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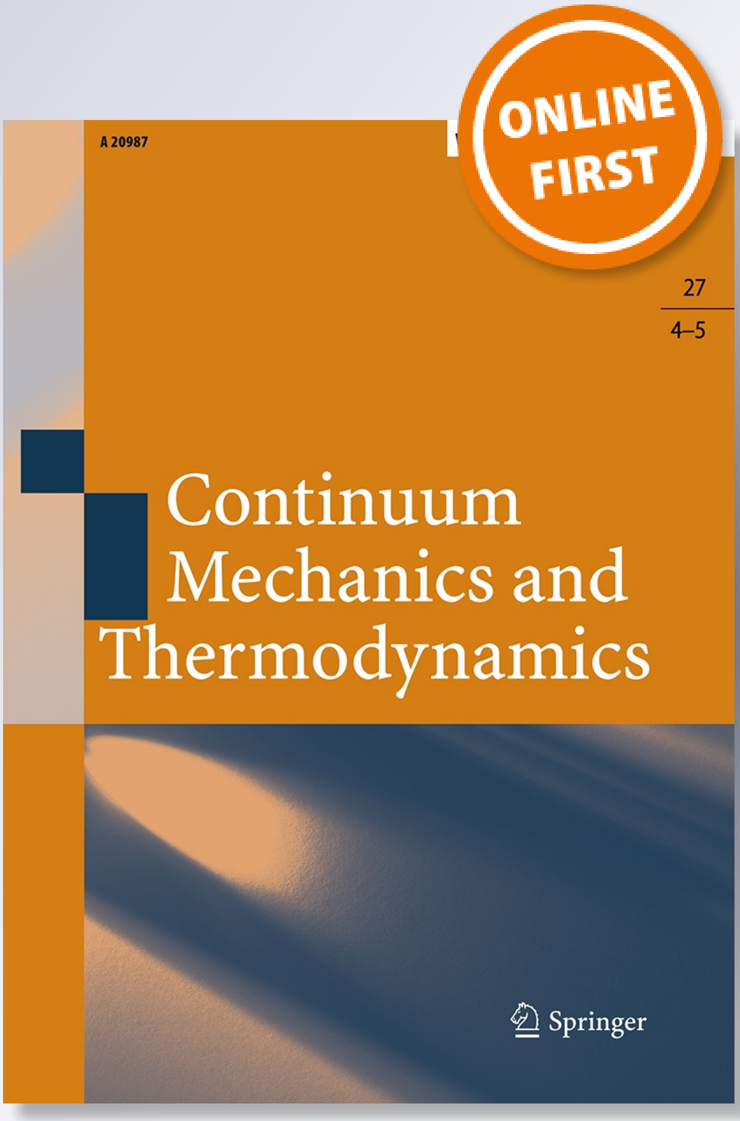

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ORIGINAL ARTICLE

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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 and 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 models for vapor–water and gas–water–vapor, respectively, are considered.

Keywords Multi-component flows · Entropy · Relaxation · Phase transition · Closure conditions · Hyperbolicity · Subcharacteristic property · Galilean invariance

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.

Our particular interest is on a two-phase flow where we consider one liquid phase and one gaseous phase. The liquid phase is assumed to consist of one species. The gaseous phase may consist of $K-1$ species where one of these species is the same as in the liquid phase but in a different aggregate state. To model this flow, we use a K component model where in each point all $K-1$ species are present with one species in both aggregate states. Only a species that is present in both aggregate states can undergo a phase change. Typical applications

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are evaporation and drying processes as can be observed in daily live, e.g., cooking pot or puddle, or formation of clouds. A technical application is the spherical collapse of a laser-induced bubble at elevated temperatures to investigate the influence of the amount of non-condensable gas inside the bubble; see [17,35,39].

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 [37]. Here our interest is on multi-component fluids derived from an ensemble averaging procedure of Drew [7]. A comprehensive introduction to these models can be found in the classical book of Drew and Passman [8].

Baer and Nunziato [4] 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 [33] 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 chemical potentials into equilibrium mass transfer between the phases can be modeled; see Abgrall et al. [31,34] or Zein et al. [38].

There are simplified models available in the literature that can be derived from the above general model by assuming zero relaxation times; see [20]. 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 chemical potential; 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 [37] and the references cited therein.

Typically, reduced models suffer from some shortcomings. 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 Hérard; see Remark 7 in [18]. For instance, the Saurel–Abgrall approach [33] fits into this class.

Characteristic for models based on ensemble averaging is the problem to close the set of equations; i.e., finding 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 subcharacteristic 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 [3,12,32,37] and three-phase models [5,18]. Here we do not confine ourselves to two and three components but on an arbitrary number of components. Drew and Passmann [8] 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 Sect. 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 Sect. 3. Neglecting viscosity and heat conduction some mathematical properties of the models are investigated. In particular, we verify hyperbolicity and the subcharacteristic condition; see Sect. 4. Furthermore, a physical meaningful model should be Galilean invariant. This is investigated in Sect. 5. In Sect. 6, we are concerned with the entropies corresponding to the non-equilibrium model and the mixture model. From the second law of thermodynamics, we derive constraints for the definition of the interfacial velocity and pressures. In Sect. 7, 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 second 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 Hérard [18], the fluid equations for each component can be written as

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

$$\partial_t (\alpha_k \rho_k \boldsymbol{v}_k) + \nabla \cdot (\alpha_k \rho_k \boldsymbol{v}_k \boldsymbol{v}_k^T + \alpha_k p_k \boldsymbol{I}) = -\sum_{l=1}^{K} P_{k,l} \nabla \alpha_l + \nabla \cdot (\alpha_k \boldsymbol{T}_k) + \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}, \tag{2.3}$$

$$\partial_t (\alpha_k \rho_k E_k) + \nabla \cdot (\alpha_k \rho_k \boldsymbol{v}_k (E_k + p_k/\rho_k)) = -\sum_{l=1}^{K} P_{k,l} \boldsymbol{V}_I \cdot \nabla \alpha_l + \nabla \cdot (\alpha_k \left(\boldsymbol{v}_k \cdot \boldsymbol{T}_k - \boldsymbol{q}_k\right)) + S_{\alpha\rho E,k}, \tag{2.4}$$

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 [8], 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

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

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.,

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

The source terms $S_{\alpha,k}$, $S_{\rho,k}$, $\boldsymbol{S}_{\rho v,k}$ 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.,

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

These depend on the specific components at hand discussed in Sect. 7.

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

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

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

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

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

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

$$\partial_t\, (\rho\, \boldsymbol{v}) + \nabla \cdot (\rho\, \boldsymbol{v}\, \boldsymbol{v}^T + p\, \boldsymbol{I}) = \nabla \cdot \boldsymbol{T} - \nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \rho_k\, (\boldsymbol{v} - \boldsymbol{v}_k)\, (\boldsymbol{v} - \boldsymbol{v}_k)^T \right), \tag{2.16}$$

$$\begin{aligned} &\partial_t\, (\rho\, E) + \nabla \cdot (\rho\, \boldsymbol{v}\, (E + p/\rho)) \\ &= \nabla \cdot (\boldsymbol{v} \cdot \boldsymbol{T} - \boldsymbol{q}) - \nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \boldsymbol{T}_k\, (\boldsymbol{v}_k - \boldsymbol{v}) \right) - \nabla \cdot \left(\sum_{k=1}^{K} \alpha_k\, \rho_k\, (H_k - H)\, (\boldsymbol{v}_k - \boldsymbol{v}) \right). \end{aligned} \tag{2.17}$$

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 [8], pp. 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.,

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

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 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), e.g., [26,38].

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

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

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

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

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

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

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

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

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

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

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

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

with the relaxation term

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

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

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

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

$$\begin{aligned}\partial_t\, e + \boldsymbol{v} \cdot \nabla\, e + \frac{1}{\rho} \sum_{k=1}^{K} \alpha_k p_k \nabla \cdot \boldsymbol{v}_k &= \frac{1}{\rho} \sum_{l,k=1}^{K} P_{k,l}\,(\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla\, \alpha_l \\ &\quad - \frac{1}{\rho} \sum_{k=1}^{K} \alpha_k \rho_k e_k (\boldsymbol{v}_k - \boldsymbol{v}) + \frac{1}{\rho} \sum_{k=1}^{K} \sum_{i,l=1}^{d} \frac{\partial\, v_{k,l}}{\partial\, x_i} \alpha_k (\boldsymbol{T}_k)_{l,i} \\ &\quad - \frac{1}{\rho} \nabla \cdot \boldsymbol{q} - \frac{1}{\rho} \sum_{k=1}^{K} (\boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} - S_{\alpha\rho,k} u_k). \end{aligned} \tag{3.11}$$

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

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

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

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

4 Mathematical properties: hyperbolicity and subcharacteristic condition

Neglecting viscosity and heat conduction as well as relaxation processes in the fluid equations introduced in Sect. 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. We conclude this section with a note on the symmetrization of the hyperbolic system.

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

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

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

$$\boldsymbol{A}_{k,n} := \begin{pmatrix} \frac{\rho_k}{\alpha_k}\, (v_{k,n} - V_{I,n})\, (\boldsymbol{e}_{k,K-1}^T (1 - \delta_{k,K}) - \boldsymbol{1}_{K-1}^T\, \delta_{k,K}) \\ \boldsymbol{n} \boldsymbol{\beta}_k^T \\ \frac{\rho_k}{\alpha_k}\, (v_{k,n} - V_{I,n})\, \boldsymbol{\gamma}_k^T \end{pmatrix}, \tag{4.8}$$

$$\boldsymbol{B}_{k,n} := \begin{pmatrix} v_{k,n} & \rho_k\, \boldsymbol{n}^T & 0 \\ \boldsymbol{0}_d & v_{k,n}\, \boldsymbol{I}_d & \frac{1}{\rho_k}\, \boldsymbol{n} \\ 0 & \rho_k\, c_k^2 \boldsymbol{n}^T & v_{k,n} \end{pmatrix}. \tag{4.9}$$

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 their components $l = 1, \ldots, K-1$ as

$$\beta_{k,l} := \frac{1}{\alpha_k \rho_k} \left((P_{k,l} - p_k)(1 - \delta_{k,l}) - (P_{k,K} - p_k)(1 - \delta_{k,K}) \right), \tag{4.10}$$

$$\gamma_{k,l} := C_{k,l}^2 (1 - \delta_{k,l}) - C_{k,K}^2 (1 - \delta_{k,K}) \tag{4.11}$$

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

$$v_{k,n} := \boldsymbol{v}_k \cdot \boldsymbol{n}, \quad V_{I,n} := \boldsymbol{V}_I \cdot \boldsymbol{n}. \tag{4.12}$$

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

$$\det(\boldsymbol{B}_n - \lambda\,\boldsymbol{I}) = \det(V_{n,I}\,\boldsymbol{I}_{K-1} - \lambda\,\boldsymbol{I}_{K-1}) \prod_{k=1}^{K} \det(\boldsymbol{B}_{k,n} - \lambda\,\boldsymbol{I}_{d+2}) = 0 \tag{4.13}$$

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

$$\det(\boldsymbol{B}_{k,n} - \lambda\,\boldsymbol{I}_{d+2}) = (v_{k,n} - \lambda)^d\,((v_{k,n} - \lambda)^2 - c_k^2) \tag{4.14}$$

Hence, we obtain the following eigenvalues:

$$\lambda_{I,k} = V_{I,n},\ k = 1, \ldots, K-1 \tag{4.15}$$

$$\lambda_{k,i} = v_{k,n},\ k = 1, \ldots, K,\ i = 1, \ldots, d \tag{4.16}$$

$$\lambda_{k,\pm} = v_{k,n} \pm c_k,\ k = 1, \ldots, K. \tag{4.17}$$

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

$$\boldsymbol{R}_n := \begin{pmatrix} \boldsymbol{R}_{I,n}^0 & & & \\ \boldsymbol{R}_{I,n}^1 & \boldsymbol{R}_{1,n} & & \\ \vdots & & \ddots & \\ \boldsymbol{R}_{I,n}^K & & & \boldsymbol{R}_{K,n} \end{pmatrix}, \quad \boldsymbol{L}_n := \begin{pmatrix} \boldsymbol{L}_{I,n}^0 & & & \\ \boldsymbol{L}_{I,n}^1 & \boldsymbol{L}_{1,n} & & \\ \vdots & & \ddots & \\ \boldsymbol{L}_{I,n}^K & & & \boldsymbol{L}_{K,n} \end{pmatrix} \tag{4.18}$$

with blocks

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

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

Here the matrices $\boldsymbol{R}_n$ and $\boldsymbol{L}_n$ are composed of the right and left eigenvectors in their 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 subproblems 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 (4.16) and (4.17) are

$$\boldsymbol{r}_{k,d} = (1, \boldsymbol{0}_d^T, 0)^T,\ \boldsymbol{r}_{k,i} = (0, \boldsymbol{t}_i^T, 0)^T,\ \boldsymbol{r}_{k,\pm} = (1, \pm c_k/\rho_k \boldsymbol{n}^T, c_k^2)^T, \tag{4.19}$$

$$\boldsymbol{l}_{k,d} = (1, \boldsymbol{0}_d^T, -c_k^{-2})^T,\ \boldsymbol{l}_{k,i} = (0, \boldsymbol{t}_i^T, 0)^T,\ \boldsymbol{l}_{k,\pm} = 0.5 c_k^{-2}(1, \pm c_k \rho_k \boldsymbol{n}^T, 1)^T \tag{4.20}$$

for $i = 1, \ldots, d-1$. Thus, there exists an eigenvalue decomposition of the matrix $\boldsymbol{B}_{k,n}$, i.e.,

$$\boldsymbol{L}_{k,n} \boldsymbol{B}_{k,n} \boldsymbol{R}_{k,n} = \boldsymbol{\Lambda}_{k,n}, \tag{4.21}$$

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

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

$$\boldsymbol{L}_{k,n} := \frac{1}{2c_k^2} \begin{pmatrix} 0 & 0 & \ldots & 0 & 2c_k^2 & 0 \\ -c_k \rho_k \boldsymbol{n} & 2c_k^2 \boldsymbol{t}_1 & \ldots & 2c_k^2 \boldsymbol{t}_{d-1} & \boldsymbol{0}_d & c_k \rho_k \boldsymbol{n} \\ 1 & 0 & \ldots & 0 & -2 & 1 \end{pmatrix}^T, \tag{4.23}$$

$$\boldsymbol{\Lambda}_{k,n} := \begin{pmatrix} v_{k,n} - c_k & \boldsymbol{0}_d^T & 0 \\ \boldsymbol{0}_d & v_{k,n} \boldsymbol{I}_d & \boldsymbol{0}_d \\ 0 & \boldsymbol{0}_d^T & v_{k,n} + c_k \end{pmatrix}. \tag{4.24}$$

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

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

for $k = 1, \ldots, K$. 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 $\boldsymbol{R}^k_{I,n}$. For its representation, we introduce

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

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

$$\boldsymbol{R}^0_{I,n} := \kappa_0\,\boldsymbol{I}_{K-1}, \tag{4.25}$$

$$\boldsymbol{R}^k_{I,n} := \kappa_k\,\rho_k \begin{pmatrix} \alpha_k c^2_k\boldsymbol{\beta}^T_k - (\delta^n_k)^2\boldsymbol{\gamma}^T_k \\ -\boldsymbol{n}(\alpha_k\boldsymbol{\beta}^T_k - \boldsymbol{\gamma}^T_k)\delta^n_k/\rho_k \\ -\sigma_k(\boldsymbol{e}^T_{i,K-1}(1-\delta_{k,K}) - \boldsymbol{1}^T_{K-1}\delta_{k,K}) + \alpha_k\boldsymbol{\beta}^T_k - \boldsymbol{\gamma}^T_k \end{pmatrix} \tag{4.26}$$

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

$$\sigma_k \neq 0 \quad \forall\, k = 1, \ldots, K, \tag{4.27}$$

holds. This condition is referred to as the *non-resonance condition*; see [6] 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

$$\boldsymbol{L}_{k,n} = \boldsymbol{R}^{-1}_{k,n},\ \ k = 1, \ldots, K, \tag{4.28}$$

$$\boldsymbol{L}^0_{I,n} = (\boldsymbol{R}^0_{I,n})^{-1} = \kappa^{-1}_0\,\boldsymbol{I}_{K-1}, \tag{4.29}$$

$$\boldsymbol{L}^K_{I,n} = -\boldsymbol{L}_{k,n}\boldsymbol{R}^K_{I,n}(\boldsymbol{R}^0_{I,n})^{-1} = -\kappa^{-1}_0\,\boldsymbol{L}_{k,n}\boldsymbol{R}^K_{I,n}, \quad k = 1, \ldots, K, \tag{4.30}$$

and we obtain for the right eigenvectors

$$\boldsymbol{r}_{I,l} := \kappa_0\left((\overline{\boldsymbol{r}}^0_{I,l})^T, (\overline{\boldsymbol{r}}^1_{I,l})^T, \ldots, (\overline{\boldsymbol{r}}^K_{I,l})^T\right)^T, \quad l = 1, \ldots, K-1. \tag{4.31}$$

where $\overline{\boldsymbol{r}}^0_{I,l} = \boldsymbol{e}_{l,K-1}$ and $\overline{\boldsymbol{r}}^k_{I,l} = (\overline{x}_{k,l}, \overline{\boldsymbol{y}}^T_{k,l}, \overline{z}_{k,l})^T$ is determined by the components

$$\overline{z}_{k,l} = \rho_k\left(\alpha_k c^2_k\beta_{k,l} - (\delta^n_k)^2\gamma_{k,l}\right)/(\alpha_k\sigma_k), \tag{4.32}$$

$$\overline{\boldsymbol{y}}_{k,l} = -\boldsymbol{n}\left(\alpha_k\beta_{k,l} - \gamma_{k,l}\right)\delta^n_k/(\alpha_k\sigma_k), \tag{4.33}$$

$$\overline{x}_{k,l} = \left(-\sigma_k(\delta_{k,l}(1-\delta_{k,K}) - \delta_{k,K}) + \alpha_k\beta_{k,l} - \gamma_{k,l}\right)\rho_k/(\alpha_k\sigma_k). \tag{4.34}$$

These are well defined also in case of $\alpha_k = 0$ or $\sigma_k = 0$. Similar to (4.31), the left eigenvectors are then given by

$$\boldsymbol{l}_{I,l} := \left((\boldsymbol{l}^1_{I,0})^T, (\boldsymbol{l}^1_{I,l})^T, \ldots, (\boldsymbol{l}^K_{I,l})^T\right)^T, \quad l = 1, \ldots, K-1. \tag{4.35}$$

with

$$\boldsymbol{l}^0_{I,l} = \prod_{k=1}^{K}(\alpha_k\sigma_k)^{-1}\,\boldsymbol{e}_{l,K-1}, \quad \boldsymbol{l}^k_{I,l} = \frac{\rho_k}{2c^2_k\alpha_k\sigma_k}(a^l_k, 0, \ldots, 0, b^l_k, c^l_k)^T$$

and

$$
\begin{aligned}
a_k^l &:= -c_k(\alpha_k\beta_{k,l}-\gamma_{k,l})\delta_k^n + \sigma_k(\delta_{k,l}(1-\delta_{k,K}) - \delta_{k,K}) - \alpha_k\beta_{k,l}+\gamma_{k,l},\\
b_k^l &:= 2c_k^2((\delta_k^n)^2\gamma_{k,l}-\alpha_k c_k^2\beta_{k,l}) - 2\sigma_k(\delta_{k,l}(1-\delta_{k,K}) - \delta_{k,K}) + 2(\alpha_k\beta_{k,l}-\gamma_{k,l}),\\
c_k^l &:= c_k(\alpha_k\beta_{k,l} - \gamma_{k,l})\delta_k^n + \sigma_k(\delta_{k,l}(1-\delta_{k,K}) - \delta_{k,K}) - \alpha_k\beta_{k,l}+\gamma_{k,l}.
\end{aligned}
$$

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 $\boldsymbol{B}_n$

$$\boldsymbol{L}_n\boldsymbol{B}_n\boldsymbol{R}_n = \boldsymbol{\Lambda}_n \tag{4.36}$$

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 $\boldsymbol{B}_{k,n}\boldsymbol{R}_{I,n}^k = \boldsymbol{R}_{I,n}^k\boldsymbol{\Lambda}_{0,n} - \boldsymbol{A}_{k,n}\boldsymbol{R}_{I,n}^0$. To conclude the investigation on the hyperbolicity, we summarize the findings in the following theorem.

Theorem 1 (Hyperbolicity) *Let the interfacial pressures satisfy the conditions* (2.5) *and* (2.14). *Let the interfacial velocity* $\boldsymbol{V}_I$ *be chosen such that for arbitrary normal direction* $\boldsymbol{n}$ *the normal interfacial velocity* $v_{I,n}$ *does not coincide with one of the eigenvalues* $\lambda_{k,i}$ *and* $\lambda_{k,\pm}$ *of* $\boldsymbol{B}_n$*; i.e., the non-resonance condition* (4.27) *is satisfied. 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* (4.36).

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 [3,37] in case of a seven-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. A starting point is the evolution equations (2.21), (2.22) and (2.23). The corresponding first-order system then reads

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

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

$$\partial_t\,p + \sum_{i=1}^{d}\left(v_i\,\frac{\partial\,p}{\partial\,x_i} + \rho\,c^2\,\frac{\partial\,v_i}{\partial\,x_i}\right) = 0, \tag{4.39}$$

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

$$\partial_t\,\boldsymbol{w} + \boldsymbol{B}_n(\boldsymbol{w})\,\frac{\partial\,\boldsymbol{w}}{\partial\,\xi} = \boldsymbol{0} \tag{4.40}$$

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

$$\boldsymbol{B}_n := \begin{pmatrix} v_n & \rho\,\boldsymbol{n}^T & 0\\ \boldsymbol{0}_d & v_n\,\boldsymbol{I}_d & \frac{1}{\rho}\,\boldsymbol{n}\\ 0 & \rho\,c^2\boldsymbol{n}^T & v_n \end{pmatrix}. \tag{4.41}$$

The normal component of the velocity is defined as

$$v_n := \boldsymbol{v} \cdot \boldsymbol{n}. \tag{4.42}$$

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:

$$\lambda_\pm = v_n \pm c, \quad \lambda_i = v_n,\ i = 1, \ldots, d. \tag{4.43}$$

With regard to a stable numerical discretization of the non-equilibrium model in the limit of vanishing relaxation terms, the so-called subcharacteristic condition, see Whitham [36] and Liu [24], has to hold true. For this purpose, we evaluate the eigenvalues (4.15), (4.16) and (4.17) with respect to an equilibrium state; i.e.,(2.18), (2.19) and (2.20) hold,

$$\overline{\lambda}_{I,k} = \overline{V}_{I,n} = \overline{\boldsymbol{v}}_I \cdot \boldsymbol{n} = \overline{\boldsymbol{v}} \cdot \boldsymbol{n} = \overline{v}_n, \quad k = 1, \ldots, K-1 \tag{4.44}$$

$$\overline{\lambda}_{k,i} = \overline{v}_{k,n} = \overline{\boldsymbol{v}}_k \cdot \boldsymbol{n} = \overline{\boldsymbol{v}} \cdot \boldsymbol{n} = \overline{v}_n, \quad k = 1, \ldots, K,\ i = 1, \ldots, d \tag{4.45}$$

$$\overline{\lambda}_{k,\pm} = \overline{v}_{k,n} \pm c_k = \overline{v}_n \pm c_k, \quad k = 1, \ldots, K. \tag{4.46}$$

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

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

A straight forward estimate gives

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

In the second estimate, we use that

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

This immediately implies that the following theorem holds true.

Theorem 2 (Subcharacteristic condition) *Let α_k, ρ_k and c_k, $k = 1, \ldots, K$ be non-negative. Then, the eigenvalues (4.15), (4.16), (4.17) and (4.44), (4.45), (4.46) 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 subcharacteristic condition*

$$\overline{\lambda}_i \in \left[\min\left(\min_k \overline{\lambda}_{I,k},\ \min_{k,i} \overline{\lambda}_{k,i}\right), \max\left(\max_k \overline{\lambda}_{I,k},\ \max_{k,i} \overline{\lambda}_{k,i}\right)\right] = \{\overline{v}_n\},$$
$$\overline{\lambda}_\pm \in \left[\min_k \overline{\lambda}_{k,\pm}, \max_k \overline{\lambda}_{k,\pm}\right].$$

Note that similar results have been proven recently by Flatten and Lund [11] for a hierarchy of two-phase relaxation models.

4.3 Symmetrization

From Kato's theorem [21], it follows that there exists a local-in-time smooth solution to the Cauchy problem of the projected system (4.6), if the problem is symmetrizable; i.e., there exists a symmetric positive definite matrix $\boldsymbol{P}_n = \boldsymbol{P}_n(\boldsymbol{w})$ such that the matrix $\boldsymbol{P}_n \boldsymbol{B}_n$ is symmetric. To construct such a symmetrizer, we first observe that the matrix

$$\boldsymbol{P}_k = \begin{pmatrix} 1 & \boldsymbol{0}_d^T & -1/c_k^2 \\ \boldsymbol{0}_d & 0.5(\rho_k/c_k)^2\, \boldsymbol{I}_d & \boldsymbol{0}_d \\ -1/c_k^2 & \boldsymbol{0}_d^T & 1.5/c_k^4 \end{pmatrix}.$$

is a symmetrizer of the phasic problem

$$\partial_t\, \boldsymbol{w}_k + \boldsymbol{B}_{k,n}(\boldsymbol{w}_k)\, \frac{\partial\, \boldsymbol{w}_k}{\partial\, \xi} = \boldsymbol{0}.$$

We then make the following ansatz for a symmetrizer of (4.6):

$$\boldsymbol{P}_n = \begin{pmatrix} K\; P_{\alpha,n} \boldsymbol{I}_{K-1} & \boldsymbol{P}_{1,\alpha,n}^T & \cdots & \boldsymbol{P}_{K,\alpha,n}^T \\ \boldsymbol{P}_{1,\alpha,n} & \boldsymbol{P}_1 & & \\ \vdots & & \ddots & \\ \boldsymbol{P}_{K,\alpha,n} & & & \boldsymbol{P}_K \end{pmatrix},$$

where

$$\boldsymbol{P}_{k,\alpha,k} = \boldsymbol{L}_{k,n}^T \left(\boldsymbol{\Lambda}_{k,n} - V_{I,n} \boldsymbol{I}_{d+2}\right)^{-1} \boldsymbol{R}_{k,n} \boldsymbol{A}_{k,n}$$

with $\boldsymbol{A}_{k,n}$, $\boldsymbol{R}_{k,n}$, $\boldsymbol{L}_{k,n}$ and $\boldsymbol{\Lambda}_{k,n}$ defined by (4.8), (4.22), (4.23) and (4.24). Note that $\boldsymbol{P}_{k,\alpha,n}$ is well defined if the non-resonance condition (4.27) holds true. Obviously, $\boldsymbol{P}_n$ is symmetric. It turns out that $\boldsymbol{P}_n \boldsymbol{B}_n$ is symmetric whenever $\boldsymbol{P}_{k,\alpha,n}^T \boldsymbol{A}_{k,n}$ is symmetric. The latter holds true provided that $\boldsymbol{P}_{k,n}^T \boldsymbol{R}_{k,n} = \boldsymbol{L}_{k,n}^T$. This condition is only satisfied in the one-dimensional case, i.e., $d = 1$. It remains to verify that $\boldsymbol{P}_n$ is positive definite. For this purpose, we have to verify for any $\boldsymbol{a} = (\boldsymbol{a}_\alpha^T, \boldsymbol{a}_1^T, \ldots, \boldsymbol{a}_K^T)^T \neq \boldsymbol{0}$ with $\boldsymbol{a}_\alpha \in \mathbb{R}^{K-1}$, $\boldsymbol{a}_k \in \mathbb{R}^{d+2}$, $k = 1, \ldots, K$ that $\boldsymbol{a}^T \boldsymbol{P}_n \boldsymbol{a}$ is positive. A straightforward calculus yields

$$\boldsymbol{a}^T \boldsymbol{P}_n \boldsymbol{a} = P_{\alpha,n} \sum_{k=1}^{K-1} \sum_{i=1}^{K-1} \left(a_{\alpha,i} + (\boldsymbol{P}_{k,\alpha,n}^T \boldsymbol{a}_k)_i / P_{\alpha,n}\right)^2 + \sum_{k=1}^{K} P_{\alpha,n}^{-1} \boldsymbol{a}_k^T\, \boldsymbol{Q} \boldsymbol{a}_k$$

with $\boldsymbol{Q} := P_{\alpha,n} \boldsymbol{P}_k - \boldsymbol{P}_{k,\alpha,n} \boldsymbol{P}_{k,\alpha,n}^T$. Since $\boldsymbol{P}_k$ is symmetric positive definite, the Cholesky decomposition $\boldsymbol{P}_k = \boldsymbol{C}_k \boldsymbol{C}_k^T$ exists. Furthermore, the matrix $\boldsymbol{E}_k := \boldsymbol{C}_k^{-1} \boldsymbol{P}_{k,\alpha,n}^T \boldsymbol{P}_{k,\alpha,n} \boldsymbol{C}_k^T$ is symmetric, and thus, there exists an orthogonal matrix $\boldsymbol{T}_k$ such that $\boldsymbol{T}_k \boldsymbol{E}_k \boldsymbol{T}_k^T = \boldsymbol{D}_k$ where $\boldsymbol{D}_k$ is a diagonal matrix with the eigenvalues μ_i^k of $\boldsymbol{E}_k$ as entries. Then, we obtain

$$\boldsymbol{a}_k^T\, \boldsymbol{Q} \boldsymbol{a}_k = \boldsymbol{b}_k^T (P_{\alpha,n} \boldsymbol{I}_{d+2} - \boldsymbol{D}_k) \boldsymbol{b}_k = \sum_{i=1}^{d+2} b_{k,i}^2 \left(P_{\alpha,n} - \mu_i^k\right)$$

with $\boldsymbol{b}_k := \boldsymbol{T}_k^T \boldsymbol{C}_k^T \boldsymbol{a}_k$. Choosing $P_{\alpha,n} > \max_{i,k} \left\{|\mu_i^k|\right\} > 0$ the term $\boldsymbol{a}_k^T\, \boldsymbol{Q} \boldsymbol{a}_k$ is non-negative and is positive for $\boldsymbol{a}_k \neq \boldsymbol{0}$. Thus, we have finally verified that in the one-dimensional case the matrix $\boldsymbol{P}_n$ is a symmetrizer of (4.6) provided the non-resonance condition (4.27) holds true. This generalizes the result in [6] for a two-phase model.

5 Frame invariance, objectivity and Galilean transformation

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. [8, p. 31 ff], and [23]: 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

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

To rewrite the fluid equations in terms of the general Euclidean change of frame, we introduce the change of variables

$$f(t, \boldsymbol{x}) = f(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))), \tag{5.4}$$

$$\boldsymbol{u}(t, \boldsymbol{x}) = \boldsymbol{u}(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))), \tag{5.5}$$

$$\boldsymbol{T}(t, \boldsymbol{x}) = \boldsymbol{T}(t^* - a, \boldsymbol{x}_0 + \boldsymbol{Q}^T(t)(\boldsymbol{x}^* - \boldsymbol{x}_0^*(t))). \tag{5.6}$$

It is well known that the fluid equations for a single phase are not invariant under a general Euclidean frame of change. 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

$$\dot{\boldsymbol{x}}_0 = 0,\ \ \dot{\boldsymbol{Q}} = \boldsymbol{0}\ \ \text{ equiv. }\ \ \boldsymbol{Q} = const,\ \ \ \boldsymbol{x}_0^*(t) = \boldsymbol{c}_0 + \boldsymbol{c}_1 t,\ \ \boldsymbol{c}_1, \boldsymbol{c}_2 = const \tag{5.7}$$

in (5.1). For this transformation, the velocity vector is still not objective, but the acceleration and the rotation tensor are objective.

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 $S_{\alpha\rho E,k}$. For this purpose, we apply a Galilean frame of change to the fluid equations (2.2), (2.3), (2.4) and (2.7). A detailed derivation can be found in [29]. Here we will confine ourselves to the main results. First of all, we derive from the evolution equation (2.7) of the volume fractions assuming that the volume fractions are objective, i.e., $\alpha_k^* = \alpha_k$,

$$\partial_{t^*}\,\alpha_k^* + \boldsymbol{V}_I^* \cdot \nabla_{\boldsymbol{x}^*}\,\alpha_k^* = S^*_{\alpha^*,k},\quad k = 1, \ldots, K, \tag{5.8}$$

where the interfacial velocity and the source term are given as

$$\boldsymbol{V}_I^* := \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q}\boldsymbol{V}_I + \dot{\boldsymbol{Q}}(\boldsymbol{x} - \boldsymbol{x}_0) = \dot{\boldsymbol{x}}_0^* + \boldsymbol{Q}\boldsymbol{V}_I = \boldsymbol{c}_1 + \boldsymbol{Q}\boldsymbol{V}_I, \tag{5.9}$$

$$S^*_{\alpha^*,k} := S_{\alpha,k}. \tag{5.10}$$

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

$$\partial_{t^*}\,(\alpha_k^*\,\rho_k^*) + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^*\,\rho_k^*\,\boldsymbol{v}_k^*) = S^*_{\alpha^*\rho^*,k}, \tag{5.11}$$

with source term

$$S^*_{\alpha^*\rho^*,k} := S_{\alpha\rho,k}. \tag{5.12}$$

Note that (5.8) and (5.11) 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 incorporate (5.11). 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

$$\partial_{t^*}\,(\alpha_k^*\,\rho_k^*\,\boldsymbol{v}_k^*) + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^*\,\rho_k^*\,\boldsymbol{v}_k{}^*\,\boldsymbol{v}_k^{*T} + \alpha_k^*\,p_k^*\,\boldsymbol{I}) = -\sum_{l=1}^{K} P_{k,l}^*\,\nabla_{\boldsymbol{x}^*}\,\alpha_l^* + \nabla_{\boldsymbol{x}^*} \cdot (\alpha_k^*\,\boldsymbol{T}_k^*) + \boldsymbol{S}^*_{\alpha^*\rho^*\boldsymbol{v}^*,k}, \tag{5.13}$$

with source term

$$\boldsymbol{S}^*_{\alpha^*\rho^*\boldsymbol{v}^*,k} := S_{\alpha\rho,k}\,\dot{\boldsymbol{x}}_0^* + \boldsymbol{Q}\,\boldsymbol{S}_{\alpha\rho\boldsymbol{v},k}. \tag{5.14}$$

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

$$e^*_{kin,k} = e_{kin,k} + \dot{\boldsymbol{x}}^*_0 \cdot \boldsymbol{v}^*_k - \frac{1}{2}(\dot{\boldsymbol{x}}^*_0)^2, \quad e_{kin,k} := \frac{1}{2}\boldsymbol{v}^2_k. \tag{5.15}$$

Thus, the total energy and the total enthalpy are

$$E_k := e_k + \frac{1}{2}\boldsymbol{v}^2_k = E^*_k - \dot{\boldsymbol{x}}^*_0 \cdot \boldsymbol{v}^*_k + \frac{1}{2}(\dot{\boldsymbol{x}}^*_0)^2, \quad E^*_k := e^*_k + \frac{1}{2}(\boldsymbol{v}^*_k)^2, \tag{5.16}$$

$$H_k := E_k + \frac{p_k}{\rho_k} = H^*_k - \dot{\boldsymbol{x}}^*_0 \cdot \boldsymbol{v}^*_k + \frac{1}{2}(\dot{\boldsymbol{x}}^*_0)^2, \quad H^*_k := E^*_k + \frac{p^*_k}{\rho^*_k}, \tag{5.17}$$

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) and incorporating (5.11), (5.13), the energy equation (2.4) in the Galilean frame becomes

$$\begin{aligned} &\partial_{t^*}(\alpha^*_k\,\rho^*_k\,E^*_k) + \nabla_{\boldsymbol{x}^*} \cdot (\alpha^*_k\,\rho^*_k\,\boldsymbol{v}^*_k\,(E^*_k + p^*_k/\rho^*_k)) \\ &\quad = -\sum_{l=1}^{K} P^*_{k,l}\,\boldsymbol{V}^*_I \cdot \nabla_{\boldsymbol{x}^*}\,\alpha^*_l + \nabla_{\boldsymbol{x}^*} \cdot \left(\alpha^*_k\,\left(\boldsymbol{v}^*_k \cdot \boldsymbol{T}^*_k - \boldsymbol{q}^*_k\right)\right) + S^*_{\alpha^*\rho^*E^*,k}, \end{aligned} \tag{5.18}$$

with source term

$$S^*_{\alpha^*\rho^*E^*,k} := S_{\alpha\rho E,k} + \boldsymbol{Q}\boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} \cdot \dot{\boldsymbol{x}}^*_0 + \frac{1}{2}\,(\dot{\boldsymbol{x}}^*_0)^2 S_{\alpha\rho,k}. \tag{5.19}$$

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 $\boldsymbol{q}^*_k = \boldsymbol{Q}\boldsymbol{q}_k$.

Finally, we conclude with summarizing our findings in the following

Theorem 3 (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., the viscosity coefficient $\overline{\mu}_k$, the heat conduction coefficient $\overline{\lambda}_k$ introduced in Sect. 6.3.1, are objective,*
4. *the source terms (5.10), (5.12), (5.14), (5.19) are invariant under a Galilean transformation, i.e.,*

$$S^*_{\alpha^*,k} = S_{\alpha^*,k}, \;\; S^*_{(\alpha\rho)^*,k} = S_{(\alpha\rho)^*,k}, \;\; \boldsymbol{S}^*_{(\alpha\rho\boldsymbol{v})^*,k} = \boldsymbol{S}_{(\alpha\rho\boldsymbol{v})^*,k}, \;\; S^*_{(\alpha\rho E)^*,k} = S_{(\alpha\rho E)^*,k}. \tag{5.20}$$

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 $\dot{\boldsymbol{x}}^*_0 + \boldsymbol{Q}\boldsymbol{V}_I$ and total energy (5.16) is Galilean invariant. This also holds true for the system without the source terms as well as for the mixture model and the equilibrium model because the latter are derived from the non-equilibrium model by summation.

6 Thermodynamical properties: second 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 second 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.,

$$\begin{aligned}
&\frac{\partial^2 e_k}{\partial^2 \tau_k}(\tau_k, s_k) \geq 0, \ \frac{\partial^2 e_k}{\partial^2 s_k}(\tau_k, s_k) \geq 0, \\
&\frac{\partial^2 e_k}{\partial^2 \tau_k}(\tau_k, s_k)\frac{\partial^2 e_k}{\partial^2 s_k}(\tau_k, s_k) \geq \left(\frac{\partial^2 e_k}{\partial \tau_k \partial s_k}(\tau_k, s_k)\right)^2.
\end{aligned}$$

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

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

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

$$\begin{aligned}
\partial_t s_k + \boldsymbol{v}_k \cdot \nabla s_k = \frac{1}{\alpha_k \rho_k T_k} \Bigg(&\sum_{l=1}^{K} P_{k,l} \left(\boldsymbol{v}_k - \boldsymbol{V}_I\right) \cdot \nabla \alpha_l + p_k (\boldsymbol{v}_k - \boldsymbol{V}_I) \cdot \nabla \alpha_k \\
&+ \alpha_k \sum_{i,l=1}^{d} \frac{\partial v_{k,l}}{\partial x_i} (\boldsymbol{T}_k)_{l,i} - \nabla \cdot (\alpha_k \boldsymbol{q}_k) + S_{s,k} \Bigg)
\end{aligned} \tag{6.6}$$

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)

$$\begin{aligned}
&\partial_t\left(\alpha_k\rho_k s_k\right)+\nabla\cdot\left(\alpha_k\rho_k s_k\boldsymbol{v}_k\right)+\nabla\cdot\left(\frac{1}{T_k}\alpha_k\boldsymbol{q}_k\right)\\
&\quad=\frac{1}{T_k}\left(\sum_{l=1}^{K}P_{k,l}\left(\boldsymbol{v}_k-\boldsymbol{V}_I\right)\cdot\nabla\alpha_l+p_k(\boldsymbol{v}_k-\boldsymbol{V}_I)\cdot\nabla\alpha_k+\alpha_k\sum_{i,l=1}^{d}\frac{\partial\, v_{k,l}}{\partial\, x_i}(\boldsymbol{T}_k)_{l,i}-\alpha_k\frac{1}{T_k}\boldsymbol{q}_k\cdot\nabla T_k\right)\\
&\qquad+S_{\alpha\rho s,k}
\end{aligned}\tag{6.8}$$

with the relaxation term

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

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

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

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

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

Note that the total entropy of a homogeneous mixture is determined by the sum of ρs and the non-negative mixture entropy, [27], p. 320. We discuss the mixture entropy in the context of the relaxation terms for chemical potentials for a three-component mixture; see Sect. 7.3.2.

6.3 Entropy production

According to the second 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

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

where $\overline{\mu}_k$ denotes the viscosity coefficient of component k. Thus, the components of this symmetric tensor are

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

Then, we compute for the entropy production term (6.13)

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

with

$$\begin{aligned} \Gamma &:= \sum_{i=1}^{d} \left(2 \left(\frac{\partial v_{k,i}}{\partial x_i} \right)^2 - \sum_{j=1, j \neq i}^{d} \frac{\partial v_{k,j}}{\partial x_j} \frac{\partial v_{k,i}}{\partial x_i} \right) \\ &= \begin{cases} 2 \left(\frac{\partial v_{k,1}}{\partial x_1} \right)^2, & d = 1 \\ \left(\frac{\partial v_{k,1}}{\partial x_1} \right)^2 + \left(\frac{\partial v_{k,2}}{\partial x_2} \right)^2 + \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,2}}{\partial x_2} \right)^2, & d = 2 \\ \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,2}}{\partial x_2} \right)^2 + \left(\frac{\partial v_{k,2}}{\partial x_2} - \frac{\partial v_{k,3}}{\partial x_3} \right)^2 + \left(\frac{\partial v_{k,1}}{\partial x_1} - \frac{\partial v_{k,3}}{\partial x_3} \right)^2, & d = 3 \end{cases} . \end{aligned}$$

Obviously, the following theorem holds true.

Theorem 4 (Entropy production due to viscosity) *The viscous stress tensors are determined by* (6.15). *Let the temperatures* T_k *and the viscosity coefficients* $\overline{\mu}_k$, $k = 1, \ldots, K$ *be non-negative. Then, the production terms* (6.13) *are non-negative. In addition, assuming the saturation condition* (2.1), *then 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

$$\boldsymbol{q}_k = -\overline{\lambda}_k \nabla T_k, \tag{6.16}$$

where $\overline{\lambda}_k$ denotes the heat conduction coefficient of component k. Then, the entropy production term (6.14) reads

$$\Delta_k = \frac{1}{T_k^2} \overline{\lambda}_k \nabla T_k \cdot \nabla T_k.$$

From this, we directly conclude

Theorem 5 (Entropy production due to heat conduction) *The heat fluxes are determined by* (6.16). *Let the temperatures* T_k *and the heat conduction coefficients* $\overline{\lambda}_k$, $k = 1, \ldots, K$ *be non-negative. Then, the production terms* (6.14) *are non-negative. In addition, assuming the saturation condition* (2.1), *the entropy production due to heat conduction* $\sum_{k=1}^{K} \alpha_k \Delta_k$ *is non-negative.*

Note that Theorems 4 and 5 are counterparts of the results of Guillemaud [16] in case of a two-component model.

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

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

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

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

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.,

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

This is motivated by Gallouët et al. [12] and Hérard [18] for a two-phase and a three-phase model, respectively. Then, we may rewrite the velocity differences in (6.17) as

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

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

$$\begin{aligned}&\sum_{k=1}^{i} \frac{1}{T_k} \big((P_{k,l} - p_k)(1 - \delta_{l,k}) - (P_{k,K} - p_k)\big) \sum_{j=i+1}^{K} \beta_j \\ &+ \left(\sum_{k=i+1}^{K-1} \frac{1}{T_k} \big((P_{k,l} - p_k)(1 - \delta_{l,k}) - (P_{k,K} - p_k)\big) + \frac{1}{T_K}(P_{K,l} - p_K) \right) \sum_{j=1}^{i} (-\beta_j) = 0 \end{aligned} \qquad (6.19)$$

or, equivalently,

$$\begin{aligned}&\sum_{k=1,\neq l}^{i} \left(\frac{1}{T_k} \sum_{j=i+1}^{K} \beta_j \right) P_{k,l} - \sum_{k=1}^{i} \left(\frac{1}{T_k} \sum_{j=i+1}^{K} \beta_j \right) P_{k,K} \\ &\quad - \sum_{k=i+1,\neq l}^{K-1} \left(\frac{1}{T_k} \sum_{j=1}^{i} \beta_j \right) P_{k,l} + \sum_{k=i+1}^{K-1} \left(\frac{1}{T_k} \sum_{j=1}^{i} \beta_j \right) P_{k,K} - \frac{1}{T_K} \sum_{j=1}^{i} \beta_j P_{K,l} \\ &\quad = - \sum_{k=1}^{i} \frac{1}{T_k} p_k \delta_{l,k} \sum_{j=i+1}^{K} \beta_j + \left(\sum_{k=i+1}^{K-1} \frac{1}{T_k} p_k \delta_{l,k} - \frac{1}{T_K} p_K \right) \sum_{j=1}^{i} \beta_j \end{aligned} \qquad (6.20)$$

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

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

These equations are equivalent to

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

Then, (6.20) and (6.22) form a linear system for the interfacial pressures. To solve the system, it is convenient to rewrite it in blockwise form

$$\boldsymbol{A}_l \boldsymbol{\Lambda}_l \boldsymbol{P}_l + \boldsymbol{B} \boldsymbol{\Lambda}_K \boldsymbol{P}_K = \boldsymbol{d}_l, \quad l = 1, \ldots, K-1 \tag{6.23}$$

for the unknowns $\boldsymbol{P}_l := (P_{1,l}, \ldots, P_{l-1,l}, P_{l+1,l}, \ldots, P_{1,K})^T, l = 1, \ldots, K$ with matrix $\boldsymbol{\Lambda}_l = \operatorname{diag}(T_1^{-1}, \ldots, T_{l-1}^{-1}, T_{l+1}^{-1}, \ldots, T_K^{-1})$ assuming positive temperatures T_k, and $\boldsymbol{A}_l = (\boldsymbol{a}^1, \ldots, \boldsymbol{a}^{l-1}, \boldsymbol{a}^{l+1}, \ldots, \boldsymbol{a}^K)$ and $\boldsymbol{B} = (\boldsymbol{b}^1, \ldots, \boldsymbol{b}^{K-1})$ in $\mathbb{R}^{K \times (K-1)}$ defined by the columns

$$\begin{aligned} \boldsymbol{a}^k &= (-c_1, \ldots, -c_{k-1}, c^k, \ldots, c^{K-1}, T_k)^T \in \mathbb{R}^K, \quad k = 1, \ldots, K, \\ \boldsymbol{b}^k &= (c_1, \ldots, c_{k-1}, -c^k, \ldots, -c^{K-1}, T_k)^T \in \mathbb{R}^K, \quad k = 1, \ldots, K-1 \end{aligned}$$

and right-hand side $d_{l,i} = c_i(p_l/T_l - P_K/T_K)$, $1 \le i \le l-1$ and $d_{l,i} = c_i(p_l/T_l - P_K/T_K) - p_l/T_l$, $l \le i \le K-1$. Here we define $c_k := \sum_{j=1}^{k} \beta_j$, $c^k := \sum_{j=k+1}^{K} \beta_j$. Note that by the convexity assumption (6.18), it holds $c_k + c^k = 1$, $k = 1, \ldots, K$. Manipulating the rows and columns of (6.23), we obtain the equivalent system $\overline{\boldsymbol{A}}\, \overline{\boldsymbol{P}} = \overline{\boldsymbol{d}}$ with

$$\overline{\boldsymbol{A}} = \begin{pmatrix} \overline{\boldsymbol{A}}_1 & & & \overline{\boldsymbol{B}} \\ & \overline{\boldsymbol{A}}_2 & & \overline{\boldsymbol{B}} \\ & & \ddots & \vdots \\ & & \overline{\boldsymbol{A}}_{K-1} & \overline{\boldsymbol{B}} \end{pmatrix} \overline{\boldsymbol{S}}, \quad \overline{\boldsymbol{P}} = \overline{\boldsymbol{S}}^{-1} \begin{pmatrix} \boldsymbol{S}^{-1} \overline{\boldsymbol{P}}_1 \\ \boldsymbol{S}^{-1} \overline{\boldsymbol{P}}_2 \\ \vdots \\ \boldsymbol{S}^{-1} \overline{\boldsymbol{P}}_K \end{pmatrix}, \quad \overline{\boldsymbol{r}} = \begin{pmatrix} \boldsymbol{L}\boldsymbol{d}_1 \\ \boldsymbol{L}\boldsymbol{d}_2 \\ \vdots \\ \boldsymbol{L}\boldsymbol{d}_{K-1} \end{pmatrix}$$

with $\overline{\boldsymbol{A}}_l = \boldsymbol{L} \boldsymbol{A}_l \boldsymbol{\Lambda}_l \boldsymbol{S}$, $\boldsymbol{B} = \boldsymbol{L} \boldsymbol{B} \boldsymbol{\Lambda}_K \boldsymbol{S}$ and Frobenius matrices

$$\boldsymbol{S} = \boldsymbol{I}_{K-1} - \sum_{j=1}^{K-2} \boldsymbol{e}_{j+1} \otimes \boldsymbol{e}_j, \quad \boldsymbol{L} = \boldsymbol{I}_K + \sum_{j=1}^{K-1} (T_{j+1} - T_j) \boldsymbol{e}_j \otimes \boldsymbol{e}_K$$

and the transpose of a Frobenius matrix

$$\overline{\boldsymbol{S}} = \boldsymbol{I}_{(K-1)K} + \sum_{k=1}^{K-1} \left(\sum_{j=1}^{k-2} \boldsymbol{e}_{j'(k,j)} \otimes \boldsymbol{e}_{j'(K,j)} + \sum_{j=k}^{K-2} \boldsymbol{e}_{j'(k,j)} \otimes \boldsymbol{e}_{j'(K,j+1)} + \boldsymbol{e}_{j'(k,K-1)} \otimes \boldsymbol{e}_{j'(K,K-1)} \right)$$

with indices $j'(k, j) = j + (k-1)(K-1)$. Here we make the convention that in case of $K = 2$ empty sums in $\overline{\boldsymbol{S}}$ and $\boldsymbol{S}$ correspond to zero matrices. Since the determinant of Frobenius matrices is one, it follows that $\det(\overline{\boldsymbol{A}}) = \left(\hat{T} / \prod_{k=1}^{K} T_k\right)^{K-1}$ with $\hat{T} = \sum_{k=1}^{K} \beta_k T_k$. Thus, the system has a unique solution. This can be determined by successively solving the subsystems $\check{\boldsymbol{A}}_l \check{\boldsymbol{P}}_l = \check{\boldsymbol{r}}_l$, $l = 1, \ldots, L-1$ with $\check{\boldsymbol{A}}_l = (\check{\boldsymbol{a}}_1^l, \ldots, \check{\boldsymbol{a}}_{K-1}^l, \check{\boldsymbol{b}}_l)^T$ with $\check{\boldsymbol{a}}_k^l = \boldsymbol{e}_k$, $k = 1, \ldots, l-2$, $\check{\boldsymbol{a}}_{l-1}^l = \boldsymbol{e}_{l-1} + \boldsymbol{e}_l$, $\check{\boldsymbol{a}}_k^l = \boldsymbol{e}_{k+1}$, $k = l, \ldots, K-2$, $\check{\boldsymbol{a}}_{K-1}^l = (-c_1, \ldots, -c_{K-1}, \hat{T})^T$ and $\check{\boldsymbol{b}}_k^l = -\boldsymbol{e}_k$, $k = l-1, l$ and $\check{\boldsymbol{b}}_k^l = \boldsymbol{0}$ otherwise. The right-hand side is determined by $\check{\boldsymbol{r}}_l = \overline{\boldsymbol{r}}_l + \boldsymbol{e}_{l-1} \overline{P}_{l-1+(K-2)K}$. A tedious calculation finally gives the unique solution to the system (6.20) and (6.22), and we conclude with the following.

Theorem 6 (Entropy production due to interfacial states) *Let the assumptions* (2.5) *and* (2.14) *hold true. If the temperatures T_k are all positive, then for any convex combination* (6.18) *for the interfacial velocity $\boldsymbol{V}_I$ there uniquely exist interfacial pressures*

$$P_{k,l} = \frac{1}{\hat{T}} \left(\beta_k p_l T_k + p_k \sum_{j=1, \neq k}^{K} \beta_j T_j \right), \quad \hat{T} := \sum_{k=1}^{K} \beta_k T_k \tag{6.24}$$

solving the linear system (6.20) *and* (6.22)*, and thus, the production term $\Pi = \sum_{k=1}^{K} \Pi_k$ vanishes. In particular, the interfacial pressures are all positive and it holds*

$$P_I = \sum_{k=1}^{K} p_k \sum_{j=1, \neq k}^{K} \beta_j T_j / \hat{T}. \tag{6.25}$$

Since by means of the linear system (6.20) and (6.22), the interfacial pressures $P_{k,l}$ depend on the convex combination (6.18) for the interfacial velocity $\boldsymbol{V}_I$, and the second law of thermodynamics does not uniquely characterize interfacial velocity. There are several options discussed in the literature for two-component and three-component models, cf. [12,18,32]. We comment on this in Sect. 7.4.

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

$$S_{\alpha\rho s,k} = \frac{1}{T_k}\left(p_k S_{\alpha,k} + (u_k - g_k) S_{\alpha\rho,k} - \boldsymbol{v}_k \cdot \boldsymbol{S}_{\alpha\rho\boldsymbol{v},k} + S_{\alpha\rho E,k}\right), \tag{6.26}$$

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

$$g_k = e_k + p_k/\rho_k - T_k s_k \tag{6.27}$$

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

$$S_{\rho s,k} \geq 0,\ \ k = 1, \ldots, K \ \text{or} \ \sum_{k=1}^{K} S_{\alpha\rho s,k} \geq 0. \tag{6.28}$$

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

6.4 Thermodynamic stability

According to Menikoff and Plohr [25], thermodynamic stability of a single component k requires that e_k is a convex function of the specific volume τ_k and the specific entropy s_k; see also Sect. 6.1. In [15], p. 99 ff, it is proven that this holds true, if the entropy $U_k := -\rho_k s_k$ is a convex function of $\boldsymbol{u}_k := (\rho_k, \rho_k \boldsymbol{v}_k^T, \rho_k E_k)^T$. In the following, we will verify that

$$U(\boldsymbol{u}) := -\sum_{k=1}^{K} \alpha_k \rho_k s_k = -\rho s \tag{6.29}$$

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 $\boldsymbol{\alpha} := (\alpha_1, \ldots, \alpha_{K-1})^T$. For this purpose, we extend the proof in [32], Appendix A, for a two-phase model to our K-component model.

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)

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

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

$$\frac{\partial U}{\partial \alpha_l}(\boldsymbol{u}) = U_l(\boldsymbol{u}_l) - U_K(\boldsymbol{u}_K) - \frac{\partial U_l}{\partial \boldsymbol{u}_l}(\boldsymbol{u}_l) \cdot \boldsymbol{u}_l + \frac{\partial U_K}{\partial \boldsymbol{u}_K}(\boldsymbol{u}_K) \cdot \boldsymbol{u}_K, \ \frac{\partial U}{\partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) = \frac{\partial U_l}{\partial \boldsymbol{u}_l}(\boldsymbol{u}_l). \tag{6.30}$$

The Hessian of U is determined by the second-order derivatives

$$\begin{aligned}
\frac{\partial^2 U}{\partial \alpha_k \partial \alpha_l}(\boldsymbol{u}) &= \delta_{k,l} \frac{1}{\alpha_l} \boldsymbol{u}_l^T \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l) \boldsymbol{u}_l + \frac{1}{\alpha_K} \boldsymbol{u}_K^T \frac{\partial^2 U_K}{\partial^2 \boldsymbol{u}_K}(\boldsymbol{u}_K) \boldsymbol{u}_K, \quad k, l = 1, \ldots, K, \\
\frac{\partial^2 U}{\partial \alpha_k \partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) &= -\frac{1}{\alpha_l} (\delta_{k,l} - \delta_{K,l}) \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l) \boldsymbol{u}_l, l = 1, \ldots, K, \quad k = 1, \ldots, K-1, \\
\frac{\partial^2 U}{\partial \alpha_k \boldsymbol{u}_k \partial \alpha_l \boldsymbol{u}_l}(\boldsymbol{u}) &= \frac{1}{\alpha_l} \delta_{k,l} \frac{\partial^2 U_l}{\partial^2 \boldsymbol{u}_l}(\boldsymbol{u}_l), \quad k, l = 1, \ldots, K.
\end{aligned}$$

For a compact representation of the Hessian, we introduce the notation

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

According to the above second-order derivatives, these are determined by

$$\boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} = \frac{1}{\alpha_K}\boldsymbol{u}_K^T\boldsymbol{U}_K''\boldsymbol{u}_K\boldsymbol{1}_{K-1} + \operatorname{diag}\left(\left(\frac{1}{\alpha_k}\boldsymbol{u}_k^T\boldsymbol{U}_k''\boldsymbol{u}_k\right)_{k=1,\ldots,K-1}\right), \tag{6.31}$$

$$\boldsymbol{U}_{\alpha_k\boldsymbol{u_k},\alpha_k\boldsymbol{u_k}} = \frac{1}{\alpha_k}\boldsymbol{U}_k'', \tag{6.32}$$

$$\boldsymbol{U}_{\alpha_k\boldsymbol{u_k},\boldsymbol{\alpha}} = \left(-\frac{1}{\alpha_k}(\delta_{k,l}-\delta_{K,k})\boldsymbol{U}_k''\boldsymbol{u}_k\right)_{l=1,\ldots,K-1} = \boldsymbol{U}^T_{\boldsymbol{\alpha},\alpha_k\boldsymbol{u}_k}, \tag{6.33}$$

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

$$\boldsymbol{U}''(\boldsymbol{u}) = \begin{pmatrix}
\boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}} & \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_1\boldsymbol{u_1}} & \cdots & \boldsymbol{U}_{\boldsymbol{\alpha},\alpha_1\boldsymbol{u_K}}\\
\boldsymbol{U}_{\alpha_1\boldsymbol{u_1},\boldsymbol{\alpha}} & \boldsymbol{U}_{\alpha_1\boldsymbol{u_1},\alpha_1\boldsymbol{u_1}} & & \\
\vdots & & \ddots & \\
\boldsymbol{U}_{\alpha_K\boldsymbol{u_K},\boldsymbol{\alpha}} & & & \boldsymbol{U}_{\alpha_1\boldsymbol{u_K},\alpha_K\boldsymbol{u_K}}
\end{pmatrix}. \tag{6.34}$$

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 (6.34) of the Hessian

$$\boldsymbol{x}^T\boldsymbol{U}''\boldsymbol{x} = \boldsymbol{a}^T\boldsymbol{U}_{\boldsymbol{\alpha},\boldsymbol{\alpha}}\boldsymbol{a} + \sum_{k=1}^{K}\boldsymbol{a}^T\boldsymbol{U}_{\boldsymbol{\alpha},\alpha_k\boldsymbol{u_k}}\boldsymbol{b}_k + \sum_{k=1}^{K}\boldsymbol{b}_k^T\left(\boldsymbol{U}_{\alpha_k\boldsymbol{u_k},\boldsymbol{\alpha}}\boldsymbol{a} + \boldsymbol{U}_{\alpha_k\boldsymbol{u_k},\alpha_k\boldsymbol{u_k}}\boldsymbol{b}_k\right). \tag{6.35}$$

By means of (6.31), (6.32) and (6.33), we determine

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

Incorporating this into (6.35), 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 (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.*

6.5 Remarks on entropy–entropy flux pairs

From a mathematical point of view, the concept of entropy–entropy flux pairs, cf. [14], 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

$$\partial_t \boldsymbol{u} + \sum_{i=1}^{d} \boldsymbol{A}_i(\boldsymbol{u})\partial_{x_i} \boldsymbol{u} = \boldsymbol{S}(\boldsymbol{u}), \quad \boldsymbol{A}_i(\boldsymbol{u}) := \frac{\partial \boldsymbol{f}_i}{\partial \boldsymbol{u}}(\boldsymbol{u}) \tag{6.36}$$

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

$$\partial_t\, U(\boldsymbol{u}) + \sum_{i=1}^{d} \partial_{x_i}\, \boldsymbol{F}_i(\boldsymbol{u}) \le 0 \tag{6.37}$$

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

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T\, \boldsymbol{A}_i(\boldsymbol{u}) = \nabla_{\boldsymbol{u}} F_i(\boldsymbol{u})^T, \; i = 1, \ldots, d. \tag{6.38}$$

Due to these conditions, we infer for smooth solutions of (6.36) the entropy equation

$$\partial_t\, U(\boldsymbol{u}) + \sum_{i=1}^{d} \partial_{x_i}\, F_i(\boldsymbol{u}) = \nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T\, \boldsymbol{S}(\boldsymbol{u}), \tag{6.39}$$

Obviously, the entropy inequality (6.37) holds if and only if the entropy production is negative, i.e.,

$$\nabla_{\boldsymbol{u}} U(\boldsymbol{u})^T\, \boldsymbol{S}(\boldsymbol{u}) \le 0. \tag{6.40}$$

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

$$U(\boldsymbol{u}) := -\sum_{k=1}^{K} \alpha_k \rho_k s_k = -\rho s, \quad F_i(\boldsymbol{u}) := -\sum_{k=1}^{K} \alpha_k \rho_k s_k v_{k,i}, \; i = 1, \ldots, d. \tag{6.41}$$

In [29], it has been proven that the entropy–entropy flux pairs (U, F_i) satisfy the compatibility conditions (6.38), if the conditions (6.17) hold. Furthermore, it was shown that inequality (6.40) is equivalent to $S_{\rho s} \ge 0$ provided that the entropies $s_k = s_k(\tau_k, e_k), k = 1, \ldots, K$, are concave functions; i.e., (6.4) holds.

7 Relaxation model

The non-equilibrium model presented in Sect. 2.1 allows for different values for velocities, pressures, temperatures and 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 [33] or Lallemand et al. [22] for mechanical relaxation terms and Métayer et al. [26] for pressure, temperature and Gibbs free energy relaxation terms. Typically, it is assumed that pressure and velocity relax instantaneously, see [33], whereas the thermal relaxation and the relaxation of chemical potentials are much slower; see Zein [37]. For particular applications, the orders of the relaxation times can be precised, for instance in the barotropic case, cf. [2].

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 (6.28). Note that for all relaxation processes, the corresponding source terms satisfy the constraint (5.20) due to Galilean invariance.

7.1 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 [33] for a two-phase model according to [37] by introducing a pressure average that we choose as the mixture pressure. The pressure relaxation terms then read

$$S^{p}_{\alpha,k} := \theta_p\, \alpha_k\, (p_k - p),\ S^{p}_{\alpha\rho,k} := 0,\ \boldsymbol{S}^{p}_{\alpha\rho\boldsymbol{v},k} := \boldsymbol{0},\ S^{p}_{\alpha\rho E,k} := \theta_p\, \alpha_k\, p(p - p_k). \tag{7.1}$$

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

$$S^{v}_{\alpha,k} = S^{v}_{\alpha\rho,k} := 0,\ \boldsymbol{S}^{v}_{\alpha\rho\boldsymbol{v},k} := \theta_v\, \alpha_k\, \rho_k\, (\boldsymbol{v} - \boldsymbol{v}_k),\ S^{v}_{\alpha\rho E,k} := \theta_v\, \alpha_k\, \rho_k\, \boldsymbol{v} \cdot (\boldsymbol{v} - \boldsymbol{v}_k) \tag{7.2}$$

with the velocity relaxation parameter θ_v. For more details on mechanical relaxation, see Baer and Nunziato [4] or Baer [10] for two-phase models.

Obviously, the mechanical relaxation terms (7.1) and (7.2) 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 (6.26) and (7.1), (7.2) the entropy production terms

$$S^{v}_{\alpha\rho s,k} = \theta_v \frac{\alpha_k \rho_k}{T_k} (\boldsymbol{v} - \boldsymbol{v}_k)^2, \quad S^{p}_{\alpha\rho s,k} = \theta_p \frac{\alpha_k}{T_k} (p - p_k)^2. \tag{7.3}$$

This immediately implies

Theorem 8 (Entropy production due to mechanical relaxation) *Let* $\rho_k \geq 0$, $T_k > 0$ *and the relaxation parameters* $\theta_p, \theta_v \geq 0$. *Then, the entropy production due to mechanical relaxation is non-negative, i.e.,*

$$S^{p,v}_{\alpha\rho s,k} \geq 0,\ k = 1, \ldots, K \quad \text{and} \quad \sum_{k=1}^{K} S^{p,v}_{\alpha\rho s,k} \geq 0. \tag{7.4}$$

7.2 Thermal relaxation

For the modeling of *temperature relaxation*, we follow in principal Zein [37]. First of all, we introduce a general class of temperature relaxation models

$$S^{T}_{\alpha,k} := \theta_T \frac{Q_k}{\kappa_k},\ S^{T}_{\alpha\rho,k} := 0,\ \boldsymbol{S}^{T}_{\alpha\rho\boldsymbol{v},k} := \boldsymbol{0},\ S^{T}_{\alpha\rho E,k} := \theta_T\, Q_k, \tag{7.5}$$

with the relaxation parameter θ_T and

$$Q_k = \gamma_k (\hat{T} - T_k). \tag{7.6}$$

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

$$\sum_{k=1}^{K} Q_k = 0 \quad \text{and} \quad \sum_{k=1}^{K} \frac{Q_k}{\kappa_k} = 0. \tag{7.7}$$

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

$$\hat{T} = \sum_{k=1}^{K} \beta^{T}_{k}\, T_k \tag{7.8}$$

with coefficients

$$\beta_k^T = \gamma_k / \gamma, \quad \gamma := \sum_{k=1}^{K} \gamma_k. \tag{7.9}$$

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

$$\sum_{k=1}^{K} \beta_k^T = 1. \tag{7.10}$$

For instance, we may choose (a) $\gamma_k = \alpha_k$. Then, $\beta_k^T = \alpha_k$ and $\hat{T}$ coincides with the mixture temperature (6.10). In case of (b) $\gamma_k = 1$ or (c) $\gamma_k = K$, we compute $\beta_k^T = 1/K$ 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 (6.26) and (7.5) the entropy production term

$$S_{\rho s,k}^T = \theta_T \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1 \right). \tag{7.11}$$

Thus, the entropy production due to thermal relaxation becomes

$$S_{\rho s}^T := \sum_{k=1}^{K} S_{\alpha \rho s,k}^T = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1 \right) = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k + \theta_T \sum_{k=1}^{K} \frac{p_k}{T_k \kappa_k} Q_k. \tag{7.12}$$

We note that by the definitions (7.6) and (7.9) of Q_k and β_k, respectively, the relation

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

holds. Here we employ (7.8) and (7.10) to compute the difference $\hat{T} - T_k = \sum_{l=1}^{K} \beta_l^T (T_l - T_k)$. Furthermore, we observe that for any b_k and $a_{k,l} = -a_{l,k}$, $l, k = 1, \dots, k$ 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 $a_{k,l} = \beta_k^T \beta_l^T (T_l - T_k)$, we thus conclude with

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

Obviously, the sum is non-negative whenever the temperatures are positive. Thus, the first term on the right-hand side of (7.12) is non-negative. To ensure that the second term is also non-negative, we rewrite the sum by means of the conservation constraints (7.7) 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

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

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

$$\kappa_k = \frac{T_K p_k - T_k p_K}{a_k T_k T_K Q_k}, \quad k = 1, \ldots, K-1. \tag{7.13}$$

The missing parameter κ_K is determined by the conservation constrains (7.7) as

$$\kappa_K = -Q_K \left(\sum_{k=1}^{K-1} \frac{Q_k}{\kappa_k} \right)^{-1}. \tag{7.14}$$

Finally, we summarize our results in the following

Theorem 9 (Entropy production due to thermal relaxation) *Let the temperatures and the relaxation parameter be strictly positive, i.e., $T_k > 0$ and $\theta_T > 0$. Let Q_k satisfy (7.6) where $\hat{T}$ is defined as convex combination (7.8) of the temperatures T_k with coefficients β_k satisfying (7.9) and (7.10). Then, the mixture entropy production due to thermal relaxation is non-negative, i.e.,*

$$S^T_{\rho s} = \theta_T \sum_{k=1}^{K} \frac{1}{T_k} Q_k \left(\frac{p_k}{\kappa_k} + 1 \right) \geq 0, \tag{7.15}$$

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 (7.13) and (7.14) with non-negative coefficients a_k. It also holds in case of pressure equilibrium, i.e., $p_1 = \cdots = p_K = p$, and constant parameters $\kappa_1 = \cdots = \kappa_K = \kappa$.

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., $S^T_{\alpha,k} = 0$. 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 [37], 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 models can be found in Zein [37] and Zein et al. [38], respectively. Note that the coefficient κ in [37] results in a non-negative entropy production if the pressures are at equilibrium. In the non-equilibrium case, (7.15) cannot be proven to hold.

In the thermal relaxation model considered by Saleh [32], there is no relaxation term accounted for in the evolution equations for the volume fractions, i.e., $S^T_{\alpha,k} = 0$. 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 (7.12) does not exist.

7.3 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.

7.3.1 Chemical potential relaxation for two-component mixtures

For a two-component mixture ($K = 2$), the relaxation of chemical potentials is modeled according to [37] by

$$\begin{gathered} S^\mu_{\alpha,1} := \theta_\mu \frac{\dot{m}}{\varrho},\ S^\mu_{\alpha\rho,1} := \theta_\mu \dot{m},\ \boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},1} := \theta_\mu \dot{m} \hat{\boldsymbol{v}},\ S^\mu_{\alpha\rho E,1} := \theta_\mu \dot{m} \left(\epsilon + \frac{\hat{\boldsymbol{v}}^2}{2} \right), \\ S^\mu_{\alpha,2} := -S^\mu_{\alpha,1},\ S^\mu_{\alpha\rho,2} := -S^\mu_{\alpha\rho,1},\ \boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},2} := -\boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},1},\ S^\mu_{\alpha\rho E,2} := -S^\mu_{\alpha\rho E,1}, \end{gathered} \tag{7.16}$$

with the relaxation parameter θ_μ. Similar to the interfacial velocity (6.18), we choose for the velocity $\hat{\boldsymbol{v}}$ a convex combination

$$\hat{\boldsymbol{v}} = \sum_{k=1}^{K} \beta_k^v \boldsymbol{v}_k, \quad \beta_k^v \in [0,1], \quad \sum_{k=1}^{K} \beta_k^v = 1. \tag{7.17}$$

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 (6.26) and (7.16) as

$$S^{\mu}_{\alpha\rho s,k} = (-1)^{k+1}\theta_\mu\, \dot{m}\, \frac{1}{T_k}\left(\epsilon + \frac{1}{2}(\hat{\boldsymbol{v}} - \boldsymbol{v}_k)^2 - g_k + \frac{p_k}{\varrho}\right), \quad k = 1, 2. \tag{7.18}$$

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 $\hat{\boldsymbol{v}}$ the entropy production due to the sum of the phasic entropies

$$S^{\mu}_{\rho s} = \theta_\mu\, \dot{m}\, \sum_{k=1}^{2}(-1)^{k+1}\frac{1}{T_k}\left(\epsilon + \frac{1}{2}(\hat{\boldsymbol{v}} - \boldsymbol{v}_k)^2 - g_k + \frac{p_k}{\varrho}\right) \tag{7.19}$$

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

$$\boldsymbol{v}_1 = \cdots = \boldsymbol{v}_K = \boldsymbol{v}, \quad p_1 = \cdots = p_K = p, \quad T_1 = \cdots = T_K = T, \tag{7.20}$$

the entropy production term becomes

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

as was already proven in [37]. Obviously, this term is non-negative if

$$\dot{m} = a(g_2 - g_1) \tag{7.21}$$

with $a \geq 0$. This is an agreement with the kinetic relation in [9].

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

$$\sum_{k=1}^{2}(-1)^{k+1}\frac{1}{T_k}\left(\epsilon + \frac{1}{2}(\hat{\boldsymbol{v}} - \boldsymbol{v}_k)^2 - g_k + \frac{p_k}{\varrho}\right) = b\,(g_2 - g_1) \tag{7.22}$$

for some non-negative b. Note that for the parameters ϵ and ϱ in [37], this condition does not hold true. To verify (7.22), we proceed in three steps to determine $\hat{\boldsymbol{v}}$, ϵ and ϱ:

1. The velocity $\hat{\boldsymbol{v}}$ is chosen in such a way that the velocity terms in (7.19) vanish:

$$\frac{1}{T_1}(\hat{\boldsymbol{v}} - \boldsymbol{v}_1)^2 - \frac{1}{T_2}(\hat{\boldsymbol{v}} - \boldsymbol{v}_2)^2 = 0. \tag{7.23}$$

   This is reasonable because the entropy production (7.19) 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 velocity $\hat{\boldsymbol{v}}$ is assumed to be a convex combination of the single-component velocities, i.e., $\hat{\boldsymbol{v}} = \beta_1^v \boldsymbol{v}_1 + \beta_2^v \boldsymbol{v}_2$ with $\beta_2^v = 1 - \beta_1^v$ according to (7.17), we derive from (7.23)

$$\beta_1^v := \frac{\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_2^v := \frac{\sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}}. \tag{7.24}$$

2. In the next step, we determine ϵ such that

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

   resulting in

$$\epsilon = c\,\frac{g_2 T_1 + g_1 T_2}{T_1 + T_2}.$$

1. Finally, we determine ϱ such that

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

   resulting in

$$\varrho = \frac{1}{d}\,\frac{T_1 + T_2}{g_2 T_1 + g_1 T_2}\,\frac{p_2 T_1 - p_1 T_2}{T_1 - T_2}.$$

   Choosing

$$d = \frac{1}{2}\operatorname{sign}\left(\frac{p_2 T_1 - p_1 T_2}{T_1 - T_2}\right), \qquad c = 1 - d, \tag{7.25}$$

then with the above choice of $\hat{\boldsymbol{v}}$, ϵ and ϱ, we obtain (7.22) 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 $g/2$ and $2p/g$, respectively, assuming that the pressure relaxes faster than the Gibbs free energy. Again we conclude with the following.

Theorem 10 (Entropy production due to relaxation of Gibbs free energies) *At mechanical and thermal equilibrium, i.e.,* (7.20) *holds, the mixture entropy production due to relaxation of Gibbs free energies is non-negative, i.e.,*

$$S^\mu_{\rho s} \geq 0, \tag{7.26}$$

if the mass flux is chosen as the kinetic relation (7.21) *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* (7.22) *holds.*

7.3.2 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

$$\begin{aligned}
&S^\mu_{\alpha,1} := \theta_\mu \frac{\dot{m}}{\varrho_1},\ S^\mu_{\alpha\rho,1} := \theta_\mu\,\dot{m},\ \boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},1} := \theta_\mu\,\dot{m}\,\hat{\boldsymbol{v}},\ S^\mu_{\alpha\rho E,1} := \theta_\mu\,\dot{m}\left(\epsilon_1 + \frac{\hat{\boldsymbol{v}}^2}{2}\right),\\
&S^\mu_{\alpha,2} := \theta_\mu \frac{\dot{m}}{\varrho_2},\ S^\mu_{\alpha\rho,2} := -\theta_\mu\,\dot{m},\ \boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},2} := -\theta_\mu\,\dot{m}\,\hat{\boldsymbol{v}},\ S^\mu_{\alpha\rho E,2} := -\theta_\mu\,\dot{m}\left(\epsilon_2 + \frac{\hat{\boldsymbol{v}}^2}{2}\right),\\
&S^\mu_{\alpha,3} := -\theta_\mu\,\dot{m}\left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2}\right),\ S^\mu_{\alpha\rho,3} := 0,\ \boldsymbol{S}^\mu_{\alpha\rho\boldsymbol{v},3} := \boldsymbol{0},\ S^\mu_{\alpha\rho E,3} := \theta_\mu\,\dot{m}\,(\epsilon_2 - \epsilon_1)\,,
\end{aligned} \tag{7.27}$$

with the relaxation parameter θ_μ and $\hat{\boldsymbol{v}}$ given by (7.17). For details on the physics, see the book of Müller and Müller [28]. Again we note that the conservation constraints (2.13) are satisfied. Furthermore, the entropy production terms can be determined by (6.26) and(7.16)

$$
\begin{aligned}
S^{\mu}_{\alpha\rho s,1} &= \theta_\mu \, \dot m \, \frac{1}{T_1}\left(\epsilon_1 + \frac{1}{2}(\hat{\boldsymbol v} - \boldsymbol v_1)^2 - g_1 + \frac{p_1}{\varrho_1}\right),\\
S^{\mu}_{\alpha\rho s,2} &= -\theta_\mu \, \dot m \, \frac{1}{T_2}\left(\epsilon_2 + \frac{1}{2}(\hat{\boldsymbol v} - \boldsymbol v_2)^2 - g_2 - \frac{p_2}{\varrho_2}\right),\\
S^{\mu}_{\alpha\rho s,3} &= \theta_\mu \, \dot m \, \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3(\frac{1}{\varrho_1} + \frac{1}{\varrho_2})\right).
\end{aligned}
\tag{7.28}
$$

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

$$
S^{\mu}_{\rho s} = \dot m \, \theta_\mu \left(\sum_{k=1}^{2} \frac{(-1)^{k+1}}{T_k}\left(\epsilon_k + \frac{1}{2}(\hat{\boldsymbol v} - \boldsymbol v_k)^2 - g_k - (-1)^k \frac{p_k}{\varrho_k}\right) + \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3\left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2}\right)\right)\right).
\tag{7.29}
$$

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 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., (7.21) holds. Similar to the two-component case, see Sect. (7.3.1), we may enforce a non-negative entropy production by choosing the parameters ϵ_k and ϱ_k such that the condition

$$
\sum_{k=1}^{2} \frac{(-1)^{k+1}}{T_k}\left(\epsilon_k + \frac{1}{2}(\boldsymbol V_I - \boldsymbol v_k)^2 - g_k - (-1)^k \frac{p_k}{\varrho_k}\right) + \frac{1}{T_3}\left(\epsilon_2 - \epsilon_1 - p_3\left(\frac{1}{\varrho_1} + \frac{1}{\varrho_2}\right)\right) = b\,(g_2 - g_1)
\tag{7.30}
$$

holds for some non-negative b analogously to (7.22). Note that the parameters ϵ_k and ϱ_k in [37,39] do not satisfy this condition.

As already assumed in the two-component mixture, we expect that the entropy production of the three-component mixture (7.28) should not depend on any velocity. This assumption gives us a condition for the velocity $\hat{\boldsymbol v}$ and delivers us the same result as above (7.24):

$$
\beta_1^v := \frac{\sqrt{T_2}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_2^v := \frac{\sqrt{T_1}}{\sqrt{T_1} + \sqrt{T_2}}, \quad \beta_3^v := 0.
\tag{7.31}
$$

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 Sect. 6.2, in the total entropy we also have to account for the mixture entropy given by

$$
S_M = - \sum_{k=1,3} \alpha_k \rho_k \frac{\kappa_b}{m_k} \ln\left(\frac{\alpha_k}{\alpha_1 + \alpha_3}\right),
\tag{7.32}
$$

with κ_b the Boltzmann constant and m_k the mass of a single molecule of component k; see [27, p. 54, 298, 320]. Moreover, the chemical potential of the vapor phase is now given by

$$
\mu_1 = g_1 + \frac{\kappa_b T}{m_1} \ln\left(\frac{\alpha_1}{\alpha_1 + \alpha_3}\right)
\tag{7.33}
$$

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.,

$$\dot{m} = a(\mu_2 - \mu_1) \tag{7.34}$$

with $a \geq 0$ that again is an agreement with the kinetic relation in [9].

For a homogeneous mixture, the entropy production (7.29) reduces to

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

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

$$S^{\mu}_{S_M} = -\frac{1}{T}\,\dot{m}\,\theta_\mu\,\frac{\kappa_b T}{m_1}\ln\left(\frac{\alpha_1}{\alpha_1 + \alpha_3}\right). \tag{7.35}$$

Then, the total entropy production is given by

$$S^{\mu}_{\rho s} + S^{\mu}_{S_M} = \frac{1}{T}\,\dot{m}\,\theta_\mu\,(\mu_2 - \mu_1)\,. \tag{7.36}$$

Thus, we conclude with the following theorem.

Theorem 11 (Entropy production due to relaxation of chemical potentials) *For a homogeneous mixture, the total entropy production is non-negative, i.e.,*

$$S^{\mu}_{\rho s} + S^{\mu}_{S_M} \geq 0, \tag{7.37}$$

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.

7.4 Remarks on the closure of the interfacial velocity

According to the ansatz (6.18) for the interfacial velocity, we have some freedom in the choice of the parameters β_k. One option might be the velocity $\hat{\boldsymbol{v}}$ determined in Sect. 7.3. However, these are state dependent, i.e., $\beta_k^v = \beta_k^v(\boldsymbol{w})$; see (7.24) and (7.31). As a consequence, the linear field associated with the eigenvalue $\lambda_{I,i}$, $i = 1, \ldots, K-1$ will not be linearly degenerated, i.e.,

$$\boldsymbol{r}_{I,i} \cdot \nabla_{\boldsymbol{w}} \lambda_{I,i} = \kappa_0 \left(\frac{\partial V_{I,n}}{\partial \alpha_i} + \sum_{k=1}^{K} \left(\overline{x}_{k,i} \frac{\partial V_{I,n}}{\partial \rho_k} + \overline{\boldsymbol{y}}_{k,i} \cdot \nabla_{\boldsymbol{v}_k} V_{I,n} + \overline{z}_{k,i} \frac{\partial V_{I,n}}{\partial p_k} \right) \right) \neq 0.$$

Since the non-equilibrium model contains non-conservative products in the phasic momentum and energy equations, see Eqs. (2.3) and (2.4), there is no way to cope with these terms in case of genuinely nonlinear fields. If fields associated with the non-conservative products only occur in linearly degenerated fields, then Riemann invariants of the associated field can be enforced, and thus, the exact solution of the Riemann problem exists as has been verified for Baer–Nunziato-type models in [13]. Therefore, it is suggested in [12] and [18] to determine the interfacial velocity such that the associated field is linearly degenerated. Obviously, at mechanical and thermal equilibrium this field is linearly degenerate for arbitrary convex combinations (6.18) provided that $\beta_k \neq \beta_k(\alpha)$ because $\overline{\boldsymbol{y}}_{k,i} = \boldsymbol{0}, \overline{x}_{k,i} = \overline{z}_{k,i} = \partial\beta_k/\partial\alpha_i = 0$. At non-equilibrium, this no longer holds true. To derive appropriate closing conditions in this case, we extend the ansatz of Saleh [eqn. (4.3.40)] [32], in case of a two-phase mixture. For this purpose, we introduce another arbitrary but fixed convex combination $\sum_{k=1}^{K} c_k = 1$ with constant coefficients $c_k \in [0, 1]$. Then, we define the coefficients β_k in (6.18) as

$$\beta_k := \frac{c_k \alpha_k \rho_k}{\hat{\rho}}, \quad \hat{\rho} := \sum_{k=1}^{K} c_k \alpha_k \rho_k.$$

By a straightforward calculation using (4.32), (4.33) and (4.34), we can verify that $\boldsymbol{r}_{I,i} \cdot \nabla_{\boldsymbol{w}} \lambda_{I,i}$ vanishes. Then, the interfacial pressure and velocity are given by

$$P_I = \sum_{k=1}^{K} p_k (1 - c_k \alpha_k \rho_k T_k / (\hat{\rho} \hat{T})), \quad \boldsymbol{V}_I = \sum_{i=1}^{K} c_i \alpha_i \rho_i \boldsymbol{v}_i \Bigg/ \sum_{k=1}^{K} c_k \alpha_k \rho_k. \tag{7.38}$$

For special choices of $\boldsymbol{c} \in [0, 1]^K$, these interfacial values coincide with those in the literature in case of two and three components. For instance, choosing $\boldsymbol{c} = \boldsymbol{e}_i$ for some $i \in \{1, \ldots, K\}$, we obtain

$$P_I = \sum_{k=1, \neq i}^{K} p_k, \quad \boldsymbol{V}_I = \boldsymbol{v}_i. \tag{7.39}$$

For $i = 1$, these coincide with those given in [12] and [18] for $K = 2$ and $K = 3$, respectively. In case of uniform coefficients $c_k = 1/K, k = 1, \ldots, K$, the interfacial pressure and velocity are given by

$$P_I = \sum_{k=1}^{K} p_k (1 - \alpha_k \rho_k T_k / (\rho \hat{T})), \quad \boldsymbol{V}_I = \sum_{i=1}^{K} \alpha_i \rho_i \boldsymbol{v}_i \Bigg/ \sum_{k=1}^{K} \alpha_k \rho_k = \boldsymbol{v}. \tag{7.40}$$

where ρ and $\boldsymbol{v}$ are the density and the velocity of the mixture, see (2.10), respectively.

Obviously, the interfacial states (7.38) do not satisfy (7.23) for an arbitrary non-equilibrium state meaning that (7.26) and (7.37) might not hold in general; i.e., the second law of thermodynamics might be violated. To overcome this contradiction, it is recommended in [19] to use different interfacial velocities for the convective system and the relaxation terms. This is admissible because the conservation constraint (2.13) is satisfied for any convex combination (6.18). Moreover, the source term cannot be derived from the ensemble averaging procedure, see [8], Chapter 11, but the averaged model has to be closed by modeling these terms appropriately. Therefore, we are free to choose another velocity in the chemical relaxation model. Note that in the Drew–Passman model, different interfacial velocities have been introduced in the evolution equations for volume fraction, momentum and energy; see [8], formulae (11.8), (11.39) and (11.41).

8 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 models. In particular, the corresponding eigenvalues satisfy the subcharacteristic 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 [30]. 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 [33] 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 [38] and [17,39] 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.

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