

A consistent kinetic model for a two-component mixture of polyatomic molecules

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Abstract

We consider a multi component gas mixture with translational and internal energy degrees of freedom assuming that the number of particles of each species remains constant. We will illustrate the derived model in the case of two species, but the model can be easily generalized to multiple species. The two species are allowed to have different degrees of freedom in internal energy and are modelled by a system of kinetic ES-BGK equations featuring two interaction terms to account for momentum and energy transfer between the species. We prove consistency of our model: conservation properties, positivity of the temperature, H-theorem and convergence to a global equilibrium in the form of a global Maxwell distribution. Thus, we are able to derive the usual macroscopic conservation laws. For numerical purposes we apply the Chu reduction to the developed model for polyatomic gases and give an application for a gas consisting of a mono atomic and a diatomic species.

Keywords: multi-fluid mixture, kinetic model, ES-BGK approximation, polyatomic molecules

AMS subject classification: 35Q20; 35Q79; 82C40; 65Z05

1 Introduction

In this paper we shall concern ourselves with a kinetic description of gas mixtures for polyatomic molecules. In the case of mono atomic molecules and two species this is traditionally done via the Boltzmann equation for the density distributions f_1 and f_2 , see for example [10, 11]. Under certain assumptions the complicated interaction terms of the Boltzmann equation can be simplified by a so called BGK approximation, consisting of a collision frequency multiplied by the deviation of the distributions from local Maxwellians. This approximation should be constructed in a way such that it has the same main properties of the Boltzmann equation namely conservation of mass, momentum and energy, further it should have an H-theorem with its entropy inequality and the equilibrium must still be Maxwellian. BGK models give rise to efficient numerical computations, which are asymptotic preserving, that is they remain efficient even approaching the hydrodynamic regime [4, 5, 12–14, 22]. Evolution of a polyatomic gas is

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very important in applications, for instance air consists of a gas mixture of polyatomic molecules. But, most kinetic models modelling air deal with the case of a mono atomic gas consisting of only one species.

In the literature one can find two types of models for polyatomic molecules using the classical description of physics. We do not take into account quantum mechanical effects, for this see for example [17]. In classical thermodynamics, there are models which contain a sum of collision terms on the right-hand side corresponding to the elastic and inelastic collisions. Examples are the models of Rykov [23], Holway [15] and Morse [21]. The other type of models contain only one collision term on the right-hand side taking into account both elastic and inelastic interactions. Examples for this are Bernard, Iollo, Puppo [6] or the model by Bisi and Caceres [7] modelling chemical interactions. In this paper we want to extend the model of Bernard, Iollo and Puppo [6] from one species of molecules to a gas mixture of polyatomic molecules. In contrast to mono atomic molecules, in a polyatomic gas energy is not entirely stored in the kinetic energy of its molecules but also in their rotational and vibrational modes. For simplification we present the model in the case of two species. We do not consider chemical reactions. For models which include chemical reactions, see for example [1]. We allow the two species to have different degrees of freedom in internal energy. For example, we may consider a mixture consisting of a mono atomic and a diatomic gas. In addition, we want to model it via an ES-BGK approach in order to reproduce the correct Boltzmann hydrodynamic regime close to the asymptotic continuum limit. The presence of a tensor in the attractors should allow to overcome the well known problem of incorrect Prandtl number (analogously to paper [3] for a single gas) but the proof is still lacking. At least, we will propose a model which is consistent in the special case of a mono-atomic single gas. The ES-BGK approximation was suggested by Holway in the case of one species [15]. The H-Theorem of this model then was proven in [3]. Brull and Schneider relate this model to a minimization problem in [8].

The outline of the paper is as follows: in section 2 we will present the extension of the BGK model for polyatomic molecules from [6] to two species of polyatomic molecules. In section 3, we extend it to an ES-BGK model and check if it is well-defined. In sections 3.1 to 3.4 we prove the conservation properties and the H-theorem. We show the positivity of all temperatures and quantify the structure of the equilibrium. In section 4, we compare our model with an other model presented in the literature from [3] which considers an ES-BGK model for one species of polyatomic molecules. In section 5.1 we apply the method of Chu reduction to our model in order to reduce the complexity of the variables for the rotational and vibrational energy degrees of freedom for numerical purposes. In section 5.2 we give an application in the case of a mono atomic and a diatomic molecule.

2 The BGK approximation

In this section we first want to motivate how our model with several coupled equations will look like. For the convenience of the reader, we will summarize all this equations again at the end of the section such that one sees the whole model at a glance. For simplicity in the following we consider a mixture composed of two different species. Let $x \in \mathbb{R}^d$ and $v \in \mathbb{R}^d$, $d \in \mathbb{N}$ be the phase space variables and $t \geq 0$ the time. Let M be the total number of different rotational and vibrational degrees of freedom and l_k the number of internal degrees of freedom of species k , $k=1,2$. Note that the sum $l_1 + l_2$ is not necessarily equal to M , because the two species could both have the same

internal degree of freedom. Then $\eta \in \mathbb{R}^M$ is the variable for the internal energy degrees of freedom, $\eta_k \in \mathbb{R}^M$ coincides with η in the components corresponding to the internal degrees of freedom of species k and is zero in the other components. For example, we can consider two species both composed of molecules consisting of two atoms, such that the molecules have rotational degrees of freedom in addition to the three translational degrees of freedom. In general, a molecule consisting of two atoms has three possible axes around which it can rotate. But since the energy needed to rotate the molecule around the axes parallel to the line connecting the two atoms is very high (see for example [16]), this does not occur, so we have two rotational degrees of freedom. In this example we have $M = l_1 = l_2 = 2$.

Since we want to describe two different species, our kinetic model has two distribution functions $f_1(x, v, \eta_{l_1}, t) > 0$ and $f_2(x, v, \eta_{l_2}, t) > 0$. Furthermore we relate the distribution functions to macroscopic quantities by mean-values of f_k , $k = 1, 2$ as follows

$$\int f_k(v, \eta_{l_k}) \begin{pmatrix} 1 \\ v \\ \eta_k \\ m_k |v - u_k|^2 \\ m_k |\eta_k - \bar{\eta}_k|^2 \\ m_k (v - u_k(x, t)) \otimes (v - u_k(x, t)) \end{pmatrix} dv d\eta_{l_k} =: \begin{pmatrix} n_k \\ n_k u_k \\ n_k \bar{\eta}_k \\ dn_k T_k^t \\ l_k n_k T_k^r \\ \mathbb{P}_k \end{pmatrix}, \quad k = 1, 2, \quad (2.1)$$

where n_k is the number density, u_k the mean velocity, T_k^t the mean temperature of the translation, T_k^r the mean temperature of the internal energy degrees of freedom for example rotation or vibration and \mathbb{P}_k the pressure tensor of species k , $k = 1, 2$. Note that in this paper we shall write T_k^t and T_k^r instead of $k_B T_k^t$ and $k_B T_k^r$, where k_B is Boltzmann's constant. In the following, we will require $\bar{\eta}_k = 0$, which means that the energy in rotations clockwise is the same as in rotations counter clockwise. Similar for vibrations.

The distribution functions are determined by two equations to describe their time evolution. Furthermore we only consider binary interactions. So the particles of one species can interact with either themselves or with particles of the other species. In the model this is accounted for by introducing two interaction terms in both equations. These considerations allow us to write formally the system of equations for the evolution of the mixture. The following structure containing a sum of the collision operators is also given in [10, 11].

We are interested in a BGK approximation of the interaction terms. This leads us to define equilibrium distributions not only for each species itself but also for the two interspecies distributions. Then the model can be written as:

$$\begin{aligned} \partial_t f_1 + \nabla_x \cdot (v f_1) &= \nu_{11} n_1 (M_1 - f_1) + \nu_{12} n_2 (M_{12} - f_1), \\ \partial_t f_2 + \nabla_x \cdot (v f_2) &= \nu_{22} n_2 (M_2 - f_2) + \nu_{21} n_1 (M_{21} - f_2), \end{aligned} \quad (2.2)$$

with the Maxwell distributions

$$\begin{aligned} M_k(x, v, \eta_{l_k}, t) &= \frac{n_k}{\sqrt{2\pi \frac{\Lambda_k}{m_k}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}^{l_k}} \exp\left(-\frac{|v - u_k|^2}{2 \frac{\Lambda_k}{m_k}} - \frac{|\eta_k|^2}{2 \frac{\Theta_k}{m_k}}\right), \\ M_{kj}(x, v, \eta_{l_k}, t) &= \frac{n_{kj}}{\sqrt{2\pi \frac{\Lambda_{kj}}{m_k}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_{kj}}{m_k}}^{l_k}} \exp\left(-\frac{|v - u_{kj}|^2}{2 \frac{\Lambda_{kj}}{m_k}} - \frac{|\eta_{kj}|^2}{2 \frac{\Theta_{kj}}{m_k}}\right), \end{aligned} \quad (2.3)$$

for $j, k = 1, 2, j \neq k$, where $\nu_{11}n_1$ and $\nu_{22}n_2$ are the collision frequencies of the particles of each species with itself, while $\nu_{12}n_2$ and $\nu_{21}n_1$ are related to interspecies collisions. In this model, the collision frequencies between interspecies operators can be taken different allowing molecular mass discrepancies. This point is relevant for example in the context of plasma physics, because the mass ratio between electrons and ions is very small. To be flexible in choosing the relationship between the collision frequencies, we now assume the relationship

$$\nu_{12} = \varepsilon \nu_{21}, \quad 0 < \frac{l_1}{l_1 + l_2} \varepsilon \leq 1. \quad (2.4)$$

The restriction $\frac{l_1}{l_1 + l_2} \varepsilon \leq 1$ is without loss of generality. If $\frac{l_1}{l_1 + l_2} \varepsilon > 1$, exchange the notation 1 and 2 and choose $\frac{1}{\varepsilon}$. In addition, we assume that all collision frequencies are positive.

Since rotational/vibrational and translational degrees of freedom relax at a different rate, T_k^t and T_k^r will first relax to partial temperatures Λ_k and Θ_k respectively. Conservation of internal energy then requires that at each time

$$\frac{d}{2} n_k \Lambda_k = \frac{d}{2} n_k T_k^t + \frac{l_k}{2} n_k T_k^r - \frac{l_k}{2} n_k \Theta_k, \quad k = 1, 2. \quad (2.5)$$

Thus, Λ_k can be written as a function of Θ_k . In equilibrium we expect the two temperatures Λ_k and Θ_k to coincide, so we close the system by adding the equations

$$\begin{aligned} \partial_t M_k + v \cdot \nabla_x M_k = & \frac{\nu_{kk} n_k}{Z_r^k} \frac{d + l_k}{d} (\widetilde{M}_k - M_k) + \nu_{kk} n_k (M_k - f_k) \\ & + \nu_{kj} n_j (M_{kj} - f_k), \end{aligned} \quad (2.6)$$

for $j, k = 1, 2, j \neq k$, where Z_r^k are given parameters corresponding to the different rates of decays of translational and rotational/vibrational degrees of freedom. Here M_k is given by

$$M_k(x, v, \eta_{l_k}, t) = \frac{n_k}{\sqrt{2\pi \frac{\Lambda_k}{m_k}}} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}} \exp\left(-\frac{|v - u_k|^2}{2 \frac{\Lambda_k}{m_k}} - \frac{|\eta_{l_k}|^2}{2 \frac{\Theta_k}{m_k}}\right), \quad k = 1, 2, \quad (2.7)$$

and \widetilde{M}_k is given by

$$\widetilde{M}_k = \frac{n_k}{\sqrt{2\pi \frac{T_k}{m_k}}} \exp\left(-\frac{m_k |v - u_k|^2}{2 T_k} - \frac{m_k |\eta_{l_k}|^2}{2 T_k}\right), \quad k = 1, 2. \quad (2.8)$$

where T_k is the total equilibrium temperature and is given by

$$T_k := \frac{d \Lambda_k + l_k \Theta_k}{d + l_k} = \frac{d T_k^t + l_k T_k^r}{d + l_k}. \quad (2.9)$$

The second equality follows from (2.5). If we multiply (2.6) by $|\eta_{l_k}|^2$, integrate with respect to v and η_{l_k} and use (2.9), we obtain

$$\begin{aligned} \partial_t (n_k \Theta_k) + \nabla_x \cdot (n_k \Theta_k u_k) = & \frac{\nu_{kk} n_k}{Z_r^k} n_k (\Lambda_k - \Theta_k) + \nu_{kk} n_k n_k (\Theta_k - T_k^r) \\ & + \nu_{kj} n_j n_k (\Theta_{kj} - T_k^r), \quad k = 1, 2. \end{aligned} \quad (2.10)$$

We obtained a macroscopic equation which describes the relaxation of the temperature Θ_k towards the temperature Λ_k and the relaxation of Θ_k towards the rotational and vibrational temperature T_k^r and of T_k^r relaxing towards the mixture temperature Θ_{kj} in accordance with equation (2.2). Note that equation (2.10) together with mass, momentum and total energy conservation, is equivalent to (2.6). In addition, (2.2) and (2.6) are consistent. If we multiply the equations for species k of (2.2) and (2.6) by v and integrate with respect to v and η_{lk} , we get in both cases for the right-hand side

$$\nu_{kj}n_jn_k(u_{jk} - u_k),$$

and if we compute the total internal energy of both equations, we obtain in both cases

$$\frac{1}{2}\nu_{kj}n_kn_j[d\Lambda_{jk} + l_j\Theta_{jk} - (d\Lambda_j + l_j\Theta_j)].$$

We will see this in section 3.1 in theorem 3.1.1.

We recall that we assume that the mean values of the momentum due to the internal degrees of freedom $\bar{\eta}_1$, $\bar{\eta}_2$, $\bar{\eta}_{12}$ and $\bar{\eta}_{21}$ are zero. The structure of the collision terms ensures that at equilibrium or when $\nu_{kj} \rightarrow \infty$ the distribution functions become Maxwell distributions. With this choice of the Maxwell distributions M_1 and M_2 have the same densities, mean velocities and internal energies as f_1 respective f_2 . This guarantees the conservation of mass, momentum and energy in interactions of one species with itself. The remaining parameters $n_{12}, n_{21}, u_{12}, u_{21}, \Lambda_{12}$, Λ_{21} , Θ_{12} and Θ_{21} will be determined further down using conservation of the number of particles, total momentum and total energy, together with some symmetry considerations. We will determine n_{12} and n_{21} in equation (3.18) using conservation of the number of particles. The velocities u_{12} and u_{21} will be determined in equations (3.19) and (3.20) by using conservation of total momentum. Last, the parameters Λ_{12} , Λ_{21} , Θ_{12} and Θ_{21} will be determined in theorem 3.1.1 and remark 2.

Now, for the convenience of the reader, we want to write down our model again that one sees on the first view which equations we want to couple. Our BGK model for two species coupled with one relaxation equation and one algebraic equation for the temperatures can be written as

$$\begin{aligned}\partial_t f_1 + \nabla_x \cdot (v f_1) &= \nu_{11}n_1(M_1 - f_1) + \nu_{12}n_2(M_{12} - f_1), \\ \partial_t f_2 + \nabla_x \cdot (v f_2) &= \nu_{22}n_2(M_2 - f_2) + \nu_{21}n_1(M_{21} - f_2),\end{aligned}$$

$$\frac{d}{dt}n_k\Lambda_k = \frac{d}{dt}n_kT_k^t + \frac{l_k}{2}n_kT_k^r - \frac{l_k}{2}n_k\Theta_k,$$

$$\begin{aligned}\partial_t(n_k\Theta_k) + \nabla_x \cdot (n_k\Theta_k u_k) &= \frac{\nu_{kk}n_k}{Z_r^k}n_k(\Lambda_k - \Theta_k) + \nu_{kk}n_kn_k(\Theta_k - T_k^r) \\ &\quad + \nu_{kj}n_jn_k(\Theta_{kj} - T_k^r),\end{aligned}$$

for $k, j = 1, 2, k \neq j$.

3 Extension to an ES-BGK model

In this section again we first want to motivate how our model with several coupled equations will look like. For the convenience of the reader, we will summarize all this

equations again at the end of the section such that one sees the whole model at a glance. It is well known that a drawback of the BGK approximation is its incapability of reproducing the correct Boltzmann hydrodynamic regime in the asymptotic continuum limit. Therefore, a modified version called ES-BGK model was suggested by Holway in the case of one species [15]. In this standard ES-BGK model, in the Maxwellian M_k , the scalar temperature T_k^t related to the distribution function f_k will be replaced by a linear combination of the temperature T_k^t and the pressure tensor \mathbb{P}_k . In the polyatomic case described in this paper the translational temperature T_k^t is different from the temperature Λ_k of the Maxwellian M_k given by (2.7). Now, we want to extend this temperature Λ_k to a tensor Λ_k^{ten} with $\text{trace}(\Lambda_k^{ten}) = n_k \Lambda_k$ such that again we can consider a linear combination of the temperature Λ_k and the tensor Λ_k^{ten} . In the BGK case described in the previous section we determined the time evolution of Θ_k by considering equation (2.6) with the Maxwellian M_k given by (2.7) and the Maxwellian \widetilde{M}_k given by (3.4.1) with the total equilibrium temperature T_k given by (2.9) which leads to a time evolution of Θ_k given by (2.10). Λ_k is then obtained by (2.5). Now, in the ES-BGK case we determine the time evolution of f_k in the ES-BGK case by

$$\partial_t f_k + \nabla_x \cdot (v f_k) = \nu_{kk} n_k (G_k(f_k) - f_k) + \nu_{kj} n_j (M_{kj}(f_k, f_j) - f_k), \quad (3.11)$$

for $k, j = 1, 2, k \neq j$. To keep it as simple as possible we only replace the collision operators which represent the collisions of a species with itself by the ES-BGK collision operator for one species suggested in [2]. The presence of a tensor in the attractors should allow to overcome the well known problem of incorrect Prandtl number (analogously to paper [2] for a single gas) but the proof is still lacking. We wanted to ensure that the is consistent with the special case of a single mono atomic gas. Other possible extensions are illustrated in the mono atomic case for gas mixtures in [20]. For further references we denote the relaxation operators by Q_{11}, Q_{12}, Q_{21} and Q_{22} . Then we define a function G_k with a linear combination Λ_k^{ES} given by

$$\Lambda_k^{ES} = (1 - \mu_k) \Lambda_k \mathbf{1}_d + \mu_k \frac{\Lambda_k^{ten}}{n_k}, \quad k = 1, 2.$$

with $\mu_k \in \mathbb{R}$, $k = 1, 2$ being free parameters which we can choose in a way to fit physical parameters in the Navier-Stokes equations like the viscosity coefficient, analogously as in the standard ES-BGK model given by

$$G_k(f_k)(x, v, \eta_k, t) = \frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ES}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}} \exp \left(-\frac{1}{2} (v - u_k) \cdot \left(\frac{\Lambda_k^{ES}}{m_k} \right)^{-1} \cdot (v - u_k) - \frac{1}{2} \frac{m_k |\eta_k|^2}{\Theta_k} \right), \quad (3.12)$$

for $k = 1, 2$.

In order to determine the time evolution of Λ_k^{ten} we consider the equation

$$\partial_t \widehat{G}_k + v \cdot \nabla_x \widehat{G}_k = \frac{\nu_{kk} n_k}{Z_r^k} \frac{d + l_k}{d} (\widetilde{G}_k - \widehat{G}_k) + \nu_{kk} n_k (G_k - f_k) + \nu_{kj} n_j (M_{kj} - f_k), \quad k = 1, 2, \quad (3.13)$$

with the extended Maxwellian \widehat{G}_k given by

$$\widehat{G}_k = \frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ten}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k^r}{m_k}}} \exp \left(-\frac{1}{2} (v - u_k) \cdot \left(\frac{\Lambda_k^{ten}}{m_k} \right)^{-1} \cdot (v - u_k) - \frac{m_k |\eta_k|^2}{2\Theta_k} \right), \quad (3.14)$$

for $k=1,2$, and the extended Maxwellian \tilde{G}_k given by

$$\tilde{G}_k = \frac{n_k}{\sqrt{\det(2\pi \frac{T_k^{ten}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k}{m_k}}^{l_k}} \exp \left(-\frac{1}{2} (v - u_k) \cdot \left(\frac{T_k^{ten}}{m_k} \right)^{-1} \cdot (v - u_k) - \frac{1}{2} \frac{m_k |\eta_{l_k}|^2}{T_k} \right). \quad (3.15)$$

The function \tilde{G}_k has the total equilibrium temperature T_k and the pressure tensor of f_k on the off-diagonals, namely

$$\begin{aligned} (T_k^{ten})_{ii} &= T_k & \text{for } i &= 1, \dots, d, \\ (T_k^{ten})_{ij} &= \frac{d}{d+l_k} \left(\frac{\mathbb{P}_k}{n_k} \right)_{ij} & \text{for } i, j &= 1, \dots, d, i \neq j. \end{aligned} \quad (3.16)$$

The factor $\frac{d}{d+l_k}$ in front of \mathbb{P}_k in the definition of T_k^{ten} has the following reason. The temperature T_k given by (2.9) is a convex combination of T_k^t and T_k^r . Now, the off-diagonal elements of T_k^{ten} have the same structure. It is a convex combination of the pressure tensor \mathbb{P}_k and the tensor corresponding to the rotational and vibrational temperature. But since the rotational effects are diagonal, we have $(T_k^{ten})_{ij} = (\frac{d}{d+l_k} \mathbb{P} + \frac{l_k}{d+l_k} 0)_{ij}$ for $i \neq j$.

We only extended Λ_k to a tensor and keep Θ_k as it is. This has the following reason. Since we assumed $\bar{\eta}_{l_k} = 0$, the microscopic velocities related to the internal degrees of freedom are symmetric and then we do not distinguish different directions as we do in the translational degrees of freedom.

Equation (3.13) leads to a time evolution of Λ_k^{ten} given by

$$\begin{aligned} \partial_t (n_k (\Lambda_k^{ten})_{ij}) + \nabla_x \cdot (n_k ((\Lambda_k^{ten})_{ij}) u_k) &= \frac{\nu_{kk} n_k}{Z_r^k} \frac{d+l_k}{d} n_k ((T_k^{ten})_{ij} - (\Lambda_k^{ten})_{ij}) \\ &+ \nu_{kk} n_k n_k ((\Lambda_k^{ES})_{ij} - (\mathbb{P}_k)_{ij}) + \nu_{kj} n_j n_k (\Theta_{kj} - T_k^{rot}) \delta_{ij}, \end{aligned} \quad (3.17)$$

The evolution of Θ_k is then obtained from (2.5).

For the convenience of the reader we want to summarize our model again. In the case of the ES-BGK model we wanted to use ES-BGK equations for the mixture coupled with a relaxation equation and an algebraic equation for the temperatures.

$$\partial_t f_k + \nabla_x \cdot (v f_k) = \nu_{kk} n_k (G_k(f_k) - f_k) + \nu_{kj} n_j (M_{kj}(f_k, f_j) - f_k),$$

$$\frac{d}{2} n_k \Lambda_k = \frac{d}{2} n_k T_k^t + \frac{l_k}{2} n_k T_k^r - \frac{l_k}{2} n_k \Theta_k,$$

$$\begin{aligned} \partial_t (n_k (\Lambda_k^{ten})_{ij}) + \nabla_x \cdot (n_k ((\Lambda_k^{ten})_{ij}) u_k) &= \frac{\nu_{kk} n_k}{Z_r^k} \frac{d+l_k}{d} n_k ((T_k^{ten})_{ij} - (\Lambda_k^{ten})_{ij}) \\ &+ \nu_{kk} n_k n_k ((\Lambda_k^{ES})_{ij} - (\mathbb{P}_k)_{ij}) + \nu_{kj} n_j n_k (\Theta_{kj} - T_k^{rot}) \delta_{ij}, \end{aligned}$$

for $k, j = 1, 2, k \neq j$.

Since G_k involves the term $(\Lambda_k^{ES})^{-1}$ and \tilde{G}_k involves the term $(T_k^{ten})^{-1}$ we have to check if Λ_k^{ES} and T_k^{ten} are invertible.

Lemma 3.0.1. *Assume that f_k and \widehat{G}_k are positive solutions to (3.11) and (3.13). Then Λ_k^{ten} and T_k^{ten} have strictly positive eigenvalues. Especially T_k^{ten} is invertible.*

Proof. Let $y \in \mathbb{R}^d \setminus \{0\}$, then

$$\begin{aligned} \langle y, \Lambda_k^{ten} y \rangle &= \sum_{i,j=1}^d y_i (\Lambda_k^{ten})_{ij} y_j = \sum_{i,j=1}^d y_i \int (v_i - u_{k,i})(v_j - u_{k,j}) \widehat{G}_k y_j dv \\ &= \int \left(\sum_{i,j=1}^d y_i (v_i - u_{k,i}) \right)^2 \widehat{G}_k dv \geq 0. \end{aligned}$$

The inequality is true since we assumed that \widehat{G} is a positive solution to (2.6).

If we use equation (2.9) and (2.5)

$$\begin{aligned} \langle y, T_k^{ten} y \rangle &= \sum_{i,j=1}^d y_i (T_k^{ten})_{ij} y_j = \sum_{\substack{i,j=1 \\ i \neq j}}^d y_i \int (v_i - u_{k,i})(v_j - u_{k,j}) f_k y_j dv + \sum_{i=1}^d y_i T_k y_j \\ &= \sum_{i,j=1}^d y_i \int (v_i - u_{k,i})(v_j - u_{k,j}) f_k y_j dv - \sum_{i=1}^d y_i T_k^t y_i + \sum_{i=1}^d y_i \frac{d\Lambda_k + l_k \Theta_k}{d + l_k} y_i \\ &= \int \left(\sum_{i,j=1}^d y_i (v_i - u_{k,i}) \right)^2 f_k dv + \sum_{i=1}^d y_i T_k^r y_i \geq 0, \end{aligned}$$

where $T_k^r > 0$ because T_k^r is defined via a positive integral of f_k , see the definition in (2.1). We even have strict inequality since $\{y_i(v - u)_i\}_{i=1}^d$ are linearly independent. \square

With the previous lemma, we can prove that Λ_k^{ES} is positive. This is the next theorem. Positivity is also proven in [2] for the one species case, but for a different variant of an ES-BGK model.

Theorem 3.0.2. *Assume that $f_k > 0$ and $-\frac{1}{d-1} \leq \mu_k \leq 1$ if $d > 1$. Then Λ_k^{ES} has strictly positive eigenvalues. Especially Λ_k^{ES} is invertible.*

Proof. Since Λ_k^{ten} is symmetric there exist an invertible matrix S_k such that $\widetilde{\Lambda_k^{ten}} = S_k \Lambda_k^{ten} S_k^{-1}$ with a diagonal matrix $\widetilde{\Lambda_k^{ten}}$. Then $\widetilde{\Lambda_k^{ES}} := S_k \Lambda_k^{ES} S_k^{-1}$ is also diagonal since

$$\widetilde{\Lambda_k^{ES}} = S_k \Lambda_k^{ES} S_k^{-1} = (1 - \mu_k) \Lambda_k \mathbf{1} + \mu_k \widetilde{\Lambda_k^{ten}}.$$

Here we can see that the eigenvalues of $\widetilde{\Lambda_k^{ES}}$ are a linear combination of Λ_k and the eigenvalues of $\widetilde{\Lambda_k^{ten}}$ which coincide with the eigenvalues of Λ_k^{ten} . We denote the eigenvalues of Λ_k^{ten} by $\lambda_{k,1}, \lambda_{k,2}, \dots, \lambda_{k,d}$. Then by definition of Λ_k and Λ_k^{ten} we have

$$d\Lambda_k = \text{Tr}(\Lambda_k^{ten}) = \lambda_{k,1} + \lambda_{k,2} + \dots + \lambda_{k,d}.$$

This means for the eigenvalues of Λ_k^{ES} denoted by $\tau_{k,i}$:

$$\tau_{k,i} = \frac{1 - \mu_k}{d} \sum_{j=1}^d \lambda_{k,j} + \mu_k \lambda_{k,i} = \frac{1 + (d-1)\mu_k}{d} \lambda_{k,i} + \frac{1 - \mu_k}{d} \sum_{j=1, j \neq i}^d \lambda_{k,j}, \quad i = 1, 2, 3.$$

Since $\lambda_{k,1}, \lambda_{k,2}, \dots, \lambda_{k,d}$ are strictly positive, the eigenvalues of Λ_k^{ES} are strictly positive, when $1 + (d-1)\mu_k$ and $1 - \mu_k$ are positive. Since we restricted μ_k to $-\frac{1}{d-1} \leq \mu_k \leq 1$ if $d > 1$, Λ_k^{ES} is strictly positive. \square

3.1 Conservation properties

Conservation of the number of particles and total momentum of the model for mixtures described in section 2 are shown in the same way as in the case of mono atomic molecules. In the extension described in section 3 these conservation properties are still satisfied since G_1 and G_2 have the same density, mean velocity and internal energy as f_1 respective f_2 . Conservation of the number of particles and of total momentum are guaranteed by the following choice of the mixture parameters:

If we assume that

$$n_{12} = n_1 \quad \text{and} \quad n_{21} = n_2, \quad (3.18)$$

we have conservation of the number of particles, see Theorem 2.1 in [19]. If we further assume that u_{12} is a linear combination of u_1 and u_2

$$u_{12} = \delta u_1 + (1 - \delta)u_2, \quad \delta \in \mathbb{R}, \quad (3.19)$$

then we have conservation of total momentum provided that

$$u_{21} = u_2 - \frac{m_1}{m_2} \varepsilon (1 - \delta)(u_2 - u_1), \quad (3.20)$$

see Theorem 2.2 in [19].

In the case of total energy we have a difference for the polyatomic case compared to the monoatomic one. So we explicitly consider this in the following theorem.

Theorem 3.1.1 (Conservation of total energy). *Assume (2.4), conditions (3.18), (3.19) and (3.20) and assume that Λ_{12} and Θ_{12} are of the following form*

$$\begin{aligned} \Lambda_{12} &= \alpha \Lambda_1 + (1 - \alpha) \Lambda_2 + \gamma |u_1 - u_2|^2, \quad 0 \leq \alpha \leq 1, \gamma \geq 0, \\ \Theta_{12} &= \frac{l_1 \Theta_1 + l_2 \Theta_2}{l_1 + l_2}. \end{aligned} \quad (3.21)$$

Then we have conservation of total energy

$$\begin{aligned} & \int \frac{m_1}{2} (|v|^2 + |\eta_1|^2) (Q_{11}(f_1, f_1) + Q_{12}(f_1, f_2)) dv d\eta_1 \\ & + \int \frac{m_2}{2} (|v|^2 + |\eta_2|^2) (Q_{22}(f_2, f_2) + Q_{21}(f_2, f_1)) dv d\eta_2 = 0, \end{aligned}$$

provided that

$$\begin{aligned} \Lambda_{21} + \frac{l_2}{d} \Theta_{21} &= \left[\frac{1}{d} \varepsilon m_1 (1 - \delta) \left(\frac{m_1}{m_2} \varepsilon (\delta - 1) + \delta + 1 \right) - \varepsilon \gamma \right] |u_1 - u_2|^2 \\ &+ \varepsilon (1 - \alpha) \Lambda_1 + (1 - \varepsilon (1 - \alpha)) \Lambda_2 + \frac{1}{d} \varepsilon \frac{l_1 l_2}{l_1 + l_2} \Theta_1 + \frac{1}{d} (l_2 - \varepsilon \frac{l_1 l_2}{l_1 + l_2}) \Theta_2. \end{aligned} \quad (3.22)$$

Proof. Using the definition of the energy exchange of species 1 and equation (2.5), we obtain

$$F_{E_{1,2}} := \int \frac{m_1}{2} (|v|^2 + |\eta_1|^2) [Q_{11}(f_1, f_2) + Q_{12}(f_1, f_2)] dv d\eta_1$$

$$\begin{aligned}
&= \varepsilon \nu_{21} \frac{1}{2} n_2 n_1 m_1 (|u_{12}|^2 - |u_1|^2) + \frac{d}{2} \varepsilon \nu_{21} n_1 n_2 (\Lambda_{12} - T_1^t) + \frac{l_1}{2} \varepsilon \nu_{21} n_1 n_2 (\Theta_{12} - T_1^r) \\
&= \varepsilon \nu_{21} \frac{1}{2} n_2 n_1 m_1 (|u_{12}|^2 - |u_1|^2) + \frac{d}{2} \varepsilon \nu_{21} n_1 n_2 (\Lambda_{12} - \Lambda_1) + \frac{l_1}{2} \varepsilon \nu_{21} n_1 n_2 (\Theta_{12} - \Theta_1).
\end{aligned}$$

Next, we will insert the definitions of u_{12} , Λ_{12} and Θ_{12} given by (3.19) and (3.21). Analogously the energy exchange of species 2 towards 1 is

$$F_{E_{2,1}} = \nu_{21} \frac{1}{2} n_2 n_1 m_2 (|u_{21}|^2 - |u_2|^2) + \frac{d}{2} \nu_{21} n_1 n_2 (\Lambda_{21} - \Lambda_2) + \frac{l_2}{2} \nu_{21} n_1 n_2 (\Theta_{21} - \Theta_2).$$

Substitute u_{21} with (3.20) and $\Lambda_{21} + \frac{l_2}{d} \Theta_{21}$ from (3.22). This permits to rewrite the energy exchange as

$$\begin{aligned}
F_{E_{1,2}} &= \varepsilon \nu_{21} \frac{1}{2} n_2 n_1 m_1 (1 - \delta) [(u_1 + u_2) - \delta(u_2 - u_1)](u_1 - u_2) \\
&+ \frac{1}{2} \varepsilon \nu_{21} n_1 n_2 \left[(1 - \alpha) d (\Lambda_2 - \Lambda_1) + \frac{l_1 l_2}{l_1 + l_2} (\Theta_2 - \Theta_1) + \gamma d |u_1 - u_2|^2 \right], \tag{3.23}
\end{aligned}$$

$$\begin{aligned}
F_{E_{2,1}} &= \frac{1}{2} \nu_{21} m_2 n_1 n_2 \left[\left(\left(1 - \frac{m_1}{m_2} \varepsilon (1 - \delta) \right)^2 - 1 \right) |u_2|^2 + \left(\frac{m_1}{m_2} \varepsilon (\delta - 1) \right)^2 |u_1|^2 \right. \\
&+ 2 \left(1 - \frac{m_1}{m_2} \varepsilon (1 - \delta) \right) \frac{m_1}{m_2} \varepsilon (1 - \delta) u_1 \cdot u_2 \left. \right] + \frac{1}{2} \nu_{21} n_1 n_2 [\varepsilon (1 - \alpha) d (\Lambda_1 - \Lambda_2) \\
&+ \varepsilon \frac{l_1 l_2}{l_1 + l_2} (\Theta_1 - \Theta_2) + \left(\varepsilon m_1 (1 - \delta) \left(\frac{m_1}{m_2} \varepsilon (\delta - 1) + \delta + 1 \right) - \varepsilon \gamma d \right) |u_1 - u_2|^2]. \tag{3.24}
\end{aligned}$$

Adding these two terms, we see that the total energy is conserved. \square

Remark 1. *The energy flux between the two species is zero if and only if $u_1 = u_2$, $\Lambda_1 = \Lambda_2$, $\Theta_1 = \Theta_2$ provided that $\alpha, \delta < 1$ and $\gamma > 0$.*

Remark 2. *From conservation of total energy we get only one condition on $\Lambda_{21} + \frac{l_2}{d} \Theta_{21}$ given by (3.22), but not an explicit formula for Λ_{21} and Θ_{21} . In order to keep the model symmetric we again separate the temperatures corresponding to the translational part and the one corresponding to the rotational and vibrational part and choose*

$$\begin{aligned}
\Lambda_{21} &= \varepsilon (1 - \alpha) \Lambda_1 + (1 - \varepsilon (1 - \alpha)) \Lambda_2 \\
&+ \left[\frac{1}{d} \varepsilon m_1 (1 - \delta) \left(\frac{m_1}{m_2} \varepsilon (\delta - 1) + \delta + 1 \right) - \varepsilon \gamma \right] |u_1 - u_2|^2, \tag{3.25}
\end{aligned}$$

$$\Theta_{21} = \left(1 - \varepsilon \frac{l_1}{l_1 + l_2} \right) \Theta_2 + \varepsilon \frac{l_1}{l_1 + l_2} \Theta_1. \tag{3.26}$$

Remark 3. *If $l_1 = l_2$, we have $\Theta_{12} = \frac{1}{2} (\Theta_1 + \Theta_2)$. We then find $\Theta_{21} = \Theta_{12}$ if the two species have the same interspecies collision frequency ($\varepsilon = 1$).*

Remark 4. *The fact that we only consider the two species case is just for simplicity. We can also extend the model to more than two species, because we assume that we only have binary interactions. So if we consider collision terms given by*

$$\nu_{ii} n_i (G_i - f_i) + \sum_{j \neq i}^N \nu_{ij} n_j (G_{ij} - f_i), \quad i = 1, \dots, N,$$

we expect that we have conservation of total momentum and total energy in every interaction of species i with species j . This means we require

$$\int \left(\frac{v}{v^2} \right) \nu_{ij} n_j (G_{ij} - f_i) dv + \int \left(\frac{v}{v^2} \right) \nu_{ji} n_i (G_{ji} - f_j) dv = 0,$$

for every $i, j = 1, \dots, N$, $i \neq j$ and so it reduces to the two species case.

3.2 Positivity of the temperatures

Theorem 3.2.1. *Assume that $f_1(x, v, \eta_{l_1}, t), f_2(x, v, \eta_{l_2}, t) > 0$. Then all temperatures $\Lambda_1, \Lambda_2, \Theta_1, \Theta_2$, and $\Lambda_{12}, \Theta_{12}$ given by (3.21), and $\Lambda_{21}, \Theta_{21}$ determined by (3.25), (3.26) are positive provided that*

$$0 \leq \gamma \leq \frac{m_1}{d} (1 - \delta) \left[\left(1 + \frac{m_1}{m_2} \varepsilon \right) \delta + 1 - \frac{m_1}{m_2} \varepsilon \right]. \quad (3.27)$$

Proof. The temperatures $\Lambda_1, \Lambda_2, \Theta_1, \Theta_2, \Lambda_{12}, \Theta_{12}$ and Θ_{21} are positive by definition because they are integrals or convex combinations of positive functions. So the only thing to check is when the temperature Λ_{21} in (3.25) is positive. This is done in [19] for $d = 3$, so we skip the proof here. The resulting condition is given by (3.27). \square

Remark 5. *Since $\gamma \geq 0$ is a non-negative number, so the right-hand side of the inequality in (3.27) must be non-negative. This condition is equivalent to*

$$\frac{\frac{m_1}{m_2} \varepsilon - 1}{1 + \frac{m_1}{m_2} \varepsilon} \leq \delta \leq 1. \quad (3.28)$$

Note that we have to assume that the distribution function f_1 and f_2 are positive. In [18], positivity of the distribution function for the model described in [19] for mono atomic molecules is proven. This method can be extended to the model described in this paper for polyatomic molecules.

3.3 The structure of equilibrium

Theorem 3.3.1 (Equilibrium). *Assume $f_1, f_2 > 0$ with f_1 and f_2 independent of x and t . Assume the conditions (3.18), (3.19), (3.20), (3.21) and (3.22), $\delta \neq 1, \alpha \neq 1, l_1, l_2 \neq 0$, so that all temperatures are positive.*

Then f_1 and f_2 are Maxwell distributions with equal mean velocities $u_1 = u_2 = u_{12} = u_{21}$ and temperatures $T := T_1^r = T_2^r = T_1^t = T_2^t = \Lambda_1 = \Lambda_2 = \Theta_1 = \Theta_2 = \Theta_{12} = \Theta_{21} = \Lambda_{12} = \Lambda_{21}$. This means f_k is given by

$$M_k(x, v, \eta_{l_k}, t) = \frac{n_k}{\sqrt{2\pi \frac{T}{m_k}}} \frac{1}{\sqrt{2\pi \frac{T}{m_k}}} \exp\left(-\frac{|v - u|^2}{2 \frac{T}{m_k}} - \frac{|\eta_{l_k}|^2}{2 \frac{T}{m_k}}\right), \quad k = 1, 2.$$

Proof. Equilibrium means that $f_1, f_2, \Lambda_1, \Lambda_2, \Theta_1, \Theta_2$ are independent of x and t . Thus in equilibrium the right-hand side of the equations (3.11) and (3.13) have to be zero. In particular,

$$(\nu_{11} n_1 + \nu_{12} n_2) f_1 = \nu_{11} n_1 G_1 + \nu_{12} n_2 M_{12}, \quad (3.29)$$

$$(\nu_{22}n_2 + \nu_{21}n_1)f_2 = \nu_{22}n_2G_2 + \nu_{21}n_1M_{21}. \quad (3.30)$$

Since the right-hand side of (3.11) and the right-hand side of (3.13) have to be zero, the difference of the right-hand side of (3.11) and the right-hand side of (3.13) has to be equal to zero. If we compute the translational temperature of this difference, we obtain

$$\Lambda_1^{ten} = T_1^{ten}, \quad (3.31)$$

$$\Lambda_2^{ten} = T_2^{ten}. \quad (3.32)$$

Especially, from the diagonal part of (3.31) and (3.32) we can deduce

$$\Lambda_1 = \Theta_1, \quad (3.33)$$

$$\Lambda_2 = \Theta_2. \quad (3.34)$$

When we consider the moment of the velocity of (3.29), we get

$$(\nu_{11}n_1 + \nu_{12}n_2)u_1 = \nu_{11}n_1u_1 + \nu_{12}n_2u_{12}.$$

Substituting $u_{12} = \delta u_1 + (1 - \delta)u_2$, we have

$$u_1 = u_2, \quad (3.35)$$

for $\delta \neq 1$.

Using (3.33), (3.34) and (3.35), the temperatures of the mixture Maxwellians (3.21) and (3.25), (3.26) simplify to

$$\Lambda_{12} = \alpha\Lambda_1 + (1 - \alpha)\Lambda_2, \quad \Theta_{12} = \frac{l_1}{l_1 + l_2}\Lambda_1 + \frac{l_2}{l_1 + l_2}\Lambda_2, \quad (3.36)$$

$$\Lambda_{21} = \varepsilon(1 - \alpha)\Lambda_1 + (1 - \varepsilon(1 - \alpha))\Lambda_2, \quad \Theta_{21} = \varepsilon\frac{l_1}{l_1 + l_2}\Lambda_1 + (1 - \varepsilon\frac{l_1}{l_1 + l_2})\Lambda_2. \quad (3.37)$$

When we consider the moments of the translational and the rotational and vibrational temperatures of (3.29) and (3.30), we get

$$(\nu_{11}n_1 + \nu_{12}n_2)T_1^t = (\nu_{11}n_1 + \nu_{12}n_2\alpha)\Lambda_1 + \nu_{12}n_2(1 - \alpha)\Lambda_2, \quad (3.38)$$

$$(\nu_{11}n_1 + \nu_{12}n_2)T_1^r = (\nu_{11}n_1 + \nu_{12}n_2\frac{l_1}{l_1 + l_2})\Lambda_1 + \nu_{12}n_2\frac{l_2}{l_1 + l_2}\Lambda_2, \quad (3.39)$$

$$(\nu_{22}n_2 + \nu_{21}n_1)T_2^t = \nu_{22}n_2\Lambda_2 + \nu_{21}n_1\Lambda_{21}, \quad (3.40)$$

$$(\nu_{22}n_2 + \nu_{21}n_1)T_2^r = \nu_{22}n_2\Lambda_2 + \nu_{21}n_1\Theta_{21}, \quad (3.41)$$

where we used the definitions of the mixture velocities and temperatures (3.18), (3.19), (3.20), (3.21) and equations (3.33), (3.34) and (3.35). Analogue, equations (2.5) simplify to

$$\frac{d + l_1}{2}\Lambda_1 = \frac{d}{2}T_1^t + \frac{l_1}{2}T_1^r, \quad (3.42)$$

$$\frac{d + l_2}{2}\Lambda_2 = \frac{d}{2}T_2^t + \frac{l_2}{2}T_2^r. \quad (3.43)$$

Inserting (3.38) and (3.39) in (3.42), we obtain

$$\frac{d}{2}\left(\frac{\nu_{11}n_1 + \nu_{12}n_2\alpha}{\nu_{11}n_1 + \nu_{12}n_2}\Lambda_1 + \frac{\nu_{12}n_2(1 - \alpha)}{\nu_{11}n_1 + \nu_{12}n_2}\Lambda_2\right) + \frac{l_1}{2}\left(\frac{\nu_{11}n_1 + \nu_{12}n_2\frac{l_1}{l_1 + l_2}}{\nu_{11}n_1 + \nu_{12}n_2}\Lambda_1 + \frac{\nu_{12}n_2\frac{l_2}{l_1 + l_2}}{\nu_{11}n_1 + \nu_{12}n_2}\Lambda_2\right)$$

$$= \frac{d+l_1}{2} \Lambda_1,$$

which, provided $d\alpha + l_1 \frac{l_1}{l_1+l_2} \neq d+l_1$, is equivalent to

$$\Lambda_1 = \Lambda_2. \quad (3.44)$$

This condition is equivalent to $d(1-\alpha) + \frac{l_1 l_2}{l_1+l_2} \neq 0$ which is satisfied since $\alpha \neq 1, l_1, l_2 \neq 0$. With (3.44) we can deduce from (3.38) and (3.39) that

$$T_1^t = \Lambda_1 \quad \text{and} \quad T_1^r = \Lambda_1. \quad (3.45)$$

Condition (3.37) together with (3.44) leads to

$$\Lambda_{21} = \Theta_{21} = \Lambda_1. \quad (3.46)$$

Inserting (3.44) and (3.46) in (3.40) and (3.41) leads to

$$T_2^t = T_2^r = \Lambda_1. \quad (3.47)$$

If we compute the pressure tensor of (3.29) using that all temperatures are equal to Λ_1 we obtain

$$(\nu_{11}n_1 + \nu_{12}n_2) \frac{\mathbb{P}_1}{n_1} = \nu_{11}n_1(1-\mu_1)\Lambda_1 \mathbf{1} + \nu_{11}n_1\mu_1\Lambda_1^{ten} + \nu_{12}n_2\Lambda_1 \mathbf{1}.$$

Using (3.16), (3.31) and (3.45), we have that

$$\frac{d}{d+l_k} \frac{\mathbb{P}_1}{n_1} + \frac{l_k}{d+l_k} \Lambda_1^{rot} \mathbf{1}_d = \Lambda_1^{ten} = T_1^{ten}$$

and therefore

$$(\nu_{11}n_1(1-\mu_1 \frac{d}{d+l_k}) + \nu_{12}n_2) \frac{\mathbb{P}_1}{n_1} = (\nu_{11}n_1(1-\mu_1 \frac{d}{d+l_k}) + \nu_{12}n_2) \Lambda_1 \mathbf{1},$$

for $j \neq i$, which shows that the pressure tensor of f_1 is diagonal since $\mu_1 \leq 1$. Similar for $\frac{\mathbb{P}_2}{n_2}$ using (3.30), (3.32) and (3.45).

So all in all, in equilibrium we get that f_1 and f_2 are Maxwell distributions with equal mean velocities $u_1 = u_2 = u_{12} = u_{21}$ and temperatures $T_1^r = T_2^r = T_1^t = T_2^t = \Lambda_1 = \Lambda_2 = \Theta_1 = \Theta_2 = \Theta_{12} = \Theta_{21} = \Lambda_{12} = \Lambda_{21}$. \square

Definition 3.3.1. *If f_1 and f_2 are Maxwell distributions with equal mean velocities $u = u_1 = u_2$ and temperatures $T = T_1^r = T_2^r = T_1^t = T_2^t = \Lambda_1 = \Lambda_2 = \Theta_1 = \Theta_2$, then we say that f_1 and f_2 are in local equilibrium.*

Note that for $\alpha = 1$ or $\delta = 1$, we have no exchange of momentum and energy of the two species, so we do not expect a relaxation towards a common equilibrium. So in the following, we always assume $\alpha, \delta \neq 1$.

3.4 H-Theorem

In this section we will prove that our model admits an entropy with an entropy inequality. For this, we have to prove an inequality on the term $\int \ln f_k (G_k - f_k) dv d\eta_k$ coupled with the right-hand side of equation (3.13) and an inequality on $\nu_{12}n_2 \int (M_{12} - f_1) \ln f_1 dv d\eta_{l_1} + \nu_{21}n_1 \int (M_{21} - f_2) \ln f_2 dv d\eta_{l_2}$ coupled with the right-hand side of equation (3.13). We prove the first one in subsection 3.4.1 and the second one in subsection 3.4.2.

3.4.1 H-Theorem for the one species relaxation terms

Remark 6. From the definition of the moments of $f_k, k=1,2$ in (2.1) and the definitions of the extended Maxwellians $G_k, k=1,2$ in (3.12), we see that the pressure tensors and the temperatures, do not coincide. Now, we consider extended Maxwellians $\bar{G}_k, k=1,2$ which have the same moments as $f_k, k=1,2$. Then from the case of one species ES-BGK model we know that

$$\int \bar{G}_k \ln \bar{G}_k dv d\eta_{l_k} \leq \int f_k \ln f_k dv d\eta_{l_k},$$

for $k=1,2$, see equations (20) and (21) in [2] in the mono atomic case. The polyatomic case is analogously to the mono atomic case.

Lemma 3.4.1. Assume that $f_1, f_2 > 0$. As in remark 6 let \bar{G}_k be the extended Maxwellians with the same moments as $f_k, k=1,2$ and \hat{G}_k the Maxwellians defined by (3.14). Then we have

$$\begin{aligned} \int \tilde{G}_k \ln \tilde{G}_k dv d\eta_{l_k} &\leq \int \bar{G}_k \ln \bar{G}_k dv d\eta_{l_k}, \quad k=1,2, \\ \int \hat{G}_k \ln \hat{G}_k dv d\eta_{l_k} &\geq \int G_k \ln G_k dv d\eta_{l_k}, \quad k=1,2, \\ \int G_k \ln G_k dv d\eta_{l_k} &\geq \int M_k \ln M_k dv d\eta_{l_k}, \quad k=1,2. \end{aligned}$$

Proof. The proof of the second inequality is analogously to the proof in the mono atomic case of equation (21) in [2]. So we only prove the first and the third one. Using that

$$\begin{aligned} \ln M_k &= \ln \left(\frac{n_k}{\sqrt{2\pi \frac{\Lambda_k}{m_k}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}^{l_k}} \right) - \frac{|v-u_k|^2}{2 \frac{\Lambda_k}{m_k}} - \frac{|\eta_{l_k}|^2}{2 \frac{\Theta_k}{m_k}}, \\ \ln \bar{G}_k &= \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{\mathbb{P}_k}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k^r}{m_k}}^{l_k}} \right) - \frac{1}{2} (v-u_k) \cdot \left(\frac{\mathbb{P}_k}{m_k} \right)^{-1} \cdot (v-u_k) - \frac{|\eta_{l_k}|^2}{2 \frac{T_k^r}{m_k}}, \\ \ln \tilde{G}_k &= \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{T_k^{ten}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k}{m_k}}^{l_k}} \right) - \frac{1}{2} (v-u_k) \cdot \left(\frac{T_k^{ten}}{m_k} \right)^{-1} \cdot (v-u_k) - \frac{|\eta_{l_k}|^2}{2 \frac{T_k}{m_k}}, \quad \text{and} \\ \ln G_k &= \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ES}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}^{l_k}} \right) - \frac{1}{2} m_k (v-u_k) \cdot (\Lambda_k^{ES})^{-1} \cdot (v-u_k) - \frac{|\eta_{l_k}|^2}{2 \frac{\Theta_k}{m_k}}, \end{aligned}$$

we compute the integrals and obtain that the required inequalities are equivalent to

$$\begin{aligned} \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{T_k^{ten}}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k}{m_k}}^{l_k}} \right) &\leq \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{\mathbb{P}_k}{m_k})}} \frac{1}{\sqrt{2\pi \frac{T_k^r}{m_k}}^{l_k}} \right), \\ \ln \left(\frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ES}}{m_k})}} \right) &\geq \ln \left(\frac{n_k}{\sqrt{2\pi \frac{\Lambda_k}{m_k}}^d} \right). \end{aligned}$$

This is equivalent to the conditions

$$\begin{aligned} \ln \det(T_k^{ten}) + l_k \ln T_k &\geq \ln \det \mathbb{P}_k + l_k \ln T_k^r, \\ (\Lambda_k)^d &\geq \det(\Lambda_k^{ES}). \end{aligned} \tag{3.48}$$

We first look at the first inequality. If we insert the expression for T_k given by (2.9) and use the concavity of \ln , we obtain

$$\ln \det(T_k^{ten}) + l_k \frac{l_k}{d+l_k} \ln T_k^r + l_k \frac{d}{d+l_k} \ln T_k^t \geq \ln \det \mathbb{P}_k + l_k \ln T_k^r. \quad (3.49)$$

Now we use the Brunn-Minkowsky inequality (inequality (27) in [2]) given by

$$\det(aA + (1-a)B) \geq (\det A)^a (\det B)^{1-a},$$

for $0 \leq a \leq 1$ and A, B positive symmetric matrices. Since we can write T_k^{ten} as

$$T_k^{ten} = \frac{d}{d+l_k} \mathbb{P}_k + \frac{l_k}{d+l_k} T_k^r \mathbf{1}_d,$$

we can apply the Brunn-Minkowsky inequality on (3.49) and obtain

$$\begin{aligned} \frac{d}{d+l_k} \ln \det \mathbb{P}_k + d \frac{l_k}{d+l_k} \ln T_k^r + l_k \frac{l_k}{d+l_k} \ln T_k^r + l_k \frac{d}{d+l_k} \ln T_k^t \\ \geq \ln \det \mathbb{P}_k + l_k \ln T_k^r \end{aligned}$$

So it remains to show that

$$(T_k^t)^d \geq \det \mathbb{P}_k.$$

This inequality has the same structure as the second inequality in (3.48). So we prove only the second inequality in (3.48). We observe that $\text{trace}(\Lambda_k^{ES}) = d\Lambda_k$, so we have to show

$$\left(\frac{\text{trace}(\Lambda_k^{ES})}{d} \right)^d \geq \det(\Lambda_k^{ES}).$$

Let $\lambda_1, \dots, \lambda_d$ the eigenvalues of the symmetric positive matrix Λ_k^{ES} , then this inequality is equivalent to

$$\left(\frac{\lambda_1 + \dots + \lambda_d}{d} \right)^d \geq \lambda_1 \cdots \lambda_d.$$

This is true since it is the inequality of arithmetic and geometric means. \square

Lemma 3.4.2 (Contribution to the H-theorem from the one species relaxation terms). *Assume $f_1, f_2 > 0$. Then*

$$\int \ln f_k (G_k - f_k) dv d\eta_{l_k} + \int \ln \widehat{G}_k (\widetilde{G}_k - \widehat{G}_k) dv d\eta_{l_k} \leq 0, \quad k=1,2,$$

with equality if and only if $M_k = f_k$ and $\Lambda_k = \Theta_k = T_k^r = T_k^t$.

Proof. Since the function $H(x) = x \ln x - x$ is strictly convex for $x > 0$, we have $H'(f)(g - f) \leq H(g) - H(f)$ with equality if and only if $g = f$. So

$$(g - f) \ln f \leq g \ln g - f \ln f + f - g. \quad (3.50)$$

Apply (3.50) on both terms of

$$S_k(f_k) := \int \ln f_k (G_k - f_k) dv d\eta_{l_k} + \int \ln \widehat{G}_k (\widetilde{G}_k - \widehat{G}_k) dv d\eta_{l_k}.$$

Then we obtain

$$\begin{aligned} S_k(f_k) \leq & \int G_k \ln G_k dv d\eta_{l_k} - \int f_k \ln f_k dv d\eta_{l_k} - \int G_k dv d\eta_{l_k} + \int f_k dv d\eta_{l_k} \\ & + \left[\int \tilde{G}_k \ln \tilde{G}_k dv d\eta_{l_k} - \int \hat{G}_k \ln \hat{G}_k dv d\eta_{l_k} - \int \tilde{G}_k dv d\eta_{l_k} + \int \hat{G}_k dv d\eta_{l_k} \right], \end{aligned}$$

with equality if and only if $f_k = G_k$ and $G_k = \tilde{G}_k$ from which we can deduce $f_k = M_k$ by computing macroscopic quantities of $f_k = G_k$ and $G_k = \tilde{G}_k$. Since f_k , G_k , \tilde{G}_k and \hat{G}_k have the same density, we obtain

$$S(f_k) \leq \int G_k \ln G_k dv d\eta_{l_k} - \int f_k \ln f_k dv d\eta_{l_k} + \left[\int \tilde{G}_k \ln \tilde{G}_k dv d\eta_{l_k} - \int \hat{G}_k \ln \hat{G}_k dv d\eta_{l_k} \right]. \quad (3.51)$$

According to the second part of lemma 3.4.1, we obtain

$$S(f_k) \leq \int \tilde{G}_k \ln \tilde{G}_k dv d\eta_{l_k} - \int f_k \ln f_k dv d\eta_{l_k}. \quad (3.52)$$

Here we have equality if and only if $G_k = \tilde{G}_k$, which means $\Lambda_k = \Theta_k$. Now, using the first part of lemma 3.4.1 and remark 6, we can estimate $\int \tilde{G}_k \ln \tilde{G}_k dv d\eta_{l_k}$ by $\int f_k \ln f_k dv d\eta_{l_k}$. So, all in all, we obtain $S_k(f_k) \leq 0$ with equality if and only if $f_k = M_k$ and $\Lambda_k = \Theta_k = T_k^r = T_k^t$. □

3.4.2 H-Theorem for mixtures of polyatomic molecules

Define $\frac{1}{z_k} := \frac{1}{Z_k^r} \frac{d+l_k}{d}$, $k=1,2$ and the total entropy

$$H(f_1, f_2) = \int (f_1 \ln f_1 + 3z_1 \hat{G}_1 \ln \hat{G}_1) dv d\eta_{l_1} + \int (f_2 \ln f_2 + 3z_2 \hat{G}_2 \ln \hat{G}_2) dv d\eta_{l_2}. \quad (3.53)$$

We start with an inequality which is used to prove lemma 3.5. Lemma 3.5 is then needed to prove the H-theorem in theorem 3.5

Lemma 3.4.3. *Assume $f_1, f_2 > 0$. Assume the relationship between the collision frequencies (2.4), the conditions for the interspecies Maxwellians (3.18), (3.19), (3.20), (3.21) and (3.22) and the positivity of all temperatures, then*

$$\varepsilon \frac{d}{2} \ln \Lambda_{12} + \varepsilon \frac{l_1}{2} \ln \Theta_{12} + \frac{d}{2} \ln \Lambda_{21} + \frac{l_2}{2} \ln \Theta_{21} \geq \frac{d}{2} \varepsilon \ln \Lambda_1 + \frac{d}{2} \ln \Lambda_2 + \frac{l_1}{2} \varepsilon \ln \Theta_1 + \frac{l_2}{2} \ln \Theta_2. \quad (3.54)$$

Proof. First we consider the part $E_1 := \frac{d}{2} \ln \Lambda_{12} + \frac{l_1}{2} \ln \Theta_{12}$. We insert the definitions of Λ_{12} and Θ_{12} into E_1 and use the monotonicity of \ln to drop the velocity term. Then we obtain

$$E_1 \geq \frac{d}{2} \ln(\alpha \Lambda_1 + (1-\alpha) \Lambda_2) + \frac{l_1}{2} \ln\left(\frac{l_1}{l_1+l_2} \Theta_1 + \frac{l_2}{l_1+l_2} \Theta_2\right).$$

Now we use that \ln is concave and get

$$E_1 \geq \frac{d}{2} \alpha \ln \Lambda_1 + \frac{d}{2} (1-\alpha) \ln \Lambda_2 + \frac{l_1}{2} \frac{l_1}{l_1+l_2} \ln \Theta_1 + \frac{l_1}{2} \frac{l_2}{l_1+l_2} \ln \Theta_2. \quad (3.55)$$

Doing the same with the second part $E_2 := \frac{d}{2} \ln \Lambda_{21} + \frac{l_2}{2} \ln \Theta_{21}$ using that $\frac{l_1}{l_1+l_2} \varepsilon \leq 1$, we obtain

$$E_2 \geq \frac{d}{2} \varepsilon (1-\alpha) \ln \Lambda_1 + \frac{d}{2} (1-\varepsilon(1-\alpha)) \ln \Lambda_2 + \frac{l_2}{2} \varepsilon \frac{l_1}{l_1+l_2} \ln \Theta_1 + \frac{l_2}{2} (1-\varepsilon \frac{l_1}{l_1+l_2}) \ln \Theta_2. \quad (3.56)$$

Multiplying (3.55) by ε and adding (3.56), we get

$$\varepsilon E_1 + E_2 \geq \frac{d}{2} \varepsilon \ln \Lambda_1 + \frac{d}{2} \ln \Lambda_2 + \frac{l_1}{2} \varepsilon \ln \Theta_1 + \frac{l_2}{2} \ln \Theta_2.$$

which is the required inequality. \square

Lemma 3.4.4. *Assume $f_1, f_2 > 0$. Assume the relationship between the collision frequencies (2.4), the conditions for the interspecies Maxwellians (3.18), (3.19), (3.20), (3.21) and (3.22) and the positivity of all temperatures. Then*

$$\begin{aligned} & \nu_{12} n_2 \int M_{12} \ln M_{12} dv d\eta_{l_1} + \nu_{21} n_1 \int M_{21} \ln M_{21} dv d\eta_{l_2} \\ & \leq \nu_{12} n_2 \int M_1 \ln M_1 dv d\eta_{l_1} + \nu_{21} n_1 \int M_2 \ln M_2 dv d\eta_{l_2}. \end{aligned}$$

Proof. Using that $\ln M_{12} = \ln\left(\frac{n_2}{\sqrt{2\pi \frac{\Lambda_{12}}{m_1}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_{12}}{m_1}}^{l_1}}\right) - \frac{|v-u_{12}|^2}{2 \frac{\Lambda_{12}}{m_1}} - \frac{|\eta_{l_1}|^2}{2 \frac{\Theta_{12}}{m_1}}$,

$$\ln M_{21} = \ln\left(\frac{n_1}{\sqrt{2\pi \frac{\Lambda_{21}}{m_2}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_{21}}{m_2}}^{l_2}}\right) - \frac{|v-u_{21}|^2}{2 \frac{\Lambda_{21}}{m_2}} - \frac{|\eta_{l_2}|^2}{2 \frac{\Theta_{21}}{m_2}}$$

$\ln M_k = \ln\left(\frac{n_k}{\sqrt{2\pi \frac{\Lambda_k}{m_k}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_k}{m_k}}^{l_k}}\right) - \frac{|v-u_k|^2}{2 \frac{\Lambda_k}{m_k}} - \frac{|\eta_{l_k}|^2}{2 \frac{\Theta_k}{m_k}}$, $k=1,2$, we compute the integrals and obtain that the required inequalities are equivalent to

$$\begin{aligned} & \varepsilon \ln\left(\frac{n_1}{\sqrt{2\pi \frac{\Lambda_{12}}{m_1}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_{12}}{m_1}}^{l_1}}\right) + \ln\left(\frac{n_2}{\sqrt{2\pi \frac{\Lambda_{21}}{m_2}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_{21}}{m_2}}^{l_2}}\right) \\ & \leq \varepsilon \ln\left(\frac{n_1}{\sqrt{2\pi \frac{\Lambda_1}{m_1}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_1}{m_1}}^{l_1}}\right) + \ln\left(\frac{n_2}{\sqrt{2\pi \frac{\Lambda_2}{m_2}}^d} \frac{1}{\sqrt{2\pi \frac{\Theta_2}{m_2}}^{l_2}}\right). \end{aligned}$$

This inequality is true since after a brief manipulation of the inequality it is equivalent to lemma 3.4.3. \square

Theorem 3.4.5 (H-theorem for mixture). *Assume $f_1, f_2 > 0$. Assume $\nu_{11} n_1 \geq \nu_{12} n_2$, $\nu_{22} n_2 \geq \nu_{21} n_1$, $\alpha, \delta \neq 1, l_1, l_2 \neq 0$. Assume the relationship between the collision frequencies (2.4), the conditions for the interspecies Maxwellians (3.18), (3.19), (3.20), (3.21) and (3.22) and the positivity of all temperatures, then*

$$\begin{aligned} & \sum_{k=1}^2 [\nu_{kk} n_k \int (G_k - f_k) \ln f_k dv d\eta_{l_k} + \nu_{kk} n_k \int (\tilde{G}_k - \hat{G}_k) \ln \hat{G}_k dv d\eta_{l_k}] \\ & + \nu_{11} n_1 \int (\tilde{G}_1 - \hat{G}_1) \ln \hat{G}_1 dv d\eta_{l_1} + \nu_{22} n_2 \int (\tilde{G}_2 - \hat{G}_2) \ln \hat{G}_2 dv d\eta_{l_2} \\ & + \nu_{12} n_2 \int (M_{12} - f_1) \ln f_1 dv d\eta_{l_1} + \nu_{21} n_1 \int (M_{21} - f_2) \ln f_2 dv d\eta_{l_2} \leq 0, \end{aligned}$$

with equality if and only if f_1 and f_2 are in local equilibrium (see definition 3.3.1).

Remark 7. The inequality in the H -Theorem is still true if $l_1=0$ or $l_2=0$ which means that one species is mono atomic. In this case only the equalities with Θ_1 and Θ_2 , respectively in the local equilibrium vanish.

Proof. The fact that $\nu_{kk}n_k \int (G_k - f_k) \ln f_k dv d\eta_{l_k} + \nu_{kk}n_k \int (\tilde{G}_k - \hat{G}_k) \ln \hat{G}_k dv d\eta_{l_k} \leq 0, k=1,2$ is shown in Lemma 3.4.2. In both cases we have equality if and only if $f_1 = G_1$ with $\Lambda_1 = \Theta_1 = T_1^t = T_1^r$ and $f_2 = G_2$ with $\Lambda_2 = \Theta_2 = T_2^t = T_2^r$.

Let us define

$$S(f_1, f_2) := \nu_{11}n_1 \int (\tilde{G}_1 - \hat{G}_1) \ln \hat{G}_1 dv d\eta_{l_1} + \nu_{22}n_2 \int (\tilde{G}_2 - \hat{G}_2) \ln \hat{G}_2 dv d\eta_{l_2} \\ + \nu_{12}n_2 \int (M_{12} - f_1) \ln f_1 dv d\eta_{l_1} + \nu_{21}n_1 \int (M_{21} - f_2) \ln f_2 dv d\eta_{l_2}.$$

The task is to prove that $S(f_1, f_2) \leq 0$. Since the function $H(x) = x \ln x - x$ is strictly convex for $x > 0$, we have $H'(f)(g - f) \leq H(g) - H(f)$ with equality if and only if $g = f$. So

$$(g - f) \ln f \leq g \ln g - f \ln f + f - g. \quad (3.57)$$

Consider now $S(f_1, f_2)$ and apply the inequality (3.57) to each of the terms in S .

$$S \leq \nu_{11}n_1 \left[\int \tilde{G}_1 \ln \tilde{G}_1 dv d\eta_{l_1} - \int \hat{G}_1 \ln \hat{G}_1 dv d\eta_{l_1} + \int \hat{G}_1 dv d\eta_{l_1} - \int \tilde{G}_1 dv d\eta_{l_1} \right] \\ + \nu_{12}n_2 \left[\int M_{12} \ln M_{12} dv d\eta_{l_1} - \int f_1 \ln f_1 dv d\eta_{l_1} + \int f_1 dv d\eta_{l_1} - \int M_{12} dv d\eta_{l_1} \right] \\ + \nu_{21}n_1 \left[\int M_{21} \ln M_{21} dv d\eta_{l_2} - \int f_2 \ln f_2 dv d\eta_{l_2} + \int f_2 dv d\eta_{l_2} - \int M_{21} dv d\eta_{l_2} \right] \\ + \nu_{22}n_2 \left[\int \tilde{G}_2 \ln \tilde{G}_2 dv d\eta_{l_2} - \int \hat{G}_2 \ln \hat{G}_2 dv d\eta_{l_2} + \int \hat{G}_2 dv d\eta_{l_2} - \int \tilde{G}_2 dv d\eta_{l_2} \right],$$

with equality if and only if $f_1 = M_{12}$, $f_2 = M_{21}$, $\tilde{G}_1 = \hat{G}_1$ and $\tilde{G}_2 = \hat{G}_2$. Combining this with the condition for equality of the single collision term $f_1 = G_1$ with $\Lambda_1 = \Theta_1 = T_1^t = T_1^r$ and $f_2 = G_2$ with $\Lambda_2 = \Theta_2 = T_2^t = T_2^r$, we get that we have equality if and only if we are in local equilibrium (see definition 3.3.1). Since $\hat{G}_1, \tilde{G}_1, f_1$ and M_{12} have the same density and $\hat{G}_2, \tilde{G}_2, M_{21}$ and f_2 have the same density, too, the right-hand side reduces to

$$S \leq \nu_{11}n_1 \left[\int \tilde{G}_1 \ln \tilde{G}_1 dv d\eta_{l_1} - \int \hat{G}_1 \ln \hat{G}_1 dv d\eta_{l_1} \right] \\ + \nu_{12}n_2 \left[\int M_{12} \ln M_{12} dv d\eta_{l_1} - \int f_1 \ln f_1 dv d\eta_{l_1} \right] \\ + \nu_{21}n_1 \left[\int M_{21} \ln M_{21} dv d\eta_{l_2} - \int f_2 \ln f_2 dv d\eta_{l_2} \right] \\ + \nu_{22}n_2 \left[\int \tilde{G}_2 \ln \tilde{G}_2 dv d\eta_{l_2} - \int \hat{G}_2 \ln \hat{G}_2 dv d\eta_{l_2} \right].$$

According to the second part of lemma 3.4.1, we obtain

$$S \leq \nu_{11}n_1 \left[\int \tilde{G}_1 \ln \tilde{G}_1 dv d\eta_{l_1} - \int G_1 \ln G_1 dv d\eta_{l_1} \right] \\ + \nu_{12}n_2 \left[\int M_{12} \ln M_{12} dv d\eta_{l_1} - \int f_1 \ln f_1 dv d\eta_{l_1} \right]$$

$$\begin{aligned}
& +\nu_{21}n_1\left[\int M_{21}\ln M_{21}dv d\eta_{l_2}-\int f_2\ln f_2dv d\eta_{l_2}\right] \\
& +\nu_{22}n_2\left[\int \tilde{G}_2\ln \tilde{G}_2dv d\eta_{l_2}-\int G_2\ln G_2dv d\eta_{l_2}\right].
\end{aligned}$$

According to lemma 3.4.4, the last part of lemma 3.4.1 and the assumption that $\nu_{kk}n_k \geq \nu_{kj}n_j$, $k, j=1, 2, k \neq j$, we get

$$\begin{aligned}
S & \leq \nu_{11}n_1\left[\int \tilde{G}_1\ln \tilde{G}_1dv d\eta_{l_1}-\int G_1\ln G_1dv d\eta_{l_1}\right] \\
& +\nu_{12}n_2\left[\int G_1\ln G_1dv d\eta_{l_1}-\int f_1\ln f_1dv d\eta_{l_1}\right] \\
& +\nu_{21}n_1\left[\int G_2\ln G_2dv d\eta_{l_2}-\int f_2\ln f_2dv d\eta_{l_2}\right] \\
& +\nu_{22}n_2\left[\int \tilde{G}_2\ln \tilde{G}_2dv d\eta_{l_2}-\int G_2\ln G_2dv d\eta_{l_2}\right] \\
& \leq \nu_{12}n_2\left[\int \tilde{G}_1\ln \tilde{G}_1dv d\eta_{l_1}-\int f_1\ln f_1dv d\eta_{l_1}\right] \\
& +\nu_{21}n_1\left[\int \tilde{G}_2\ln \tilde{G}_2dv d\eta_{l_2}-\int f_2\ln f_2dv d\eta_{l_2}\right].
\end{aligned}$$

which leads to $S \leq 0$ using the first part of lemma 3.4.1 and remark 6. □

Using the definition (3.53), we can compute

$$\begin{aligned}
& \partial_t H(f_1, f_2) + \nabla_x \cdot \int (f_1 \ln f_1 + 2z_1 \hat{G}_1 \ln \hat{G}_1) v dv d\eta_{l_1} \\
& + \nabla_x \cdot \int (f_2 \ln f_2 + 2z_2 \hat{G}_2 \ln \hat{G}_2) v dv d\eta_{l_2} = S(f_1, f_2) + R(f_1, f_2),
\end{aligned}$$

by multiplying the BGK equation for species 1 by $\ln f_1$, the BGK equation for the species 2 by $\ln f_2$, equations (3.13) by $3z_k \ln G_k$ and sum the integrals with respect to v and η_{l_1} and η_{l_2} , respectively. The remaining term $R(f_1, f_2)$ can be bounded by zero from below by an explicit computation assuming that Λ_k and Θ_k are bounded from below and above and assume that $T_k^{rot} \geq \tilde{C}\Theta_k$ for an appropriate \tilde{C} and z_k small enough. The additional estimate $T_k^{rot} \geq \tilde{C}\Theta_k$ helps to indicate how to choose the initial data of the artificial temperature Θ_k .

Corollary 3.4.6 (Entropy inequality for mixtures). *Assume $f_1, f_2 > 0$, Λ_k and Θ_k are bounded from below and above and $T_k^{rot} \geq \tilde{C}\Theta_k$ for an appropriate \tilde{C} and z_k small enough. Assume relationship (2.4), the conditions (3.18), (3.19), (3.20), (3.21) and (3.22) and the positivity of all temperatures (3.27), then we have the following entropy inequality*

$$\begin{aligned}
& \partial_t (H(f_1, f_2)) \\
& + \nabla_x \cdot \left(\int v(f_1 \ln f_1 + 3z_1 \hat{G}_1 \ln \hat{G}_1) v dv d\eta_{l_1} + \int v(f_2 \ln f_2 + 3z_2 \hat{G}_2 \ln \hat{G}_2) v dv d\eta_{l_2} \right) \leq 0,
\end{aligned}$$

with equality if and only if f_1 and f_2 are in local equilibrium (see definition 3.3.1).

Remark 8. *By computing the integrals*

$$\int \widehat{G}_k \ln \widehat{G}_k dv d\eta_{l_k} \quad \text{and} \quad \int v \widehat{G}_k \ln \widehat{G}_k dv d\eta_{l_k} \quad \text{for } k=1,2,$$

we see that

$$\partial_t \left[\int \widehat{G}_1 \ln \widehat{G}_1 dv d\eta_{l_1} + \int \widehat{G}_2 \ln \widehat{G}_2 dv d\eta_{l_2} \right] + \nabla_x \cdot \left[\int v \widehat{G}_1 \ln \widehat{G}_1 dv d\eta_{l_1} + \int v \widehat{G}_2 \ln \widehat{G}_2 dv d\eta_{l_2} \right] \leq 0,$$

is equivalent to

$$\partial_t (\det(\Lambda_1^{ten}) \Theta_1^{l_1} + \det(\Lambda_2^{ten}) \Theta_2^{l_2}) + \nabla_x \cdot ((\det(\Lambda_1^{ten}) \Theta_1^{l_1} + \det(\Lambda_2^{ten}) \Theta_2^{l_2}) u_k) \leq 0,$$

so we could also consider the entropy

$$H(f_1, f_2) = \sum_{k=1}^2 \int f_k \ln f_k dv d\eta_{l_k} + z_1 \det(\Lambda_1^{ten}) \Theta_1^{l_1} + z_2 \det(\Lambda_2^{ten}) \Theta_2^{l_2}.$$

4 Comparison with the ES-BGK model for one species of polyatomic molecules by Andries, Le Tallec, Perlat and Perthame

We will now consider a different ES-BGK model for a single species ES-BGK model of polyatomic molecules. In [3], they consider a distribution function $f(t, x, v, I)$ depending on the position $x \in \mathbb{R}^3$, the velocity $v \in \mathbb{R}^3$ and internal energy $\varepsilon(I) = I^{\frac{2}{\delta}}$, $I \in \mathbb{R}^+$ at time t . δ denotes the number of degrees of freedom in internal energy. In [3], it is assumed that the mass of the particles is equal to 1. In the following, we assume additionally that $k_B = 1$ in this model. The mass density ρ and mean velocity u are defined as in the model described in the previous subsection integrating with respect to v and I . The energy is defined as

$$E(x, t) = \int \int \left(\frac{1}{2} |v|^2 + I^{\frac{\delta}{2}} \right) f dv dI = \frac{1}{2} \rho |u|^2 + \rho e.$$

The specific internal energy can be divided into

$$e_{tr} = \frac{1}{\rho} \int \int \frac{1}{2} |v - u|^2 f dv dI,$$

$$e_{int} = \frac{1}{\rho} \int \int I^{\frac{2}{\delta}} f dv dI,$$

and associate with this the corresponding temperatures

$$e = e_{tr} + e_{int} = \frac{3 + \delta}{2} R T_{equ},$$

$$e_{tr} = \frac{3}{2} R T_{tr},$$

$$e_{int} = \frac{\delta}{2} R T_{int},$$

and define $T_{rel} = \theta T_{equ} + (1 - \theta)T_{int}$. They consider the generalized Gaussian for the single species ES-BGK model

$$\tilde{G}[f] = \frac{\rho \Lambda_\delta}{\sqrt{\det(2\pi\mathcal{T})}} \frac{1}{RT_{rel}^{\frac{\delta}{2}}} \exp\left(-\frac{1}{2}(v-u) \cdot \mathcal{T}^{-1} \cdot (v-u) + \frac{I^{\frac{\delta}{2}}}{RT_{rel}}\right),$$

with the tensor $\mathcal{T} = (1 - \theta)((1 - \nu)RT_{tr}\mathbf{1} + \nu\Theta) + \theta RT_{equ}\mathbf{1}$ where only the translational part is replaced by a tensor. Θ denotes the pressure tensor, Λ_δ is a constant ensuring that the integral of $\tilde{G}[f]$ with respect to v and I is equal to the density ρ and R is the gas constant. The convex combination in θ takes into account that T_{tr} and T_{int} relaxes towards the common value T_{equ} . In the space-homogeneous case we see that we get the following macroscopic equations

$$\begin{aligned} \partial_t T_{tr} &= C(T_{tr}(1 - \theta) + \theta T_{equ} - T_{tr}) = C\theta(T_{equ} - T_{tr}), \\ \partial_t T_{int} &= C\theta(T_{equ} - T_{int}), \end{aligned}$$

with some coefficient C . These macroscopic equations describe a relaxation of T_{tr} and T_{int} towards T_{equ} .

In this paper, we took [6] as basis to extend it to mixtures. The main differences of the model in [3] and the model in [6] are the following. The model in [3] has one variable $I \in \mathbb{R}^+$ for all degrees of freedom in internal energy and the model in [6] has one variable $\eta \in \mathbb{R}^M$ to each degree of freedom in internal energy. Moreover, the relaxation of the translational and rotational/vibrational temperatures to a common value is done in [3] by introducing a relaxation temperature T_{rel} and in the model [6] it is done by the additional relaxation equation (3.13).

5 Applications

5.1 Chu reduction

In order to reduce the complexity of the variable for rotational and vibrational energy degrees of freedom μ_1, \dots, μ_{l_k} we apply the Chu reduction proposed in [9]. It is possible to apply the Chu reduction since $\eta_1, \dots, \eta_{l_k}$ do not appear in the transport operators in (3.11). We consider the system of equations

$$\begin{aligned} \partial_t f_1 + v \cdot \nabla_x f_1 &= \nu_{11} n_1 (G_1 - f_1) + \nu_{12} n_2 (M_{12} - f_1), \\ \partial_t f_2 + v \cdot \nabla_x f_2 &= \nu_{22} n_2 (G_2 - f_2) + \nu_{21} n_1 (M_{21} - f_2). \end{aligned} \tag{5.58}$$

Now, consider the reduced functions

$$g_1 = \int f_1 d\eta_{l_1}, \quad g_2 = \int f_2 d\eta_{l_2}.$$

Then they satisfy the equations

$$\begin{aligned} \partial_t g_1 + v \cdot \nabla_x g_1 &= \nu_{11} n_1 (\tilde{G}_1 - g_1) + \nu_{12} n_2 (\tilde{M}_{12} - g_1), \\ \partial_t g_2 + v \cdot \nabla_x g_2 &= \nu_{22} n_2 (\tilde{G}_2 - g_2) + \nu_{21} n_1 (\tilde{M}_{21} - g_2), \end{aligned} \tag{5.59}$$

where $\tilde{G}_1, \tilde{G}_2, \tilde{M}_{12}$ and \tilde{M}_{21} are given by

$$\tilde{G}_1 = \int G_1 d\eta_{l_1}, \quad \tilde{M}_{12} = \int M_{12} d\eta_{l_1}$$

$$\tilde{G}_2 = \int G_2 d\eta_{l_2}, \quad \tilde{M}_{21} = \int M_{21} d\eta_{l_2}.$$

It is possible to compute the densities

$$n_1 = \int \int f_1 d\eta_{l_1} dv = \int g_1 dv,$$

$$n_2 = \int \int f_2 d\eta_{l_2} dv = \int g_2 dv,$$

the velocities

$$u_1 = \int \int v f_1 d\eta_{l_1} dv = \int v g_1 dv,$$

$$u_2 = \int \int v f_2 d\eta_{l_2} dv = \int v g_2 dv,$$

the temperatures

$$\Lambda_1 = \frac{1}{n_1} \int |v - u_1|^2 f_1 d\eta_{l_1} dv = \frac{1}{n_1} \int |v - u_1|^2 g_1 dv,$$

$$\Lambda_2 = \frac{1}{n_2} \int |v - u_2|^2 g_2 dv,$$

$$\Theta_1 = \frac{1}{n_1} \int |\eta_{l_1}|^2 f_1 d\eta_{l_1} dv = \frac{1}{n_1} \int |\eta_{l_1}|^2 h_1 dv$$

$$\Theta_2 = \frac{1}{n_2} \int |\eta_{l_2}|^2 h_2 dv,$$

if we define the reduced functions

$$h_1 = \int |\eta_{l_1}|^2 f_1 d\eta_{l_1}, \quad h_2 = \int |\eta_{l_2}|^2 f_2 d\eta_{l_2},$$

which solve the equations

$$\begin{aligned} \partial_t h_1 + v \cdot \nabla_x h_1 &= \nu_{11} n_1 (\tilde{\tilde{G}}_1 - h_1) + \nu_{12} n_2 (\tilde{\tilde{M}}_{12} - h_1), \\ \partial_t h_2 + v \cdot \nabla_x h_2 &= \nu_{22} n_2 (\tilde{\tilde{G}}_2 - h_2) + \nu_{21} n_1 (\tilde{\tilde{M}}_{21} - h_2), \end{aligned} \tag{5.60}$$

where $\tilde{\tilde{G}}_1, \tilde{\tilde{G}}_2, \tilde{\tilde{M}}_{12}$ and $\tilde{\tilde{M}}_{21}$ are given by

$$\tilde{\tilde{G}}_1 = \int |\eta_{l_1}|^2 G_1 d\eta_{l_1}, \quad \tilde{\tilde{M}}_{12} = \int |\eta_{l_1}|^2 M_{12} d\eta,$$

$$\tilde{\tilde{G}}_2 = \int |\eta_{l_2}|^2 G_2 d\eta_{l_2}, \quad \tilde{\tilde{M}}_{21} = \int |\eta_{l_2}|^2 M_{21} d\eta_{l_2}.$$

If we compute $\tilde{G}_k, \tilde{M}_{12}, \tilde{M}_{21}, \tilde{\tilde{G}}_k, \tilde{\tilde{M}}_{12}, \tilde{\tilde{M}}_{21}$ for $k=1,2$, we get

$$\begin{aligned} \tilde{G}_k(x, v, t) &= \frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ES}}{m_k})}} \exp(-m_k(v - u_k) \cdot (\Lambda_k^{ES})^{-1} \cdot (v - u_k)), \quad k=1,2, \\ \tilde{M}_{12}(x, v, t) &= \frac{n_1}{\sqrt{2\pi \frac{\Lambda_{12}}{m_1}}} \exp(-\frac{|v - u_{12}|^2}{2 \frac{\Lambda_{12}}{m_1}}), \\ \tilde{M}_{21}(x, v, t) &= \frac{n_2}{\sqrt{2\pi \frac{\Lambda_{21}}{m_2}}} \exp(-\frac{|v - u_{21}|^2}{2 \frac{\Lambda_{21}}{m_2}}), \end{aligned} \tag{5.61}$$

$$\begin{aligned}
\widetilde{\widetilde{G}}_k(x, v, t) &= \frac{n_k}{\sqrt{\det(2\pi \frac{\Lambda_k^{ES}}{m_k})}} \exp(-m_k(v - u_k) \cdot (\Lambda_k^{ES})^{-1} \cdot (v - u_k)) \Theta_k, \quad k=1,2, \\
\widetilde{\widetilde{M}}_{12}(x, v, t) &= \frac{n_1}{\sqrt{2\pi \frac{\Lambda_{12}}{m_1}}} \exp(-\frac{|v - u_{12}|^2}{2 \frac{\Lambda_{12}}{m_1}}) \Theta_{12}, \\
\widetilde{\widetilde{M}}_{21}(x, v, t) &= \frac{n_2}{\sqrt{2\pi \frac{\Lambda_{21}}{m_2}}} \exp(-\frac{|v - u_{21}|^2}{2 \frac{\Lambda_{21}}{m_2}}) \Theta_{21},
\end{aligned} \tag{5.62}$$

We are able to compute all the six Maxwell distributions because we can compute all moments by the previous computation.

5.2 A mixture consisting of a mono and a diatomic gas

We consider now the special case of two species, one species is mono-atomic and has only translational degrees of freedom $l_1 = 0$, the other one is diatomic and has in addition two rotational degrees of freedom $l_2 = 2$ and both have the number of degrees of freedom in translations given by d with $d \in \mathbb{N}$. In this case the total number of rotational degrees of freedom is $M = l_1 + l_2 = 2$ since in sum we have two possible rotations. Our variables for the rotational energy degrees of freedom are $\eta \in \mathbb{R}^2$, $\eta_{l_1} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$, $\eta_{l_2} = \eta$, since η_k coincides with η in the components corresponding to the rotational degrees of freedom of species k and is zero in the other components. So our distribution function $f_1(x, v, t)$ of species 1 depends on x, v , and t and our distribution function $f_2(x, v, \eta, t)$ of species 2 depends on x, v, η and t . The moments of f_1 are given by

$$\int f_1(v) \begin{pmatrix} 1 \\ v \\ m_1 |v - u_1|^2 \\ m_1(v - u_1(x, t)) \otimes (v - u_1(x, t)) \end{pmatrix} dv =: \begin{pmatrix} n_1 \\ n_1 u_1 \\ dn_1 T_1^t \\ \mathbb{P}_1 \end{pmatrix} \tag{5.63}$$

and the moments of species 2 are given by

$$\int f_2(v, \eta) \begin{pmatrix} 1 \\ v \\ \eta \\ m_2 |v - u_2|^2 \\ m_2 |\eta|^2 \\ m_2(v - u_2(x, t)) \otimes (v - u_2(x, t)) \end{pmatrix} dv d\eta =: \begin{pmatrix} n_2 \\ n_2 u_2 \\ 0 \\ dn_2 T_2^t \\ l_2 n_2 T_k^r \\ \mathbb{P}_2 \end{pmatrix}. \tag{5.64}$$

The third equality is an assumption. We could also consider a general $\bar{\eta}$. Our model reduces to

$$\begin{aligned}
\partial_t f_1 + \nabla_x \cdot (v f_1) &= \nu_{11} n_1 (G_1(f_1) - f_1) + \nu_{12} n_2 (M_{12}(f_1, f_2) - f_1), \\
\partial_t f_2 + \nabla_x \cdot (v f_2) &= \nu_{22} n_2 (G_2(f_2) - f_2) + \nu_{21} n_1 (M_{21}(f_1, f_2) - f_2),
\end{aligned} \tag{5.65}$$

with the modified Maxwellians

$$\begin{aligned}
G_1(f_1)(x, v, t) &= \frac{n_1}{\sqrt{\det(2\pi \frac{\Lambda_1^{ES}}{m_1})}} \exp \left(-\frac{1}{2}(v - u_1) \cdot \left(\frac{\Lambda_1^{ES}}{m_1} \right)^{-1} \cdot (v - u_1) \right), \\
G_2(f_2)(x, v, \eta, t) &= \frac{n_2}{\sqrt{\det(2\pi \frac{\Lambda_2^{ES}}{m_2})}} \frac{1}{\sqrt{2\pi \frac{\Theta_2}{m_2} l_2}} \exp \left(-\frac{1}{2}(v - u_2) \cdot \left(\frac{\Lambda_2^{ES}}{m_2} \right)^{-1} \cdot (v - u_2) - \frac{1}{2} \frac{m_2 |\eta|^2}{\Theta_2} \right), \\
M_{12}(x, v, t) &= \frac{n_{12}}{\sqrt{2\pi \frac{\Lambda_{12}}{m_1} d}} \exp \left(-\frac{|v - u_{12}|^2}{2 \frac{\Lambda_{12}}{m_1}} \right), \\
M_{21}(x, v, \eta, t) &= \frac{n_{21}}{\sqrt{2\pi \frac{\Lambda_{21}}{m_2} d}} \frac{1}{\sqrt{2\pi \frac{\Theta_{21}}{m_2} l_2}} \exp \left(-\frac{|v - u_{21}|^2}{2 \frac{\Lambda_{21}}{m_2}} - \frac{|\eta|^2}{2 \frac{\Theta_{21}}{m_2}} \right),
\end{aligned} \tag{5.66}$$

where

$$\begin{aligned}
\Lambda_1^{ES} &= (1 - \mu_1) T_1^t \mathbf{1}_n + \mu_1 \frac{\mathbb{P}_1}{n_1}, \\
\Lambda_2^{ES} &= (1 - \mu_2) \Lambda_2 \mathbf{1}_n + \mu_2 \frac{\Lambda_2^{ten}}{n_2},
\end{aligned}$$

with $\mu_k \in \mathbb{R}$, $k = 1, 2$. For Λ_2^{ten} we use the additional relaxation equation

$$\partial_t \widehat{G}_2 + v \cdot \nabla_x \widehat{G}_2 = \frac{\nu_{22} n_2}{Z_r^2} \frac{d+2}{d} (\widetilde{G}_2 - \widehat{G}_2) + \nu_{22} n_2 (G_2 - f_2) + \nu_{21} n_1 (M_{21} - f_2), \tag{5.67}$$

Here \widehat{G}_2 is given by

$$\widehat{G}_2 = \frac{n_2}{\sqrt{\det(2\pi \frac{\Lambda_2^{ten}}{m_2})}} \exp \left(-\frac{1}{2}(v - u_2) \cdot \left(\frac{\Lambda_2^{ten}}{m_2} \right)^{-1} \cdot (v - u_2) - \frac{m_2 |\eta|^2}{2 T_2^r} \right), \quad k = 1, 2. \tag{5.68}$$

and \widetilde{G}_2 is given by

$$\widetilde{G}_2 = \frac{n_2}{\sqrt{\det(2\pi \frac{T_2^{ten}}{m_2})}} \frac{1}{\sqrt{2\pi \frac{T_2}{m_2}}} \exp \left(-\frac{1}{2}(v - u_2) \cdot \left(\frac{T_2^{ten}}{m_2} \right)^{-1} \cdot (v - u_2) - \frac{1}{2} \frac{m_2 |\eta|^2}{T_2} \right), \tag{5.69}$$

where the components of T_2^{ten} are defined in the following way.

$$\begin{aligned}
(T_2^{ten})_{ii} &= T_2 := \frac{d}{d+2} \Lambda_2 + \frac{2}{d+2} \Theta_2 & \text{for } i = 1, \dots, d, \\
(T_2^{ten})_{ij} &= \frac{d}{d+2} (\mathbb{P}_2)_{ij} & \text{for } i, j = 1, \dots, d, i \neq j,
\end{aligned} \tag{5.70}$$

We couple this with conservation of internal energy of species 2

$$\frac{d}{2} n_2 \Lambda_2 = \frac{d}{2} n_2 T_2^t + \frac{l_2}{2} n_2 T_2^r - \frac{l_2}{2} n_2 \Theta_2. \tag{5.71}$$

If we multiply (5.67) by $|\eta|^2$ and integrate with respect to v and η , this leads to the following macroscopic equation

$$\begin{aligned} \partial_t(\Lambda_2^{ten}) + u_2 \cdot \nabla_x(\Lambda_2^{ten}) &= \frac{\nu_{22}n_2}{Z_r^2} \frac{d+2}{d} (T_2^{ten} - \Lambda_2^{ten}) + \nu_{22}n_2(\Lambda_2^{ES} - \mathbb{P}_2) \\ &\quad + \nu_{21}n_1(\Theta_{12} - T_2^r). \end{aligned} \quad (5.72)$$

If we assume that

$$\begin{aligned} n_{12} &= n_1 \quad \text{and} \quad n_{21} = n_2, \\ u_{12} &= \delta u_1 + (1 - \delta)u_2, \quad \delta \in \mathbb{R}, \end{aligned}$$

and

$$\Lambda_{12} = \alpha T_1^t + (1 - \alpha)\Lambda_2 + \gamma|u_1 - u_2|^2, \quad 0 \leq \alpha \leq 1, \gamma \geq 0, \quad (5.73)$$

we have conservation of mass, total momentum and total energy provided that

$$u_{21} = u_2 - \frac{m_1}{m_2}\varepsilon(1 - \delta)(u_2 - u_1), \quad (5.74)$$

$$\begin{aligned} \Lambda_{21} + \frac{l_2}{d}\Theta_{21} &= \left[\frac{1}{d}\varepsilon m_1(1 - \delta) \left(\frac{m_1}{m_2}\varepsilon(\delta - 1) + \delta + 1 \right) - \varepsilon\gamma \right] |u_1 - u_2|^2 \\ &\quad + \varepsilon(1 - \alpha)T_1^t + (1 - \varepsilon(1 - \alpha))\Lambda_2 + \frac{l_2}{d}\Theta_2. \end{aligned} \quad (5.75)$$

We take into account the symmetry of the temperatures and choose

$$\begin{aligned} \Lambda_{21} &= \varepsilon(1 - \alpha)\Lambda_1 + (1 - \varepsilon(1 - \alpha))\Lambda_2 \\ &\quad + \left[\frac{1}{d}\varepsilon m_1(1 - \delta) \left(\frac{m_1}{m_2}\varepsilon(\delta - 1) + \delta + 1 \right) - \varepsilon\gamma \right] |u_1 - u_2|^2, \end{aligned} \quad (5.76)$$

$$\Theta_{21} = \Theta_2. \quad (5.77)$$

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