AN ELLIPSOIDAL STATISTICAL MODEL FOR GAS MIXTURES

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Abstract. In this paper, we propose a construction of a new BGK model generalizing the Ellipsoidal Statistical Model ([2], [19]) to the context of gas mixtures. The derivation of the model is based on the introduction of relaxation coefficients associated to some moments and the resolution of a minimization problem as in ([7], [8], [10]). We obtain in this work, an ESBGK model for gas mixtures satisfying the fundamental properties of the Boltzmann collision operator (conservation laws, H theorem, equilibrium states, . . .) and that is able to give a range of Prandtl numbers including the indifferentiability situation.

Key words. Kinetic theory, gas mixtures, BGK models, moments systems

subject classifications 35Q20, 35Q35

1. Introduction   The complexity of the nonlinear Boltzmann operator suggests to introduce simpler kinetic models. Hence, the BGK model ([17]) which is a well known simplified kinetic relaxation model has been introduced. Its features are to replace the complicated integral of collisions by a relaxation model while keeping some important physical and mathematical properties of the interaction term (conservation laws, H theorem, equilibrium states, . . .). The interest of these models is that they are easier to handle numerically and less costly at a computational point of view. However the extension of the BGK model to multi-component gases meets fundamental difficulties. For example, the hydrodynamic limit is much more complicated since phenomena such as diffusion or thermal diffusion must be considered.

Many BGK models have been proposed up to now, but they are still unsatisfactory and have been constructed on the same manner. That is they must reproduce the rates of exchanges of impulsion and energy of the Boltzmann operator for Maxwell molecules between the different species. For example one polynomial model has been proposed in [13]. But its relaxation function being a polynom, the nonnegativity of the distribution function is not satisfied. However this model satisfies the indifferentiability principle stated in [13] inherited from the Boltzmann operator. That is when all the molecules have the same masses and their cross sections are equal, then the system of equations reduces to a single one by adding the distribution functions. A BGK model enjoying good mathematical properties has been derived in [1]. The main idea is to introduce only one BGK operator per species whose macrosopic parameters reproduce the interaction between each species with the others. But this model leads to uncorrect transport coefficients at the hydrodynamic limit ([21]). In [21], the authors constructed a BGK model which coincides with the Grad moments of the linearized Boltzmann operator. However the relaxation function of the model being polynomial, the nonnegativity of the distribution function is not sure.

Hence the aim of this paper is to construct a BGK model that is able to recover correct transport coefficients and enjoying good mathematical properties. The question is important because in general the authors compute the hydrodynamic limit from their own model and eventually compare with the correct fluid model ([18]). In the situation of single and monospecies a BGK model leading to the correct Prandtl number has been proposed in ([19]). This model is called Ellipsoidal Statistical Model (ESBGK). But the proof of the H theorem has been shown later on ([2]). Recently,

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a new approach of such a model has been proposed in ([7]) based on the an entropy minimization principle ([22], [23], [20]). The philosophy of the derivation consists in defining different relaxation rates associated to some moments of the distribution function. These rates intuitively describe the way in which these moments vanish for the trend to equilibrium. For example, defining a relaxation rate on the viscous stress tensor allows to reproduce viscosity and heat flux. Generally, the moment that is dissipated is considered with respect to the polynomial function that is involved in the computation of the corresponding transport coefficient that we aim to fit. In ([8]), this approach has been generalized to the polyatomic context to propose a new construction of the Ellipsoidal Statistical Model ([2]). In that case, another constraint of equalization of translational and internal temperature allows to fit simultaneously shear viscosity, volume viscosity and heat flux. In the context of gas mixtures, things are more complicated. Indeed, there are more transport coefficients, that is the Fick, Soret, Dufour, Fourier and Newton coefficients (see 4.6). In ([10]), this method has been considered for gas mixtures by deriving a BGK model that is able to recover the correct Fick law. In this situation, several relaxation parameters are involved and are shown to be directly related to the non zero eigenvalues of the diffusion part of the Onsager matrix. Moreover even if Soret, Dufour and Fourier coefficients are not correct, the structure of the fluxes is recovered. In ([9]), this model has been generalized the slow chemistry framework where the mechanical process dominates the chemical one. The BGK model is then defined as a splitting between the mechanical model of ([10]) and the chemical one constructed in ([14]). Next a Navier-Stokes system is constructed for the weak reaction regime from a Chapman-Enskog procedure and the Fick matrix is shown to be recovered by the model.

The present paper is organized as follows. In section 2, we clarify some notations and recall some backgrounds about the Boltzmann operator for gas mixtures. The third section is devoted to the construction and the fundamental properties of the ESBGK model for gas mixtures. Firstly, we introduce the set of constraints. Next, we solve a minimization problem under moments constraints and we prove that the resulting model satisfies a H theorem and the indifferentiability principle. In section 4, we perform a Chapman-Enskog expansion up to Navier-Stokes level. At this step, the two relaxation coefficients are computed in order to get an exact viscosity and an exact heat flux. Finally section 5 deals with a conclusion and perspectives to this work.

2. Notations and some backgrounds about kinetic equations for gas mixtures

2.1. Boltzmann equation for gas mixtures

In this paper, we consider a gas mixtures with p components. This mixture can be describded at the kinetic level by its distribution function $\mathbf{f} = (f_1, \ldots, f_p)$, where $f_i(t, x, v)$ represents the distribution function of the species i. Here, t corresponds to the time variable, x to the space variable and v to the velocity variable. The distribution function for the mixture evolves according to the Boltzmann equation for a p component gas

$$\forall i \in [1, p], \ \partial_t f_i + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_i = \sum_{k=1}^{k=p} Q_{ki}(f_k, f_i) := Q_i(\mathbf{f}, \mathbf{f}), \qquad (2.1)$$

where

$$Q_{ki}(f_k, f_i) = \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left(f_k(\mathbf{w}_{ki}^*) f_i(\mathbf{v}_{ki}^*) - f_k(\mathbf{w}) f_i(\mathbf{v}) \right) \sigma_{ik}(\boldsymbol{\omega}.\mathbf{V}, \|\mathbf{V}\|) \|\mathbf{V}\| \, d\mathbf{w} d\boldsymbol{\omega}.$$

Here Q_{ki} is the Boltzmann collision operator between molecules of species i and k and $\sigma_{ik} = \sigma_{ki}$ is the differential cross section which depend on the interaction potential between species i and k. Finally $\mathbf{V} = \mathbf{w} - \mathbf{v}$ is the relative velocity. The post collisional velocities are given by

$$\mathbf{v}_{ki}^* = \mathbf{v} - 2\frac{m_k}{m_i + m_k}\left((\mathbf{v} - \mathbf{w}) \cdot \boldsymbol{\omega}\right)\boldsymbol{\omega}, \quad \mathbf{w}_{ki}^* = \mathbf{w} + 2\frac{m_i}{m_i + m_k}\left((\mathbf{v} - \mathbf{w}) \cdot \boldsymbol{\omega}\right)\boldsymbol{\omega}.$$

Those equations satisfy the conservation of momentum and energy at a microscopic level

$$m_i\mathbf{v} + m_k\mathbf{w} = m_i\mathbf{v}_{ki}^* + m_k\mathbf{w}_{ki}^*, \quad m_i\left\|\mathbf{v}\right\|^2 + m_k\left\|\mathbf{w}\right\|^2 = m_i\left\|\mathbf{v}_{ki}^*\right\|^2 + m_k\left\|\mathbf{v}_{ki}^*\right\|^2.$$

2.2. Macroscopic quantities   We denote with n^i, ρ^i, u^i, E^i, T^i and E^i the macroscopic quantities representing respectively the number density, density, average velocity, energy per unit volume, energy per particle and finally temperature of a given species i. They are defined by the following relations

$$n^i = \int_{\mathbb{R}^3} f_i\,dv, \ \rho^i = m_in^i, \ n^i\mathbf{u}^i = \int_{\mathbb{R}^3} v\,f_i\,dv, \ E^i = \frac{1}{2}\rho^i(\mathbf{u}^i)^2 + n^i\mathcal{E}^i,$$

$$\mathcal{E}^i = \frac{3}{2}k_BT^i = \frac{m_i}{2n^i}\int_{\mathbb{R}^3}(v - \mathbf{u}^i)^2\,f_i\,dv,$$

where m_i represents the molecular mass of the species i and k_B is the Boltzmann constant. In the same way, we define the hydrodynamic quantities for the mixture

$$n = \sum_{k=1}^{p} n^k, \quad \rho = \sum_{k=1}^{p} \rho^k, \quad \rho\mathbf{u} = \sum_{k=1}^{p} \rho^k\mathbf{u}^k, \quad n\mathcal{E} + \frac{\rho}{2}\mathbf{u}^2 = E = \sum_{k=1}^{p} E^k, \quad \mathcal{E} = \frac{3}{2}k_BT.$$

n^i, $\mathbf{u}$ et T being given, we define the Maxwellian distribution functions as

$$\forall i \in [1, p], \ \mathcal{M}_i = \frac{n^i}{(2\pi k_BT/m_i)^{\frac{3}{2}}}\exp(-\frac{m_i(v - \mathbf{u})^2}{2k_BT}).$$

The entropy associated to the distribution function $\mathbf{f}$ of the mixture is defined by

$$\mathcal{H}(\mathbf{f}) = \sum_{i=1}^{p}\int_{\mathbb{R}^3}(f_i\ln(f_i) - f_i)\,dv. \tag{2.2}$$

2.3. Other considerations.   Using the above notations we note as $\mathbb{L}^2\left(\mathcal{M}\right)$ the set of measurable functions $\boldsymbol{\Psi} = (\psi_1, \cdots, \psi_p)$ such that:

$$\left\|\boldsymbol{\Psi}\right\|^2 := \sum_{i=1}^{i=p}\int_{\mathbb{R}^3}\psi_i^2\mathcal{M}_i < +\infty.$$

This space is equipped using its natural dot product:

$$\langle\boldsymbol{\Psi}, \boldsymbol{\Phi}\rangle = \sum_{i=1}^{i=p}\int_{\mathbb{R}^3}\psi_i\phi_i\mathcal{M}_i\,dv.$$

In the sequel we often use the dot product notation. This notation is valid both for list of p scalar functions and for p tensorial functions. For instance if $\boldsymbol{\Psi}, \boldsymbol{\Phi}$ are two lists

of p (symmetrical) tensorial functions $\psi_i, \phi_i, i \in [1, p]$, then the dot product notation $\langle \psi, \phi \rangle$ should be understood as

$$\langle \psi, \phi \rangle := \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \psi_i \otimes \phi_i \mathcal{M}_i d\mathbf{v},$$

where $\otimes$ denotes the usual tensorial product. Note also the following convention: assume that $\mathbf{V}$ is a list of p vectors and $\mathbf{T}$ a list of p square matrixes. Then a notation like $\alpha \mathbf{V}, \alpha \mathbf{T}$ (where α is a scalar) means that the scalar α is distributed on each line of the list of vectors or matrix. Besides if $\boldsymbol{\beta}$ is a vector, then a notation like $\boldsymbol{\beta} \cdot \mathbf{V}$ means that we distribute the dot product by $\boldsymbol{\beta}$ on each line of the vector $\mathbf{V}$. The same way, if $\boldsymbol{\gamma}$ is a square matrix, then a notation like $\boldsymbol{\gamma} : \mathbf{T}$ means that we distribute the (total) dot product (between matrix) by $\boldsymbol{\gamma}$ on each line of the line of $\mathbf{T}$. Finally, if $\mathbf{s}$ is a tensor and $\mathbf{S}$ a list of p tensors, then a notation like $\mathbf{s} \otimes \mathbf{S}$ means that we distribute the tensor product by $\mathbf{s}$ on the left on each line of the list $\mathbf{S}$.

DEFINITION 2.1. *The set $\mathbb{K}$ belonging to $\mathbb{L}^2(\mathcal{M})$ of the collision invariants of the Boltzmann operator (2.1) is spanned by the following list of functions:*

$$\begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \cdots, \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{pmatrix}, \begin{pmatrix} m_1 v_x \\ m_2 v_x \\ \vdots \\ m_p v_x \end{pmatrix}, \begin{pmatrix} m_1 v_y \\ m_2 v_y \\ \vdots \\ m_p v_y \end{pmatrix}, \begin{pmatrix} m_1 v_z \\ m_2 v_z \\ \vdots \\ m_p v_z \end{pmatrix}, \begin{pmatrix} m_1 \boldsymbol{v}^2 \\ m_2 \boldsymbol{v}^2 \\ \vdots \\ m_p \boldsymbol{v}^2 \end{pmatrix}. \quad (2.3)$$

This space is of dimension $p + 4$. We denote by $\boldsymbol{\phi}^l, l \in [1, p+4]$ the list of these $p+4$ elements. Contrarily to the case of monatomic gas there exists a space $\mathbb{C}$ of moments of degree 1 in velocity which is not conserved. This space is defined as follows

DEFINITION 2.2. *Let $\boldsymbol{C}_i$ be the vector whose i^{th} component is $\boldsymbol{v} - \boldsymbol{u}$ and others are 0. Denote by $\mathcal{P}_{\mathbb{K}}$ the orthogonal projection on $\mathbb{K}$ and $\mathcal{I}$ the identity operator. Then we define $\mathbb{C}$ as the space generated by the vectors $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\boldsymbol{C}_i), i \in [1, p]$.* In ([10]), we have shown the following lemma which exhibits a basis of $\mathbb{C}$.

LEMMA 2.3. *The family $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(\boldsymbol{C}_i), i \in [1, p]$ is composed of $p - 1$ independant "vectors" and as a consequence the dimension of $\mathbb{C}$ is $3(p-1)$.* For the Chapman-Enskog procedure, introduce the Sonine polynomials $\mathbb{A}$ and $\mathbf{B}$ whose i^{th} component write

$$\mathbb{A}_i = m_i \left(v \otimes v - \frac{1}{3} v^2 Id \right), \quad B_i = (v - \mathbf{u}) \left(\frac{1}{2} m_i (v - \mathbf{u})^2 - \frac{5}{2} k_B T \right). \quad (2.4)$$

3. Construction and properties of the model

3.1. Fundamental properties of kinetic operators As in ([1], [10]), the BGK model $\mathcal{R}(\mathbf{f})$ constructed in this paper consists in one operator per species as

$$\mathcal{R}(\mathbf{f}) = (\mathcal{R}_1(\mathbf{f}), \ldots, \mathcal{R}_p(\mathbf{f})). \quad (3.1)$$

We present now the fundamental properties coming from the Boltzmann operator for gas mixtures that our BGK model has to satisfy.

1. **Collisional invariants**

$$\forall \mathbf{f}, f_i \geq 0, \forall \boldsymbol{\phi}, \ \sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i(\mathbf{f}) \phi_i d\mathbf{v} = 0 \Leftrightarrow \boldsymbol{\phi} \in \mathbb{K}. \quad (3.2)$$

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2. **H-theorem:** for any list of nonnegative functions $\mathbf{f} = (f_1, \ldots, f_p)$ there holds

$$\sum_{i=1}^{i=p} \int_{\mathbb{R}^3} \mathcal{R}_i\left(\mathbf{f}\right) \ln\left(f_i\right) d\mathbf{v} \leq 0. \tag{3.3}$$

3. **Equilibrium states:** the equality holds in the above equation if and only if $\mathbf{f}$ is at thermodynamic equilibrium i.e there exists macroscopic values $n_1, \ldots, n_p$, $\mathbf{u}$, T such that

$$\forall i \in [1, p], f_i = \mathcal{M}_i.$$

In such a case we denote $\mathbf{f} = \mathcal{M}$. Moreover $\mathcal{M}$ is the only set of functions such that

$$\mathcal{R}_i\left(\mathbf{f}\right) = 0. \tag{3.4}$$

3.2. Space of constraints $\mathbf{f}$ being given, $\mathbf{G}$ is researched as the solution of an entropy minimisation problem under moments constraints. The space of constraints that is used in this paper is given in the following definition.

DEFINITION 3.1. *The space of constraints* $\mathbf{K}(\mathbf{f})$ *associated to* $\mathbf{f}$, *is defined by the set of functions* $\mathbf{g} = (g_1, \ldots, g_p)$ *s.t.* $\mathbf{g} \geq 0$ *a.e. satisfying*

$$\forall l \in \{1, p+4\}, \ \sum_{i=1}^{p} \int_{\mathbb{R}^3} \phi_i^l\left(g_i - f_i\right) dv = 0 \tag{3.5}$$

to obtain the conservation properties and the relaxation constraint

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} \lambda(g_i - f_i) \, \mathbb{A}_i(v - \mathbf{u}) \, dv = -\lambda_1 \sum_{i=1}^{p} \int_{\mathbb{R}^3} f_i \, \mathbb{A}_i(v - \mathbf{u}) \, dv, \tag{3.6}$$

where $\lambda > 0$ *and* $\lambda_1 > 0$ *are free parameters that are devoted to fit the transport coefficients. Like in ([7], [8], [10]), they are fixed during the Chapman-Enskog procedure. The constraint (3.6) can be rewritten as*

$$\frac{1}{\rho} \sum_{i=1}^{p} \int_{\mathbb{R}^3} m_i \, g_i \left(v - \mathbf{u}\right) \otimes \left(v - \mathbf{u}\right) dv = (1 - \frac{\lambda_1}{\lambda})\Theta + \frac{\lambda_1}{\lambda} T, \tag{3.7}$$

where Θ *represents the pressure tensor defined by*

$$\Theta = \sum_{i=1}^{p} \int_{\mathbb{R}^3} m_i(v - \mathbf{u}) \otimes (v - \mathbf{u}) \, f_i \, dv. \tag{3.8}$$

In order to compare our model with the one derived in ([2], [7]), we use the change of variable: $\nu = 1 - \frac{\lambda_1}{\lambda}$. *So the constraint (3.7) on* $\mathbf{g}$ *can be rewritten*

$$\frac{1}{\rho} \sum_{i=1}^{p} \int_{\mathbb{R}^3} m_i \, g_i \left(v - \mathbf{u}\right) \otimes \left(v - \mathbf{u}\right) dv = \nu\Theta + (1 - \nu)T = \tau. \tag{3.9}$$

REMARK 1. *In ([10]), the relaxation constraints (3.6) are written on a basis of* $\mathbb{C}$ *instead of the Sonine polynomials (2.4). This basis is obtained from the diagonalization of the diffusion part of the Onsager matrix.*

THEOREM 3.2. *For any nonnegative function* $\mathbf{f} = (f_1, \ldots, f_p)$ *and* $\nu \in [-\frac{1}{2}, 1[$, *the tensor* τ *defined by (3.9) is symetric defined positif and the minimization entropy problem*

$$\mathbf{G} = \min_{\mathbf{g} \in \mathbf{K}(\mathbf{f})} \mathcal{H}(\mathbf{g}) \tag{3.10}$$

has a unique solution $\mathbf{G} = (G_1, \ldots, G_p)$ *where* G_i *writes*

$$G_i = \frac{\rho_i}{\sqrt{2\pi \, det(\tau)}} \exp\left(-\frac{1}{2}\langle v - \mathbf{u}, \tau^{-1}(v - \mathbf{u})\rangle\right). \tag{3.11}$$

Conversely, if the minimization problem (3.10) has a unique solution for any nonnegative function $\mathbf{f} \in L_1^2$, *then* $\nu \in [-\frac{1}{2}, 1[$.

Proof. To prove the existence of the distribution function (3.11), we have to solve a minimization problem under moments constraints. As in ([10]), we follow the methodology of Junk ([20]). Hence we consider the set

$$\Lambda = \{(\alpha_l)_l, \, (\lambda_r)_r \, /$$

$$\int \exp\left(\sum_{l=1}^{p+3} \alpha_l \phi_i^l + \lambda_1 v_1^2 + \lambda_2 v_2^2 + \lambda_3 v_3^2 + \lambda_4 v_1 v_2 + \lambda_5 v_1 v_2 + \lambda_6 v_2 v_3\right) < +\infty\}. \tag{3.12}$$

If this set is open, then the minimization problem has a unique solution as soon as $\mathbf{K}(\mathbf{f}) \neq \emptyset$. This last condition is fullfilled because $\mathbf{G}$ defined by (3.11) belongs to $\mathbf{K}(\mathbf{f})$. Hence it remains to show that (3.12) is open. Proving this assertion is equivalent to show that the signature of the quadratic form

$$q(v) = \lambda_1 v_1^2 + \lambda_2 v_2^2 + \lambda_3 v_3^2 + \lambda_4 v_1 v_2 + \lambda_5 v_1 v_2 + \lambda_6 v_2 v_3 \tag{3.13}$$

is $(0, 3)$. Introducing the matrix associated to the quadratic form q, $M = (m_{ij})_{ij}$, the Gauss reduction of q (3.13) writes

$$q(v) = m_{11}(v_1 + \frac{m_{12}}{m_{11}}v_2 + \frac{m_{13}}{m_{11}}v_3)^2 + \alpha(v_2 + \frac{1}{\alpha}(m_{23} - \frac{m_{13}}{m_{11}})v_3)^2 + \gamma v_3^2,$$
$$m_{11} < 0, \ \alpha < 0, \ \gamma < 0, \tag{3.14}$$

where

$$\alpha = m_{22} - \frac{m_{12}^2}{m_{11}}, \quad \gamma = m_{33} - \frac{m_{13}^2}{m_{11}} - \frac{1}{\alpha}(m_{23} - \frac{m_{12}m_{13}}{m_{11}})^2.$$

Hence for $\varepsilon > 0$ small enough, we can show that the signatures of the quadratic form associated to the matrix whose terms are $m_{ij} + \varepsilon$ and $m_{ij} - \varepsilon$ is $(0, 3)$. This means that the set (3.12) is open.

The proof of the second part of the theorem is analogous to the one given in the monospecies setting. So we refer to ([7]) for more details. $\square$

3.3. H Theorem   In this section, we show that the present BGK model is entropic for $-\frac{1}{2} \leq \nu < 1$.

THEOREM 3.3. *For* $-\frac{1}{2} \leq \nu < 1$ *and* G_i *defined by (3.11), we have the following entropy dissipation property*

$$D(\mathbf{f}) = \sum_{i=1}^{p} (G_i - f_i) \ln(f_i) \, dv \leq 0.$$

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Moreover, $D(\mathbf{f}) \leq 0$ for $-\frac{1}{2} \leq \nu < 1$ with equality iff $f_i = \mathcal{M}_i$, $i = \{1, \ldots, p\}$.

Proof. The proof is similar to the one given in ([7]) but adapted to a gas mixture framework. For the sake of clarity, we give the proof in details. By using the convexity of $x \mapsto x \ln(x) - x$, we get that

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} (G_{i,\nu} - f_i) \ln f_i \, dv \leq \mathcal{H}(\mathbf{G}_\nu) - \mathcal{H}(\mathbf{f}),$$

where $G_{i,\nu}$ is the function defined in (3.11) and ν represents its dependance *w.r.t* $\nu \in [-\frac{1}{2}, 1[$. Moreover, $\mathbf{G}_{\mathbf{1}-\varepsilon}$ being the result of a minimization problem under constraints of f, $\mathcal{H}(\mathbf{G}_{\mathbf{1}-\varepsilon}) \leq \mathcal{H}(\mathbf{f})$. So

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} (G_{i,\nu} - f_i) \ln f_i \, dv \leq \mathcal{H}(\mathbf{G}_\nu) - \mathcal{H}(\mathbf{G}_{\mathbf{1}-\varepsilon}).$$

But a direct computation of $\mathcal{H}(\mathbf{G}_\nu)$ gives

$$\mathcal{H}(\mathbf{G}_\nu) = \sum_{i=1}^{p} \rho_i \ln\left(\frac{\rho_i}{\sqrt{2\pi \, det\mathcal{T}}}\right) - \frac{5}{2}\rho.$$

Moreover the set of constraints that is used for the definition of $\mathbf{G}_\nu$ are linear, the application $\nu \mapsto G_{i,\nu}$ is convex. So to obtain the entropy dissipation property, it is enough to show that $\mathcal{H}(\mathbf{G}_\nu) \leq \mathcal{H}(\mathbf{G}_{\mathbf{1}-\varepsilon})$.

$$\mathcal{H}(\mathbf{G}_\nu) - \mathcal{H}(\mathbf{G}_{\mathbf{1}-\varepsilon}) = \frac{1}{2}\rho\left(\ln(det((1-\varepsilon)\,\Theta + \varepsilon T \, Id)) - \ln(det(\nu\Theta + (1-\nu)T \, Id))\right).$$

But this term has the same sign as

$$p(\nu) = det((1-\varepsilon)\,\Theta + \varepsilon T \, Id) - det(\nu\Theta + (1-\nu)T \, Id).$$

$p(\nu)$ can be rewritten as

$$p(\nu) = \left(\prod_{i=1}^{3}(\theta_i + \varepsilon(T - \theta_i)) + \prod_{i=1}^{3}(\nu(T - \theta_i) - T)\right).$$

Hence by setting $\tilde{\theta}_i = \theta_i/T$, we get

$$p(\nu) = T^3\left(\prod_{i=1}^{3}(\tilde{\theta}_i + \varepsilon(1 - \tilde{\theta}_i)) + \prod_{i=1}^{3}(\nu(1 - \tilde{\theta}_i) - 1)\right).$$

Then

$$p(-\frac{1}{2}) = \left(\prod_{i=1}^{3}(\tilde{\theta}_i + \varepsilon(1 - \tilde{\theta}_i)) + \prod_{i=1}^{3}(-\frac{1}{2}(1 - \tilde{\theta}_i) - 1)\right).$$

Therefore after some computations

$$p(-\frac{1}{2}) = \frac{3T^3}{8}\left(3(\tilde{\theta}_1\tilde{\theta}_2\tilde{\theta}_3 - \tilde{\theta}_1\tilde{\theta}_2 - \tilde{\theta}_1\tilde{\theta}_3 - \tilde{\theta}_2\tilde{\theta}_3)\right) + \varepsilon l(\tilde{\theta}_1, \tilde{\theta}_2, \tilde{\theta}_3)$$

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with

$$l(\tilde{\theta}_1, \tilde{\theta}_2, \tilde{\theta}_3) = (1 - \tilde{\theta}_1)\tilde{\theta}_2\tilde{\theta}_3 + \tilde{\theta}_1(1 - \tilde{\theta}_2)\tilde{\theta}_3 + \tilde{\theta}_1\tilde{\theta}_2(1 - \tilde{\theta}_3)$$
$$+ \varepsilon((1 - \tilde{\theta}_1)(1 - \tilde{\theta}_2)\tilde{\theta}_3 + (1 - \tilde{\theta}_1)\tilde{\theta}_2(1 - \tilde{\theta}_3) + \tilde{\theta}_1(1 - \tilde{\theta}_2)(1 - \tilde{\theta}_3))$$
$$+ \varepsilon^2(1 - \tilde{\theta}_1)(1 - \tilde{\theta}_2)(1 - \tilde{\theta}_3).$$

By using Lagrange multipliers, we get that the maximum of $p(-\frac{1}{2})$ is obtained for $\tilde{\theta}_1 = \tilde{\theta}_2 = \tilde{\theta}_3 = 1$ and yields $p(-\frac{1}{2}) = 0$. $\square$

3.4. Indifferentiability condition   In this section, we prove that our model satisfies the indifferentiability property stated in [13] and recalled in introduction.

PROPOSITION 3.4.   *If all the molecular masses are equal ($\forall\, i \in \{1; p\}$, $m_i = m$),*

then the distribution function $\mathbf{f} = \displaystyle\sum_{i=1}^{p} f_i$ *is solution of the Ellipsoidal Statistical Model*

for monospecies ([2], [7]). Hence the model satisfies the indifferentiability principle. The proof is trivial and performed by adding term by term each component of kinetic equations.

4. Chapman-Enskog expansion

4.1. The Navier-Stokes system for gas mixtures   The Navier-Stokes system for a mixture of p components reads

$$\forall i \in [1, p]\,, \ \partial_t n^i + \nabla \cdot (n^i \mathbf{u} + \mathbf{J}_i) = 0, \tag{4.1}$$

$$\partial_t(\rho\,\mathbf{u}) + \nabla \cdot (\mathbb{P} + \rho\,\mathbf{u} \otimes \mathbf{u} + \mathbb{J}_{\mathbf{u}}) = 0, \tag{4.2}$$

$$\partial_t E + \nabla \cdot (E\mathbf{u} + \mathbb{P}\,[\mathbf{u}] + \mathbb{J}_{\mathbf{u}}\,[\mathbf{u}] + \mathbf{J}_q) = 0, \tag{4.3}$$

where $\mathbf{J}_i$, $\mathbb{J}_{\mathbf{u}}$ $\mathbf{J}_{\mathbf{q}}$ are respectively the mass, momentum and heat fluxes. These fluxes can be expressed either from thermodynamics of irreversible process (TIP) ([12]) or from the phenomenological point of view. Of course these two approaches are strictly equivalent according to the definition of the chemical potential (4.5). As it has been explained in ([10]), the Chapman-Enskog procedure leads naturally to fluxes defined from TIP assumption whereas coefficients appearing in phenomenological approach are obtained from experiments.

We firstly describe the transport coefficients obtained from the TIP point of view. In this case, mass, impulsion and energy fluxes write

$$\begin{array}{rcll} \mathbf{J}_i & = & \sum_{j=1}^{j=p} L_{ij}\nabla\left(\frac{-\mu_j}{T}\right) & + \ L_{i\mathbf{q}}\nabla\left(\frac{1}{T}\right), \\[2mm] \mathbf{J}_{\mathbf{q}} & = & \sum_{j=1}^{j=p} L_{\mathbf{q}j}\nabla\left(\frac{-\mu_j}{T}\right) & + \ L_{\mathbf{q}\mathbf{q}}\nabla\left(\frac{1}{T}\right), \\[2mm] \mathbb{J}_{\mathbf{u}} & = & & L_{\mathbf{u}\mathbf{u}}\mathbb{D}\left(\mathbf{u}\right), \end{array} \tag{4.4}$$

where

$$\mathbb{D}(\mathbf{u}) = \frac{1}{2}\left(\nabla\mathbf{u} + (\nabla\mathbf{u})^T\right) - \frac{1}{3}(\nabla \cdot \mathbf{u})\mathbb{I}$$

represents the Reynolds tensor and

$$-\frac{\mu_i}{T} = k_B\left(\ln\left(n^i\right) - \frac{3}{2}\ln\left(\frac{2\pi k_B T}{m_i}\right)\right) \tag{4.5}$$

is the chemical potential.

By using the phenomenological approach, mass and impulsion fluxes write w.r.t densities and temperature gradients as

$$\mathbf{J}_i = \sum_{j=1}^{j=p} D_{ij}\nabla n_j + D_{iT}\nabla T, \quad \mathbf{J_q} = \sum_{j=1}^{j=p} D_{\mathbf{q}j}\nabla n_j - D_{\mathbf{qq}}\nabla T, \tag{4.6}$$

where D_{ij} and D_{iT}, $D_{\mathbf{q}j}$ and $D_{\mathbf{qq}}$ respectively denote the Fick, Soret, Duffour and Fourier coefficients.

(4.4) and (4.6) are shown to be equivalent by plugging the expression (4.5) of $-\frac{\mu_i}{T}$ into (4.4).

4.2. Computation of the relaxation coefficients λ and λ_1 We determine now the coefficients λ and λ_1 in such a way that the Chapman-Enskog expansion up to order one leads to the true viscosity and the true heat flux. That is the ones that have been computed from the Boltzmann equation or that have been obtain experimentally.

Hence we consider the system of kinetic equations

$$\partial_t f_i + v \cdot \nabla f_i = \frac{\lambda}{\varepsilon}(G_i - f_i), \quad i \in \{1,\dots,p\}, \tag{4.7}$$

where ε is proportional to the Knudsen number. For each component i, the distribution function f_i is expanded according to $f_i = \mathcal{M}_i + \varepsilon f_i^{(1)} + \dots$.

For more details on Chapman-Enskog expansion for gas mixtures, we refer to ([11], [10]). According to ([10]), the fluxes write

$$\mathbf{J}_i = \langle \mathbf{f^{(1)}}, \mathbf{C_i}\rangle, \quad \mathbf{J_q} = \langle \mathbf{f^{(1)}}, \mathbf{B}\rangle, \quad \mathbb{J}_\mathbf{u} = \langle \mathbf{f^{(1)}}, \mathbb{A}\rangle. \tag{4.8}$$

From (4.7), $\mathbf{G}$ which depends on $\mathbf{f}$ is expanded around the Maxwellian distribution $\mathcal{M}$ according to

$$\mathbf{G} = \mathcal{M} + \varepsilon\mathbf{G}^{(1)} + \dots.$$

Using that $G_i(\mathcal{M}) = \mathcal{M}_i$, the expression of $G_i^{(1)}$ is given by

$$G_i^{(1)} = DG_i(\mathcal{M}).f_i^{(1)} = \lim_{\tau \to 0} \frac{G_i(\mathcal{M} + \tau\mathbf{f}^1) - \mathcal{M}_i}{\tau}. \tag{4.9}$$

So the order 0 in (4.7) leads to

$$\partial_t\mathcal{M} + v \cdot \nabla\mathcal{M} = \lambda(\mathbf{G}^{(1)} - \mathbf{f}^{(1)}). \tag{4.10}$$

But, from ([10]), we get the relation

$$(\partial_t + v.\nabla)\mathcal{M} = \Big(\sum_{j=1}^{p} k_B^{-1}(\mathcal{I} - \mathcal{P}_\mathbb{K})(C_j).\nabla(-\frac{\mu_j}{k_BT}) + \frac{1}{k_BT}\mathbb{A} : \mathbb{D}(\mathbf{u})$$

$$+ \frac{1}{k_B}\mathbf{B}.\frac{\nabla T}{T^2}\Big)\mathcal{M}, \tag{4.11}$$

the Sonine polynomial $\mathbf{B}$ has been defined in (2.4). Therefore $\mathbf{f}^{(1)}$ has the following expression

$$\mathbf{f}^{(1)} = \mathbf{G}^{(1)} - \Big(\sum_{j=1}^{p} k_B^{-1}(\mathcal{I} - \mathcal{P}_\mathbb{K})(C_j).\nabla(-\frac{\mu_j}{k_BT}) + \frac{1}{k_BT}\mathbb{A} : \mathbb{D}(\mathbf{u}) + \frac{1}{k_B}\mathbf{B}.\frac{\nabla T}{T^2}\Big)\mathcal{M}.$$

$$\tag{4.12}$$

Relation (3.6) considered at order 1 for $\mathbf{g} = \mathbf{G}$ leads to

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} \lambda (G_i^{(1)} - f_i^{(1)}) \, \mathbb{A}_i(v - \mathbf{u}) \, dv = -\lambda_1 \sum_{i=1}^{p} \int_{\mathbb{R}^3} f_i^{(1)} \, \mathbb{A}_i(v - \mathbf{u}) \, dv.$$

From orthogonality reasons, it comes that

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} f_i^{(1)} \, \mathbb{A}_i(v - \mathbf{u}) \, dv = -\frac{1}{k_B T \lambda_1} \sum_{i=1}^{p} \int_{\mathbb{R}^3} \mathbb{A}_i(v - \mathbf{u}) : \mathbb{A}_i(v - \mathbf{u}) \mathcal{M}_i \, dv \, \mathbb{D}(\mathbf{u})$$

$$= -\frac{n k_B T}{\lambda_1} \mathbb{D}(\mathbf{u}).$$

So we define λ_1 as $\lambda_1 = \frac{n k_B T}{\mu}$. By setting

$$\lambda = \frac{\lambda_1}{1 - \nu} = \frac{\rho T}{\mu(1 - \nu)}, \tag{4.13}$$

we get the relaxation operator (3.1)

$$\mathcal{R}_i(\mathbf{f}) = \frac{\rho T}{\mu(1 - \nu)} (G_i - f_i), \ i \in \{1, \dots, p\}.$$

In order to determine the heat flux, we use (4.8). Multiply (4.10) by $\mathbf{B}(v - \mathbf{u})$ and integrate. From relation (4.9) defining $\mathbf{G}^{(1)}$, we can show that

$$\int_{\mathbb{R}^3} \mathbf{G}^{(1)} \, \mathbf{B}(v - \mathbf{u}) \, dv = 0.$$

By using the orthogonality of $\mathbf{B}$ w.r.t. $\mathbb{A}$ and $(\mathcal{I} - \mathcal{P}_{\mathbb{K}})(C_j)$, it holds that

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} B_i(v - \mathbf{u}) f_i^{(1)} \, dv = -\frac{1}{3k_B \lambda} \sum_{i=1}^{p} \left(\int_{\mathbb{R}^3} B_i(v - \mathbf{u}) . B_i(v - \mathbf{u}) \mathcal{M}_i \, dv \right) \frac{\nabla T}{T^2}.$$

A direct computation gives

$$\sum_{i=1}^{p} \int_{\mathbb{R}^3} B_i(v - \mathbf{u}) . B_i(v - \mathbf{u}) \mathcal{M}_i \, dv = \frac{15}{2} k_B^3 T^3 \sum_{i=1}^{p} \frac{n^i}{m_i}.$$

Hence, from (4.4) the heat flux $L_{\mathbf{qq}}$ has the following expression

$$L_{\mathbf{qq}} = \frac{5}{2\lambda} k_B^2 T^3 \sum_{i=1}^{p} \frac{n^i}{m_i}. \tag{4.14}$$

In order to compare the model constructed in the present paper, with the monospecies model derived in ([7]), we set $\kappa = \frac{L_{\mathbf{qq}}}{T^2}$. Hence, Prandtl number writes

$$Pr = \frac{5}{2} \frac{R\mu}{\kappa} = R \frac{\lambda}{\lambda_1} \frac{n}{k_B \sum_{i=1}^{p} \frac{n^i}{m_i}}.$$

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Therefore by using the definition (4.13) of the relaxation coefficient λ and $R = k_B/m$, we get

$$Pr = \frac{R}{1-\nu} \frac{n}{k_B \sum\limits_{i=1}^{p} \dfrac{n^i}{m_i}} = \frac{1}{1-\nu} \frac{1}{\sum\limits_{i=1}^{p} \dfrac{n^i}{n} \dfrac{m}{m_i}}, \qquad (4.15)$$

where

$$m = \sum_{i=1}^{p} \frac{n^i}{n} m_i$$

represents the molecular mass of the mixture. Hence the present model is able to reach Prandtl numbers in the range

$$\left[\frac{2}{3} \frac{1}{\sum\limits_{i} \dfrac{n^i}{n} \dfrac{m}{m_i}}, +\infty\right[. \qquad (4.16)$$

Therefore for any Prandtl number in the interval (4.16), the relation (4.15) uniquely determines the coefficient λ from the value of ν.

For example, in indifferentiability situation, the relation (4.15) becomes as in ([2], [7]), $Pr = 1/(1-\nu)$. Hence $Pr = 2/3$ is obtained for $\nu = -1/2$ and this totally determines λ.

Next the other transport coefficients are computed. Their values are not correct, but the shape of the fluxes is recovered. In property 1, we collect the values of all the transport coefficients.

PROPERTY 1. *The transport coefficients are given by*

$$L_{ij} = \frac{3Tn^i}{k_B \, m_i} \delta_{ij}, \qquad L_{i\mathbf{q}} = L_{\mathbf{q}i} = 0, \qquad L_{\mathbf{q}\mathbf{q}} = \frac{5}{2\lambda} k_B^2 T^3 \sum_{i=1}^{p} \frac{n^i}{m_i}, \qquad L_{\mathbf{u}\mathbf{u}} = -\mu.$$

Proof. According to Chapmann-Enskog expansion, mass flux writes $\mathbf{J}_i = \langle \mathbf{f}^{(1)}, \mathbf{C_i} \rangle$, █ where $\mathbf{f}^{(1)}$ is computed from (4.12). But, we have $\langle \mathbb{A}, \mathbf{C}_i \rangle = 0$, $\langle \mathbb{B}, \mathbf{C}_i \rangle = 0$. Then $L_{iq} = L_{qi} = 0$ and

$$L_{ij} = -\frac{1}{k_B} \int_{\mathbb{R}^3} \mathbf{C}_i.\mathbf{C}_j \, \mathcal{M}_i \, dv = -\frac{1}{k_B} \int_{\mathbb{R}^3} (\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_i).(\mathcal{I} - \mathcal{P}_{\mathbb{K}}) (\mathbf{C}_j) \, \mathcal{M}_i \, dv.$$

So the expression of L_{ij} follows. $\square$

5. Conclusion and perspectives In this paper, we have introduced an Ellipsoidal Statistical Model for gas mixtures following the moments relaxation method introduced in ([7], [8], [10]). The resulting model fullfills two important features. Firstly, it enjoys the fundamental properties of the Boltzmann operator (H theorem, nonnegativity of the distribution function, conservation laws, indifferentiability condition, ...) which is only satisfied by few models ([1]). Moreover, its construction is based on the right hydrodynamic coefficients and the model is able to reach a certain rage of Prandl numbers. This range includes the correct Prandtl number in the situation of indifferentiability condition.

For concrete application, this methodology should be generalized to the situation of polyatomic gases in order to fit Prandtl number. Hence the following step of this work should be the derivation of an Ellipsoidal Statistical Model for polyatomic gas mixtures. For example the atmosphere can be considered as a binary mixture of Oxygen and Nitrogen. In that case, the distribution function depends on an additional continous variable, the internal energy ([5]), collecting rotational, vibrational, translational energy and belonging to $\mathbb{R}_+$. In ([8]), we have derived from the methodology described in this paper an ESBGK model for a polyatomic single gas. So by taking advantage of this work, we plan to generalize this construction to a gas mixture framework. Before this, the Chapman-Enskog expansion for polyatomic gas mixtures has to be clarified. This work is postponed to a future paper.

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