymbol{n}^T & v_n \end{pmatrix}. \tag{4.40}$$

The normal component of the velocity is defined as

$$v_n := \boldsymbol{v} \cdot \boldsymbol{n}. \tag{4.41}$$

The eigenvalues of $\boldsymbol{B}_n$ are then characterized by the roots of the characteristic polynomial

$$\det(\boldsymbol{B}_n - \lambda \boldsymbol{I}_{d+2}) = (V_n - \lambda)^d ((v_n - \lambda)^2 - c^2).$$

Hence we obtain the following eigenvalues:

$$\lambda_\pm = v_n \pm c, \quad \lambda_i = v_n, \ i = 1, \dots, d. \tag{4.42}$$

With regard to a stable numerical discretization of the non-equilibrium model in the limit of vanishing relaxation terms, the so-called sub-characteristic condition has to hold true. This condition was originally introduced by Liu [18]. For this purpose we evaluate the eigenvalues (4.14), (4.15) and (4.16) with respect to an equilibrium state, i.e.,(2.18), (2.19) and (2.20) hold,

$$\begin{aligned}
\overline{\lambda}_{I,k} &= \overline{V}_{I,n} = \overline{\boldsymbol{v}}_I \cdot \boldsymbol{n} = \overline{\boldsymbol{v}} \cdot \boldsymbol{n} = \overline{v}_n, \ k = 1, \dots, K-1 \\
\overline{\lambda}_{k,i} &= \overline{v}_{k,n} = \overline{\boldsymbol{v}}_k \cdot \boldsymbol{n} = \overline{\boldsymbol{v}} \cdot \boldsymbol{n} = \overline{v}_n, \ k = 1, \dots, K, \ i = 1, \dots, d \\
\overline{\lambda}_{k,\pm} &= \overline{v}_{k,n} \pm c_k = \overline{v}_n \pm c_k, \ k = 1, \dots, K.
\end{aligned}$$

Here the bar indicates evaluation with respect to an equilibrium state. Then by definition (3.13) and (2.10) of the mixture sound speed and the mixture density we conclude from the positivity of the densities ρ_k and the volume fractions α_k

$$\overline{c} \in [\min_{k=1,\dots,K} \overline{c}_k, \max_{k=1,\dots,K} \overline{c}_k] =: [c_{min}, c_{max}].$$

A straight forward estimation gives

$$\min_{k=1,\dots,K} \overline{\lambda}_{k,+} \le \overline{\lambda}_+ \le \max_{k=1,\dots,K} \overline{\lambda}_{k,+},$$
$$\min_{k=1,\dots,K} \overline{\lambda}_{k,-} \le \overline{\lambda}_- \le \max_{k=1,\dots,K} \overline{\lambda}_{k,-}.$$

In the second estimate we use that

$$-\overline{c} \in [-\max_{k=1,\ldots,K} \overline{c}_k, -\min_{k=1,\ldots,K} \overline{c}_k,] = [\min_{k=1,\ldots,K} -\overline{c}_k, \max_{k=1,\ldots,K} -\overline{c}_k].$$

This immediately implies that the following theorem holds true.

Theorem 4.2. *(Sub-characteristic condition) Let α_k, ρ_k and c_k, $k = 1, \ldots, K$, be non-negative. Then the eigenvalues (4.14), (4.15), (4.16) and (4.43), (4.43), (4.43) of the non-equilibrium model and the equilibrium model, respectively, evaluated with respect to an equilibrium state, i.e., (2.18), (2.19) and (2.20) hold, satisfy the sub-characteristic condition*

$$\overline{\lambda}_i \in \left[\min \left(\min_{k=1,\ldots,K-1} \overline{\lambda}_{I,k}, \min_{\substack{k=1,\ldots,K \\ i=1,\ldots,d}} \overline{\lambda}_{k,i} \right), \max \left(\max_{k=1,\ldots,K-1} \overline{\lambda}_{I,k}, \max_{\substack{k=1,\ldots,K \\ i=1,\ldots,d}} \overline{\lambda}_{k,i} \right) \right] = \{\overline{v}_n\},$$

$$\overline{\lambda}_{\pm} \in \left[\min_{k=1,\ldots,K} \overline{\lambda}_{k,\pm}, \max_{k=1,\ldots,K} \overline{\lambda}_{k,\pm} \right].$$

Note that similar results have been proven recently by Flatten and Lund [9] for a hierarchy of two-phase relaxation models.

5. Frame invariance and objectivity

Since the results of an experiment should be independent of the observer's position in the Euclidean space, a physical meaningful model should reflect this behavior. This property is referred to as frame indifference and objectivity in the literature, cf. [6], p. 31 ff, and [17]: performing the general Euclidean change of frame

$$t^* = t + a, \quad \boldsymbol{x}^* = \boldsymbol{x}_0^*(t) + \boldsymbol{Q}(t)(\boldsymbol{x} - \boldsymbol{x}_0), \tag{5.1}$$

with constant values a and $\boldsymbol{x}_0$ and $\boldsymbol{Q}$ an orthogonal matrix, i.e.,

$$\boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{Q}\boldsymbol{Q}^T = \boldsymbol{I}, \tag{5.2}$$

then a scalar f, a vector $\boldsymbol{u}$ and a tensor $\boldsymbol{T}$ are called objective, if

$$f^*(t^*, \boldsymbol{x}^*) = f(t, x), \ \boldsymbol{u}^*(t^*, \boldsymbol{x}^*) = \boldsymbol{Q}(t)\boldsymbol{u}(t, x), \ \boldsymbol{T}^*(t^*, \boldsymbol{x}^*) = \boldsymbol{Q}(t)\boldsymbol{T}(t, x)\boldsymbol{Q}^T(t). \tag{5.3}$$

From the orthogonality of $\boldsymbol{Q}$ we conclude

$$\boldsymbol{A} := \dot{\boldsymbol{Q}}\boldsymbol{Q}^T = -\boldsymbol{Q}\dot{\boldsymbol{Q}}^T = -\boldsymbol{A}^T, \tag{5.4}$$

i.e., $\boldsymbol{A}$ is a skew-symmetric matrix and it holds $A_{ii} = 0$, $A_{ij} = -A_{ji}$. Then under the general Euclidean change of frame (5.1) the velocities $\boldsymbol{v} := \dot{\boldsymbol{x}}$ and $\boldsymbol{v}^* := \dot{\boldsymbol{x}}^*$ of the different frames are linked via

$$\boldsymbol{v}^* - \dot{\boldsymbol{x}}_0^* = \boldsymbol{Q}(\boldsymbol{v} - \dot{\boldsymbol{x}}_0) + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*) \quad \text{equiv.} \quad \boldsymbol{v} - \dot{\boldsymbol{x}}_0 = \boldsymbol{Q}^T(\boldsymbol{v}^* - \dot{\boldsymbol{x}}_0^*) - \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*). \tag{5.5}$$

Thus, the velocity and the acceleration are not objective under a general Euclidean change of frame. For the rate of deformation $\boldsymbol{D}$ and the rotation tensor $\boldsymbol{W}$ defined as

$$\boldsymbol{D} := \frac{1}{2} \left(\nabla_{\boldsymbol{x}} \boldsymbol{v} + (\nabla_{\boldsymbol{x}} \boldsymbol{v})^T \right) = \boldsymbol{D}^T, \quad \boldsymbol{W} := \frac{1}{2} \left(\nabla_{\boldsymbol{x}} \boldsymbol{v} - (\nabla_{\boldsymbol{x}} \boldsymbol{v})^T \right) = -\boldsymbol{W}^T \tag{5.6}$$

we conclude from (5.1)

$$\boldsymbol{D}^* := \frac{1}{2} \left(\nabla_{\boldsymbol{x}} \boldsymbol{v}^* + (\nabla_{\boldsymbol{x}} \boldsymbol{v}^*)^T \right) = \boldsymbol{Q}\boldsymbol{D}\boldsymbol{Q}^T, \quad \boldsymbol{W}^* := \frac{1}{2} \left(\nabla_{\boldsymbol{x}} \boldsymbol{v}^* - (\nabla_{\boldsymbol{x}} \boldsymbol{v}^*)^T \right) = \boldsymbol{Q}\boldsymbol{W}\boldsymbol{Q}^T + \boldsymbol{A}^T, \tag{5.7}$$

i.e., the rate of deformation is objective but the rotation tensor is not objective under a general Euclidean change of frame.

5.1. General Euclidean change of frame

In order to rewrite the fluid equations (2.2), (2.3), (2.4) and (2.7) in terms of the general Euclidean change of frame we need some rules of calculus that will be summarized below. First of all, we determine from (5.1) the Jacobian of the transformation

$$\frac{\partial(t^*, \boldsymbol{x}^*)}{\partial(t, \boldsymbol{x})} = \begin{pmatrix} 1 & \boldsymbol{0}_d^T \\ \dot{\boldsymbol{x}}_0 + \dot{\boldsymbol{Q}}(\boldsymbol{x} - \boldsymbol{x}_0) & \boldsymbol{Q} \end{pmatrix}, \quad \frac{\partial(t, \boldsymbol{x})}{\partial(t^*, \boldsymbol{x}^*)} = \begin{pmatrix} 1 & \boldsymbol{0}_d^T \\ \dot{\boldsymbol{x}}_0 + \dot{\boldsymbol{Q}}^T(\boldsymbol{x}^* - \boldsymbol{x}_0^*)\boldsymbol{Q}^T\dot{\boldsymbol{x}}_0^* & \boldsymbol{Q}^T \end{pmatrix}. \tag{5.8}$$

Then we introduce the change of variables

$$\begin{align}
f(t, \boldsymbol{x}) &= f(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))), \tag{5.9} \\
\boldsymbol{u}(t, \boldsymbol{x}) &= \boldsymbol{u}(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))), \tag{5.10} \\
\boldsymbol{T}(t, \boldsymbol{x}) &= \boldsymbol{T}(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))). \tag{5.11}
\end{align}$$

for a scalar f, a vector $\boldsymbol{u}$ and a tensor $\boldsymbol{T}$. Next we consider the derivatives of these variable transformations. For a scalar we derive from (5.8) and (5.8)

$$\begin{align}
\frac{\partial f}{\partial t} &= \frac{\partial f}{\partial t^*} + \nabla_{\boldsymbol{x}^*} f \cdot (\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*)), \tag{5.12} \\
\nabla_{\boldsymbol{x}} f &= \boldsymbol{Q}^T \nabla_{\boldsymbol{x}^*} f. \tag{5.13}
\end{align}$$

Applying these equations componentwise we obtain for a vector

$$\begin{align}
\frac{\partial \boldsymbol{u}}{\partial t} &= \frac{\partial \boldsymbol{u}}{\partial t^*} + (\nabla_{\boldsymbol{x}^*} \boldsymbol{u})(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*)), \tag{5.14} \\
\nabla_{\boldsymbol{x}} \cdot \boldsymbol{u} &= \nabla_{\boldsymbol{x}^*} \cdot (\boldsymbol{Q}\boldsymbol{u}), \tag{5.15} \\
\nabla_{\boldsymbol{x}} \boldsymbol{u} &\equiv \left(\frac{\partial u_i}{\partial x_j} \right)_{ij} = (\nabla_{\boldsymbol{x}^*} \boldsymbol{u})\,\boldsymbol{Q}. \tag{5.16}
\end{align}$$

In particular, if $\boldsymbol{u}$ is an objective vector, i.e., $\boldsymbol{u} = \boldsymbol{Q}^T \boldsymbol{u}^*$ according to (5.3), then we have

$$\begin{align}
\frac{\partial \boldsymbol{u}}{\partial t} &= \boldsymbol{Q}^T \left(\frac{\partial \boldsymbol{u}^*}{\partial t^*} - \boldsymbol{A}\boldsymbol{u}^* + (\nabla_{\boldsymbol{x}^*} \boldsymbol{u}^*)\,\boldsymbol{Q}(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*)) \right), \tag{5.17} \\
\nabla_{\boldsymbol{x}} \boldsymbol{u} &= \boldsymbol{Q}^T (\nabla_{\boldsymbol{x}^*} \boldsymbol{u}^*)\,\boldsymbol{Q}. \tag{5.18}
\end{align}$$

Finally, we consider a tensor (matrix) $\boldsymbol{T}$ with $\boldsymbol{t}_i$ and $\boldsymbol{t}^i$ the ith column and row of $\boldsymbol{T}$, respectively. Then we obtain

$$\begin{align}
\frac{\partial \boldsymbol{T}}{\partial t} &= \frac{\partial \boldsymbol{T}}{\partial t^*} + ((\nabla_{\boldsymbol{x}^*} \boldsymbol{t}_1)(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*)), \dots, (\nabla_{\boldsymbol{x}^*} \boldsymbol{t}_d)(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*))), \tag{5.19} \\
\nabla_{\boldsymbol{x}} \cdot \boldsymbol{T} &\equiv \left(\nabla_{\boldsymbol{x}} \cdot \boldsymbol{t}^1, \dots, \nabla_{\boldsymbol{x}} \cdot \boldsymbol{t}^d \right)^T = \nabla_{\boldsymbol{x}^*} \cdot \left(\boldsymbol{T}\boldsymbol{Q}^T \right). \tag{5.20}
\end{align}$$

For $\boldsymbol{T} = f\boldsymbol{I}$ the divergence reads

$$\nabla_{\boldsymbol{x}} \cdot (f\boldsymbol{I}) = \boldsymbol{Q}^T \nabla_{\boldsymbol{x}^*} \cdot (f\boldsymbol{I}). \tag{5.21}$$

In case of an objective tensor, i.e., $\boldsymbol{T} = \boldsymbol{Q}^T \boldsymbol{T}^* \boldsymbol{Q}$ according to (5.3), we conclude from $\nabla_{\boldsymbol{x}^*} \boldsymbol{t}_m = \boldsymbol{Q}^T \left(\sum_n \nabla_{\boldsymbol{x}^*} \boldsymbol{t}_n^* Q_{nm} \right)$

$$\frac{\partial \boldsymbol{T}}{\partial t} = \boldsymbol{Q}^T \left(\frac{\partial \boldsymbol{T}^*}{\partial t^*} \boldsymbol{Q} - \boldsymbol{A}\boldsymbol{T}^*\boldsymbol{Q} + \boldsymbol{T}^*\dot{\boldsymbol{Q}} + \right. \tag{5.22}$$

$$\left. \sum_n (Q_{n1}(\nabla_{\boldsymbol{x}^*} \boldsymbol{t}_1^*)(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*)), \dots, Q_{nd}(\nabla_{\boldsymbol{x}^*} \boldsymbol{t}_d^*)(\dot{\boldsymbol{x}}_0^* + \boldsymbol{A}(\boldsymbol{x}^* - \boldsymbol{x}_0^*))) \right),$$

$$\nabla_{\boldsymbol{x}} \cdot \boldsymbol{T} = \boldsymbol{Q}^T \nabla_{\boldsymbol{x}^*} \cdot \boldsymbol{T}^*. \tag{5.23}$$

5.2. **Galilean transformation**

It is well-known that the fluid equations for a single phase are not invariant under a general Euclidean change of frame. For instance, Coriolis forces enter in case of a time-dependent rotation. However, the fluid equations are invariant under a Galilean transformation where we choose

$$\dot{\boldsymbol{x}}_0 = 0, \ \dot{\boldsymbol{Q}} = \boldsymbol{0} \quad \text{equiv.} \quad \boldsymbol{Q} = const, \quad \boldsymbol{x}_0^*(t) = \boldsymbol{c}_0 + \boldsymbol{c}_1 t, \ \boldsymbol{c}_1, \boldsymbol{c}_2 = const \tag{5.24}$$

in (5.1). For this transformation the velocity vector is still not objective but the acceleration and the rotation tensor are objective, because $\boldsymbol{A} = \boldsymbol{0}$. In the following we will confine ourselves to a Galilean transformation and derive constraints for the source terms $S_{\alpha,k}$, $S_{\alpha\rho,k}$, $S_{\alpha\rho\boldsymbol{v},k}$ and $S_{\alpha\rho E,k}$. First of all, we derive from the evolution equation (2.7) of the volume fractions using (5.12) and (5.13) and assuming that the volume fractions are objective, i.e., $\alpha_k^* = \alpha_k$,

$$\partial_{t^*} \alpha_k^* + \boldsymbol{V}_I^* \cdot \nabla_{\boldsymbol{x}^*} \alpha_k^* = S_{\alpha^*,k}^*, \ k = 1, \ldots, K, \tag{5.25}$$

where the interfacial velocity and the source term are given as

$$\boldsymbol{V}_I^* \ := \ \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q}\boldsymbol{V}_I + \dot{\boldsymbol{Q}}(\boldsymbol{x} - \boldsymbol{x}_0) = \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q}\boldsymbol{V}_I = \boldsymbol{c}_1 + \boldsymbol{Q}\boldsymbol{V}_I, \tag{5.26}$$

$$S_{\alpha^*,k}^* \ := \ S_{\alpha,k}. \tag{5.27}$$

Next we consider the evolution of mass. Assuming that the mass is objective, i.e., $\rho_k^* = \rho_k$, and using (5.12) and (5.15) we derive from (2.3)

$$\partial_{t^*} (\alpha_k^* \rho_k^*) + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^* \rho_k^* \boldsymbol{v}_k^*) = S_{\alpha^*\rho^*,k}^*, \tag{5.28}$$

with source term

$$S_{\alpha^*\rho^*,k}^* := S_{\alpha\rho,k}. \tag{5.29}$$

Note that (5.25) and (5.28) hold true for a general Euclidean change of frame (5.1). The transformation of the momentum equation (2.3) is cumbersome. It significantly simplifies in case of a Galilean transformation. Starting from (2.3) one has to employ (5.14), (5.5), (5.15), (5.13), (5.23) and incorporate (5.28). Assuming that the pressures p_k and $P_{k,l}$ and the stress tensors $\boldsymbol{T}_k$ are objective, i.e., $p_k^* = p_k$, $P_{k,l}^* = P_{k,l}$ and $\boldsymbol{T}_k^* = \boldsymbol{Q}\boldsymbol{T}_k\boldsymbol{Q}^T$, we obtain

$$\partial_{t^*} (\alpha_k^* \rho_k^* \boldsymbol{v}_k^*) + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^* \rho_k^* \boldsymbol{v}_k^* \boldsymbol{v}_k^{*T} + \alpha_k^* p_k^* \boldsymbol{I}) = -\sum_{l=1}^K P_{k,l}^* \nabla_{\boldsymbol{x}^*} \alpha_l^* + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^* \boldsymbol{T}_k^*) + \boldsymbol{S}_{\alpha^*\rho^*\boldsymbol{v}^*,k}^*, \tag{5.30}$$

with source term

$$\boldsymbol{S}_{\alpha^*\rho^*\boldsymbol{v}^*,k}^* := S_{\alpha\rho,k} \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q} \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}. \tag{5.31}$$

Finally we apply the Galilean transformation to the energy equation (2.4). Since the velocity is not an objective vector, the kinetic energy in the Galilean frame becomes

$$e_{kin,k}^* = e_{kin,k} + \dot{\boldsymbol{x}}_0^* \cdot \boldsymbol{v}_k^* - \frac{1}{2}(\dot{\boldsymbol{x}}_0^*)^2, \quad e_{kin,k} := \frac{1}{2}\boldsymbol{v}_k^2 \tag{5.32}$$

using (5.5). Thus the total energy and the total enthalpy are

$$E_k \ := \ e_k + \frac{1}{2}\boldsymbol{v}_k^2 = E_k^* - \dot{\boldsymbol{x}}_0^* \cdot \boldsymbol{v}_k^* + \frac{1}{2}(\dot{\boldsymbol{x}}_0^*)^2, \quad E_k^* := e_k^* + \frac{1}{2}(\boldsymbol{v}_k^*)^2, \tag{5.33}$$

$$H_k \ := \ E_k + \frac{p_k}{\rho_k} = H_k^* - \dot{\boldsymbol{x}}_0^* \cdot \boldsymbol{v}_k^* + \frac{1}{2}(\dot{\boldsymbol{x}}_0^*)^2, \quad H_k^* := E_k^* + \frac{p_k^*}{\rho_k^*}, \tag{5.34}$$

where we also assume objectivity of the internal energy, i.e., $e_k^* = e_k$. Again, after some tedious work of calculus using (5.2), (5.5), (5.13), (5.15) and incorporating (5.28), (5.30), the energy equation (2.4)

in the Galilean frame becomes

$$\partial_{t^*} \left(\alpha_k^* \rho_k^* E_k^* \right) + \nabla_{\boldsymbol{x}^*} \cdot \left(\alpha_k^* \rho_k^* \boldsymbol{v}_k^* \left(E_k^* + p_k^*/\rho_k^* \right) \right) = \tag{5.35}$$
$$- \sum_{l=1}^{K} P_{k,l}^* \boldsymbol{V}_I^* \cdot \nabla_{\boldsymbol{x}^*} \alpha_l^* + \nabla_{\boldsymbol{x}^*} \cdot \left(\alpha_k^* \left(\boldsymbol{v}_k^* \cdot \boldsymbol{T}_k^* - \boldsymbol{q}_k^* \right) \right) + S_{\alpha^* \rho^* E^*, k}^*,$$

with source term

$$S_{\alpha^* \rho^* E^*, k}^* := S_{\alpha \rho E, k} + \left(\boldsymbol{Q} \boldsymbol{S}_{\alpha \rho v, k} + S_{\alpha \rho, k} \dot{\boldsymbol{x}}_0^* \right) \cdot \boldsymbol{x}_0^* - \frac{1}{2} \left(\dot{\boldsymbol{x}}_0^* \right)^2 S_{\alpha \rho, k}. \tag{5.36}$$

Here we again assume objectivity of the pressure $P_{k,l}$ and the heat flux $\boldsymbol{q}_k$, i.e., $P_{k,l}^* = P_{k,l}$ and $\boldsymbol{q}_k^* = \boldsymbol{Q} \boldsymbol{q}_k$.
Thus we have proven the following

Theorem 5.1. *(Galilean Invariance) Let the following assumptions hold true*

(1) *α_k, ρ_k, p_k, e_k and $P_{k,l}$ are objective scalars,*

(2) *$\boldsymbol{q}_k$, $\boldsymbol{T}_k$ are objective vectors and tensors, respectively,*

(3) *all material parameters, e.g., μ_k, λ_k, are objective,*

(4) *the source terms (5.27), (5.29), (5.31), (5.36) are invariant under a Galilean transformation, i.e.,*

$$S_{\alpha^*, k}^* = S_{\alpha^*, k}, \ S_{(\alpha \rho)^*, k}^* = S_{(\alpha \rho)^*, k}, \ \boldsymbol{S}_{(\alpha \rho v)^*, k}^* = \boldsymbol{S}_{(\alpha \rho v)^*, k}, \ S_{(\alpha \rho E)^*, k}^* = S_{(\alpha \rho E)^*, k}. \tag{5.37}$$

Then the non-equilibrium model (2.2), (2.3), (2.4) and (2.7) with velocity $\boldsymbol{v}_k^* = \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q} \boldsymbol{v}_k$, interfacial velocity (5.26) and total energy (5.33) is Galilean invariant. This also holds true for the mixture model and the equilibrium model because they are derived from the non-equilibrium model by summation.

6. Thermodynamical properties: 2nd law of thermodynamics

From a physical point of view, a model is admissible if it is in agreement with the principles of thermodynamics. For this purpose we first derive the entropy law for the non-equilibrium model. Then we determine the entropy production terms of the mixture. To be consistent with the 2nd law of thermodynamics we have to check the sign of the entropy production terms. This will provide us with admissibility criteria for the interfacial pressures and velocity as well as the relaxation terms.

6.1. Entropy

In order to investigate thermodynamical properties of the non-equilibrium model (2.2), (2.3), (2.4) and (2.7), we assume that the entropy of each component satisfies

$$de_k = T_k ds_k - p_k d\tau_k, \tag{6.1}$$

where $\tau_k := 1/\rho_k$ is the specific volume of component k. Thus the pressure and the temperature are the partial derivatives of $e_k(\tau_k, s_k)$ that are assumed to be positive, i.e.,

$$p_k(\tau_k, s_k) = -\frac{\partial e_k}{\partial \tau_k}(\tau_k, s_k) \geq 0, \quad T_k(\tau_k, s_k) = \frac{\partial e_k}{\partial s_k}(\tau_k, s_k) \geq 0.$$

Furthermore, to ensure thermodynamical stability we assume that the Hessian of e_k is a convex function with respect to τ_k and s_k, i.e.,

$$\frac{\partial^2 e_k}{\partial^2 \tau_k}(\tau_k, s_k) \geq 0, \quad \frac{\partial^2 e_k}{\partial^2 s_k}(\tau_k, s_k) \geq 0, \quad \frac{\partial^2 e_k}{\partial^2 \tau_k}(\tau_k, s_k)\frac{\partial^2 e_k}{\partial^2 s_k}(\tau_k, s_k) \geq \left(\frac{\partial^2 e_k}{\partial \tau_k \partial s_k}(\tau_k, s_k)\right)^2.$$

Finally, the third law of thermodynamics implies

$$\tau_k \geq 0, \quad s_k \geq 0.$$

Assuming that p_k and T_k are strictly positive, then e_k becomes a monotone function in τ_k and s_k and we may change variables, i.e., $s_k = s_k(\tau_k, e_k)$ satisfying

$$T_k ds_k = de_k + p_k d\tau_k \tag{6.2}$$

with partial derivatives

$$\frac{\partial s_k}{\partial \tau_k}(\tau_k, e_k) = \frac{p_k}{T_k} > 0, \quad \frac{\partial s_k}{\partial e_k}(\tau_k, e_k) = \frac{1}{T_k} > 0. \tag{6.3}$$

It is well-known that $s_k = s_k(\tau_k, e_k)$ is a concave function, i.e., the Hessian is negative-definite

$$\frac{\partial^2 s_k}{\partial^2 \tau_k}(\tau_k, e_k) \leq 0, \quad \frac{\partial^2 s_k}{\partial^2 e_k}(\tau_k, e_k) \leq 0, \quad \frac{\partial^2 s_k}{\partial^2 \tau_k}(\tau_k, e_k)\frac{\partial^2 s_k}{\partial^2 e_k}(\tau_k, e_k) \geq \left(\frac{\partial^2 e_k}{\partial \tau_k \partial e_k}(\tau_k, e_k)\right)^2, \tag{6.4}$$

if and only if $e_k(\tau_k, s_k)$ is a convex function, i.e., thermodynamic stability holds.

6.2. Entropy equation

In order to derive the entropy equation we rewrite (6.2) as

$$T_k ds_k = de_k - \frac{p_k}{\rho_k^2} d\rho_k. \tag{6.5}$$

By means of the evolution equations (3.1) and (3.4) for the density and the internal energy we then deduce the entropy law

$$\partial_t s_k + \boldsymbol{v}_k \cdot \nabla s_k = \frac{1}{\alpha_k \rho_k T_k}\left(\sum_{l=1}^{K} P_{k,l}(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_l p_k(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_k \right. \tag{6.6}$$

$$\left. + \alpha_k \sum_{i,l=1}^{d} \frac{\partial v_{k,l}}{\partial x_i}(\boldsymbol{T}_k)_{l,i} - \nabla \cdot (\alpha_k \boldsymbol{q}_k) + S_{s,k}\right)$$

with the relaxation term

$$S_{s,k} := S_{e,k} - \frac{p_k}{\rho_k}S_{\alpha\rho,k} + p_k S_{\alpha,k}. \tag{6.7}$$

For the volume specific entropy we then obtain together with (2.2)

$$\partial_t(\alpha_k \rho_k s_k) + \nabla \cdot (\alpha_k \rho_k s_k \boldsymbol{v}_k) + \nabla \cdot (\frac{1}{T_k}\alpha_k \boldsymbol{q}_k) = \frac{1}{T_k}\left(\sum_{l=1}^{K} P_{k,l}(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_l \right. \tag{6.8}$$

$$\left. + p_k(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_k + \alpha_k \sum_{i,l=1}^{d} \frac{\partial v_{k,l}}{\partial x_i}(\boldsymbol{T}_k)_{l,i} - \alpha_k \frac{1}{T_k}\boldsymbol{q}_k \cdot \nabla T_k\right) + S_{\alpha\rho s,k}$$

with the relaxation term

$$S_{\alpha\rho s,k} := \frac{1}{T_k}S_{s,k} + s_k S_{\alpha\rho,k}. \tag{6.9}$$

Introducing the entropy of the components of the mixture

$$\rho s := \sum_{k=1}^{K} \alpha_k \rho_k s_k \tag{6.10}$$

we finally obtain with (2.12) the entropy law of the mixture

$$\partial_t \left(\rho s \right) + \nabla \cdot \left(\sum_{k=1}^{K} \alpha_k \rho_k s_k \boldsymbol{v}_k \right) + \nabla \cdot \left(\sum_{k=1}^{K} \frac{1}{T_k} \alpha_k \boldsymbol{q}_k \right) = \sum_{k=1}^{K} (\alpha_k \Sigma_k + \alpha_k \Delta_k + \Pi_k + S_{\alpha \rho s, k}), \tag{6.11}$$

where the production terms are defined as

$$\Pi_k \quad := \quad \frac{1}{T_k} \left(\sum_{l=1}^{K} P_{k,l} \left(\boldsymbol{v}_k - \boldsymbol{V}_I \right) \cdot \nabla \alpha_l + p_k (\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_k \right), \tag{6.12}$$

$$\Sigma_k \quad := \quad \frac{1}{T_k} \sum_{i,l=1}^{d} \frac{\partial v_{k,l}}{\partial x_i} (\boldsymbol{T}_k)_{l,i}, \tag{6.13}$$

$$\Delta_k \quad := \quad -\frac{1}{T_k^2} \boldsymbol{q}_k \cdot \nabla T_k. \tag{6.14}$$

Note that the total entropy of a homogeneous mixture is determined by the sum of ρs and the non-negative mixture entropy, [19], p. 320. We discuss the mixture entropy in the context of the relaxation terms for chemical potentials for a three-component mixture, see Section 8.3.2.

6.3. **Entropy production**

According to the 2nd law of thermodynamics the production terms (6.12), (6.13) and (6.14) have to be non-negative. In the subsequent sections we will derive sufficient conditions that ensure thermodynamical compatibility.

6.3.1. *Entropy production due to viscosity and heat conduction*

In order to verify the physically admissible sign of the entropy production term Σ_k we have to specify the viscous stress tensor $\boldsymbol{T}_k$ for each component. For an isotropic Newtonian fluid the stress tensor reads

$$\boldsymbol{T}_k = \mu_k \left(\nabla \boldsymbol{v}_k + \nabla \boldsymbol{v}_k{}^T - \frac{2}{3} (\nabla \cdot \boldsymbol{v}_k) \boldsymbol{I} \right). \tag{6.15}$$

Thus the components of this symmetric tensor are

$$(\boldsymbol{T}_k)_{l,i} = \mu_k \left(\frac{\partial v_{k,l}}{\partial x_i} + \frac{\partial v_{k,i}}{\partial x_l} - \frac{2}{3} \sum_{j=1}^{d} \frac{\partial v_{k,j}}{\partial x_j} \delta_{l,i} \right) = (\boldsymbol{T}_k)_{i,l}.$$

Then we compute for the entropy production term (6.13)

$$\frac{T_k}{\mu_k} \Sigma_k = 2 \sum_{i=1}^{d} \sum_{l=1}^{i-1} \left(\frac{\partial v_{k,l}}{\partial x_i} + \frac{\partial v_{k,i}}{\partial x_l} \right)^2 + \frac{2}{3} \Gamma$$

with

$$\Gamma \;\; := \;\; \sum_{i=1}^{d} \left(2 \left(\frac{\partial v_{k,i}}{\partial x_i} \right)^2 - \sum_{j=1,j\neq i}^{d} \frac{\partial v_{k,j}}{\partial x_j} \frac{\partial v_{k,i}}{\partial x_i} \right)$$

$$= \;\; \begin{cases} 2 \left(\frac{\partial v_{k,1}}{\partial x_1} \right)^2 & , d=1 \\[2mm] \left(\frac{\partial v_{k,1}}{\partial x_1} \right)^2 + \left(\frac{\partial v_{k,2}}{\partial x_2} \right)^2 + \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,2}}{\partial x_2} \right)^2 & , d=2 \\[2mm] \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,2}}{\partial x_2} \right)^2 + \left(\frac{\partial v_{k,2}}{\partial x_2} - \frac{\partial v_{k,3}}{\partial x_3} \right)^2 + \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,3}}{\partial x_3} \right)^2 & , d=3 \end{cases} .$$

Obviously, the following theorem holds true.

Theorem 6.1. *(Entropy production due to viscosity) The viscous stress tensors are determined by (6.15). Let the temperatures T_k and the viscosity coefficients μ_k, $k = 1, \ldots, K$, be non-negative. Then the production terms (6.13) are non-negative. In addition, because of the saturation condition (2.1), the entropy production due to viscosity $\sum_{k=1}^{K} \alpha_k \Sigma_k$ is non-negative.*

The heat fluxes are modeled by Fourier's law of heat conduction for a fluid with isotropic material property

$$\boldsymbol{q}_k = -\lambda_k \nabla T_k. \tag{6.16}$$

Then the entropy production term (6.14) reads

$$\Delta_k = \frac{1}{T_k^2} \lambda_k \nabla T_k \cdot \nabla T_k.$$

From this we directly conclude

Theorem 6.2. *(Entropy production due to heat conduction) The heat fluxes are determined by (6.16). Let the temperatures T_k and the heat conduction coefficients λ_k, $k = 1, \ldots, K$, be non-negative. Then the production terms (6.14) are non-negative. In addition, because of the saturation condition (2.1), the entropy production due to heat conduction $\sum_{k=1}^{K} \alpha_k \Delta_k$ is non-negative.*

6.3.2. *Interfacial velocity and pressure*

To investigate the admissibility of the production terms Π_k we first make use of the assumptions (2.5) and (2.14) for the interfacial pressures. Then these terms become

$$\Pi_k = \frac{1}{T_k} \sum_{l=1,l\neq k}^{K} (P_{k,l} - p_k) \, (\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_l.$$

Obviously, we cannot control the sign of Π_k. According to the conservation constraints (2.14) all $P_{k,l}$, $k \neq l$, are coupled. Therefore we determine the interfacial pressures $P_{k,l}$ and the interfacial velocity $\boldsymbol{V}_I$ such that the sum $\Pi := \sum_{k=1}^{K} \Pi_k$ vanishes. For this purpose we substitute $\nabla \alpha_K$ by the other gradients using (2.8). According to the saturation condition (2.1) the gradients $\nabla \alpha_k$, $k = 1, \ldots, K-1$, are linearly independent. Thus rearranging the terms in Π with respect to the $K - 1$ gradients of α_k the coefficients in front of these gradients must be zero when Π vanishes. This yields the following $K - 1$ conditions

$$\sum_{k=1,k\neq l}^{K-1} \frac{1}{T_k} \left((P_{k,l} - p_k) - (P_{k,K} - p_k) \right) (\boldsymbol{v}_k - \boldsymbol{V}_I) + \frac{1}{T_K} (P_{K,l} - p_K)(\boldsymbol{v}_K - \boldsymbol{V}_I) = \boldsymbol{0} \tag{6.17}$$

for $l = 1, \ldots, K - 1$. Next we assume that the interfacial velocity is a convex combination of the single component velocities $\boldsymbol{v}_k$, i.e.,

$$\boldsymbol{V}_I = \sum_{k=1}^{K} \beta_k \boldsymbol{v}_k, \quad \beta_k \in [0,1], \quad \sum_{k=1}^{K} \beta_k = 1. \tag{6.18}$$

This is motivated by Gallouët et al. [10] and Hèrard [14] for a two-phase and a three-phase model, respectively. Then we may rewrite the velocity differences in (6.17) as

$$\boldsymbol{v}_K - \boldsymbol{V}_I = \sum_{i=1}^{k-1} \sum_{j=1}^{i} (-\beta_j) \left(\boldsymbol{v}_i - \boldsymbol{v}_{i+1}\right) + \sum_{i=k}^{K-1} \sum_{j=i+1}^{K} \beta_j \left(\boldsymbol{v}_i - \boldsymbol{v}_{i+1}\right).$$

Rearranging (6.17) in terms of the linearly independent differences $\boldsymbol{v}_i - \boldsymbol{v}_{i+1}$, $i = 1, \ldots, K - 1$, we obtain the following conditions

$$\sum_{k=1}^{i} \frac{1}{T_k} \left((P_{k,l} - p_k)(1 - \delta_{l,k}) - (P_{k,K} - p_k) \right) \sum_{j=i+1}^{K} \beta_j + \tag{6.19}$$

$$\left(\sum_{k=i+1}^{K-1} \frac{1}{T_k} \left((P_{k,l} - p_k)(1 - \delta_{l,k}) - (P_{k,K} - p_k) \right) + \frac{1}{T_K} (P_{K,l} - p_K) \right) \sum_{j=1}^{i} (-\beta_j) = 0$$

or, equivalently,

$$\sum_{k=1}^{i} \left(\frac{1}{T_k}(1 - \delta_{l,k}) \sum_{j=i+1}^{K} \beta_j \right) P_{k,l} - \sum_{k=1}^{i} \left(\frac{1}{T_k} \sum_{j=i+1}^{K} \beta_j \right) P_{k,K} - $$

$$\sum_{k=i+1}^{K-1} \left(\frac{1}{T_k}(1 - \delta_{l,k}) \sum_{j=1}^{i} \beta_j \right) P_{k,l} + \sum_{k=i+1}^{K-1} \left(\frac{1}{T_k} \sum_{j=1}^{i} \beta_j \right) P_{k,K} - \frac{1}{T_K} \sum_{j=1}^{i} \beta_j P_{K,l} = \tag{6.20}$$

$$-\sum_{k=1}^{i} \frac{1}{T_k} p_k \delta_{l,k} \sum_{j=i+1}^{K} \beta_j + \left(\sum_{k=i+1}^{K-1} \frac{1}{T_k} p_k \delta_{l,k} - \frac{1}{T_K} p_K \right) \sum_{j=1}^{i} \beta_j$$

for $l, i = 1, \ldots, K - 1$. This gives $(K-1)^2$ equations for $(K-1)K$ unknowns $P_{k,l}$, $k, l = 1, \ldots, K$, $k \neq l$. Thus we need additional $K - 1$ equations to ensure uniqueness for fixed parameters $\beta_1, \ldots, \beta_K$. These equations are determined by the conservation constraints (2.14) that read

$$\sum_{k=1, k \neq l}^{K} P_{k,l} = P_I = const, \quad l = 1, \ldots, K. \tag{6.21}$$

These equations are equivalent to

$$\sum_{k=1, k \neq l}^{K} P_{k,l} - \sum_{k=1}^{K-1} P_{k,K} = 0, \quad l = 1, \ldots, K - 1, \tag{6.22}$$

Then (6.20) and (6.22) form a linear system for the interfacial pressures. For a two-component model, i.e., $K = 2$, the solution is given by

$$P_{1,2} = P_{2,1} = \frac{p_1 \beta_2 / T_1 + p_2 \beta_1 / T_2}{\beta_2 / T_1 + \beta_1 / T_2} = P_I. \tag{6.23}$$

20

For a three-component model Hérard [14] proved that (6.20) and (6.22) has a unique solution that is given by

$$
\begin{aligned}
P_{1,2} &= \frac{\beta_1 p_2 T_1 + \beta_2 p_1 T_2 + \beta_3 p_1 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}, \ P_{2,1} = \frac{\beta_1 p_2 T_1 + \beta_2 p_1 T_2 + \beta_3 p_2 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}, \\
P_{1,3} &= \frac{\beta_1 p_3 T_1 + \beta_2 p_1 T_2 + \beta_3 p_1 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}, \ P_{3,1} = \frac{\beta_1 p_3 T_1 + \beta_2 p_3 T_2 + \beta_3 p_1 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}, \\
P_{2,3} &= \frac{\beta_1 p_2 T_1 + \beta_2 p_3 T_2 + \beta_3 p_1 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}, \ P_{3,2} = \frac{\beta_1 p_3 T_1 + \beta_2 p_3 T_2 + \beta_3 p_2 T_3}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}
\end{aligned}
\tag{6.24}
$$

and, thus,

$$
P_I = \frac{\beta_1 T_1 (p_2 + p_3) + \beta_2 T_2 (p_1 + p_3) + \beta_3 T_3 (p_1 + p_2)}{\beta_1 T_1 + \beta_2 T_2 + \beta_3 T_3}.
\tag{6.25}
$$

As a consequence, we observe that in general $P_{k,l} = P_{l,k}$ only holds at pressure equilibrium where $P_I = 2p$. Whether there exists a unique solution to (6.20) and (6.22) for $K \geq 4$ and arbitrary convex combination (6.18) for the interfacial velocity $\boldsymbol{V}_I$ is still open. However, for the multi-component model the following result can be proven.

Theorem 6.3. *(Entropy production due to interfacial states) Let the assumptions (2.5) and (2.14) hold true. Then the production term $\Pi = \sum_{k=1}^{K} \Pi_k$ vanishes provided that the interfacial pressures $P_{k,l}$ are a solution to the linear system (6.20) and the interfacial velocity $\boldsymbol{V}_I$ satisfies (6.18).*

In particular, if we choose $\beta_1 = 1$, $\beta_2 = \ldots, \beta_K = 0$, then the interfacial pressures

$$
\begin{aligned}
&P_{k,l} = p_k, \ k = 2, \ldots, K-1, \ l = 1, \ldots, K-1 \\
&P_{1,K} = p_K, \ P_{k,K} = p_k, \ k = 2, \ldots, K-1, \\
&P_{K,l} = p_K, \ l = 1, \ldots, K-1, \\
&P_{1,l} = P_{l,K} = p_l, \ l = 2, \ldots, K-1
\end{aligned}
$$

are a solution of (6.20). Thus the interfacial pressure and the interfacial velocity are

$$
P_I = \sum_{k=2}^{K} p_k, \quad \boldsymbol{V}_I = \boldsymbol{v}_1.
\tag{6.26}
$$

Note that for $K = 2$ and $K = 3$ the interfacial states (6.26) coincide with those given in [10] and [14], respectively. In [10] another alternative is given for a two-phase model that has been proven in [23] to cancel the term Π. Since by means of the linear system (6.20) the interfacial pressures $P_{k,l}$ depend on the convex combination (6.18) for the interfacial velocity $\boldsymbol{V}_I$ there might be other options to choose the interfacial pressures, i.e., the 2nd law of thermodynamics does not uniquely characterize the interfacial pressure and interfacial velocity. In Section 8.3 we discuss another choice for the interfacial velocity.

6.3.3. *Entropy production due to relaxation*

According to the entropy law (6.8) of a single component the entropy production due to the relaxation processes is determined by

$$
S_{\alpha\rho s,k} = \frac{1}{T_k} \left(p_k S_{\alpha,k} + (u_k - g_k) S_{\alpha\rho,k} - \boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho v,k} + S_{\alpha\rho E,k} \right),
\tag{6.27}
$$

where we plug (6.7) and (3.5) into (6.9). Here the Gibbs free energy of component k is defined as

$$
g_k = e_k + p_k/\rho_k - T_k s_k
\tag{6.28}
$$

In addition to the conservation constraints (2.13) the relaxation terms (2.9) have to satisfy

$$S_{\rho s,k} \geq 0, \ k = 1,\ldots,K \text{ or } \sum_{k=1}^{K} S_{\alpha \rho s,k} \geq 0. \tag{6.29}$$

to ensure that the mixture is consistent with the 2nd law of thermodynamics.

7. Entropy-entropy flux pairs

From a mathematical point of view, the concept of entropy-entropy flux pairs, cf. [11], has been introduced to characterize a unique weak solution of an initial (boundary) value problem of (inhomogeneous) conservation laws that in quasi-conservative form reads

$$\partial_t \, \boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{A}_i(\boldsymbol{u}) \partial_{x_i} \, \boldsymbol{u} = \boldsymbol{S}(\boldsymbol{u}), \quad \boldsymbol{A}_i(\boldsymbol{u}) := \frac{\partial \, \boldsymbol{f}_i}{\partial \, \boldsymbol{u}}(\boldsymbol{u}) \tag{7.1}$$

where $\boldsymbol{u} : \mathbb{R}_+ \times \Omega \to D \subset \mathbb{R}^m$ with $\Omega \subset \mathbb{R}^d$, $\boldsymbol{f}_i : D \to \mathbb{R}^m$, $i = 1,\ldots,d$ and $\boldsymbol{S} : D \to \mathbb{R}^m$, denote the vector of m conserved quantities, the fluxes in the ith coordinate direction, $i = 1,\ldots,d$, and the source function, respectively. Motivated by thermodynamics, the entropy inequality

$$\partial_t \, U(\boldsymbol{u}) + \sum_{i=1}^{d} \partial_{x_i} \, \boldsymbol{F}_i(\boldsymbol{u}) \leq 0 \tag{7.2}$$

has to hold in a weak sense for any convex function $U : D \to \mathbb{R}$ and functions $F_i : D \to \mathbb{R}$, $i = 1,\ldots,d$, referred to as entropy and entropy flux, that satisfy the compatibility conditions

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \, \boldsymbol{A}_i(\boldsymbol{u}) = \nabla_{\boldsymbol{u}} F_i(\boldsymbol{u})^T, \ i = 1,\ldots,d. \tag{7.3}$$

Due to these conditions we infer for smooth solutions of (7.1) the entropy equation

$$\partial_t \, U(\boldsymbol{u}) + \sum_{i=1}^{d} \partial_{x_i} \, F_i(\boldsymbol{u}) = \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \, \boldsymbol{S}(\boldsymbol{u}), \tag{7.4}$$

Obviously, the entropy inequality (7.2) holds if and only if the entropy production is negative, i.e.,

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \, \boldsymbol{S}(\boldsymbol{u}) \leq 0. \tag{7.5}$$

Motivated by the entropy equation (6.11) a candidate for an entropy-entropy flux pair for our non-equilibrium model (2.2), (2.3), (2.4) and (2.7) neglecting viscosity and heat conduction is

$$U(\boldsymbol{u}) := -\sum_{k=1}^{K} \alpha_k \rho_k s_k = -\rho s, \quad F_i(\boldsymbol{u}) := -\sum_{k=1}^{K} \alpha_k \rho_k s_k v_{k,i}, \ i = 1,\ldots,d. \tag{7.6}$$

It remains to verify the convexity of U and the compatibility conditions (7.3).

7.1. Convexity of entropy function

In order to verify that U is a convex function of the quantities $\boldsymbol{u} := (\boldsymbol{\alpha}, \alpha_1 \boldsymbol{u}_1^T, \ldots, \alpha_K \boldsymbol{u}_K^T)^T$ with $\boldsymbol{\alpha} := (\alpha_1, \ldots, \alpha_{K-1})^T$ and $\boldsymbol{u}_k := (\rho_k, \rho_k \boldsymbol{v}_k^T, \rho_k E_k)^T$ we extend the proof in [23], Appendix A, for a two-phase model to our K-component model. The key idea is to employ the fact that

$$U_k(\boldsymbol{u}_k) := -\rho_k s_k$$

is a convex function of the quantities $\boldsymbol{u}_k$ of component k. In [12], p. 99 ff, it is proven that the entropy U_k is a convex function of $\boldsymbol{u}_k$, if e_k is a convex function of (τ_k, s_k).

To verify the convexity of U we need to prove that the Hessian is positive semi-definite. First of all, we note that by (2.1)

$$\frac{\partial \alpha_k}{\partial \alpha_l} = \delta_{k,l} - \delta_{k,K}, \quad \frac{\partial \boldsymbol{u}_k}{\partial \alpha_l} = -\frac{1}{\alpha_k} \boldsymbol{u}_k (\delta_{k,l} - \delta_{k,K}), \quad \frac{\partial \boldsymbol{u}_k}{\partial \alpha_l \boldsymbol{u}_l} = \frac{1}{\alpha_k} \delta_{k,l} \boldsymbol{I}_{d+2}$$

holds for $k = 1, \ldots, K$, $l = 1, \ldots, K - 1$. Then it follows for the gradient of U:

$$\frac{\partial U}{\partial \alpha_l}(\boldsymbol{u}) = U_l(\boldsymbol{u}_l) - U_K(\boldsymbol{u}_K) - \frac{\partial U_l}{\partial \boldsymbol{u}_l}(\boldsymbol{u}_l) \cdot \boldsymbol{u}_l + \frac{\partial U_K}{\partial \boldsymbol{u}_K}(\boldsymbol{u}_K) \cdot \boldsymbol{u}_K, \quad \frac{\partial U}{\partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) = \frac{\partial U_l}{\partial \boldsymbol{u}_l}(\boldsymbol{u}_l). \quad (7.7)$$

The Hessian of U is determined by the second order derivatives

$$\frac{\partial^2 U}{\partial \alpha_k \partial \alpha_l}(\boldsymbol{u}) = \delta_{k,l} \frac{1}{\alpha_l} \boldsymbol{u}_l^T \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l)\boldsymbol{u}_l + \frac{1}{\alpha_K} \boldsymbol{u}_K^T \frac{\partial^2 U_K}{\partial^2 \boldsymbol{u}_K}(\boldsymbol{u}_K)\boldsymbol{u}_K, \ k,l = 1, \ldots, K,$$

$$\frac{\partial^2 U}{\partial \alpha_k \partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) = -\frac{1}{\alpha_l}(\delta_{k,l} - \delta_{K,l}) \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l)\boldsymbol{u}_l, l = 1, \ldots, K, \ k = 1, \ldots, K-1,$$

$$\frac{\partial^2 U}{\partial \alpha_k \boldsymbol{u}_k \partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) = \frac{1}{\alpha_l} \delta_{k,l} \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l), \ k,l = 1, \ldots, K.$$

For a compact representation of the Hessian we introduce the notation

$$\boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} := \left(\frac{\partial^2 U}{\partial \alpha_k \partial \alpha_l}(\boldsymbol{u}) \right)_{l,k=1,\ldots,K-1} \in \mathbb{R}^{(K-1)\times(K-1)},$$

$$\boldsymbol{U}_{\alpha_k \boldsymbol{u_k}, \alpha_k \boldsymbol{u_k}} := \frac{\partial^2 U}{\partial \alpha_k \boldsymbol{u}_k \partial \alpha_k \boldsymbol{u}_k}(\boldsymbol{u}) \in \mathbb{R}^{(d+2)\times(d+2)},$$

$$\boldsymbol{U}_{\alpha_k \boldsymbol{u_k}, \boldsymbol{\alpha}} := \left(\frac{\partial^2 U}{\partial \alpha_k \boldsymbol{u}_k \partial \alpha_1}(\boldsymbol{u}), \ldots, \frac{\partial^2 U}{\partial \alpha_k \boldsymbol{u}_k \partial \alpha_{K-1}}(\boldsymbol{u}) \right) \in \mathbb{R}^{(d+2)\times(K-1)}.$$

According to the above second order derivatives these are determined by

$$\boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} = \frac{1}{\alpha_K} \boldsymbol{u}_K^T \boldsymbol{U}_K'' \boldsymbol{u}_K \boldsymbol{1}_{K-1} + \text{diag}\left(\left(\frac{1}{\alpha_k} \boldsymbol{u}_k^T \boldsymbol{U}_k'' \boldsymbol{u}_k \right)_{k=1,\ldots,K-1} \right), \quad (7.8)$$

$$\boldsymbol{U}_{\alpha_k \boldsymbol{u_k}, \alpha_k \boldsymbol{u_k}} = \frac{1}{\alpha_k} \boldsymbol{U}_k'', \quad (7.9)$$

$$\boldsymbol{U}_{\alpha_k \boldsymbol{u_k}, \boldsymbol{\alpha}} = \left(-\frac{1}{\alpha_k}(\delta_{k,l} - \delta_{K,k}) \boldsymbol{U}_k'' \boldsymbol{u}_k \right)_{l=1,\ldots,K-1} = \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_k \boldsymbol{u}_k}^T, \quad (7.10)$$

where $\boldsymbol{U}_k''$ denotes the Hessian of the entropy $U_k = U_k(\boldsymbol{u}_k)$ of component k. Then the Hessian can be represented as block-matrix

$$\boldsymbol{U}''(\boldsymbol{u}) = \begin{pmatrix} \boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} & \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_1 \boldsymbol{u_1}} & \cdots & \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_1 \boldsymbol{u_K}} \\ \boldsymbol{U}_{\alpha_1 \boldsymbol{u_1},\boldsymbol{\alpha}} & \boldsymbol{U}_{\alpha_1 \boldsymbol{u_1},\alpha_1 \boldsymbol{u_1}} & & \\ \vdots & & \ddots & \\ \boldsymbol{U}_{\alpha_K \boldsymbol{u_K},\boldsymbol{\alpha}} & & & \boldsymbol{U}_{\alpha_1 \boldsymbol{u_K},\alpha_K \boldsymbol{u_K}} \end{pmatrix}. \quad (7.11)$$

To verify positive semi-definiteness of the Hessian we introduce the vector $\boldsymbol{x} = (\boldsymbol{a}^T, \boldsymbol{b}_1^T, \ldots, \boldsymbol{b}_K^T)^T$ with $\boldsymbol{a} \in \mathbb{R}^{K-1}$ and $\boldsymbol{b}_k \in \mathbb{R}^{d+2}$, $k = 1, \ldots, K$. Then we obtain by the block-structure (7.11) of the Hessian

$$\boldsymbol{x}^T \boldsymbol{U}'' \boldsymbol{x} = \boldsymbol{a}^T \boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} \boldsymbol{a} + \sum_{k=1}^{K} \boldsymbol{a}^T \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_k \boldsymbol{u_k}} \boldsymbol{b}_k + \sum_{k=1}^{K} \boldsymbol{b}_k^T \left(\boldsymbol{U}_{\alpha_k \boldsymbol{u_k},\boldsymbol{\alpha}} \boldsymbol{a} + \boldsymbol{U}_{\alpha_k \boldsymbol{u_k},\alpha_k \boldsymbol{u_k}} \boldsymbol{b}_k \right). \quad (7.12)$$

By means of (7.8), (7.9) and (7.10) we determine

$$
\boldsymbol{a}^T \boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} \boldsymbol{a} = \frac{1}{\alpha_K}(a\boldsymbol{u}_K)^T \boldsymbol{U}_K''(a\boldsymbol{u}_K) + \sum_{k=1}^{K-1} \frac{1}{\alpha_k}(a_k \boldsymbol{u}_k)^T \boldsymbol{U}_k''(a_k \boldsymbol{u}_k), \quad a := \sum_{l=1}^{K-1} a_l,
$$

$$
\boldsymbol{a}^T \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_k \boldsymbol{u_k}} \boldsymbol{b}_k = -\sum_{l=1}^{K-1} \frac{1}{\alpha_k}(\delta_{k,l} - \delta_{k,K})\boldsymbol{b}_k^T \boldsymbol{U}_k''(a_l \boldsymbol{u}_k),
$$

$$
\boldsymbol{b}_k^T \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_k \boldsymbol{u_k}} \boldsymbol{a} = -\sum_{l=1}^{K-1} \boldsymbol{b}_k^T \boldsymbol{U}_{\alpha_k \boldsymbol{u}_k,\alpha_l} a_l = \frac{1}{\alpha_K}\delta_{k,K}\boldsymbol{b}_K^T \boldsymbol{U}_K''(a\boldsymbol{u}_K) - \frac{1}{\alpha_k}(1 - \delta_{k,K})\boldsymbol{b}_k^T \boldsymbol{U}_k''(a_k \boldsymbol{u}_k),
$$

$$
\boldsymbol{b}_k^T \boldsymbol{U}_{\alpha_k \boldsymbol{u_k},\alpha_k \boldsymbol{u_k}} \boldsymbol{b}_k = \frac{1}{\alpha_k}\boldsymbol{b}_k^T \boldsymbol{U}_k'' \boldsymbol{b}_k.
$$

Incorporating this into (7.12) we finally conclude after some calculus with

$$
\boldsymbol{x}^T \boldsymbol{U}'' \boldsymbol{x} = \sum_{k=1}^{K-1} \frac{1}{\alpha_k}(\boldsymbol{b}_k - a_k \boldsymbol{u}_k)^T \boldsymbol{U}_k''(\boldsymbol{b}_k - a_k \boldsymbol{u}_k) + \frac{1}{\alpha_K}(\boldsymbol{b}_K - a\boldsymbol{u}_K)^T \boldsymbol{U}_K''(\boldsymbol{b}_K - a\boldsymbol{u}_K) \geq 0,
$$

because the Hessians $\boldsymbol{U}_k''$ are assumed to be positive semi-definite. Note that for $\boldsymbol{x} \neq \boldsymbol{0}$ we cannot ensure $\boldsymbol{x}^T \boldsymbol{U}'' \boldsymbol{x}$ to be positive even if $\boldsymbol{U}_k''$ is strictly convex because all the terms $\boldsymbol{b}_k - a_k \boldsymbol{u}_k$, $k = 1, \ldots, K-1$, and $\boldsymbol{b}_K - a\boldsymbol{u}_K$ may vanish at the same time. Thus we have proven the following

Theorem 7.1. *(Convexity of entropy function) Let e_k be a convex function of (τ_k, s_k), $k = 1, \ldots, K$. Then the entropy U is a convex function of $\boldsymbol{u}$, i.e, the Hessian of U is positive semi-definite.*

7.2. Compatibility conditions

In order to verify the compatibility conditions (7.3) it is preferable to compute the derivatives in terms of primitive variables instead of conserved variables for reasons of simplicity. Therefore we first consider how an entropy-entropy flux pair transforms under a change of variables $\boldsymbol{u} = \boldsymbol{u}(\boldsymbol{w})$ with regular Jacobian

$$
\boldsymbol{T}(\boldsymbol{w}) := \left(\frac{\partial u_i}{\partial w_j}(\boldsymbol{w}) \right)_{i,j=1,\ldots,d}.
$$

Under this transformation the system of conservation laws (7.1) becomes a quasi-conservative system

$$
\partial_t \boldsymbol{w} + \sum_{i=1}^{d} \boldsymbol{B}_i(\boldsymbol{w}) \, \partial_{x_i} \boldsymbol{w} = \overline{\boldsymbol{S}}(\boldsymbol{w}) \tag{7.13}
$$

with

$$
\boldsymbol{B}_i(\boldsymbol{w}) := \boldsymbol{T}(\boldsymbol{w})^{-1} \boldsymbol{A}_i(\boldsymbol{u}(\boldsymbol{w})) \, \boldsymbol{T}(\boldsymbol{w}), \ \ \overline{\boldsymbol{S}}(\boldsymbol{w}) := \boldsymbol{T}(\boldsymbol{w})^{-1} \boldsymbol{S}(\boldsymbol{u}(\boldsymbol{w})).
$$

Introducing

$$
W(\boldsymbol{w}) := U(\boldsymbol{u}(\boldsymbol{w})), \ G_i(\boldsymbol{w}) := F_i(\boldsymbol{u}(\boldsymbol{w})), \ i = 1, \ldots, d,
$$

we conclude by a straight-forward calculation

$$
\nabla_{\boldsymbol{w}} W(\boldsymbol{w}) = (\boldsymbol{T}(\boldsymbol{w}))^T \nabla_{\boldsymbol{u}} U(\boldsymbol{u}(\boldsymbol{w})), \ \nabla_{\boldsymbol{w}} G_i(\boldsymbol{w})^T = \nabla_{\boldsymbol{u}} U(\boldsymbol{u}(\boldsymbol{w}))^T \boldsymbol{A}_i(\boldsymbol{u}(\boldsymbol{w})) \, \boldsymbol{T}(\boldsymbol{w})
$$

and, hence,

$$
\nabla_{\boldsymbol{w}} W(\boldsymbol{w})^T \boldsymbol{B}_i(\boldsymbol{w}) = \nabla_{\boldsymbol{w}} G_i(\boldsymbol{w})^T, \tag{7.14}
$$

i.e., (U, F_i) satisfies the compatibility conditions (7.3) if and only if (W, G_i) satisfies the compatibility conditions (7.14). However, the function W must not be convex although U is a convex function. This directly follows from the Hessian of W

$$\nabla_{\boldsymbol{w}\boldsymbol{w}} W(\boldsymbol{w}) = \boldsymbol{T}^T(\boldsymbol{w}) \, \nabla_{\boldsymbol{u}\boldsymbol{u}} U(\boldsymbol{u}(\boldsymbol{w})) \, \boldsymbol{T}(\boldsymbol{w}) + \sum_{l=1}^{m} \frac{\partial U}{\partial u_l}(\boldsymbol{u}(\boldsymbol{w})) \, \nabla_{\boldsymbol{w}\boldsymbol{w}} u_l(\boldsymbol{w}).$$

If the variable transformation is nonlinear, then the second term on the right-hand side must not be positive-definite.

Neglecting viscosity and heat conduction our non-equilibrium model (2.2), (2.3), (2.4) and (2.7) can be written in quasi-conservative form (7.1) for $\boldsymbol{u} = (\boldsymbol{\alpha}^T, \boldsymbol{u}_1^T, \ldots, \boldsymbol{u}_K^T)^T$ with $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_{K-1})^T$ and $\boldsymbol{u}_k = \alpha_k \rho_k (1, \boldsymbol{v}_k^T, E_k)^T$, $k = 1, \ldots, K$. Note that the notation slightly differs from the one in Section 7.1. Obviously, the non-equilibrium model cannot be written in conservative form, i.e., the corresponding matrices $\boldsymbol{A}_i$ are not Jacobians of fluxes $\boldsymbol{f}_i$. However, this does not affect the above discussion on entropy-entropy flux pairs. This non-equilibrium model is rewritten in terms of $\boldsymbol{w} = (\boldsymbol{\alpha}^T, \boldsymbol{w}_1^T, \ldots, \boldsymbol{w}_K^T)^T$ with the primitive variables $\boldsymbol{w}_k = (\rho_k, \boldsymbol{v}_k^T, e_k)^T$. The Jacobian of the transformation is given by

$$\boldsymbol{T}(\boldsymbol{w}) = \begin{pmatrix} \boldsymbol{I}_{K-1} & & \\ \boldsymbol{D}_1 & \boldsymbol{C}_1 & \\ \vdots & & \ddots \\ \boldsymbol{D}_K & & \boldsymbol{C}_K \end{pmatrix}, \qquad \begin{aligned} \boldsymbol{C}_k &:= \alpha_k \begin{pmatrix} 1 & \boldsymbol{0}_d^T & 0 \\ \boldsymbol{v}_k & \rho_k \boldsymbol{I}_d & \boldsymbol{0}_d \\ e_k + \frac{1}{2}\boldsymbol{v}_k^2 & \rho_k \boldsymbol{v}_k^T & \rho_k \end{pmatrix}, \\ \boldsymbol{D}_k &:= \rho_k \begin{pmatrix} 1 \\ \boldsymbol{v}_k \\ e_k + \frac{1}{2}\boldsymbol{v}_k^2 \end{pmatrix} (\boldsymbol{e}_{k,K-1} - \boldsymbol{1}_{K-1} \delta_{k,K})^T, \end{aligned}$$

where $\boldsymbol{e}_{k,K-1}$ is the kth unit vector in $\mathbb{R}^{K-1}$, $\boldsymbol{1}_{K-1}$ the unity vector in $\mathbb{R}^{K-1}$, $\boldsymbol{0}_d$ the zero vector in $\mathbb{R}^d$ and $\boldsymbol{I}_d$ the unity matrix in $\mathbb{R}^{d\times d}$. Obviously, the transformation is regular, if and only if the densities ρ_k, $k = 1, \ldots, K$ are positive. The quasi-conservative system corresponding to this transformation is given by (2.7), (2.2), (3.2) and (3.4) where we neglect viscosity and heat conduction. The matrices $\boldsymbol{B}_i$ in (7.13) are given by the block-matrices

$$\boldsymbol{B}_i(\boldsymbol{w}) = \begin{pmatrix} V_{I,i} \boldsymbol{I}_{K-1} & & \\ \boldsymbol{A}_{1,i} & \boldsymbol{B}_{1,i} & \\ \vdots & & \ddots \\ \boldsymbol{A}_{1,K} & & \boldsymbol{B}_{K,i} \end{pmatrix}, \qquad \begin{aligned} \boldsymbol{B}_{k,i} &:= \alpha_k \begin{pmatrix} v_{k,i} & \rho_k \boldsymbol{e}_{i,d}^T & 0 \\ \frac{1}{\rho_k}\frac{\partial p_k}{\partial \rho_k}\boldsymbol{e}_{i,d} & v_{k,i}\boldsymbol{I}_d & \frac{1}{\rho_k}\frac{\partial p_k}{\partial e_k}\boldsymbol{e}_{i,d} \\ 0 & \frac{p_k}{\rho_k}\boldsymbol{e}_{i,d}^T & v_{k,i} \end{pmatrix}, \\ \boldsymbol{A}_{k,i} &:= \rho_k \begin{pmatrix} \frac{\rho_k}{\alpha_k}(v_{k,i} - V_{I,i})(\boldsymbol{e}_{k,K-1} - \boldsymbol{1}_{K-1}\delta_{k,K})^T \\ \boldsymbol{e}_{i,d}\boldsymbol{\beta}_k^T \\ \boldsymbol{\gamma}_k^T \end{pmatrix}, \end{aligned}$$

with

$$\beta_{k,l} = \frac{1}{\alpha_k \rho_k} \left((P_{k,l}^M - p_k)(1 - \delta_{k,l}) - (P_{k,K}^M - p_k)(1 - \delta_{k,K}) \right),$$

$$\gamma_{k,l} = \frac{1}{\alpha_k \rho_k} \left((P_{k,l}^E V_{I,i} - P_{k,l}^M v_{k,i})(1 - \delta_{k,l}) - (P_{k,K}^E V_{I,i} - P_{k,K}^M v_{k,i})(1 - \delta_{k,K}) \right).$$

Then W and G_i are given by

$$W(\boldsymbol{w}) = -\sum_{k=1}^{K} \alpha_k \rho_k s_k(1/\rho_k, e_k), \ G_i(\boldsymbol{w}) = -\sum_{k=1}^{K} \alpha_k \rho_k s_k(1/\rho_k, e_k) v_{k,i}$$

25

with gradients

$$\begin{aligned}
\nabla_{\boldsymbol{\alpha}} W(\boldsymbol{w}) &= (\rho_K s_K - \rho_1 s_1, \ldots, \rho_K s_K - \rho_{K-1} s_{K-1})^T, \\
\nabla_{\boldsymbol{w_k}} W(\boldsymbol{w}) &= -(\alpha_k(s_k - p_k/(\rho_k T_k)), \boldsymbol{0}_d^T, \alpha_k \rho_k/T_k)^T, \\
\nabla_{\boldsymbol{\alpha}} G_i(\boldsymbol{w}) &= (\rho_K s_K v_{K,i} - \rho_1 s_1 v_{1,i}, \ldots, \rho_K s_K v_{K,i} - \rho_{K-1} s_{K-1} v_{K-1,i})^T, \\
\nabla_{\boldsymbol{w_k}} G_i(\boldsymbol{w}) &= -(\alpha_k v_{k,i}(s_k - p_k/(\rho_k T_k)), \alpha_k \rho_k s_k \boldsymbol{e}_{i,d}^T, \alpha_k \rho_k v_{k,i}/T_k)^T.
\end{aligned}$$

From this we compute

$$\nabla_{\boldsymbol{w}} W(\boldsymbol{w})^T \boldsymbol{B}_i(\boldsymbol{w}) = \begin{pmatrix} \nabla_{\boldsymbol{\alpha}} G_i(\boldsymbol{w}) - \boldsymbol{\Gamma}_i \\ \nabla_{\boldsymbol{w_1}} G_i(\boldsymbol{w}) \\ \vdots \\ \nabla_{\boldsymbol{w_K}} G_i(\boldsymbol{w}) \end{pmatrix}$$

with the components of $\boldsymbol{\Gamma} \in \mathbb{R}^{K-1}$ defined as

$$\Gamma_{i,l} := \frac{p_l}{T_l}(v_{l,i} - V_{I,i}) - \frac{p_K}{T_K}(v_{K,i} - V_{I,i}) - \sum_{k=1}^{K} \alpha_k \rho_k \frac{1}{T_k} \gamma_{k,l}. \tag{7.15}$$

Then we finally conclude with

Theorem 7.2. *(Compatibility of entropy-entropy flux pair) The entropy-entropy flux pairs (U, F_i) and (W, G_i) satisfy the compatibility conditions (7.3) and (7.14), respectively, if the conditions*

$$\Gamma_{i,l} = 0, \; l = 1, \ldots, K-1, \; i = 1, \ldots d \tag{7.16}$$

hold.

Note that the conditions (7.16) are equivalent to the conditions (6.17).

7.3. Entropy production

In order to ensure the entropy inequality (7.2) it remains to verify the inequality (7.5). Adopting the notation introduced in Section 7.1, the gradient of the entropy function U is determined by

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u}) = \left(\nabla_{\boldsymbol{\alpha}} U(\boldsymbol{u})^T, \nabla_{\alpha_1 \boldsymbol{u}_1} U(\boldsymbol{u})^T, \ldots, \nabla_{\alpha_K \boldsymbol{u}_K} U(\boldsymbol{u})^T \right)^T, \tag{7.17}$$

where the gradients $\nabla_{\boldsymbol{\alpha}} U(\boldsymbol{u})$ and $\nabla_{\alpha_k \boldsymbol{u}_k} U(\boldsymbol{u})$, $k = 1, \ldots, K$, are determined by (7.7). Thus, we need the gradients $\nabla_{\boldsymbol{u}_k} U_k(\boldsymbol{u}_k)$, $k = 1, \ldots, K$, that are given by

$$\frac{\partial U_k}{\partial \rho_k} = -s_k + \frac{\partial s_k}{\partial \tau_k}\frac{1}{\rho_k} + \frac{\partial s_k}{\partial e_k}(e_k - 0.5\boldsymbol{v}_k^2), \quad \frac{\partial U_k}{\partial \rho_k \boldsymbol{v}_k} = \frac{\partial s_k}{\partial e_k}\boldsymbol{v}_k, \quad \frac{\partial U_k}{\partial \rho_k E_k} = -\frac{\partial s_k}{\partial e_k}.$$

On the other hand, the vector $\boldsymbol{S}$ of the relaxation terms is defined as

$$\boldsymbol{S}(\boldsymbol{u}) := \begin{pmatrix} \boldsymbol{S_\alpha} \\ \boldsymbol{S}_1 \\ \vdots \\ \boldsymbol{S}_K \end{pmatrix}, \; \boldsymbol{S}_k(\boldsymbol{u}) := \begin{pmatrix} S_{\alpha\rho,k} \\ \boldsymbol{S}_{\alpha\rho v,k} \\ S_{\alpha\rho E,k} \end{pmatrix}, \; \boldsymbol{S}(\boldsymbol{u}) := \begin{pmatrix} \boldsymbol{S}_{\alpha,1} \\ \vdots \\ \boldsymbol{S}_{\alpha,K-1} \end{pmatrix}.$$

Thus, we obtain

$$\begin{aligned}
\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{S}(\boldsymbol{u}) &= \sum_{k=1}^{K-1} \left(\frac{\partial s_K}{\partial \tau_K} - \frac{\partial s_k}{\partial \tau_k} \right) S_{\alpha,k} + \\
&\quad \sum_{k=1}^{K} \left(\left(\frac{\partial s_k}{\partial \tau_k}\frac{1}{\rho_k} + \frac{\partial s_k}{\partial e_k}(e_k - 0.5\boldsymbol{v}_k^2) - s_k \right) S_{\alpha\rho,k} + \frac{\partial s_k}{\partial e_k}\boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho v,k} - \frac{\partial s_k}{\partial e_k}\boldsymbol{S}_{\alpha\rho E,k} \right).
\end{aligned}$$

We note that by the saturation condition (2.1) the first sum on the right-hand side can be written as

$$\sum_{k=1}^{K-1} \left(\frac{\partial s_K}{\partial \tau_K} - \frac{\partial s_k}{\partial \tau_k} \right) \boldsymbol{S}_{\alpha,k} = -\sum_{k=1}^{K} \frac{\partial s_k}{\partial \tau_k} \boldsymbol{S}_{\alpha,k}.$$

Together with (6.3) and the Gibbs free energy (6.28) we finally obtain

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{S}(\boldsymbol{u}) = -\sum_{k=1}^{K} \frac{1}{T_k} \left(p_k \boldsymbol{S}_{\alpha,k} + (0.5\boldsymbol{v}_k^2 - g_k)S_{\alpha\rho,k} - \boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho v,k} + \boldsymbol{S}_{\alpha\rho E,k} \right)$$

Because of (6.27) we thus conclude with

Theorem 7.3. *(Entropy production) If the entropies $s_k = s_k(\tau_k, e_k)$, $k = 1, \ldots, K$, satisfy (6.3), then the entropy production is determined by*

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{S}(\boldsymbol{u}) = -\sum_{k=1}^{K} S_{\alpha\rho s,k} =: -S_{\rho s} \qquad (7.18)$$

and it holds

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{S}(\boldsymbol{u}) \leq 0 \Leftrightarrow S_{\rho s} \geq 0.$$

7.4. Entropy viscosity

So far we have neglected viscosity and heat conduction. To account for these effects we have to modify (7.1) by

$$\partial_t \boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{A}_i(\boldsymbol{u}) \partial_{x_i} \boldsymbol{u} = \sum_{i=1}^{d} \boldsymbol{E}_i(\boldsymbol{u}) \partial_{x_i} \boldsymbol{u} + \boldsymbol{S}(\boldsymbol{u}), \quad \boldsymbol{E}_i(\boldsymbol{u}) := \frac{\partial \boldsymbol{f}_i^v}{\partial \boldsymbol{u}}(\boldsymbol{u}). \qquad (7.19)$$

According to the non-equilibrium model (2.2), (2.3), (2.4) and (2.7) the viscous flux reads

$$\boldsymbol{f}_i^v(\boldsymbol{u}) := \begin{pmatrix} \boldsymbol{0}_{K-1} \\ \boldsymbol{f}_{1,i}^v(\alpha_1, \alpha_1 \boldsymbol{u}_1) \\ \vdots \\ \boldsymbol{f}_{K,i}^v(\alpha_K, \alpha_K \boldsymbol{u}_K) \end{pmatrix}, \quad \boldsymbol{f}_{k,i}^v(\alpha_k, \alpha_k \boldsymbol{u}_k) := \begin{pmatrix} 0 \\ \alpha_k \boldsymbol{T}_{k,i} \\ \alpha_k(\boldsymbol{v}_k \cdot \boldsymbol{T}_{k,i} - q_{k,i}) \end{pmatrix},$$

where $\boldsymbol{T}_{k,i}$ denotes the ith column of the stress tensor $\boldsymbol{T}_k$ and $q_{k,i}$ the ith component of the heat flux $\boldsymbol{q}_k$. Hence, the Jacobian of the viscous fluxes becomes a block matrix

$$\boldsymbol{E}_i(\boldsymbol{u}) = \begin{pmatrix} \boldsymbol{0}_{K-1} & & & \\ \overline{\boldsymbol{E}}_{1,i} & \boldsymbol{E}_{1,i} & & \\ \vdots & & \ddots & \\ \overline{\boldsymbol{E}}_{K,i} & & & \boldsymbol{E}_{K,i} \end{pmatrix} \quad \text{with} \quad \overline{\boldsymbol{E}}_{k,i} := \frac{\partial \boldsymbol{f}_{k,i}^v}{\partial \boldsymbol{\alpha}}, \ \boldsymbol{E}_{k,i} := \frac{\partial \boldsymbol{f}_{k,i}^v}{\partial \alpha_k \boldsymbol{u}_k}.$$

Then the entropy equality (7.4) reads

$$\partial_t U(\boldsymbol{u}) + \sum_{i=1}^{d} \partial_{x_i} F_i(\boldsymbol{u}) = \sum_{i=1}^{d} \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{E}_i(\boldsymbol{u}) \partial_{x_i} \boldsymbol{u} + \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{S}(\boldsymbol{u}), \qquad (7.20)$$

where we apply the compatibility conditions (7.3). In the following we will rewrite the first term on the right-hand side. First of all, we note that by (7.17) and the definition of $\boldsymbol{E}_i$ it holds

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{E}_i(\boldsymbol{u}) = \left(\sum_{k=1}^{K} \nabla_{\boldsymbol{\alpha_k u_k}} U(\boldsymbol{u})^T \overline{\boldsymbol{E}}_{1,k}, \nabla_{\boldsymbol{\alpha_1 u_1}} U(\boldsymbol{u})^T \boldsymbol{E}_{1,i}, \ldots, \nabla_{\boldsymbol{\alpha_K u_K}} U(\boldsymbol{u})^T \boldsymbol{E}_{K,i} \right),$$

where due to (7.7) and (6.3) the components are determined by

$$\nabla_{\boldsymbol{\alpha}_K \boldsymbol{u}_K} U(\boldsymbol{u})^T \overline{\boldsymbol{E}}_{K,i} = \frac{1}{T_k} \boldsymbol{v}_k \cdot \frac{\partial \alpha_k \boldsymbol{T}_{k,i}}{\partial \boldsymbol{\alpha}} - \frac{1}{T_k} \frac{\partial \alpha_k (\boldsymbol{v}_k \cdot \boldsymbol{T}_{k,i} - q_{k,i})}{\partial \boldsymbol{\alpha}},$$

$$\nabla_{\boldsymbol{\alpha}_K \boldsymbol{u}_K} U(\boldsymbol{u})^T \boldsymbol{E}_{K,i} = \frac{1}{T_k} \boldsymbol{v}_k \cdot \frac{\partial \alpha_k \boldsymbol{T}_{k,i}}{\partial \alpha_k \boldsymbol{u}_k} - \frac{1}{T_k} \frac{\partial \alpha_k (\boldsymbol{v}_k \cdot \boldsymbol{T}_{k,i} - q_{k,i})}{\partial \alpha_k \boldsymbol{u}_k}.$$

Hence, we obtain

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{E}_i \frac{\partial \boldsymbol{u}}{\partial x_i} = \sum_{k=1}^{K} \left(\frac{\partial}{\partial x_i} \left(\frac{\alpha_k q_{k,i}}{T_k} \right) + \frac{\alpha_k q_{k,i}}{T_k^2} \frac{\partial T_k}{\partial x_i} - \alpha_k \frac{1}{T_k} \sum_{l=1}^{d} (T_k)_{l,i} \frac{\partial v_{k,l}}{\partial x_i} \right).$$

Summing over all directions $i = 1, \ldots, d$ we finally obtain the entropy viscosity

$$\sum_{i=1}^{d} \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{E}_i(\boldsymbol{u}) \partial_{x_i} \boldsymbol{u} = \nabla_{\boldsymbol{x}} \cdot \left(\sum_{k=1}^{K} \frac{\alpha_k}{T_k} \boldsymbol{q}_k \right) + \sum_{k=1}^{K} \frac{\alpha_k}{T_k^2} \boldsymbol{q}_k \cdot \nabla_{\boldsymbol{x}} T_k - \sum_{k=1}^{K} \frac{\alpha_k}{T_k} \sum_{i,l=1}^{d} (T_k)_{l,i} \frac{\partial v_{k,l}}{\partial x_i}.$$

Thus, the following theorem holds.

Theorem 7.4. *(Entropy viscosity production) If the entropies $s_k = s_k(\tau_k, e_k)$, $k = 1, \ldots, K$, satisfy (6.3), then the entropy viscosity is determined by*

$$\sum_{i=1}^{d} \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T \boldsymbol{E}_i(\boldsymbol{u}) \partial_{x_i} \boldsymbol{u} = -\sum_{i=1}^{d} \partial_{x_i} F_i^v(\boldsymbol{u}) - \sum_{k=1}^{K} \alpha_k (\Delta_k + \Sigma_k), \tag{7.21}$$

where the entropy viscosity flux is defined as

$$F_i^v(\boldsymbol{u}) := -\sum_{k=1}^{K} \frac{\alpha_k}{T_k} q_{k,i}, \ i = 1, \ldots, d$$

and the entropy production due to viscosity Σ_k and heat conduction Δ_k are determined by (6.13) and (6.14), respectively. In particular, the entropy viscosity production is non-positive, i.e.,

$$-\sum_{k=1}^{K} \alpha_k (\Delta_k + \Sigma_k) \leq 0$$

provided that Σ_k and Δ_k are non-negative.

Obviously, the entropy equality (7.20) coincides with (6.11) except for the sign due to (7.6), (7.18) and (7.21). Note that $\Sigma_k \geq 0$ and $\Delta_k \geq 0$ hold under the assumptions of Theorem 7.4.

8. Relaxation model

The non-equilibrium model presented in Section 2.1 allows for different values for velocities, pressures, temperatures as well as chemical potentials at the same point. Therefore one has to introduce a relaxation mechanism, that drives all these quantities into equilibrium. Typically it is distinguished between mechanical and thermal relaxation processes that relax either pressures and velocities or temperatures and chemical potentials to equilibrium.

The relaxation terms are of major importance when dealing with interface problems, see for instance Saurel and Abgrall [24] or Lallemand et al. [16] for mechanical relaxation terms. Typically, it is assumed that pressure and velocity relax instantaneously, see [24], whereas the thermal relaxation and the relaxation of chemical potentials are much slower, see Zein [26].

Note that in the equilibrium model the equilibrium state is characterized by vanishing relaxation terms rather than the transient relaxation process itself. Since the equilibrium state does not depend on the order of relaxation, the relaxation times have not to be known explicitly.

In the subsequent sections we present the relaxation terms for mechanical, thermal and chemical potential relaxation. For each relaxation process we verify the constraints due to conservation (2.13) and entropy production (6.29). Note that for all relaxation processes the corresponding source terms satisfy the constraint (5.37) due to Galilean invariance.

8.1. **Mechanical relaxation**

The *pressure relaxation* implies volume variations, that induce energy variations due to the interfacial pressure work. Here we extend the pressure relaxation vector given in [24] for a two-phase model according to [26] by introducing a pressure average that we choose as the mixture pressure. The pressure relaxation terms then read

$$S^p_{\alpha,k} := \theta_p \, \alpha_k \, (p_k - p), \ S^p_{\alpha\rho,k} := 0, \ \boldsymbol{S}^p_{\alpha\rho\boldsymbol{v},k} := \boldsymbol{0}, \ S^p_{\alpha\rho E,k} := \theta_p \, \alpha_k \, p(p - p_k). \tag{8.1}$$

Here θ_p denotes the pressure relaxation parameter. Similarly the *velocity relaxation* terms read

$$S^v_{\alpha,k} = S^v_{\alpha\rho,k} := 0, \ \boldsymbol{S}^v_{\alpha\rho\boldsymbol{v},k} := \theta_v \, \alpha_k \, \rho_k \, (\boldsymbol{v} - \boldsymbol{v}_k), \ S^v_{\alpha\rho E,k} := \theta_v \, \alpha_k \, \rho_k \, \boldsymbol{v} \cdot (\boldsymbol{v} - \boldsymbol{v}_k) \tag{8.2}$$

with the velocity relaxation parameter θ_v. For more details on mechanical relaxation see Baer and Nunziato [3] or Baer [8] for two-phase models.

Obviously, the mechanical relaxation terms (8.1) and (8.2) satisfy the conservation constraints (2.13) as can be validated by the definition of the mixture pressure and the mixture velocity (2.10) and the saturation condition (2.1). Furthermore we determine by (6.27) and (8.1), (8.2) the entropy production terms

$$S^v_{\alpha\rho s,k} = \theta_v \frac{\alpha_k \rho_k}{T_k} (\boldsymbol{v} - \boldsymbol{v}_k)^2, \quad S^p_{\alpha\rho s,k} = \theta_p \frac{\alpha_k}{T_k} (p - p_k)^2. \tag{8.3}$$

This immediately implies

Theorem 8.1. *(Entropy production due to mechanical relaxation) Let $\rho_k \geq 0$, $T_k > 0$ and the relaxation parameters θ_p, $\theta_v \geq 0$. Then the entropy production due to mechanical relaxation is non-negative, i.e.,*

$$S^{p,v}_{\alpha\rho s,k} \geq 0, \ k = 1,\ldots,K \quad \text{and} \quad \sum_{k=1}^{K} S^{p,v}_{\alpha\rho s,k} \geq 0. \tag{8.4}$$

8.2. **Thermal relaxation**

For the modeling of *temperature relaxation* we follow in principal Zein [26]. First of all, we introduce a general class of temperature relaxation models

$$S^T_{\alpha,k} := \theta_T \frac{Q_k}{\kappa_k}, \ S^T_{\alpha\rho,k} := 0, \ \boldsymbol{S}^T_{\alpha\rho\boldsymbol{v},k} := \boldsymbol{0}, \ S^T_{\alpha\rho E,k} := \theta_T \, Q_k, \tag{8.5}$$

with the relaxation parameter θ_T and

$$Q_k = \gamma_k(\hat{T} - T_k). \tag{8.6}$$

According to the conservation constraint (2.13) the terms Q_k have to satisfy

$$\sum_{k=1}^{K} Q_k = 0 \quad \text{and} \quad \sum_{k=1}^{K} \frac{Q_k}{\kappa_k} = 0. \tag{8.7}$$

In order to guarantee the first constraint, we choose for $\hat{T}$ the following expression

$$\hat{T} = \sum_{k=1}^{K} \beta_k T_k \tag{8.8}$$

with coefficients

$$\beta_k = \gamma_k / \gamma, \quad \gamma := \sum_{k=1}^{K} \gamma_k. \tag{8.9}$$

Obviously, $\hat{T}$ is a convex combination of the temperatures T_k because

$$\sum_{k=1}^{K} \beta_k = 1. \tag{8.10}$$

For instance, we may choose (a) $\gamma_k = \alpha_k$. Then $\beta_k = \alpha_k$ and $\hat{T}$ coincides with the mixture temperature (6.10). In case of (b) $\gamma_k = 1$ or (c) $\gamma_k = K$ we compute $\beta_k = 1/K$ and $\hat{T}$ is given as the averaged mixture $\hat{T} = \sum_{k=1}^{K} T_k / K$. For these three cases we obtain (a) $Q_k = \alpha_k(\hat{T} - T_k)$, (b) $Q_k = (\hat{T} - T_k)$ and (c) $Q_k = \sum_{l=1}^{K}(T_l - T_k)$, respectively.

Next we determine by (6.27) and (8.5) the entropy production term

$$S_{\rho s,k}^{T} = \theta_T \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1 \right). \tag{8.11}$$

Thus the entropy production due to thermal relaxation becomes

$$S_{\rho s}^{T} := \sum_{k=1}^{K} S_{\alpha \rho s,k}^{T} = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1 \right) = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k + \theta_T \sum_{k=1}^{K} \frac{p_k}{T_k \kappa_k} Q_k. \tag{8.12}$$

We note that by the definitions (8.6) and (8.9) of Q_k and β_k, respectively, the relation

$$\sum_{k=1}^{K} \frac{1}{T_k} Q_k = \gamma \sum_{k,l=1}^{K} \frac{1}{T_k} \beta_k \beta_l (T_l - T_k)$$

holds. Here we employ (8.8) and (8.10) to compute the difference $\hat{T} - T_k = \sum_{l=1}^{K} \beta_l(T_l - T_k)$. Furthermore we observe that for any b_k and $a_{k,l} = -a_{l,k}$, $l, k = 1, \ldots, k$ we have

$$\sum_{k,l=1}^{K} b_k a_{k,l} = \sum_{k=2}^{K} b_k \sum_{l=1}^{k-1} a_{k,l} + \sum_{k=1}^{K-1} b_k \sum_{l=k+1}^{K} a_{k,l} = \sum_{k=1}^{K-1} \sum_{l=k+1}^{K} (b_k - b_l) a_{k,l}.$$

Choosing $b_k = 1/T_k$ and $a_{k,l} = \beta_k \beta_l(T_l - T_k)$ we thus conclude with

$$\sum_{k=1}^{K} \frac{1}{T_k} Q_k = \gamma \sum_{k=1}^{K-1} \sum_{l=k+1}^{K} \beta_k \beta_l \frac{(T_k - T_l)^2}{T_k T_l}.$$

Obviously, the sum is non-negative whenever the temperatures are positive. Thus the first term on the right-hand side of (8.12) is non-negative. To ensure that the second term is also non-negative, we rewrite the sum by means of the conservation constraints (8.7) as

$$\sum_{k=1}^{K} \frac{p_k}{T_k \kappa_k} Q_k = \sum_{k=1}^{K-1} \left(\frac{p_k}{T_k} - \frac{p_K}{T_K} \right) \frac{1}{\kappa_k} Q_k.$$

and choose κ_k such that

$$\left(\frac{p_k}{T_k} - \frac{p_K}{T_K}\right)\frac{1}{\kappa_k} = a_k Q_k, \quad k = 1, \ldots, K-1$$

holds for some positive parameters a_k, i.e.,

$$\kappa_k = \frac{T_K p_k - T_k p_K}{a_k T_k T_K Q_k}, \quad k = 1, \ldots, K-1. \tag{8.13}$$

The missing parameter κ_K is determined by the conservation constrains (8.7) as

$$\kappa_K = -Q_K \left(\sum_{k=1}^{K-1} \frac{Q_k}{\kappa_k}\right)^{-1}. \tag{8.14}$$

Finally we summarize our results in the following

Theorem 8.2. *(Entropy production due to thermal relaxation) Let the temperatures and the relaxation parameter be non-negative, i.e., $T_k > 0$ and $\theta_T > 0$. Let Q_k satisfy (8.6) where $\hat{T}$ is defined as convex combination (8.8) of the temperatures T_k with coefficients β_k satisfying (8.9) and (8.10). Then the mixture entropy production due to thermal relaxation is non-negative, i.e.,*

$$S_{\rho s}^T = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1\right) \geq 0, \tag{8.15}$$

provided that the condition

$$\sum_{k=1}^{K} \frac{p_k}{T_k \kappa_k} Q_k \geq 0$$

holds. In particular, this condition holds for the parameters κ_k determined by (8.13) and (8.14) with non-negative coefficients a_k. It also holds in case of pressure equilibrium, i.e., $p_1 = \ldots = p_K = p$, and constant parameters $\kappa_1 = \ldots = \kappa_K = \kappa$.

When the temperature relaxation approaches thermal equilibrium, the parameters κ_k, $k = 1, \ldots, K-1$, tend to $\kappa_k = p/(a_k \gamma_k T^2)$ provided that the pressure relaxes faster to its equilibrium state. If the pressure is not at equilibrium when thermal equilibrium is reached, then $\kappa_k = \infty$, i.e., $S_{\alpha,k}^T = 0$. However, it is widely accepted that the mechanical relaxation proceeds faster than the thermal relaxation.

Finally we conclude with some remarks on existing relaxation models. In [26] a constant parameter $\kappa_k = \kappa$ is chosen such that pressure stays at equilibrium during the temperature relaxation. More details on its definition in case of a two-phase and a three-phase model can be found in Zein [26] and Zein et al. [27], respectively. Note that the coefficient κ in [26] results in a non-negative entropy production if the pressures are at equilibrium. In the non-equilibrium case (8.15) cannot be proven to hold.

In the thermal relaxation model considered by Saleh [23] there is no relaxation term accounted for in the evolution equations for the volume fractions, i.e., $S_{\alpha,k}^T = 0$. This fits into our model when choosing $a_k = 0$, i.e., $\kappa_k = \infty$, for $k = 1, \ldots, K$. Then the investigation of the entropy production simplifies because the second term on the right-hand side in (8.12) does not exist.

8.3. Chemical potential relaxation

Mass transfer between different phases of the same substance occurs, whenever these phases are not in chemical equilibrium. This physical matter of fact is the decisive factor for the idea to model the mass transfer by relaxation of the chemical potentials. The mass transfer is driven by the difference of the chemical potentials. It is obvious, that from now on it is necessary to identify the phases.

8.3.1. *Chemical potential relaxation for two-component mixtures*

For a two-component mixture ($K = 2$) the relaxation of chemical potentials is modeled according to [26] by

$$S_{\alpha,1}^{\mu} := \theta_\mu \frac{\dot{m}}{\varrho}, \; S_{\alpha\rho,1}^{\mu} := \theta_\mu \dot{m}, \; \boldsymbol{S}_{\alpha\rho\boldsymbol{v},1}^{\mu} := \theta_\mu \dot{m} \boldsymbol{V}_I, \; S_{\alpha\rho E,1}^{\mu} := \theta_\mu \dot{m} \left(\epsilon + \frac{\boldsymbol{V}_I^2}{2} \right), \tag{8.16}$$

$$S_{\alpha,2}^{\mu} := -\theta_\mu \frac{\dot{m}}{\varrho}, \; S_{\alpha\rho,2}^{\mu} := -\theta_\mu \dot{m}, \; \boldsymbol{S}_{\alpha\rho\boldsymbol{v},2}^{\mu} := -\theta_\mu \dot{m} \boldsymbol{V}_I, \; S_{\alpha\rho E,2}^{\mu} := -\theta_\mu \dot{m} \left(\epsilon + \frac{\boldsymbol{V}_I^2}{2} \right),$$

with the relaxation parameter θ_μ. Since for a two-component mixture the Gibbs free energy coincides with the chemical potential, chemical equilibrium is achieved, if the Gibbs free energies of the two components coincide, i.e., $g_1 = g_2$.

Obviously, the conservation constraints (2.13) are satisfied. Note that due to these constraints we are not allowed to introduce ϵ_k and ϱ_k differently for each component $k = 1, 2$. Furthermore, the entropy production terms are determined by (6.27) and (8.16) as

$$S_{\alpha\rho s,k}^{\mu} = (-1)^{k+1} \theta_\mu \dot{m} \frac{1}{T_k} \left(\epsilon + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_k)^2 - g_k + p_k/\varrho \right), \quad k = 1, 2. \tag{8.17}$$

These terms may become negative also when θ_μ, $\dot{m}$ and T_k are positive. However, for an appropriate choice of ϵ, ϱ and $\boldsymbol{V}_I$ the entropy production due to the sum of the phasic entropies

$$S_{\rho s}^{\mu} = \theta_\mu \dot{m} \left(\frac{1}{T_1} \left(\epsilon + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_1)^2 - g_1 + p_1/\varrho \right) - \frac{1}{T_2} \left(\epsilon + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_2)^2 - g_2 + p_2/\varrho \right) \right) \tag{8.18}$$

can be verified to be non-negative. For this purpose, we first note that in case of mechanical and thermal equilibrium, i.e.,

$$\boldsymbol{v}_1 = \ldots = \boldsymbol{v}_K = \boldsymbol{v}, \quad p_1 = \ldots = p_K = p, \quad T_1 = \ldots = T_K = T, \tag{8.19}$$

the entropy production term becomes

$$S_{\rho s}^{\mu} = \frac{1}{T} \dot{m} \, \theta_\mu \, (g_2 - g_1)$$

as was already proven in [26]. Obviously this term is non-negative if

$$\dot{m} = a(g_2 - g1) \tag{8.20}$$

with $a \geq 0$. This is an agreement with the kinetic relation in [7].

At mechanical and thermal non-equilibrium we may enforce a non-negative entropy production by choosing the parameters ϵ and ϱ such that

$$\frac{1}{T_1} \left(\epsilon + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_1)^2 - g_1 + p_1/\varrho \right) - \frac{1}{T_2} \left(\epsilon + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_2)^2 - g_2 + p_2/\varrho \right) = b \, (g_2 - g_1) \tag{8.21}$$

for some non-negative b. Note that for the parameters ϵ and ϱ in [26] this condition does not hold true. To verify (8.21) we proceed in three steps to determine $\boldsymbol{V}_I$, ϵ and ϱ:

(1) The interfacial velocity $\boldsymbol{V}_I$ is chosen in such a way, that the velocity terms in (8.18) vanish:

$$\frac{1}{T_1}(\boldsymbol{V}_I - \boldsymbol{v}_1)^2 - \frac{1}{T_2}(\boldsymbol{V}_I - \boldsymbol{v}_2)^2 = 0. \tag{8.22}$$

This is reasonable because the entropy production (8.18) should be a product of the relaxed mass flux $\theta_\mu \dot{m}$ and an interfacial entropy s_I that should not depend on any velocity. Because the interfacial velocity is assumed to be a convex combination of the single component

32

velocities, i.e. $\boldsymbol{V}_I = \beta_1 \boldsymbol{v}_1 + \beta_2 \boldsymbol{v}_2$ with $\beta_2 = 1 - \beta_1$ according to (6.18), we derive from (8.22)

$$\beta_1 := \frac{\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_2 := \frac{\sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}}. \tag{8.23}$$

Then the interfacial pressures are determined by (6.23) as

$$P_{1,2} = P_{2,1} = \frac{p_1 \sqrt{T_2} + p_2 \sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}} = P_I. \tag{8.24}$$

(2) In the next step we determine ϵ such that

$$\frac{1}{T_1} \left(\epsilon - \frac{g_1}{2} \right) - \frac{1}{T_2} \left(\epsilon - \frac{g_2}{2} \right) = b_\epsilon (g_2 - g_1), \quad \text{with} \quad b_\epsilon = (T_1 + T_2)^{-1}$$

resulting in

$$\epsilon = \frac{g_2 T_1 + g_1 T_2}{2(T_1 + T_2)}.$$

(3) Finally we determine ϱ such that

$$\frac{1}{T_1} \left(p_1/\varrho - \frac{g_1}{2} \right) - \frac{1}{T_2} \left(p_2/\varrho - \frac{g_2}{2} \right) = b_\varrho (g_2 - g_1), \quad \text{with} \quad b_\varrho = (T_1 + T_2)^{-1}$$

resulting in

$$\varrho = \frac{2(T_1 + T_2)(p_2 T_1 - p_1 T_2)}{(T_1 - T_2)(g_2 T_1 + g_1 T_2)}.$$

With the above choice of $\boldsymbol{V}_I$, ϵ and ϱ we thus obtain (8.21) with $b = b_\epsilon + b_\varrho = ((T_1 + T_2)/2)^{-1}$ the reciprocal of the mean temperature of the components. Note that in the equilibrium case ϵ and ϱ tend to g and $2p/g$, respectively, assuming that the pressure relaxes faster than the Gibbs free energy. Thus, for states close to pressure equilibrium ϱ is positive. For arbitrary non-equilibrium states one may determine positive ϱ and ϵ depending on the local state. Since the derivation is complicate we do not give the details here.

Thus we conclude with the following theorem.

Theorem 8.3. *(Entropy production due to relaxation of Gibbs free energies) At mechanical and thermal equilibrium, i.e., (8.19) holds, the mixture entropy production due to relaxation of Gibbs free energies is non-negative, i.e.,*

$$S_{\rho s}^\mu \geq 0, \tag{8.25}$$

if the mass flux is chosen as the kinetic relation (8.20) and the relaxation parameter θ_μ as well as the equilibrium temperature T are positive. In the non-equilibrium case, the entropy production is non-negative, if the parameters ϵ and ϱ are chosen such that (8.21) holds.

8.3.2. *Chemical potential relaxation for three-component mixtures*

Exemplarily, we consider three components, i.e., $K = 3$, with water vapor ($k = 1$), liquid water ($k = 2$) and inert gas ($k = 3$). Then the vector for relaxation of chemical potentials is given by

$$S_{\alpha,1}^\mu := \theta_\mu \frac{\dot{m}}{\varrho_1}, \; S_{\alpha\rho,1}^\mu := \theta_\mu \dot{m}, \; \boldsymbol{S}_{\alpha\rho\boldsymbol{v},1}^\mu := \theta_\mu \dot{m} \boldsymbol{V}_I, \; S_{\alpha\rho E,1}^\mu := \theta_\mu \dot{m} \left(\epsilon_1 + \frac{\boldsymbol{V}_I^2}{2} \right),$$

$$S_{\alpha,2}^\mu := \theta_\mu \frac{\dot{m}}{\varrho_2}, \; S_{\alpha\rho,2}^\mu := -\theta_\mu \dot{m}, \; \boldsymbol{S}_{\alpha\rho\boldsymbol{v},2}^\mu := -\theta_\mu \dot{m} \boldsymbol{V}_I, \; S_{\alpha\rho E,2}^\mu := -\theta_\mu \dot{m} \left(\epsilon_2 + \frac{\boldsymbol{V}_I^2}{2} \right),$$

$$S_{\alpha,3}^\mu := -\theta_\mu \dot{m} \left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2} \right), \; S_{\alpha\rho,3}^\mu := 0, \; \boldsymbol{S}_{\alpha\rho\boldsymbol{v},3}^\mu := \boldsymbol{0}, \; S_{\alpha\rho E,3}^\mu := \theta_\mu \dot{m} \left(\epsilon_2 - \epsilon_1 \right), \tag{8.26}$$

with the relaxation parameter θ_μ. For details on the physics see the book of Müller and Müller [20]. Again we note that the conservation constraints (2.13) are satisfied. Furthermore the entropy production terms can be determined by (6.27) and (8.16)

$$
\begin{aligned}
S^\mu_{\alpha\rho s,1} &= \theta_\mu \dot{m} \frac{1}{T_1}\left(\epsilon_1 + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_1)^2 - g_1 + p_1/\varrho_1\right), \\
S^\mu_{\alpha\rho s,2} &= -\theta_\mu \dot{m} \frac{1}{T_2}\left(\epsilon_2 + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_2)^2 - g_2 - p_2/\varrho_2\right), \\
S^\mu_{\alpha\rho s,3} &= \theta_\mu \dot{m} \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3(1/\varrho_1 + 1/\varrho_2)\right).
\end{aligned}
\tag{8.27}
$$

These terms may become negative also when θ_μ, $\dot{m}$ and T_k are non-negative. For the sum of the phasic entropy production $S^\mu_{\rho s} = S^\mu_{\rho s,1} + S^\mu_{\rho s,2} + S^\mu_{\rho s,3}$ we obtain

$$
S^\mu_{\rho s} = \dot{m}\,\theta_\mu \left(\sum_{k=1}^2 \frac{(-1)^{k+1}}{T_k}\left(\epsilon_k + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_k)^2 - g_k - (-1)^k \frac{p_k}{\varrho_k}\right) + \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3\left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2}\right)\right)\right).
\tag{8.28}
$$

In the following we distinguish between a non-homogeneous and a homogeneous mixture, respectively.

Non-homogeneous mixture. In a non-homogeneous mixture velocity, pressure and temperature are not necessarily in equilibrium. Therefore we need not to account for the mixture entropy. Thus, the chemical potentials and the Gibbs free energies of water vapor and liquid water, respectively, coincide, i.e., $g_k = \mu_k$, $k = 1, 2$, and the mass flux is proportional to the difference in the Gibbs free energies, i.e., (8.20) holds. Similar to the two-component case, see Section (8.3.1), we may enforce a non-negative entropy production by choosing the parameters ϵ_k and ϱ_k such that the condition

$$
\sum_{k=1}^2 \frac{(-1)^{k+1}}{T_k}\left(\epsilon_k + \frac{1}{2}(\boldsymbol{V}_I - \boldsymbol{v}_k)^2 - g_k - (-1)^k \frac{p_k}{\varrho_k}\right) + \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3\left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2}\right)\right) = b\,(g_2 - g_1)
\tag{8.29}
$$

holds for some non-negative b analogously to (8.21). Note that the parameters ϵ_k and ϱ_k in [26, 28] do not satisfy this condition.

As already assumed in the two-component mixture, we expect that the entropy production of the three-component mixture (8.27) should not depend on any velocity. This assumption gives us a condition for the interfacial velocity $\boldsymbol{V}_I$ and delivers us the same result as above (8.23):

$$
\beta_1 := \frac{\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_2 := \frac{\sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_3 := 0.
$$

From (6.24) and (6.25) we then conclude for the interfacial pressures

$$
\begin{aligned}
P_{1,2} &= P_{2,1} = \frac{p_2\sqrt{T_1} + p_1\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad P_{3,1} = P_{3,2} = p_3, \\
P_{1,3} &= \frac{p_3\sqrt{T_1} + p_1\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad P_{2,3} = \frac{p_2\sqrt{T_1} + p_3\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \\
P_I &= \frac{(p_2 + p_3)\sqrt{T_1} + (p_1 + p_3)\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}.
\end{aligned}
\tag{8.30}
$$

The remaining parameters ϵ_k, ϱ_k, $k = 1, 2$, can be determined similar to the two-component case. We omit details here.

Homogeneous mixture. In a homogeneous mixture velocity, pressure and temperature are in equilibrium. Therefore, as already mentioned in Section 6.2, in the total entropy we also have to account for the mixture entropy given by

$$S_M = -\sum_{k=1,3} \alpha_k \rho_k \frac{\kappa_b}{m_k} \ln\left(\frac{\alpha_k}{\alpha_1 + \alpha_3}\right), \tag{8.31}$$

with κ_b the Boltzmann constant and m_k the mass of a single molecule of component k, see [19], p. 54, 298, 320. Moreover, the chemical potential of the vapor phase is now given by

$$\mu_1 = g_1 + \frac{\kappa_b T}{m_1} \ln\left(\frac{\alpha_1}{\alpha_1 + \alpha_3}\right) \tag{8.32}$$

i.e., it does not coincide with its Gibbs free energy. Note that for vanishing third component, i.e., $\alpha_3 = 0$, the chemical potential of the vapor phase reduces to the vapor Gibbs free energy. Again, the chemical potential of the liquid phase equals its Gibbs free energy, i.e., $\mu_2 = g_2$. In chemical equilibrium the chemical potentials of the vapor and the liquid phase equal each other. Accordingly, the mass flux is now a function of $\mu_2 - \mu_1$, i.e.,

$$\dot{m} = a(\mu_2 - \mu_1) \tag{8.33}$$

with $a \geq 0$ that again is an agreement with the kinetic relation in [7].

For a homogeneous mixture the entropy production (8.28) reduces to

$$S_{\rho s}^\mu = \frac{1}{T} \dot{m}\,\theta_\mu\,(g_2 - g_1) = \frac{1}{T} \dot{m}\,\theta_\mu\left(\mu_2 - \mu_1 + \frac{\kappa_b T}{m_1} \ln\left(\frac{\alpha_1}{\alpha_1 + \alpha_3}\right)\right).$$

Analogously to Section 6.2, we determine the entropy production of the mixture entropy S_M

$$S_{S_M}^\mu = -\frac{1}{T} \dot{m}\,\theta_\mu\,\frac{\kappa_b T}{m_1} \ln\left(\frac{\alpha_1}{\alpha_1 + \alpha_3}\right). \tag{8.34}$$

Then the total entropy production is given by

$$S_{\rho s}^\mu + S_{S_M}^\mu = \frac{1}{T} \dot{m}\,\theta_\mu\,(\mu_2 - \mu_1). \tag{8.35}$$

Thus we conclude with the following theorem.

Theorem 8.4. *(Entropy production due to relaxation of chemical potentials) For a homogeneous mixture the total entropy production is non-negative, i.e.,*

$$S_{\rho s}^\mu + S_{S_M}^\mu \geq 0, \tag{8.36}$$

if the relaxation parameter θ_μ as well as the equilibrium temperature T are positive.

Finally we would like to remark that the above procedure for a particular three-component mixture can be extended to a multi-component mixture.

9. Conclusion

In the present work we discussed some properties of a non-equilibrium multi-component model of Baer-Nunziato type taking into account viscosity and heat conduction. This model is non-conservative due to exchange terms between different components. However, these terms vanish in the mixture model derived from the non-equilibrium model by averaging over all components and the resulting equilibrium model, i.e., the mixture model as well as the equilibrium model are conservative. Furthermore, the first order model, i.e., neglecting viscosity and heat conduction, could be verified to be hyperbolic, i.e., all eigenvalues are real and there exists a family of linearly independent eigenvectors provided that the non-resonance condition is satisfied and none of the components of the mixture vanishes. This

holds true for both the non-equilibrium and the equilibrium model. In particular, the corresponding eigenvalues satisfy the sub-characteristic condition.

The main interest was on the derivation of closure conditions for the relaxation model as well as the interfacial pressures and the interfacial velocity. These were set up by verifying the second law of thermodynamics. It turned out that the pressures and the interfacial velocity can be chosen such that their contribution in the entropy law of the mixture vanishes. However, this does not characterize a unique choice for the interfacial pressures and the interfacial velocity because a physically reasonable choice of the interfacial velocities could not be derived so far in the general case of $K > 2$ components. The entropy production due to mechanical relaxation could be proven to be non-negative. The entropy production due to thermal and chemical relaxation is non-negative when assuming mechanical and thermal equilibrium, respectively. In the non-equilibrium case, sufficient conditions are given that pose constraints on the relaxation parameters to ensure a non-negative entropy production. Finally, we obtained constraints for the relaxation terms to ensure Galilean invariance.

We conclude with some remarks on the numerical discretization of the multi-component model. The main difficulty arises from the non-conservative products in the momentum equation (2.3) and the energy equation (2.4) as well as the evolution equation for the volume fractions (2.7). A popular approach to deal with those products is based upon so-called path-conservative schemes, see [21]. However, it was verified by Abgrall and Karni [1] that path-conservative schemes may not be able, in general, to compute correctly the solution of non-conservative hyperbolic problems. In case of a stiffened gas equation of state for the single components one may employ the Saurel-Abgrall trick [24] that couples the discretization of the evolution equations of the volume fractions with the discretization of the fluid equations of the components resulting in a non-conservative finite volume discretization. Numerical results for inviscid computations have been reported in [27] and [28, 13] for two-phase fluids and three-phase fluids. There are many other publications available in the literature using different discretizations, see the aforementioned publications and citations therein.

Bibliography

[1] R. Abgrall and S. Karni. A comment on the computation of non-conservative products. *J. Comput. Phys.*, 229:2759–2763, 2010.

[2] N. Andrianov. *Analytical and numerical investigation of two-phase flows*. PhD thesis, Otto-von-Guericke University, Magdeburg, 2003.

[3] M.R. Baer and J.W. Nunziato. A two-phase mixture theory of the deflagration-to-detonation transition (DDT) in reactive granular materials. *Int. J. Multiphase Flows*, 12:861–889, 1986.

[4] F. Coquel, J.-M. Hérard, K. Saleh, and N. Seguin. Two properties of two-velocity two-pressure models for two-phase flows. *Int. J. Multiphase Flows*, 12(3):593–600, 2014.

[5] D. Drew. Mathematical modeling of two-phase flow. *Ann. Rev. Fluid Mech.*, 15:261–291, 1983.

[6] D.A. Drew and S.L. Passman. *Theory of Multicomponent Fluids*, volume 135 of *Applied Mathematical Sciences*. Springer, 1999.

[7] W. Dreyer, F. Duderstadt, M. Hantke, and G. Warnecke. Bubbles in liquids with phase transition. part 1: On phase change of a single vapor bubble in liquid water. *Contin. Mech. Thermodyn.*, 24:461–483, 2012.

[8] P. Embid and M. Baer. Mathematical analysis of a two-phase continuum mixture theory. *Contin. Mech. Thermodyn.*, 4:279–312, 1992.

[9] T. Flåtten and H. Lund. Relaxation two-phase flow models and the subcharacteristic condition. *Mathematical Models and Methods in Applied Sciences*, 21(12):2379–2407, 2011.

[10] T. Gallouët, J.-M. Hérard, and N. Seguin. Numerical modelling of two-phase flows using the two-fluid two-pressure approach. *Mathematical Models and Methods in Applied Sciences*, 14(5):663–700, 2004.

[11] E. Godlewski and P.-A. Raviart. *Hyperbolic systems of conservation laws*, volume 3-4 of *Mathématiques & Applications (Paris)*. Springer, 1991.

[12] E. Godlewski and P.-A. Raviart. *Numerical approximation of hyperbolic systems of conservation laws*. New York, NY: Springer, 1996.

[13] E. Han, M. Hantke, and S. Müller. Modeling of multi-component flows with phase transition and application to collapsing bubbles. IGPM Preprint 409, RWTH Aachen University, 2014.

[14] J.-M. Hérard. A three-phase flow model. *Mathematical and Computer Modelling*, 45:732–755, 2007.

[15] A. Kapila, R. Menikoff, J. Bdzil, S. Son, and D. Stewart. Two-phase modelling of DDT in granular materials: Reduced equations. *Phys. Fluid*, 13:3002–3024, 2001.

[16] M.H. Lallemand, A. Chinnayya, and O. Le Metayer. Pressure relaxation procedures for multiphase compressible flows. *International Journal for Numerical Methods in Fluids*, 49(1):1–56, 2005.

[17] I. Liu and R. Sampaio. On objectivity and the principle of material frame-indifference. In A. Cardona, P.H. Kohan, R.D. Quinteros, and M.A. Storti, editors, *Mecánica Computacional Vol XXXI*, pages 1553–1569, 2012. Salta, Argentina, 13-16 November 2012.

[18] T.-P. Liu. Hyperbolic conservation laws with relaxation. *Commun. Math. Phys*, 108:153–175, 1987.

[19] I. Müller. *Thermodynamics*. Pitman, London, 1985.

[20] I. Müller and W. Müller. *Fundamentals of Thermodynamics and Applications*. Springer-Verlag, Berlin, 2009.

[21] C. Parés. Numerical methods for nonconservative hyperbolic systems: A theoretical framework. *SIAM Journal on Numerical Analysis*, 44(1):300–321, 2006.

[22] M.G. Rodio and R. Abgrall. An innovative phase transition modeling for reproducing cavitation. part 1: Formulation of a 5-equations model and theoretical generalization to six and seven-equations models. submitted to International Journal of Heat and Mass Transfer, September 6, 2014, 2014.

[23] K. Saleh. *Analyse et Simulation Numérique par Relaxation d'Écoulements Diphasiques Compressibles*. PhD thesis, Université Pierre et Marie Curie, Paris, 2012.

[24] R. Saurel and R. Abgrall. A multiphase Godunov method for compressible multifluid and multiphase flows. *J. Comput. Phys.*, 150(2):425–467, 1999.

[25] R. Saurel, F. Petitpas, and R. Abgrall. Modelling phase transition in metastable liquids: Application to cavitation and flashing flows. *J. Fluid Mech.*, 607:313–350, 2008.

[26] A. Zein. *Numerical methods for multiphase mixture conservation laws with phase transition.* PhD thesis, Otto-von-Guericke University, Magdeburg, 2010.

[27] A. Zein, M. Hantke, and G. Warnecke. Modeling phase transition for compressible two-phase flows applied to metastable liquids. *J. Comput. Phys.*, 229(8):2964–2998, 2008.

[28] A. Zein, M. Hantke, and G. Warnecke. On the modelling and simulation of a laser-induced cavitation bubble. *Int. J. Num. Meth. Fluids.*, 73(2):172–203, 2013.