

An Ellipsoidal Statistical Model for a monoatomic and polyatomic gas mixture

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Abstract

This paper is devoted to the derivation of an Ellipsoidal Statistical model for a mixture constituted by both monoatomic and polyatomic gases. The non translational degrees of freedom are described by a continuous variable and each polyatomic component is allowed to have its own internal degrees of freedom. The construction of the model is based on the moment relaxed method that has been developed in previous works that is generalized in the present paper to a more general setting. More precisely, this method is based on the introduction of free parameters and on the resolution of an entropy minimisation problem. The resulting model satisfies conservation properties and a H theorem. Next, by performing a Chapman-Engskog expansion, the model is shown to recover the right heat transfer coefficient, the shear viscosity and the volume viscosity.

Key words: Kinetic theory, ESBGK model, Polyatomic gas mixture

Subject of classification: 35Q20, 35Q35

1 Introduction

In the context of atmospheric reentry, it is necessary to use kinetic models, because in high altitude the Knudsen number can be of order 1. However most of the kinetic models that have been constructed up to now have been developed only for a monoatomic single gas. But in the upper atmosphere the air is made of molecules like molecular oxygen (O_2) and molecular nitrogen (N_2) which are both diatomic. Moreover the atomic oxygen (O), the atomic nitrogen (N), and the diatomic nitrogen (NO) monoxide are also present. Therefore a kinetic description involving in the same time polyatomic and monoatomic gases is necessary. For this modelling, each polyatomic components are represented by a distribution function $f(t, x, v, I)$ depending on time t , space x , velocity v and on a continuous quantum number I ([1]). This last variable collects in particular vibrational and rotational modes. In ([15]), the authors proposed a Boltzmann like collision operator for a single polyatomic gas that is based on the Borgnakke-Larsen procedure ([14]). This means that in each binary interaction, a fraction of the ingoing total energy is attributed to the internal energy of the outgoing pair of molecules and then randomly distributed between the two single particles. This operator is shown to satisfy the right conservation laws and a H theorem. In [25], an existence theorem is proved for the nonlinear collision operator ([15]) in the space homogeneous case. Starting from this model, a compressible Euler system with a general internal energy law has been derived in ([20]) for a single gas. The generalisation of the collision operator in the context of a polyatomic reacting gas mixture has been performed in ([21]) together with the derivation of a compressible

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Euler system. In ([6]), a Navier-Stokes system has been rigorously constructed starting from a Boltzmann model in the context of a mixture of any monoatomic and any polyatomic components. In particular, in the case of Maxwellian and diatomic molecules explicit transport coefficients are computed. In ([4]), the authors derive a two temperature Navier-Stokes system for a polyatomic gas.

In some applications, the complicated Boltzmann collision operator has to be simplified into a BGK model. The principle is to replace the complicated integral operator by a relaxation model while keeping some important physical and mathematical properties: Maxwellian equilibrium states, conservation laws, H theorem. However in the mixture case, even for monoatomic gases, things are not clear. For example, the hydrodynamic limit is much more complicated to handle because there are several transport coefficients and interspecies phenomena like thermal diffusion have to be considered. There are mainly two families of BGK models for gas mixtures. The first type is based on a unique Maxwellian attractor per species ([2], [16]). The interactions between the particles are modelled by fictitious macroscopic quantities. In particular, in ([2]), these quantities are chosen in order to reproduce the same momentum and energy exchange terms per species like for Maxwell molecules. Moreover [2], is generalized to reactive gas mixtures in ([17], [11] [27]). So when the chemical reactions stop, the model derived in ([17], [11] [27]) correspond to ([2]). In ([40]), the Shakhov model and the ESBGK are improved by introducing fictitious macroscopic velocities in the model. The second type of BGK model is made by a sum of BGK models which reproduce the Boltzmann structure ([5], [13]). In particular, in ([29]), the authors propose a BGK model that is able to reproduce Coulombian cross-sections which is more appropriate for plasma physics applications.

In the present paper, we consider polyatomic gas mixtures. More precisely, we aim to derive from an entropy minimisation problem a BGK model that enables to recover in the same time the shear viscosity, the volume viscosity and the thermal conductivity coefficient for a mixture of any number monoatomic components and any number of polyatomic components. The question is crucial because in general the authors compute the hydrodynamic limit and eventually compare a posteriori with some existing models. So even if the structure of the fluxes is recovered, the values of the transport coefficients are not correct. By using this minimisation principle, an Ellipsoidal Statistical Model (ESBGK model) ([3], [34]), has been constructed in the monoatomic case in ([18]) and in the polyatomic case in ([19]) for a single gas. Next this technique has been transported to a monoatomic gas mixture ([16], [17]). In ([31]), the authors propose an ESBGK model for a binary polyatomic mixture. In ([36], [37], [41]), existence theorems are proved for the ESBGK model. Hence the main novelty of this paper is the rigorous construction of an Ellipsoidal Statistical Model for a monoatomic and polyatomic gas mixture.

The internal energy variable can also be discrete. For example, a first paper ([33]) incorporates discrete internal degrees of energy in a BGK model. These energies correspond in this model to a vibrational energy. Moreover, in ([26]), the hydrodynamic limit is studied up to Navier-Stokes system including chemical reactions by starting from a collisional model. In particular, transport coefficients are explicitly computed. Moreover, BGK models have also been derived ([7], [12], [38]) for discrete energy variable. In particular, in ([38]), a generalisation of ([17]) is performed to the polyatomic setting within the formalism of ([26]).

Concerning some applications of such models, we refer to ([24], [32]). In particular, in ([32]) the authors highlight different types of shock profiles that are specific to a polyatomic framework.

The paper is organised as follows. In section 2, the notations that are used in this paper are precised. In particular, hydrodynamic quantities are defined. In section 3, the ESBGK is

constructed by solving an entropy minimisation problem. The model is next shown to satisfy a H theorem and an indifferenciability principle. In section 4, a Chapman-Enskog expansion is performed for the present model and a compressible Navier-Stokes system is obtained. In this part, the relaxation coefficients are determined in order to fit the thermal conductivity coefficient, the shear viscosity and the volume viscosity. Some concluding remarks and perspectives are summarized in section 5.

2 Notations

In the present paper, we consider a mixture of A monoatomic components and B polyatomic components. For $i \in \{1, \dots, A\}$, $f_i(t, x, v_i, I_i)$ represents the distribution function of the i^{th} component where v_i and I_i are respectively the velocity and the continuous quantum number of the i^{th} species. The indexes of species are $S_m = \{1, \dots, A\}$ and $S_p = \{A + 1, \dots, A + B\}$. The sets of quantum numbers are

$$\begin{aligned} \mathcal{Q}_i &= \{0\} & \text{if } i \in S_m, \\ \mathcal{Q}_i &= [0, +\infty[& \text{if } i \in S_p \end{aligned}$$

and the associated integration measures dI_i are defined by

$$\begin{aligned} dI_i &= \delta_i & \text{if } i \in S_m, \\ dI_i &= m_+ & \text{if } i \in S_p, \end{aligned}$$

where δI_i is the Dirac distribution and m_+ the Lebesgue measure over \mathbb{R}_+ .

Next, we introduce for $i \in S$, δ_i as the number of internal degrees of freedom for species i . This parameter collects rotational and vibrational modes. For $i \in S_m$, $\delta_i = 0$ and we use the convention $f_i(t, x, v_i, 0) = f_i(t, x, v_i)$ in order to be consistent with the monospecies case. In this context, I_i^{2/δ_i} represents the internal energy of the i^{th} species.

Next, we recall the definition of macroscopic quantities:

The number density of species i (at time t and space x) is given by

$$n_i = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} f_i dv_i dI_i.$$

$n = \sum_{i \in S} n_i$ represents the total number density.

The mass density of species $i \in S$ (at time t and point x)

$$\rho_i = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i f_i dv_i dI_i,$$

where m_i represents the molecular mass of species i .

$\rho = \sum_{i \in S} m_i n_i$ represents the total mass density.

The momentum of species $i \in S$ (at time t and point x)

$$\rho_i u_i = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i v_i f_i dv_i dI_i.$$

$\rho u = \sum_{i \in S} \rho_i u_i$ represents the total momentum.

The total energy of species $i \in S$ (at time t and point x)

$$\rho_i e_i = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} (m_i |v_i - u|^2 + I_i^{2/\delta_i}) f_i dv_i dI_i.$$

Next, the macroscopic internal energy is splitted into a translational and an internal part. So we define the macroscopic translational energy of species $i \in S$ (at time t and point x)

$$\rho_i e_{i,tr} = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \frac{1}{2} m_i (v - u_i)^2 f_i dv_i dI_i, \quad i \in S.$$

The macroscopic internal energy of species $i \in S$ (at time t and point x) writes

$$\rho_i e_{i,int} = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} I_i^{2/\delta_i} f_i dv_i dI_i.$$

The total energy for the mixture reads

$$\rho e = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \left(\frac{1}{2} m_i (v_i - u)^2 + I_i^{2/\delta_i} \right) f_i dv_i dI_i = \rho e_{tr} + \rho e_{int}, \quad (2.1)$$

where

$$e_{tr} = \sum_{i \in S} c_i e_{i,tr}, \quad e_{int} = \sum_{i \in S} c_i e_{i,int}, \quad c_i = \frac{\rho_i}{\rho}. \quad (2.2)$$

e_{tr} represents the translational energy for the mixture and e_{int} represents the internal energy for the mixture.

We define δ as the number of internal degrees of freedom for the mixture

$$\delta = \sum_{i \in S} c_i \delta_i. \quad (2.3)$$

Temperatures are associated to each energy e , e_{tr} , e_{int} defined in (2.1, 2.2) by $e = \frac{3+\delta}{2} k_B T_{eq}$, $e_{tr} = \frac{3}{2} k_B T_{tr}$, $e_{int} = \frac{\delta}{2} k_B T_{int}$. Hence T_{eq} writes

$$T_{eq} = \frac{\frac{3}{2} T_{tr} + \frac{\delta}{2} T_{int}}{\frac{3}{2} + \frac{\delta}{2}}. \quad (2.4)$$

Moreover δ_i is related to $e_{i,int}$ by $e_{i,int} = \frac{\delta_i}{2} k_B T_{int}$. So, the relation (2.2) defining e_{int} in function of $e_{i,int}$ is consistent with the definition of δ given in (2.3)

Remark 1. In ([21], [6]), the authors use in kinetic models $\varphi_i f_i$ instead of f_i . In that case, $\varphi_i f_i$ represents the effective distribution function of species i . This means that in the definitions of macroscopic quantities, a weight measure φ_i appears. Moreover, in the Boltzmann operator the cross sections have to be modified accordingly into effective cross sections. We refer to ([6]) for more details and to ([22]) where a comparison of the two formalisms is presented.

Introduce the natural scalar product ([26])

$$\langle\langle\phi, \psi\rangle\rangle = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \phi_i \psi_i dv_i dI_i, \quad (2.5)$$

where ϕ and ψ are tensors. Consider the vector distribution function \mathbf{f} by

$$\mathbf{f} = (f_j)_{j \in S}.$$

and the family of polynomials $(\Psi^{\mathbf{l}})_{\mathbf{l} \in \mathbf{S}}$, Ψ^{mm} and Ψ^{en}

$$\Psi^{\mathbf{l}} = (\delta_{lj})_{j \in S}, \quad \mathbf{l} \in \mathbf{S}, \quad \Psi^{\text{mm}} = (m_j v_j)_{j \in S}, \quad \Psi^{\text{en}} = \left(\frac{1}{2} m_j |v_j - u_j|^2 + I_j^{2/\alpha_j}\right)_{j \in S}.$$

Then, according to the notation (2.5), the macroscopic quantities write

$$\rho_i = \langle\langle \mathbf{f}, \Psi^{\mathbf{l}} \rangle\rangle, \quad \rho u = \langle\langle \mathbf{f}, \Psi^{\text{mm}} \rangle\rangle, \quad \rho e = \langle\langle \mathbf{f}, \Psi^{\text{en}} \rangle\rangle$$

and the Boltzmann entropy is defined by

$$\mathcal{H}(\mathbf{f}) = \langle\langle \mathbf{f} \ln(\mathbf{f}) \rangle\rangle. \quad (2.6)$$

The stationary states $\mathcal{M} = (\mathcal{M}_i)_{i \in S}$ of the collision operator presented in ([6]) read

$$\mathcal{M}_i = \frac{n_i}{\mathcal{Q}_i^{\text{tr}} \mathcal{Q}_i^{\text{int}}} \exp\left(-\frac{m_i |v_i - u|^2 + 2I_i^{2/\delta_i}}{2k_B T}\right), \quad v_i \in \mathbb{R}^3, \quad I_i \in \mathcal{Q}_i, \quad i \in S \quad (2.7)$$

with

$$\mathcal{Q}_i^{\text{tr}} = \left(\frac{2\pi k_B T}{m_i}\right)^{\frac{3}{2}}, \quad \mathcal{Q}_i^{\text{int}} = \int_{\mathcal{Q}_i} \exp\left(-\frac{I_i^{2/\delta_i}}{k_B T}\right) dI_i. \quad (2.8)$$

3 Construction of an ESBGK model

The aim of this section is to construct an ESBGK model

$$\partial_t f_i + v \cdot \nabla_x f_i = \lambda(G_i - f_i), \quad i \in S,$$

where, the function G_i is constructed according to an entropy minimisation principle. The steps of the construction are the following. We firstly define the space of constraints (section 3.2), next the entropy minimisation problem is solved (section 3.3). Finally the model is shown to satisfy a H theorem (section 3.4) and an indiffereability principle (section 3.5)

3.1 Important families of polynomials

In this section, we define polynomials that will be involved in the definition of the space of constraints and in the computation of the hydrodynamic limit. Let us define

$$\Psi^{\text{pr}} = (\Psi_j^{\text{pr}})_{j \in S} = \left(m_j ((v_j - u) \otimes (v_j - u) - \frac{1}{3} |v_j - u|^2 I_d)\right)_{j \in S}, \quad (3.9)$$

where I_d represents the identity matrix on \mathbb{R}^3 ,

$$\begin{aligned}\Psi^{\text{int}} = (\Psi_j^{\text{int}})_{j \in S} &= \left(\frac{\delta}{\delta(3+\delta)} \frac{1}{2} m_j |v_j - u|^2 - \frac{2}{(3+\delta)} I_j^{2/\delta_j} \right)_{j \in S} \\ &= \left(\frac{1}{3} m_j |v_j - u|^2 - \frac{2}{(3+\delta)} \left(m_j \frac{|v_j - u|^2}{2} + I_j^{2/\delta_j} \right) \right)_{j \in S},\end{aligned}\quad (3.10)$$

$$\Psi^{\text{tr}} = (\Psi_j^{\text{tr}})_{j \in S} = \left(\frac{1}{2} m_j |v_j - u|^2 \right)_{j \in S}, \quad (3.11)$$

$$\Psi^\lambda = (\Psi_j^\lambda)_{j \in S} = \left(\left(m_j \frac{(v_j - u)^2}{2} - \frac{5}{2} k_B T + I_j^{\frac{2}{\delta_j}} - k_B T \frac{\delta_j}{2} \right) (v_j - u) \right)_{j \in S}. \quad (3.12)$$

For any $j \in S$,

$$\Psi^{\mathbf{D}j} = (\Psi_i^{\mathbf{D}j})_{i \in S} = \frac{1}{p_i} (\delta_{ij} - \frac{\rho_i}{\rho}) (v_i - u), \quad i \in S,$$

where $p_i = n_i k_B T$ represents the species partial pressure of the i^{th} species.

3.2 Space of constraints

We define now the set constraints, in order to prescribe some properties to the BGK operator that we aim to construct. The principle is to guarantee firstly the classical conservation properties (mass, total momentum, total energy). But also some supplementary moments have to be relaxed with a correct rate in order to recover correct transport coefficients. So, \mathbf{f} being given, $K(\mathbf{f})$ is defined as the set of functions $\mathbf{g} = (g_j)_{j \in S}$ s.t. $g_j \geq 0$ for $j \in S$ and satisfying the constraints

$$\langle \langle \mathbf{g} - \mathbf{f}, \Psi^{\mathbf{1}} \rangle \rangle = 0, \quad \mathbf{1} \in S \cup \{mm, en\}, \quad (3.13)$$

$$\lambda \langle \langle \mathbf{g} - \mathbf{f}, \Psi^{\mathbf{Pr}} \rangle \rangle = -\lambda_1 \langle \langle \mathbf{f}, \Psi^{\mathbf{Pr}} \rangle \rangle, \quad (3.14)$$

$$\lambda \langle \langle \mathbf{g} - \mathbf{f}, \Psi^{\text{int}} \rangle \rangle = -\lambda_2 \langle \langle \mathbf{f}, \Psi^{\text{int}} \rangle \rangle. \quad (3.15)$$

The constraints (3.13) impose the conservation of mass, momentum and total energy for the resulting model. The relation (3.14) has been introduced in ([18]) for a single monoatomic gas and generalised next ([19], [16]). This constraint means more precisely that the solution of the homogeneous BGK model tends to an isotropic distribution function as time tends to infinity. The constraint (3.15) implies that the distribution function tends to a distribution function whose translational and internal macroscopic temperatures are equal. This relation has been introduced in ([19]). Hence the constraints (3.14, 3.15) are consistent with the fact that the distribution function tends to the Maxwellian (2.7, 2.8) when time tends to infinity.

In order to solve a entropy minimisation problem, the constraints (3.14, 3.15) should be recast in a more convenient form. So, by using (3.13, 3.11, 3.10), it comes that

$$\langle \langle \mathbf{g} - \mathbf{f}, \Psi^{\text{int}} \rangle \rangle = \frac{2}{3} \langle \langle \mathbf{g} - \mathbf{f}, \Psi^{\text{tr}} \rangle \rangle$$

So, the equation (3.15) can be rewritten as

$$\frac{2}{3}\langle\langle\mathbf{g}, \Psi^{\text{tr}}\rangle\rangle = \frac{2}{3}\left(1 - \frac{\lambda_2}{\lambda}\right)\langle\langle\mathbf{f}, \Psi^{\text{tr}}\rangle\rangle + \frac{\lambda_2}{\lambda}\frac{2}{3+\delta}\langle\langle\mathbf{f}, \Psi^{\text{en}}\rangle\rangle.$$

Hence by using the definition e and e_{tr} given in (2.2, 2.1), the previous relation yields

$$\frac{2}{3}\langle\langle\mathbf{g}, \Psi^{\text{tr}}\rangle\rangle = \frac{2}{3}\left(1 - \frac{\lambda_2}{\lambda}\right)\rho e_{tr} + \frac{\lambda_2}{\lambda}\frac{2}{3+\delta}\rho e. \quad (3.16)$$

But as $e = \frac{3+\delta}{2}k_B T_{eq}$ and $e_{tr} = \frac{3}{2}k_B T_{tr}$ and by setting $\theta = \frac{\lambda_2}{\lambda}$, the relation (3.16) reads

$$\langle\langle\mathbf{g}, \Psi^{\text{tr}}\rangle\rangle = \frac{3}{2}(1 - \theta)\rho k_B T_{tr} + \frac{3}{2}\theta\rho k_B T_{eq}. \quad (3.17)$$

From the definition (3.9) of Ψ^{Pr} , the relation (3.14) gives

$$\sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i(v_i - u) \otimes (v_i - u) g_i dv_i dI_i = \frac{2}{3}\langle\langle\mathbf{g}, \Psi^{\text{tr}}\rangle\rangle I_d + \left(1 - \frac{\lambda_1}{\lambda}\right)\langle\langle\mathbf{f}, \Psi^{\text{Pr}}\rangle\rangle.$$

Moreover by setting

$$\frac{\lambda_1}{\lambda} = 1 - \nu(1 - \theta) \quad (3.18)$$

and by using the relation (3.17), we get

$$\langle\langle\mathbf{g}, \Psi^{\text{Pr}}\rangle\rangle = ((1 - \theta)\rho k_B T_{tr} + \theta\rho k_B T_{eq}) I_d + \nu(1 - \theta)\langle\langle\mathbf{f}, \Psi^{\text{tr}}\rangle\rangle.$$

Hence by using the relation

$$\langle\langle\mathbf{f}, \Psi^{\text{Pr}}\rangle\rangle = \rho\Theta,$$

where Θ represents the pressure tensor, we get the relation

$$\langle\langle\mathbf{g}, \Psi^{\text{Pr}}\rangle\rangle = \rho\mathcal{T}, \quad (3.19)$$

with

$$\mathcal{T} = (1 - \theta)[(1 - \nu)k_B T_{tr} I_d + \nu\Theta] + \theta k_B T_{eq} I_d. \quad (3.20)$$

Hence, $K(\mathbf{f})$ is constituted by distribution functions \mathbf{g} satisfying (3.13, 3.17, 3.19, 3.20). In the next steps of the paper, we will consider this version of $K(\mathbf{f})$.

3.3 Entropy minimisation problem

In this section we consider the variational problem

Find a solution to the minimisation problem

$$\mathbf{G} = \operatorname{argmin}_{\mathbf{g} \in K(\mathbf{f})} \mathcal{H}(\mathbf{g}), \quad (3.21)$$

where $K(\mathbf{f})$ is the set of function \mathbf{g} s.t $g_i \geq 0$ and s.t. the constraints (3.13, 3.17, 3.19, 3.20) are satisfied. We recall that \mathcal{H} is the Boltzmann entropy defined in (2.6).

Theorem 3.1. Let $\mathbf{f} = (f_j)_{j \in S}$, be a nonnegative function, $\nu \in [-1/2, 1[$, $\theta \in [0, 1]$. Then the tensor \mathcal{T} defined in (3.20) is symmetric positive definite and the minimization problem (3.21) admits a unique solution $\mathbf{G} = (G_j)_{j \in S}$, s.t.

$$G_i = \frac{n_i(k_B T)^{(3+\delta_i)/2}}{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{int} \sqrt{\det(\mathcal{T})(k_B T_{rel})^{\frac{\delta_i}{2}}}} \exp \left(-\frac{m_i}{2} \langle \mathcal{T}^{-1}(v_i - u), (v_i - u) \rangle - \frac{I_i^{\frac{\delta_i}{2}}}{k_B T_{rel}} \right), \quad i \in S \quad (3.22)$$

where

$$T_{rel} = \theta T_{eq} + (1 - \theta) T_{int}. \quad (3.23)$$

Proof. First of all, by arguing as in ([19]), we can show that $\mathcal{T} \in S_3^+(\mathbb{R})$ is equivalent to $\theta \in [0, 1]$ and $\nu \in [-1/2, 1[$. In ([3]) it is only proved that $\mathcal{T} \in S_3^+(\mathbb{R})$ implies that $\theta \in [0, 1]$ and $\nu \in [-1/2, 1[$. Moreover, in this proof, we follow the approach of Junk ([30]) that has been generalized to a mixture setting in ([28]). So, we proceed as in ([16], [17], [18], [19]). Let $v_{i,1}, v_{i,2}, v_{i,3}$ be the three components of v_i . Hence, we consider the set

$$\mathcal{L} = \{(\lambda_l)_{l \in S}, (\alpha_r)_{r \in \{1, \dots, 3\}}, (\beta_s)_{s \in \{1, \dots, 6\}}, \gamma, / \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \exp \left(\sum_{l \in S} \lambda_l \Psi_i^l + \sum_{r=1}^3 \alpha_r v_{i,r} + \sum_{s=1}^3 \beta_s v_{i,s}^2 + \beta_4 v_{i,1} v_{i,2} + \beta_5 v_{i,1} v_{i,3} + \beta_6 v_{i,2} v_{i,3} + \gamma I_i^{2/\delta_i} \right) dv_i dI_i < +\infty \}.$$

Let us show that \mathcal{L} is open by proceeding as in ([16]). Let $(\lambda_l)_{l \in S}, (\alpha_r)_{r \in \{1, \dots, 3\}}, (\beta_s)_{s \in \{1, \dots, 6\}}, \gamma \in \mathcal{L}$. In that case, $\gamma < 0$ and the signature of the quadratic form

$$q(v_i) = \beta_1 v_{i,1}^2 + \beta_2 v_{i,1}^2 + \beta_1 v_{i,3}^2 + \beta_4 v_{i,1} v_{i,2} + \beta_5 v_{i,1} v_{i,3} + \beta_6 v_{i,2} v_{i,3}$$

is (0, 3). Hence the Gauss reduction of the quadratic form writes

$$q(v_i) = \beta_1 \left(v_{i,1} + \frac{\beta_4}{2\beta_1} v_{i,2} + \frac{\beta_5}{2\beta_1} v_{i,3} \right)^2 + \alpha_1 \left(v_{i,2} + \frac{1}{2\alpha} \left(\beta_6 - \frac{\beta_4\beta_5}{2\beta_1} \right) v_{i,3} \right)^2 + \alpha_2 v_{i,3}^2,$$

with $\beta_1 < 0$, $\alpha_1 < 0$, $\alpha_2 < 0$ where

$$\alpha_1 = \beta_2 - \frac{\beta_4^2}{4\beta_1} \quad \alpha_2 = \beta_2 - \frac{\beta_5^2}{4\beta_1} + \frac{1}{4\alpha} \left(\beta_6 - \frac{\beta_4\beta_5}{2\beta_1} \right).$$

Therefore by proceeding in the same way, we can prove that for $\varepsilon > 0$ small enough, the signature of the quadratic form whose terms are $\beta_j + \varepsilon$ and $\beta_j - \varepsilon$ is still (0, 3). Moreover, ε can be chosen such as $\gamma + \varepsilon < 0$ and $\gamma - \varepsilon < 0$. So \mathcal{L} is open. Moreover, \mathcal{L} is non empty.

Hence according to ([28], [30]), the solution $\mathbf{G} = (G_i)_{i \in S}$ of the minimisation problem (3.21) reads

$$G_i = \alpha_i \exp(-m_i \langle v_i - u, \mathcal{A}(v_i - u) \rangle - a I_i^{\frac{\delta_i}{2}}), \quad i \in S,$$

where $\mathcal{A} \in \mathcal{M}_3(\mathbb{R})$, $\alpha_i \in \mathbb{R}$, $a \in \mathbb{R}$. Next we aim to determine these parameters.

By using constraint (3.13), we get

$$\alpha_i = \det(\mathcal{A})^{1/2} n_i \frac{(k_B T)^{(3+\delta_i)/2}}{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{int}} a^{\delta_i/2}, \quad i \in S. \quad (3.24)$$

A straightforward computation gives

$$\int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u) \otimes (v_i - u) G_i dv_i dI_i = \alpha_i \frac{1}{2} \mathcal{A}^{-1} \frac{1}{a^{\frac{\delta_i}{2}}} \frac{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{int}}{T^{(3+\delta_i)/2}} = \frac{1}{2} n_i \mathcal{A}^{-1}.$$

Hence by comparing the two previous expressions with the relations (3.19, 3.20) we get $\mathcal{A} = \frac{1}{2} \mathcal{T}^{-1}$. So (3.24) implies

$$\alpha_i = \frac{n_i}{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{int}} \frac{1}{\sqrt{\det(\mathcal{T})}} (k_B T)^{(3+\delta_i)/2} a^{\delta_i/2}, \quad i \in S.$$

By combining (3.13) and (3.16), it comes that

$$\frac{2}{3} \left(e - \sum_{i \in S} \alpha_i m_i \int_{\mathbb{R}^3 \times \mathcal{Q}_i} I_i^{\frac{2}{\delta_i}} \exp\left(-\frac{m_i}{2} \langle v - u, \mathcal{T}^{-1}(v - u) \rangle - a I_i^{\frac{2}{\delta_i}}\right) dv_i dI_i \right) = (1 - \theta) \frac{2}{3} \rho e_{tr} + \theta \rho e. \quad (3.25)$$

A straightforward computation gives that

$$\left(\sum_{i \in S} \int_{\mathcal{Q}_i} I_i^{\frac{2}{\delta_i}} \exp(-a I_i^{\frac{2}{\delta_i}}) dI_i \right) a^{\frac{\delta_i}{2}} T^{\frac{\delta_i}{2}} \rho_i \frac{1}{\mathcal{Q}_i^{int}} = \frac{1}{a} \sum_{i \in S} \frac{\delta_i}{2} \rho_i.$$

Hence the relation (3.25) gives

$$\frac{2}{3} \left(e - \frac{1}{a} \sum_{i \in S} \frac{\delta_i}{2} \frac{\rho_i}{\rho} \right) = (1 - \theta) \frac{2}{3} e_{tr} + \theta \frac{2}{3 + \delta} e.$$

So

$$\frac{1}{a} \frac{\delta}{3} = \frac{2}{3} e - (1 - \theta) \frac{2}{3} e_{tr} - \theta \frac{2}{3 + \delta} e.$$

By using that $e = e_{tr} + e_{int}$, we get

$$\frac{1}{a} \frac{\delta}{3} = \left(\frac{2}{3} - \frac{2}{3 + \delta} \right) \theta e + \frac{2}{3} (1 - \theta) e_{int}.$$

As $\frac{2}{3} - \frac{2}{3 + \delta} = \frac{2\delta}{3(3 + \delta)}$, the previous relation gives $a = \frac{1}{k_B T_{rel}}$ where T_{rel} has been defined in (3.23) and we recover that G_i is given by (3.22). \square

3.4 H theorem

Theorem 3.2. *For all $-\frac{1}{2} \leq \nu < 1$ and $\theta \in [0, 1]$, we denote by $G_i^{\nu, \theta}$ the expression of G_i given by (3.22) and by $\mathbf{G}^{\nu, \theta}$ the vector $\mathbf{G}^{\nu, \theta} = (G_i^{\nu, \theta})_{i \in S}$. Hence, the entropy dissipation satisfies*

$$D(\mathbf{f}) = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} (G_i^{\nu, \theta} - f_i) \ln(f_i) dv_i dI_i \leq 0.$$

Moreover $D(\mathbf{f}) \leq 0$ for $-\frac{1}{2} \leq \nu < 1$ and $0 \leq \theta \leq 1$ with equality iff $\mathbf{f} = \mathcal{M}$, where \mathcal{M} is given by (2.7).

Proof. By using the convexity of $x \ln(x)$, it holds that

$$\langle\langle \mathbf{G}^{\nu,\theta} - \mathbf{f}, \ln(\mathbf{f}) \rangle\rangle \leq \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} (G_i^{\nu,\theta} \ln(G_i^{\nu,\theta}) - f_i \ln(f_i)) dv_i dI_i.$$

By using the minimisation problem for $\nu = 1$ and $\theta = 0$, we get

$$\sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} G_i^{1,0} \ln(G_i^{1,0}) dv_i dI_i \leq \mathcal{H}(\mathbf{f}),$$

where we have used for $G_i^{1,0}$ the previous notation. So

$$\langle\langle \mathbf{G}^{\nu,\theta} - \mathbf{f}, \ln(\mathbf{f}) \rangle\rangle \leq \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \left(G_i^{\nu,\theta} \ln(G_i^{\nu,\theta}) - G_i^{1,0} \ln(G_i^{1,0}) \right) dv_i dI_i.$$

Moreover a straightforward computation gives ([3]),

$$\int_{\mathbb{R}^3 \times \mathcal{Q}_i} (G_i^{\nu,\theta} \ln(G_i^{\nu,\theta}) - G_i^{1,0} \ln(G_i^{1,0})) dv_i dI_i = \rho_i \ln \left(\frac{\rho_i}{\sqrt{(2\pi\mathcal{T})(k_B T_{rel})^{\frac{\delta_i}{2}}}} \right) - \frac{3}{2} \rho_i, \quad i \in S \quad (3.26)$$

we get

$$\langle\langle \mathbf{G}^{\nu,\theta} - \mathbf{f}, \ln(\mathbf{f}) \rangle\rangle \leq \frac{1}{2} \rho \ln \left(\frac{\det(\Theta) T_{int}^\delta}{\det(\mathcal{T}) T_{rel}^\delta} \right).$$

The end of the proof is inspired fom ([18]). Consider $\lambda_1, \lambda_2, \lambda_3$ the eigenvalues of Θ . Hence, we have to study the sign of

$$p(\nu, \theta) = \ln \left(\prod_{i=1}^3 \lambda_i T_{int}^\delta \right) - \ln \left(\det \left((1-\theta)((1-\nu)T_{tr}I_d + \nu\Theta) + \theta T_{eq}I_d \right) T_{rel}^\delta \right).$$

By using that $tr(\Theta) = 3T_{tr}$, the maximum of p is reached by $\lambda_1 = \lambda_2 = \lambda_3 = T_{tr}$. Then, we have to study the sign of

$$\begin{aligned} \ln((T_{tr})^3 T_{int}^{\frac{\delta}{2}}) - \ln \left(\left((1-\theta)T_{tr} + \theta T_{eq}I_d \right)^3 T_{rel}^\delta \right) &= 3 \ln(T_{tr}) + \delta \ln(T_{int}) \\ &\quad - 3 \ln((1-\theta)T_{tr} + \theta T_{eq}) - \delta \ln(T_{rel}). \end{aligned}$$

Then, by using the concavity of \ln , we get

$$\begin{aligned} &3 \ln(T_{tr}) + \delta \ln(T_{int}) - 3(1-\theta) \ln(T_{tr}) - 3\theta \ln(T_{eq}) - \delta \ln(T_{rel}) \\ &\leq 3 \ln(T_{tr}) + \delta \ln(T_{int}) - 3(1-\theta) \ln(T_{tr}) - 3\theta \ln(T_{eq}) - \delta \theta \ln(T_{eq}) - \delta(1-\theta)T_{int}. \end{aligned}$$

So,

$$\begin{aligned} &3 \ln(T_{tr}) + \delta \ln(T_{int}) - 3(1-\theta) \ln(T_{tr}) - 3\theta \ln(T_{eq}) - \delta \ln(T_{rel}) \\ &\leq 3\theta \ln(T_{tr}) + \delta \theta \ln(T_{int}) - \theta(3+\delta) \ln(T_{eq}). \end{aligned}$$

Therefore, by using the definition (2.4) of T_{eq} and the concavity of \ln , we get that the right-hand side of the previous inequality is negative.

When $D(\mathbf{f}) = 0$, from previously we get $\Theta = T_{tr}I_d$. Moreover, we obtain $\mathcal{H}(\mathbf{f}) = \mathcal{H}(\mathbf{G}^{1,0})$ and $\mathcal{H}(\mathbf{f}) = \mathcal{H}(\mathbf{G}^{\nu,\theta})$. By uniqueness of the minimisation problem, \mathbf{f} is the Gaussian distribution satisfying $\mathbf{f} = \mathbf{G}^{1,0}$. Hence from (3.26), we get $T_{int} = T_{rel}$. So $T_{int} = T_{tr} = T_{eq}$. So $\mathbf{f} = \mathcal{M}$, where \mathcal{M} is given by (2.7). \square

3.5 Indifferentiability principle

In this section, we show that our model satisfies the indifferentiability principle stated in ([2]) for an inert monoatomic gas mixture. This means that when all the molecular masses are equal, the distribution function that is obtained by adding all the species satisfies the single gas version of the present BGK model. In this paper, we aim to compare the present model with the single gas BGK models ([18], [19]).

If $S = S_m$, we consider a monoatomic mixture and we recover the model of ([16]). Therefore the distribution function $\mathbf{f} = \sum_{i \in S_m} f_i$ is solution of the Ellipsoidal Statistical Model for monospecies ([3], [18]).

In the case, where the mixture is purely polyatomic ($S = S_p$), the distribution function $\mathbf{f} = \sum_{i \in S_p} f_i$ is solution of the polyatomic Ellipsoidal Statistical Model for monospecies ([3], [19]) when all the molecular masses are equal.

4 Chapman-Enskog expansion

This section is devoted to the derivation of the Navier-Stokes system starting from the ESBGK model obtained in Theorem 3.1. More precisely, we consider the system

$$\partial_t f_i + v \cdot \nabla_x f_i = \frac{\lambda}{\tau} (G_i - f_i), \quad i \in S, \quad (4.27)$$

where τ is proportional to the Knudsen number. In this process, the relaxation coefficients λ , λ_1 and λ_2 are adjusted in order to fit the shear viscosity, the volume viscosity and the heat conductivity coefficient.

4.1 Euler system

Starting from (4.27), we can derive the compressible Euler system as in ([21]). Hence, we get

$$\partial_t \rho_i + \nabla \cdot (\rho_i u) = 0, \quad i \in S,$$

$$\partial_t (\rho u) + \nabla_x \cdot (\rho u \otimes u + p I_d) = 0,$$

$$\partial_t \left(\frac{1}{2} \rho u^2 + \mathcal{E} \right) + \nabla_x \cdot \left(u \left(\frac{1}{2} \rho u^2 + \mathcal{E} + p \right) \right) = 0,$$

where the internal energy \mathcal{E} per unit volume is defined by

$$\mathcal{E} = nk_B \left(\frac{3}{2} + \frac{\delta}{2} \right)$$

and $p = nk_B T$ represents the thermodynamic pressure.

The non conservative form of the Euler system writes

$$\partial_t n_i + (u \cdot \nabla) n_i + n_i \nabla \cdot u = 0, \quad i \in S,$$

$$\partial_t u + u \cdot \nabla u + \frac{\nabla p}{\rho} = 0,$$

$$\partial_t T + 2 \frac{\sum_{i \in S} n_i}{3 \sum_{i \in S} n_i + \sum_{i \in S} \delta_i n_i} T \nabla \cdot u + u \cdot \nabla T = 0.$$

4.2 Derivation of the Navier-Stokes Fourier system

4.2.1 Computation of the expansion

$\mathbf{f} = (f_i)_{i \in S}$ is expanded around a Maxwellian $\mathcal{M} = (\mathcal{M}_i)_{i \in S}$ as

$$f_i = \mathcal{M}_i + \tau \mathcal{M}_i f_i^1 + \mathcal{O}(\tau^2), \quad (4.28)$$

with

$$\langle \langle \mathcal{M} \mathbf{f}^1, \Psi^l \rangle \rangle = 0, \quad l \in S \cup \{\mathbf{mm}, \mathbf{en}\}. \quad (4.29)$$

Moreover G_i satisfies for any $i \in S$,

$$G_i = \mathcal{M}_i + \tau G_i^1 + \mathcal{O}(\tau^2), \quad (4.30)$$

with

$$G_i^1 = DG_i(\mathcal{M}) \cdot \mathcal{M} \mathbf{g} = \lim_{\tau \rightarrow 0} \frac{G_i(\mathcal{M} + \tau \mathcal{M} \mathbf{g}) - \mathcal{M}_i}{\tau}.$$

Moreover, it can be proved that $\mathbf{G}^1 = (G_i^1)_{i \in S}$ satisfies

$$\langle \langle \mathbf{G}^1, \Psi^l \rangle \rangle = \mathcal{O}(\tau), \quad l \in S \cup \{\mathbf{mm}, \mathbf{en}\}.$$

Introduce (4.28) into (4.27) leads to

$$f_i^1 = \frac{G_i^1}{\mathcal{M}_i} - \frac{1}{\lambda} (\partial_t \mathcal{M}_i + v \cdot \nabla_x \mathcal{M}_i) \frac{1}{\mathcal{M}_i} + \mathcal{O}(\tau). \quad (4.31)$$

A direct computation gives

$$\begin{aligned} \frac{1}{\mathcal{M}_i} (\partial_t \mathcal{M}_i + v \cdot \nabla_x \mathcal{M}_i) &= \sum_{j \in S} \Psi_i^{D_j} \cdot \nabla p_j + \frac{1}{k_B T} \Psi_i^{pr} : \nabla_x u + \Psi_i^\lambda \cdot \frac{\nabla T}{k_B T^2} \\ &+ \left(\frac{2}{k_B T} \Lambda \left(\frac{\delta_i}{2} k_B T - I_i^{\frac{2}{\delta_i}} \right) + \frac{2}{k_B T} \left(\frac{1}{3} - \Lambda \right) \left(m_i \frac{(v_i - u)^2}{2} - \frac{3}{2} k_B T \right) \right) \nabla \cdot u, \end{aligned} \quad (4.32)$$

with

$$\Lambda = \frac{\sum_{j \in S} n_j}{3 \sum_{j \in S} n_j + \sum_{j \in S} n_j \delta_j}.$$

Finally, by using (4.32) $\mathbf{f}^1 = (f_i^{(1)})_{i \in S}$ defined by (4.31) reads for $i \in S$

$$\begin{aligned} f_i^{(1)} &= \frac{G_i^1}{\mathcal{M}_i} - \frac{1}{\lambda} \left(\sum_{j \in S} \Psi_i^{D_j} \cdot \nabla p_j - \frac{1}{k_B T} \Psi_i^{pr} : \nabla_x u - \Psi_i^\lambda \cdot \frac{\nabla T}{k_B T^2} \right) \\ &- \left(2 \frac{\Lambda}{k_B T} (k_B T \frac{\delta_i}{2} - I_i^{\frac{\delta_i}{2}}) + \frac{2}{k_B T} (\frac{1}{3} - \Lambda) (m_i \frac{(v_i - u)^2}{2} - \frac{3}{2} k_B T) \right) \nabla \cdot u. \end{aligned} \quad (4.33)$$

4.2.2 Macroscopic equations and computation of the fluxes

In this section, the fluxes are computed and the relaxation parameters λ , λ_1 and λ_2 are fixed during the procedure.

By performing a Chapman-Engskog expansion we get

$$\begin{aligned} \partial \rho_i + \nabla \cdot (\rho_i u) + \nabla \cdot \mathbf{D}^{(i)} &= 0, \\ \partial_t (\rho u) + \nabla \cdot (\rho u \otimes u + p I_d) + \nabla \cdot \mathbf{\Pi} &= 0, \end{aligned}$$

$$\partial_t \left(\rho \frac{u^2}{2} + \mathcal{E} \right) + \nabla \cdot \left(\left(\rho \frac{u^2}{2} + \mathcal{E} + p \right) u \right) + \nabla \cdot \mathcal{Q} = 0,$$

where we have introduced the diffusion fluxes

$$\mathbf{D}^{(i)} = \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \mathcal{M}_i f_i^{(1)} m_i v_i dv_i dI_i, \quad i \in S,$$

where we have introduced the the pressure tensor

$$\mathbf{\Pi} = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i v_i \otimes v_i \mathcal{M}_i f_i^{(1)} dv_i dI_i,$$

the heat flux \mathcal{Q}

$$\mathcal{Q} = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \left(m_i \frac{v_i^2}{2} + I_i^{\frac{\delta_i}{2}} \right) v_i \mathcal{M}_i f_i^{(1)} dv_i dI_i.$$

As in ([26]), the diffusion velocity can be introduced as $\mathcal{V}_i = \frac{\mathbf{D}^{(i)}}{\rho_i}$. Hence using the expression (4.33) of $f_i^{(1)}$ and according to evenness properties

$$\begin{aligned} \mathbf{D}^{(i)} &= - \frac{\sqrt{k_B T}}{\lambda} \sum_{j \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \frac{n_i}{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{tr}} \exp \left(- m_i \frac{(v_i - u)^2 + 2 I_i^{2/\delta_i}}{2 k_B T} \right) \Psi_i^{D_j} \cdot \nabla p_j m_i (v_i - u) dv_i dI_i \\ &- \frac{1}{3} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i \frac{n_i}{\mathcal{Q}_i^{tr} \mathcal{Q}_i^{tr}} \exp \left(- \frac{m_i (v - u)^2 + 2 I_i^{2/\delta_i}}{2 k_B T} \right) (v_i - u) \Psi_i^\lambda \cdot \frac{\nabla T}{k_B T^2} dv_i dI_i. \end{aligned}$$

Moreover a direct computation gives

$$- \frac{1}{3} \int_{\mathbb{R}^3} m_i \frac{n_i}{\mathcal{Q}_i^{tr}} \exp \left(- m_i \frac{(v - u)^2}{2 k_B T} \right) \left(m_i \frac{(v_i - u)^2}{2} - \frac{5}{2} k_B T \right) (v_i - u)^2 dv_i = - \frac{n_i}{3} \left(\frac{15}{2} - \frac{15}{2} \right) = 0.$$

So, $\mathbf{D}^{(i)}$ writes

$$\mathbf{D}^{(i)} = -\frac{\sqrt{k_B T}}{\lambda p_i} \sum_{j \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i \frac{n_i}{\mathcal{Q}_i^{tr}} \exp\left(-m_i \frac{(v_i - u)^2}{2T}\right) \left(\delta_{ij} - \frac{m_j n_i}{\rho}\right) (v_i - u)^2 dv_i dI_i \nabla p_j.$$

So

$$\mathbf{D}^{(i)} = -\frac{\sqrt{k_B T}}{\lambda} n \sum_{j \in S} \left(\delta_{ij} - \frac{m_j n_i}{\rho}\right) \frac{\nabla p_j}{p}. \quad (4.34)$$

Then by comparison with [26], the species multicomponent diffusion coefficient D_{ij} for $i, j \in S$ reads

$$D_{ij} = \frac{\sqrt{k_B T} n}{\lambda} \sum_{j \in S} \left(\delta_{ij} - \frac{m_j n_i}{\rho}\right),$$

where λ will be fixed during the computation of κ .

Moreover, according to (4.34), the model gives a Soret effect that is equal to 0. Indeed, we can show that

$$\langle\langle \Psi^{\mathbf{D}_i}, \mathcal{M} \mathbf{f}^1 \rangle\rangle = \frac{1}{\rho_i} \mathbf{D}^{(i)}. \quad (4.35)$$

More precisely, formula (4.35) is obtained by developping $\langle\langle \Psi^{\mathbf{D}_i}, \mathcal{M} \mathbf{f}^1 \rangle\rangle$ as

$$\langle\langle \Psi^{\mathbf{D}_i}, \mathcal{M} \mathbf{f}^1 \rangle\rangle = \sum_{j \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_j} \frac{1}{p_j} \left(\delta_{ij} - \frac{\rho_j}{\rho}\right) (v_j - u) \mathcal{M}_j f_j^{(1)} dv_j dI_j.$$

So by using the orthogonality relation for the momentum (4.29), we get (4.35). Therefore,

$$\frac{1}{\rho_i} \mathbf{D}^{(i)} = \nu_i = \sum_{j \in S} D_{ij} \frac{\nabla p_j}{p} - \theta_i \frac{\nabla T}{T},$$

with

$$\theta_i = \frac{1}{3} \langle\langle \Psi^{\mathbf{D}_i}, \Psi^\lambda \mathcal{M} \rangle\rangle.$$

θ_i represents the thermal diffusion coefficient ([26]) and yields 0 in the present case. This term correspond to the Soret effect.

Next, by using the constraint (3.15) and the expansions (4.28, 4.30), it holds that

$$\sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v - u)^2 \lambda (G_i^1 - \mathcal{M}_i f_i^{(1)}) dv_i = -\lambda_2 \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \mathcal{M}_i f_i^{(1)} dv_i dI_i.$$

Moreover by using (4.31), it comes that

$$-\lambda_2 \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \mathcal{M}_i f_i^{(1)} dv_i dI_i = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} (\partial_t \mathcal{M}_i + v \cdot \nabla \mathcal{M}_i) m_i (v_i - u)^2 dv_i dI_i.$$

Hence from (4.32), it holds that

$$\begin{aligned}
& -\lambda_2 \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \mathcal{M}_i f_i^{(1)} dv_i dI_i \\
= & - \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \left(2\Lambda \left(\frac{\delta_i}{2} - \frac{I_i^{\frac{2}{\delta_i}}}{k_B T} \right) + 2 \left(\frac{1}{3} - \Lambda \right) \left(m_i \frac{(v_i - u)^2}{2k_B T} - \frac{3}{2} \right) \right) \mathcal{M}_i dv_i dI_i \nabla \cdot u.
\end{aligned}$$

A straightforward computation gives

$$\int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \left(\frac{\delta_i}{2} - \frac{I_i^{\frac{2}{\delta_i}}}{k_B T} \right) \mathcal{M}_i dv_i dI_i = 0,$$

and

$$\sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i \frac{(v_i - u)^2}{T} \left(m_i \frac{(v_i - u)^2}{2k_B T} - \frac{3}{2} \right) \mathcal{M}_i dv_i dI_i = 3 \sum_{i \in S} n_i.$$

So

$$-\lambda_2 \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u)^2 \mathcal{M}_i f_i^{(1)} dv_i dI_i = -6k_B T \sum_{i \in S} n_i \left(\frac{1}{3} - \Lambda \right) \nabla \cdot u.$$

Then by comparing with the viscous stress tensor, it holds that the second viscosity η satisfies

$$\eta = \frac{2}{\lambda_2} k_B T \sum_{i \in S} n_i \left(\frac{1}{3} - \Lambda \right) = \frac{2nk_B T}{\lambda_2} \left(\frac{1}{3} - \Lambda \right).$$

and can be adjusted from λ_2 . Due to orthogonality relations (4.29), $\mathbf{\Pi}$ reads

$$\mathbf{\Pi} = \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} m_i (v_i - u) \otimes (v_i - u) \mathcal{M}_i f_i^{(1)} dv_i dI_i.$$

Next, we insert the expansion (4.28) into the constraint (3.14). So

$$\langle \langle \mathbf{\Psi}^{\text{pr}}, \mathbf{G}^1 - \mathcal{M}\mathbf{f}^{(1)} \rangle \rangle = -\lambda_1 \langle \langle \mathbf{\Psi}^{\text{pr}}, \mathcal{M}\mathbf{f}^{(1)} \rangle \rangle.$$

Hence by using the relation (4.33) together with orthogonality relations, it comes that

$$\langle \langle \mathbf{\Psi}^{\text{pr}}, \mathcal{M}\mathbf{f}^{(1)} \rangle \rangle = -\frac{1}{\lambda_1} \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \Psi_i^{\text{pr}} : \Psi_i^{\text{pr}} \mathcal{M}_i dv_i dI_i \frac{1}{2} \left(\nabla u + \nabla u^t - \frac{2}{3} \nabla \cdot u \right).$$

So

$$\langle \langle \mathbf{\Psi}^{\text{pr}}, \mathcal{M}\mathbf{f}^{(1)} \rangle \rangle = -\frac{nk_B T}{\lambda_1} \frac{1}{2} \left(\nabla u + \nabla u^t - \frac{2}{3} \nabla \cdot u I_d \right).$$

Then the viscosity μ , satisfies $\mu = \frac{nk_B T}{\lambda_1}$ and can be adjusted from λ_1 .

Next, the heat flux writes

$$\mathcal{Q} = \mathbf{\Pi}u + \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \left(m_i \frac{(v_i - u)^2}{2} + I_i^{\frac{2}{\delta_i}} \right) (v_i - u) \mathcal{M}_i f_i^{(1)} dv_i dI_i.$$

Therefore, it comes that

$$\mathcal{Q} = \mathbf{\Pi}u + \langle\langle \Psi^\lambda, \mathcal{M}\mathbf{f}^{(1)} \rangle\rangle + \sum_{i \in S} k_B T \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \mathcal{M}_i f_i^{(1)} \left(\frac{5}{2} + \frac{\delta_i}{2} \right) (v_i - u) dv_i dI_i.$$

Hence by introducing the enthalpy $h_i = \left(\frac{5}{2}T + \frac{\delta_i}{2}T \right) \frac{k_B}{m_i}$ of i^{th} species, with the convention that $\delta_i = 0$ for $i \in S_m$, it holds that

$$\mathcal{Q} = \mathbf{\Pi}u + \langle\langle \Psi^\lambda, \mathcal{M}\mathbf{f}^{(1)} \rangle\rangle + \sum_{i \in S} h_i \mathbf{D}^{(i)}.$$

By using the expression of $\mathcal{M}_i f_i^{(1)}$ together with orthogonality properties, it holds that

$$\begin{aligned} \mathcal{Q} &= \mathbf{\Pi}u - \frac{1}{\lambda} \sum_{i \in S} \int_{\mathbb{R}^3 \times \mathcal{Q}_i} \sum_{j \in S} (\Psi_i^{D_j} \cdot \nabla p_j) \left(\frac{1}{2} m_i (v_i - u)^2 - \frac{5}{2} k_B T + I_i^{\frac{2}{\delta_i}} - \frac{\delta_i}{2} k_B T \right) (v_i - u) \mathcal{M}_i dv_i dI_i \\ &\quad - \frac{1}{3\lambda} \langle\langle \Psi^\lambda, \mathcal{M}\Psi^\lambda \rangle\rangle \frac{\nabla T}{k_B T^2} + \sum_{i \in S} h_i \mathbf{D}^{(i)}. \end{aligned}$$

Moreover, a direct computation gives

$$\langle\langle \Psi^\lambda, \mathcal{M}\Psi^\lambda \rangle\rangle = (k_B T)^3 \sum_{i \in S} \left(\frac{5}{2} + \frac{\delta_i}{2} \right) \frac{n_i}{m_i}.$$

So, the expression of \mathcal{Q} yields

$$\mathcal{Q} = \mathbf{\Pi}u - \frac{k_B^2 T}{\lambda} \sum_{i \in S} \left(\frac{5}{2} + \frac{\delta_i}{2} \right) \frac{n_i}{m_i} \nabla T + \sum_{i \in S} h_i \mathbf{D}^{(i)} - \frac{1}{3\lambda} \sum_{j \in S} \langle\langle \Psi^{D_j}, \Psi^\lambda \mathcal{M} \rangle\rangle \nabla p_j.$$

But, as $\langle\langle \Psi^{D_j}, \Psi^\lambda \mathcal{M} \rangle\rangle = 0$, \mathcal{Q} writes finally

$$\mathcal{Q} = \mathbf{\Pi}u - \frac{k_B^2 T}{\lambda} \sum_{i \in S} \left(\frac{5}{2} + \frac{\delta_i}{2} \right) \frac{n_i}{m_i} \nabla T + \sum_{i \in S} h_i \mathbf{D}^{(i)}. \quad (4.36)$$

So

$$\kappa = \frac{k_B^2 T}{\lambda} \sum_{i \in S} \left(\frac{5}{2} + \frac{\delta_i}{2} \right) \frac{n_i}{m_i}.$$

Hence, the heat conductivity coefficient can be obtained from λ . Moreover, the relation (4.36) implies that the Duffour effect yields 0 which is consistent with the fact that the Soret effect is equal to 0. This point comes from the fact that $\langle\langle \Psi^{D_j}, \Psi^\lambda \mathcal{M} \rangle\rangle = 0$.

4.3 Comparison with the Ellipsoidal Statistical Model

According to (3.18), λ satisfies the relation

$$\lambda = \frac{\lambda_1}{(1 - \nu + \theta\nu)} = \frac{nk_B T}{\mu(1 - \nu + \theta\nu)}$$

and the relaxation operator reads

$$\frac{nk_B T}{\mu(1-\nu+\theta\nu)}(G_i - f_i), \quad i \in S.$$

Therefore, we obtain a generalisation of the Ellipsoidal Statistical Model for a mixture of any monoatomic components and any polyatomic components.

Define the mixture enthalpy h by the relation ([26])

$$h = \sum_{i \in S} \frac{\rho_i}{\rho} h_i = \frac{1}{\rho} \sum_{i \in S} n_i k_B \left(\frac{5}{2} T + \frac{\delta_i}{2} T \right).$$

Hence, the constant pressure specific heat c_p reads ([1])

$$c_p = \frac{\partial}{\partial T} h = \sum_{i \in S} \frac{\rho_i}{\rho} h_i = \frac{1}{\rho} \sum_{i \in S} n_i k_B \left(\frac{5}{2} + \frac{\delta_i}{2} \right). \quad (4.37)$$

The Prandtl number can be defined by $Pr = \frac{c_p \mu}{\kappa}$. So by using the definition of μ , the definition (4.37) of c_p and the definition of λ , we obtain

$$Pr = \frac{n \lambda}{\rho \lambda_1} \frac{\sum_{i \in S} n_i \left(\frac{5}{2} + \frac{\delta_i}{2} \right)}{\sum_{i \in S} \frac{n_i}{m_i} \left(\frac{5}{2} + \frac{\delta_i}{2} \right)} = \frac{n}{\rho} \frac{\sum_{i \in S} n_i \left(\frac{5}{2} + \frac{\delta_i}{2} \right)}{\sum_{i \in S} \frac{n_i}{m_i} \left(\frac{5}{2} + \frac{\delta_i}{2} \right)} \frac{1}{(1-\nu+\theta\nu)}, \quad (4.38)$$

where $\theta \in [0, 1]$ and $\nu \in [-\frac{1}{2}, 1]$ is chosen according to Theorem 3.2.

We remark that in case of indifferentiability, when all the molecular masses are equal, the formula (4.38) reduces to

$$Pr = \frac{1}{(1-\nu+\theta\nu)}$$

as in ([3], [18]). For some comparisons with values of Prandtl number, we refer to ([22]).

5 Conclusion

We have built up an Ellipsoidal Statistical Model for a mixture of any component of monoatomic and polyatomic gases, where the non-translational degrees of freedom are modeled by a continuous variable. The construction is based on the resolution of an entropy minimisation problem under moments constraints and generalizes the papers ([18], [19], [17], [16]). The resulting model is made of a unique attractor and reproduces the correct equilibrium states of ([6]). Moreover, it is consistent with the correct conservation laws, recovers the H theorem and satisfies an indifferentiability principle. We have next developed a Chapman-Enskog expansion in the spirit of ([6]) and a Navier-Stokes system has been derived. The structure of the fluxes has been of course recovered. During the procedure, the free parameters have been fixed in order to fit the shear viscosity, the volume viscosity and the thermal heat conductivity.

As a perspective, we planned to design a BGK model for a mixture of any component of monoatomic and polyatomic gases in the spirit of ([17]) with a continuous non-translational energy variable. Moreover, we aim to generalise this work to discrete energies by proceeding like in ([38]). The case of fitting the Fick matrix in the context of a mixture of monoatomic and polyatomic components for a continuous energy variable is left in perspective.

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