Mesoscopic Boltzmann model equations for thermally perfect gases

J. Mathiaud[1], L. Mieussens[2]

[1]Centre Lasers Intenses et Applications, Université de Bordeaux-CNRS-CEA,UMR 5107, F-33400 Talence, France. (`julien.mathiaud@u-bordeaux.fr`)

[2]Univ. Bordeaux, Bordeaux INP, CNRS, IMB, UMR 5251, F-33400 Talence, France. (`Luc.Mieussens@math.u-bordeaux.fr`)

Abstract

We propose a way to derive Bhatnagar-Gross-Krook and Fokker-Planck models of the Boltzmann equation for rarefied flows of thermally perfect gases. These models can allow for various internal energies (rotation, vibration, electronic), which is required for high temperature flows, like in atmospheric reentry problems. However, our models do not contain any internal degrees of freedom: instead, they are accounted for by a mesoscopic approach. The molecular velocity is the only kinetic variable in the models, that makes their computational complexity similar to that of simple monoatomic gases. Moreover, we prove that these models satisfy conservation and entropy properties (H-theorem), and we derive their corresponding compressible Euler and Navier-Stokes asymptotics. gases.

Keywords: Fokker-Planck model, Bhatnagar-Gross-Krook model, H-theorem, Rarefied Gas Dynamics, thermally perfect gases

Contents

1 Introduction

Gas flows in high altitude aerodynamics, in low pressure devices, or in micro systems, are often in a rarefied regime: the mean free path of gas molecules is of the same order of magnitude as a relevant macroscopic length scale. In such cases, the flow cannot be accurately described by the macroscopic Navier-Stokes equations. Instead, the Boltzmann equation of gas kinetic theory is a more relevant model. This equation was first derived by Boltzmann for a monoatomic gas, and later extended to mixtures [1], then to polyatomic molecules with internal energy and to gases with chemical reactions [2].

Numerical simulations of rarefied gas flows is a difficult task, due to the large number of degrees of freedom of gas molecules. The Direct Simulation Monte Carlo (DSMC) is the most frequently used method for such simulations [3, 4, 5, 6] : it combines deterministic transport of particles and stochastic collision algorithms that make it partially independent of the number of degrees of freedom of gas molecules. However, it is interesting to use other methods, especially for the transitional regime, between rarefied and continuous regimes, in which the number of molecules can be too large for DSMC. It can also be difficult for DSMC to capture small thermal fluctuations in gas micro flows due to a large statistical numerical noise. For such problems, it is attractive to directly solve the Boltzmann equation itself [7]: it gives very accurate numerical methods, but generally limited to simple monoatomic gases. In particular, simulating polyatomic gases is still nowadays much too computationally expensive with such deterministic methods.

However, the Boltzmann equation can be strongly simplified: the idea of model equations like Bhatnagar-Gross-Krook (BGK) [8] or Fokker-Plank models [9] is to simplify the collision process, while the transport process and gas surface interactions are not modified. In the BGK model, collisions are taken into account by a relaxation of the distribution function to the Maxwellian equilibrium. In the Fokker-Planck model, collisions are modeled by a diffusion process of the molecular velocity. With some further modifications [10, 11, 12, 13], it can be shown analytically that these model equations give the same solution as the Boltzmann equation in the dense regime, and

numerical simulations show that they are often sufficiently accurate in rarefied regimes, for a much lower computational cost than that of Boltzmann based numerical methods.

These models have recently been extended to more complex gases: polyatomic gases with rotational [14, 15] and vibrational nonequilibrium [5, 6, 16, 17, 18, 19, 20, 21]. However, these models are still computationally expensive due to the large number of degrees of freedom induced by the polyatomic structure of gas molecules. But a very interesting feature of these model equations is that their mathematical structure permits a reduction of this complexity: the internal energy variables can be easily eliminated by a simple integration (this reduction was proposed in [22] for a reduced model in a one dimensional shock wave problem), which leads to a reduced model that has more or less the same complexity as a model for a monoatomic gas, while it still accounts for molecular energy transfers between internal modes. These reduced models can then be viewed as intermediate models between fully kinetic Boltzmann like models and Navier-Stokes like fluid models.

While mathematical results for existence and uniqueness of solutions of such models is a very difficult task (see [23] for instance), there is a very simple tool that gives some nonlinear stability: the so called H-theorem, originally proved by Boltzmann for his equation. This theorem gives a non linear functional (related to the macroscopic entropy of thermodynamics) that satisfies a local dissipation law. Since most of BGK and Fokker-Planck like models satisfy such an H-theorem, reduced models naturally inherit this property: the integration process with respect to the internal variables is compatible with the H-theorem, since it is mainly based on convexity arguments.

In this paper, we show that these reduced models can be derived a priori, without any reduction of a fully kinetic model. Here, we only use the functional relation between the internal energy of the gas and its temperature, which is generally given by statistical physics, thermodynamics or by measurements. This approach does not require a precise description of the internal structure of gas molecules: it can then be applied to any polyatomic thermally perfect gas for which degrees of freedom of rotation or vibration (with harmonic or anharmonic oscillator model) can be activated. Consequently, these models can now be viewed as *direct* mesoscopic models, and not only as reduced models. Moreover, we are able to prove that these models satisfy an H-theorem. This is indeed the main innovation of our paper: we derive a general entropy functional for our models that does not require to know the entropy functional of a superior fully kinetic model.

The outline of our paper is as follows. In section 2, we introduce relations between internal energy of the gas and its temperature, we define a corresponding macroscopic entropy, we define the distribution functions of mass and energy required to describe the gas at a kinetic level, and we introduce our kinetic entropy functional on which our models are based on. In section 3 and 4, we propose BGK and Fokker-Planck models for these distributions. In section 5, we derive the macroscopic Euler and Navier-Stokes limits of these models. In section 6, our models are extended to take into account independent internal energies: the gas is then described with a distribution function for each internal energy. Our last section 7 is devoted to conclusion and perspectives.

3

2 Thermally perfect gas: energies, entropies, and distribution functions

2.1 Some elements of thermodynamics of thermally perfect gases

A thermally perfect gas is a gas satisfying the perfect gas law $P = \rho RT$ where P is the pressure, ρ the density and T the temperature, with R the gas constant per unit mass. Its energy e depends on the temperature, either linearly, like for polyatomic rotating molecules, or non linearly, like for vibrating molecules. Its heat capacities are constant (for linear energy) or temperature dependent (for non linear energy).

For instance, for rotating diatomic molecules, the specific energy reads $e(T) = \frac{5}{2}RT$ while for vibrational diatomic molecules in case of the harmonic oscillator model, it reads $e(T) = \frac{5}{2}RT + \frac{RT_0}{\exp(T_0/T)-1}$, where T_0 is the characteristic vibrational temperature. If the electronic energy has to be taken into account, $e(T)$ is obtained directly from spectroscopic measurements.

In order to develop general BGK and Fokker-Planck models that can allow for such temperature dependence of the specific energy in non equilibrium flows, we need to define different temperatures for translational and internal degrees of freedom. Then from now on, we assume a general temperature law of specific energy e, and we assume that it can be decomposed into

$$e(T) = e_{tr}(T) + e_{int}(T),$$

where $e_{tr}(T) = \frac{3}{2}RT$ is the translational kinetic energy (the energy associated to movement in the three directions of space), while $e_{int}(T)$ is some given energy that corresponds to the internal degrees of freedom of molecules. Moreover we also assume that e_{int} is an increasing function of T, and hence e is an increasing function too. Consequently, we can define the inverse functions $\mathbb{T}_{int}$, $\mathbb{T}_{tr}$, and $\mathbb{T}$ that map any given energy E to the corresponding temperatures. In other words, for any energy E, we define the temperatures

$$T_{int} = \mathbb{T}_{int}(E), \qquad T_{tr} = \mathbb{T}_{int}(E), \quad \text{and} \quad T = \mathbb{T}(E), \tag{1}$$

such that $e_{int}(T_{int}) = E$, $e_{tr}(T_{tr}) = E$ and $e(T) = E$. We shall also need the specific heat corresponding to the internal energy, which is defined by

$$c_v^{int}(T) = \frac{de_{int}(T)}{dT}, \tag{2}$$

so that the global specific heat is $c_v(T) = \frac{de(T)}{dT} = \frac{3}{2}R + c_v^{int}(T)$.

We also define the corresponding specific entropies s_{tr} and s_{int} by

$$\frac{ds_{tr}}{dE} = \frac{1}{\mathbb{T}_{tr}(E)}, \quad \text{and} \quad \frac{ds_{int}}{dE} = \frac{1}{\mathbb{T}_{int}(E)}, \tag{3}$$

see some expressions for rotational and vibrational case in section 6.4. The global entropy is defined by $ds = ds_{tr} + ds_{int} - Rd\rho/\rho$, and since at equilibrium, $T_{tr} = T_{int} = T$, these definitions are compatible with the usual Gibbs relation $ds = \frac{de}{T} - R\frac{d\rho}{\rho}$.

We now have all the necessary tools to construct our BGK and Fokker-Planck models.

2.2 Reduced distribution functions and local equilibrium

We define $F(t, x, v)$ the mass density of molecules with position x and velocity v, and $G(t, x, v)$ their internal energy density. In other words, the mass and internal energy of molecules in a volume element dx around x with velocity in dv around v are $F dx dv$ and $G dx dv$, respectively.

The macroscopic mass density ρ, velocity u, and energy densities ρE_{tr}, ρE_{int}, and ρE are defined by

$$
\rho = \langle F \rangle, \qquad \rho u = \langle v F \rangle,
$$
$$
\rho E_{tr} = \left\langle \frac{1}{2} |v - u|^2 F \right\rangle, \quad \rho E_{int} = \langle G \rangle, \tag{4}
$$
$$
\rho E = \left\langle \frac{1}{2} |v - u|^2 F \right\rangle + \langle G \rangle,
$$

where we use the notation $\langle \psi \rangle = \int \psi \, dv$ for any velocity dependent function ψ. The equilibrium temperature is defined by

$$
T = \mathbb{T}(E). \tag{5}
$$

At equilibrium, the mass and internal energy distributions are Maxwellian: we have $F = M[F, G]$ and $G = e_{int}(T) M[F, G]$, where

$$
M[F, G](v) = \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{|u - v|^2}{2RT} \right). \tag{6}
$$

2.3 Reduced vs fully kinetic models

Usually, mass and energy densities F and G are obtained by reduction of a single mass density that depends on internal microscopic energy modes. For instance, in case of rotational and discrete vibrational energy modes, one can define the kinetic mass density $\mathcal{F}(t, x, v, \varepsilon, i)$ such that

$$
F(t, x, v) = \sum_{i=0}^{+\infty} \int_{\mathbb{R}^3} \mathcal{F}(t, x, v, \varepsilon, i) \, d\varepsilon \quad \text{and} \quad G(t, x, v) = \sum_{i=0}^{+\infty} \int_{\mathbb{R}^3} (\varepsilon + iRT_0) \mathcal{F}(t, x, v, \varepsilon, i) \, d\varepsilon.
$$

While the fully kinetic distribution $\mathcal{F}$ is obviously more accurate than reduced distributions F and G, we point out other elements of comparisons between both descriptions:

- Macroscopic quantities: the macroscopic quantities ρ, u, T corresponding to $\mathcal{F}$ are the same as that given by F and G.

- Computational cost: a fully kinetic model for $\mathcal{F}$ requires to discretize a huge phase space: at least 8-dimensional for x, v, ε and i, and even more in case of electronic energy levels. This is why a deterministic simulation based on phase space discretization of the fully kinetic model is still nowadays computationally too expensive, even with modern large scale computers. At the contrary, using a reduced model for a deterministic simulation is possible, for the same computational cost as a simple monoatomic gas flow simulation (see [24]): indeed, the reduced model corresponding to F and G (see sections 3 and 4) requires to discretize the usual position-velocity phase space, which is 6-dimensional only.

5

- Information loss: only higher order moments with respect to the internal energy variables cannot be defined with F and G. But these moments are generally not quantities of interest in practical applications. Moreover, even if some solid wall interaction models with internal energy exchanges can be taken into account only with a fully kinetic distribution, standard diffuse and Maxwell boundary conditions are compatible with reduced distributions.

Finally, we mention that the novelty of our approach is that we derive reduced models *directly*, without using any fully kinetic model. These models can be viewed as direct mesoscopic models. Our approach is guided by the macroscopic energy laws of perfect gases, and is independent of continuous or discrete representations of microscopic energy levels.

2.4 Conservation and entropy

Standard Gaussian integrals (see section B) show that the local equilibrium distributions have the same moments as F and G, as it is stated in the following proposition.

Proposition 2.1 (Conservation properties)**.**

$$\langle M[F,G]\rangle = \rho, \qquad \langle vM[F,G]\rangle = \rho u,$$

$$\left\langle \frac{1}{2}|v-u|^2 M[F,G]\right\rangle = \rho E_{tr}, \quad \langle e_{int}(T)M[F,G]\rangle = \rho E_{int},$$

$$\left\langle \frac{1}{2}|v-u|^2 M[F,G]\right\rangle + \langle e_{int}(T)M[F,G]\rangle = \rho E.$$

We now define an entropy functional as a function of F and G and we state some of its useful properties in the following proposition.

Proposition 2.2 (Entropy)**.** *The entropy functional $\mathcal{H}(F,G)$ is*

$$\mathcal{H}(F,G) = \langle H(F,G)\rangle, \quad where \quad H(F,G) = F\log(F) - F\frac{1}{R}s_{int}\left(\frac{G}{F}\right). \tag{7}$$

1. *The partial derivatives of H are:*

$$D_1H(F,G) = 1+\log(F)+\frac{G}{R\mathbb{T}_{int}(G/F)F} - \frac{1}{R}s_{int}\left(\frac{G}{F}\right), \quad D_2H(F,G) = -\frac{1}{R\mathbb{T}_{int}(G/F)}. \tag{8}$$

2. *We note $\mathbb{H} = \begin{pmatrix} D_{11}H(F,G) & D_{12}H(F,G) \\ D_{12}H(F,G) & D_{22}H(F,G) \end{pmatrix}$ the Hessian matrix of H. Its components are*

$$D_{11}H(F,G) = \frac{1}{F} + \frac{G^2}{F^3 c_v^{int}(\mathbb{T}_{int}(G/F))R\mathbb{T}_{int}^2(G/F)},$$

$$D_{12}H(F,G) = D_{21}H(F,G) = -\frac{G}{F^2 c_v^{int}(\mathbb{T}_{int}(G/F))R\mathbb{T}_{int}^2(G/F)}$$

$$D_{22}H(F,G) = \frac{1}{c_v^{int}(\mathbb{T}_{int}(G/F))R\mathbb{T}_{int}^2(G/F)F}.$$

Moreover, the second order derivatives satisfy the following equalities:

$$\begin{aligned} FD_{11}H(F,G) + GD_{21}H(F,G) &= 1, \\ FD_{12}H(F,G) + GD_{22}H(F,G) &= 0. \end{aligned} \tag{9}$$

6

3. The function $(F, G) \mapsto H(F, G)$ is convex.

Proof. First, note that even if G/F is velocity dependent, it has the dimension of a specific energy, and hence the expressions $s_{int}(G/F)$ and $\mathbb{T}_{int}(G/F)$ make sense (see equations (1) and (3)). Points 1 and 2 are given by direct computations. The Hessian matrix is positive definite (its trace and determinant are positive) so that H is convex. $\qquad\square$

Remark 2.1. One can note that since s_{int} was defined up to a constant, the entropy is defined up to a linear term, which is proportional to the mass. Since the mass is naturally conserved in our models, this additional term plays no role in the proof of the H-theorem.

Proposition 2.3 (Minimization of $\mathcal{H}$)**.** *Let (F, G) be a couple of reduced distributions, ρ, ρu, and ρE its moments as defined by (4), and T its equilibrium temperature as defined by (5). Let $\mathcal{S}$ be the convex set defined by*

$$\mathcal{S} = \left\{ (F_1, G_1) \geq 0 \text{ such that } \langle F_1 \rangle = \rho, \quad \langle v F_1 \rangle = \rho u, \quad \left\langle \frac{1}{2}|v - u|^2 F_1 + G_1 \right\rangle = \rho E \right\}.$$

1. The minimum of $\mathcal{H}$ on $\mathcal{S}$ is obtained for the couple $(M[F, G], e_{int}(T) M[F, G])$, where $M[F, G]$ is the Maxwellian distribution defined in (6), while $e_{int}(T)$ is the specific internal energy at temperature T.

2. The following inequalities hold

$$0 \geq H\big(M[F, G], e_{int}(T) M[F, G]\big) - H(F, G)$$
$$\geq D_1 H(F, G)\big(M[F, G] - F\big) + D_2 H(F, G)\big(e_{int}(T) M[F, G] - G\big)$$

Proof. First, the set $\mathcal{S}$ is clearly convex, and it is non empty, since $(M[F, G], e_{int}(T) M[F, G])$ realizes the moments ρ, ρu, and ρE (see proposition 2.1), and hence belongs to $\mathcal{S}$. Now, we define the following Lagrangian

$$\mathcal{L}(F_1, G_1, \alpha, \beta, \gamma) = \langle H(F_1, G_1) \rangle - \alpha(\langle F_1 \rangle - \rho)$$
$$- \beta \cdot (\langle v F_1 \rangle - \rho u) - \gamma \left(\left\langle \frac{1}{2}|v - u|^2 F_1 + G_1 \right\rangle - \rho E \right)$$

for $(F_1, G_1) \in \mathcal{S}$, $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^3$, $\gamma \in \mathbb{R}$. The entropy functional $\mathcal{H}$ can reach a minimum of $\mathcal{S}$ when $\mathcal{L}$ has its first order partial derivatives equal to zero. This minimum is then characterized by the following relations:

$$D_1 H(F_1, G_1) = \alpha + \beta \cdot v + \gamma \frac{1}{2}|v|^2, \tag{10}$$

$$D_2 H(F_1, G_1) = \gamma, \tag{11}$$

$$\langle F_1 \rangle - \rho = 0, \quad , \langle v F_1 \rangle - \rho u = 0, \quad \left\langle \frac{1}{2}|v - u|^2 F_1 + G_1 \right\rangle - \rho E = 0, \tag{12}$$

where $D_1 H$ and $D_2 H$ are defined in (8).

Relation (11) gives $\mathbb{T}_{int}(G/F) = -1/(R\gamma)$ and hence γ is non positive. Since $\mathbb{T}_{int}$ is a one-to-one function, this gives $G/F = e_{int}(-1/(R\gamma))$. Then relation (10) shows that there exists real numbers a, b, and one vector $c \in \mathbb{R}^3$, independent of v, such that:

$$F_1 = a \exp\left(c \cdot v + b|v - u|^2\right).$$

It is then standard to use equations (12) to get $F_1 = M[F, G]$ and $G_1 = e_{int}(T)M[F, G]$.

Finally point 2 is a direct consequence of the convexity of H and of the minimization property. $\square$

3 A reduced BGK model for thermally perfect gases

3.1 The model

The evolution of mass and energy distributions can be simply modeled by the BGK approach [8, 25]: we assume that F and G relax to their local equilibrium $M[F, G]$ and $e_{int}(T)M[F, G]$ with the same relaxation time τ, and this gives

$$
\begin{aligned}
\partial_t F + v \cdot \nabla_x F &= \frac{1}{\tau}\left(M[F, G] - F\right), \\
\partial_t G + v \cdot \nabla_x G &= \frac{1}{\tau}(e_{int}(T)M[F, G] - G),
\end{aligned}
\tag{13}
$$

where ρ, u, T, and $M[F, G]$ are defined in (4–6).

We mention that similar models were recently obtained to take vibrational energy into account: the same reduced model can be found in [26], and a microscopic (non reduced) ES-BGK model is proposed in [19]. In this last case, if the model is reduced and the Prandtl number is taken as 1, we get the same reduced BGK model as (13). However, in these papers, the authors are not able to prove any H-theorem (only a local entropy dissipation can be proved). This is due to the fact that their models are derived from a microscopic model with continuous vibrational energy that does not has any entropy functional. Here, our derivation allows us to prove a H-theorem, as it is shown below.

3.2 Properties of the reduced model

System (13) naturally satisfies local conservation laws of mass, momentum, and energy. Moreover, the H-theorem holds with the entropy functional $\mathcal{H}$. Indeed, we have the

Proposition 3.1. *The reduced BGK system (13) satisfies the H-theorem*

$$\partial_t \mathcal{H}(F, G) + \nabla_x \cdot \langle v H(F, G)\rangle \leq 0,$$

where $\mathcal{H}(F, G)$ is the entropy functional defined in (7).

Proof.

By differentiation we get

$$\partial_t \mathcal{H}(F,G) + \nabla_x \cdot \langle v H(F,G)\rangle$$
$$= \langle D_1 H(F,G)(\partial_t F + v \nabla_x F) + D_2 H(F,G)(\partial_t G + v \nabla_x G)\rangle$$
$$= \frac{1}{\tau} \langle D_1 H(F,G)(M[F,G] - F) + D_2 H(F,G)(e_{int}(T)M[F,G] - G)\rangle$$
$$\leq 0$$

where we have used (13) to replace the transport terms by relaxation ones, and point 2 of proposition 2.3 to obtain the inequality. $\square$

4 A Fokker-Planck model for thermally perfect gases

Here, we derive a reduced Fokker-Planck model, by analogy with the reduced BGK model (13) and by using our previous work [15] on a Fokker-Planck model for polyatomic gases. We remind that the original Fokker-Planck model for monoatomic gas can be derived from the Boltzmann collision operator under the assumption of small velocity changes through collisions and additional equilibrium assumptions (see [9]). In practice, the agreement of this model with the Boltzmann equation is observed even when the gas is far from equilibrium (see [12], for instance).

4.1 A reduced Fokker-Planck model

Now, the evolution of the mass and internal energy distributions F and G is governed by the following model

$$\partial_t F + v \cdot \nabla_x F = D_F(F,G),$$
$$\partial_t G + v \cdot \nabla_x G = D_G(F,G),$$
(14)

with

$$D_F(F,G) = \frac{1}{\tau} \left(\nabla_v \cdot ((v-u)F + RT\nabla_v F) \right),$$
$$D_G(F,G) = \frac{1}{\tau} \left(\nabla_v \cdot ((v-u)G + RT\nabla_v G) \right) + \frac{2}{\tau} \left(e_{int}(T)F - G \right),$$
(15)

where the temperature is defined in (4). The elastic collisions are accounted for by the drift-diffusion terms that make F and G relax to the local equilibrium, while the energy exchanges induced by inelastic collisions are accounted for by the relaxation term.

4.2 Properties of the reduced model

Using direct calculations and dissipation properties as in [15] we can prove the following proposition.

Proposition 4.1. *The collision operator conserves the mass, momentum, and energy:*

$$\langle (1,v)D_F(F,G)\rangle = 0 \quad \text{and} \quad \left\langle \frac{1}{2}|v|^2 D_F(F,G) + D_G(F,G) \right\rangle = 0,$$

the entropy functional $\mathcal{H}(F,G)$ *satisfies the H-theorem:*

$$\partial_t \mathcal{H}(F,G) + \nabla_x \cdot \langle v H(F,G)\rangle = \mathcal{D}(F,G) \leq 0,$$

9

and we have the equilibrium property

$$(D_F(F,G) = 0 \ and \ D_G(F,G) = 0) \Leftrightarrow (F = M[F,G] \ and \ G = e_{int}(T)M[F,G]).$$

Proof. The conservation property is the consequence of direct integration of (15). The equilibrium property can be proved as follows.

To make the notations simpler, $M[F,G]$ will be simply denoted by M in the following. Then the collision operators can be written in the compact form

$$D_F(F,G) = \frac{1}{\tau}\nabla_v \cdot \left(M\nabla_v \frac{F}{M}\right),$$

$$D_G(F,G) = \frac{1}{\tau}\nabla_v \cdot \left(M\nabla_v \frac{G}{M}\right) + \frac{2}{\tau}\left(e_{int}(T)F - G\right).$$

For $D_F(F,G)$, a simple integration by part gives

$$\left\langle D_F(F,G)\frac{F}{M}\right\rangle = -\frac{1}{\tau}\left\langle \left(\nabla_v \frac{F}{M}\right)^T M\nabla_v \frac{F}{M}\right\rangle,$$

and the integral in the right-hand side is a positive definite form. Consequently, if $D_F(F,G) = 0$, we necessarily have $\nabla_v(F/M) = 0$, and hence $F = M$.

For the equilibrium property of G, the proof is a bit more complicated. First, we have

$$\left\langle D_G(F,G)\frac{G}{e_{int}(T)M}\right\rangle = -\frac{1}{\tau e_{int}(T)}\left\langle \left(\nabla_v \frac{G}{M}\right)^T M\nabla_v \frac{G}{M}\right\rangle + \left\langle \frac{2}{\tau}\left(e_{int}(T)F - G\right)\frac{G}{e_{int}(T)M}\right\rangle.$$

Consequently, if $D_G(F,G) = 0$, the right-hand side of the previous relation vanishes, and since $F = M$, we get

$$\frac{1}{e_{int}(T)}\left\langle \left(\nabla_v \frac{G}{M}\right)^T M\nabla_v \frac{G}{M}\right\rangle = 2\left\langle \left(e_{int}(T)M - G\right)\frac{G}{e_{int}(T)M}\right\rangle$$

$$= -2\left\langle \left(e_{int}(T)M - G\right)^2 \frac{1}{e_{int}(T)M}\right\rangle + 2\left\langle e_{int}(T)M - G\right\rangle$$

$$\leq 2\left\langle e_{int}(T)M - G\right\rangle = 2\rho(e_{int}(T) - E_{int}).$$

Now we can observe that $\rho e_{int}(T) - E_{int} = 0$. Indeed, note that $F = M$ implies $E_{tr} = e_{tr}(T)$, and therefore we have

$$e_{int}(T) - E_{int} = (e_{int}(T) + e_{tr}(T)) - (E_{int} + E_{tr}),$$
$$= e(T) - E = 0,$$

by definition of T (see (1)). Consequently, we obtain

$$\frac{1}{e_{int}(T)}\left\langle \left(\nabla_v \frac{G}{M}\right)^T M\nabla_v \frac{G}{M}\right\rangle \leq 0,$$

and again this gives $G = e_{int}(T)M$, which concludes the proof of the equilibrium property.

The proof of the H-theorem is much longer. First, by differentiation one gets that the quantity $\mathcal{D}(F, G) = \partial_t \mathcal{H}(F, G) + \nabla_x \cdot \langle v H(F, G) \rangle$ satisfies:

$$
\begin{aligned}
\mathcal{D}(F, G) &= \langle D_1 H(F, G)(\partial_t F + v \cdot \nabla_x F) + D_2 H(F, G)(\partial_t G + v \cdot \nabla_x G) \rangle \\
&= \langle D_1 H(F, G) D_F(F, G) + D_2 H(F, G) D_G(F, G) \rangle,
\end{aligned}
\tag{16}
$$

from (13). Then the proof is based on the convexity of $H(F, G)$: while for the BGK model we only used the first derivatives of H, we now use the positive-definiteness of the Hessian matrix of H. To do so we integrate by parts $\mathcal{D}(F, G)$ and multiply it by τ so that:

$$
\begin{aligned}
\tau \mathcal{D}(F, G) = &- \sum_{i=1}^{3} \langle (\partial_{v_i} F) D_{11} H(F, G) \left((v_i - u_i) F + RT \partial_{v_i} F \right) \rangle \\
&- \sum_{i=1}^{3} \langle (\partial_{v_i} G) D_{21} H(F, G) \left((v_i - u_i) F + RT \partial_{v_i} F \right) \rangle \\
&- \sum_{i=1}^{3} \langle (\partial_{v_i} F) D_{12} H(F, G) \left((v_i - u_i) G + RT \partial_{v_i} G \right) \rangle \\
&- \sum_{i=1}^{3} \langle (\partial_{v_i} G) D_{22} H(F, G) \left((v_i - u_i) G + RT \partial_{v_i} G \right) \rangle \\
&- 2 \left\langle (e_{int}(T) F - G) \frac{1}{R \mathbb{T}_{int}(G/F)} \right\rangle
\end{aligned}
\tag{17}
$$

To use the positive definiteness of the Hessian matrix $\mathbb{H}$ of H, we introduce the following vector:

$$
V_i = ((v_i - u_i) F + RT \partial_{v_i} F, (v_i - u_i) G + RT \partial_{v_i} G)
$$

so that the partial derivatives of F and G read

$$
(\partial_{v_i} F, \partial_{v_i} G) = \frac{1}{RT} V_i - \left(\frac{v_i - u_i}{RT} F, \frac{v_i - u_i}{RT} G \right).
$$

This is used in (17) to get

$$
\begin{aligned}
\tau \mathcal{D}(F, G) = &\sum_{i=1}^{3} \left\langle \left(\frac{v_i - u_i}{RT} F \right) D_{11} H(F, G) \left((v_i - u_i) F + RT \partial_{v_i} F \right) \right\rangle \\
&+ \sum_{i=1}^{3} \left\langle \left(\frac{v_i - u_i}{RT} G \right) D_{21} H(F, G) \left((v_i - u_i) F + RT \partial_{v_i} F \right) \right\rangle \\
&+ \sum_{i=1}^{3} \left\langle \left(\frac{v_i - u_i}{RT} F \right) D_{12} H(F, G) \left((v_i - u_i) G + RT \partial_{v_i} G \right) \right\rangle \\
&+ \sum_{i=1}^{3} \left\langle \left(\frac{v_i - u_i}{RT} G \right) D_{22} H(F, G) \left((v_i - u_i) G + RT \partial_{v_i} G \right) \right\rangle \\
&- \sum_{i=1}^{3} \langle V_i^T \mathbb{H} V_i \rangle \\
&- 2 \left\langle (e_{int}(T) F - G) \frac{1}{R \mathbb{T}_{int}(G/F)} \right\rangle.
\end{aligned}
$$

Now this expression can be considerably simplified by using property (9), and we get

$$
\begin{aligned}
\tau \mathcal{D}(F, G) \;=\;& \sum_{i=1}^{3} \left\langle \left(\frac{v_i - u_i}{RT} \right) \left((v_i - u_i)F + RT \partial_{v_i} F \right) \right\rangle \\
& - \sum_{i=1}^{3} V_i^t \mathbb{H} V_i - 2 \left\langle (e_{int}(T)F - G) \frac{1}{R \mathbb{T}_{int}(G/F)} \right\rangle .
\end{aligned}
$$

Then the first two terms are simplified by using an integration by parts to get

$$
\tau \mathcal{D}(F, G) = \frac{2}{RT} (\rho E_{tr} - \frac{3}{2} \rho RT) - \sum_{i=1}^{3} V_i^t \mathbb{H} V_i - 2 \left\langle (e_{int}(T)F - G) \frac{1}{R \mathbb{T}_{int}(G/F)} \right\rangle .
$$

By using (1), the first term is equal to $\frac{2}{RT} \rho(e_{int}(T) - E_{int}) = \frac{2}{RT} \langle e_{int}(T)F - G \rangle$ (this is equivalent to $E = e(T)$, which is true by definition of T). The terms with the Hessian are clearly negative, since $\mathbb{H}$ is positive definite (see the proof of proposition 2.2). Then we have

$$
\tau \mathcal{D}(F, G) \leq \frac{2}{RT} \langle e_{int}(T)F - G \rangle - 2 \left\langle (e_{int}(T)F - G) \frac{1}{R \mathbb{T}_{int}(G/F)} \right\rangle ,
$$

that can be factorized to find

$$
\tau \mathcal{D}(F, G) \leq 2 \left\langle (e_{int}(T)F - G) \left(\frac{1}{RT} - \frac{1}{R \mathbb{T}_{int}(G/F)} \right) \right\rangle .
$$

We can now prove that the integrand of the right-hand side is non-positive. Indeed, assume for instance that the second factor is non-positive, that is to say $\frac{1}{RT} - \frac{1}{R \mathbb{T}_{int}(G/F)} \leq 0$. Then $T \geq \mathbb{T}_{int}(G/F)$, and since e_{int} is an increasing function of the temperature (see section 2.1), we get $e_{int}(T) \geq e_{int}(\mathbb{T}_{int}(G/F)) = G/F$. This is equivalent to $e_{int}(T)F - G \geq 0$, that is to say the first factor of the integrand is non-negative. We get the same result in the opposite case. Consequently, we have proved $\tau \mathcal{D}(F, G) \leq 0$, which concludes the proof. $\qquad \square$

5 Hydrodynamic limits for reduced models

With a convenient scaling, the relaxation time τ of the reduced BGK model (13) and the Fokker-Planck model (14)) is replaced by $\mathrm{Kn}\,\tau$, where Kn is the Knudsen number, which can be defined as a ratio between the mean free path and a macroscopic length scale. It is then possible to look for macroscopic models derived from BGK and Fokker-Planck reduced models, in the asymptotic limit of small Knudsen numbers. For convenience, these models are re-written below in non-dimensional form. The BGK model is:

$$
\begin{aligned}
\partial_t F + v \cdot \nabla_x F &= \frac{1}{\mathrm{Kn}\,\tau} \left(M[F, G] - F \right), \\
\partial_t G + v \cdot \nabla_x G &= \frac{1}{\mathrm{Kn}\,\tau} (e_{int}(T) M[F, G] - G),
\end{aligned}
\tag{18}
$$

where $M[F, G]$ can be defined by (6) with $R = 1$. Similarly, the relations in section 2.1 between the translational, internal, and total energies and the temperature, have to be read with $R = 1$ in

non-dimensional variables. The Fokker-Planck model is

$$\partial_t F + v \cdot \nabla_x F = D_F(F, G),$$
$$\partial_t G + v \cdot \nabla_x G = D_G(F, G), \tag{19}$$

with

$$D_F(F, G) = \frac{1}{\text{Kn}\,\tau} \left(\nabla_v \cdot \left((v - u)F + T\nabla_v F \right) \right),$$
$$D_G(F, G) = \frac{1}{\text{Kn}\,\tau} \left(\nabla_v \cdot \left((v - u)G + T\nabla_v G \right) \right) + \frac{2}{\text{Kn}\,\tau} \left(e_{int}(T)F - G \right). \tag{20}$$

The conservation laws are obtained by multiplying the equation for F in (18) by 1, v, and $\frac{1}{2}|v|^2$ and then by integrating with respect to v. The equation for G is simply integrated and added to the last equation. Conservation property 2.1 then gives

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$
$$\partial_t(\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla \cdot P(f) = 0, \tag{21}$$
$$\partial_t \mathcal{E} + \nabla \cdot \mathcal{E} u + \nabla \cdot (P(f)u) + \nabla \cdot q(f) = 0,$$

where $\mathcal{E} = \langle \frac{1}{2}|v|^2 F + G \rangle_v$ is the total energy density, $P(f) = \langle (v - u) \otimes (v - u)F \rangle$ is the pressure tensor, and $q(f) = \langle \frac{1}{2}|v - u|^2(v - u)F + (v - u)G \rangle$ is the heat flux. The same conservation equations are obtained for the Fokker-Planck model (19), for which we use proposition 4.1.

Then with standard asymptotic analysis, we can prove that two asymptotic macroscopic models can be derived from our kinetic equations. These models are presented in the following two propositions: the first one for the compressible Euler asymptotics, the second one for the compressible Navier-Stokes asymptotics. These two propositions are proved in appendix A.

Proposition 5.1. *The mass, momentum, and energy densities of the solutions of the reduced BGK (18) and Fokker-Planck (19) models satisfy the Euler equations up to $O(\text{Kn})$:*

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$
$$\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p = O(\text{Kn}), \tag{22}$$
$$\partial_t \mathcal{E} + \nabla \cdot (\mathcal{E} + p)u = O(\text{Kn}).$$

The non-conservative form of these equations is

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$
$$\rho(\partial_t u + (u \cdot \nabla)u) + \nabla p = O(\text{Kn}), \tag{23}$$
$$\partial_t T + u \cdot \nabla T + \frac{T}{c_v(T)} \nabla_x \cdot u = O(\text{Kn}),$$

where $c_v(T) = \frac{d}{dT}e(T)$ is the heat capacity at constant volume.

Proposition 5.2. *The moments of the solution of the BGK and Fokker-Planck kinetic models (18) and (19) satisfy the compressible Navier-Stokes equations up to $O(\text{Kn}^2)$:*

$$\partial_t \rho + \nabla \cdot \rho u = 0,$$
$$\partial_t \rho u + \nabla \cdot (\rho u \otimes u) + \nabla p = \nabla \cdot \sigma + O(\text{Kn}^2), \tag{24}$$
$$\partial_t \mathcal{E} + \nabla \cdot (\mathcal{E} + p)u = -\nabla \cdot q + \nabla \cdot (\sigma u) + O(\text{Kn}^2),$$

13

where the viscous stress tensor and the heat flux are given by

$$\sigma = \mu\big(\nabla u + (\nabla u)^T - \frac{2}{3}\nabla \cdot uI\big) + \zeta \nabla \cdot uI, \quad and \quad q = -\kappa \nabla T, \tag{25}$$

and the values of the viscosity and heat transfer coefficients (in dimensional variables) are:

$$\begin{aligned} \mu &= \tau p, \quad and \quad \kappa = \mu c_p(T) \quad for\ BGK, \\ \mu &= \frac{1}{2}\tau p, \quad and \quad \kappa = \frac{2}{3}\mu c_p(T) \quad for\ Fokker\text{-}Planck, \end{aligned} \tag{26}$$

while the volume viscosity coefficient is $\zeta = \mu(\frac{2}{3} - \alpha)$, with $\alpha = \frac{c_p(T)}{c_v(T)} - 1$ for both models, and $c_p(T) = \frac{d}{dT}(e(T) + p/\rho) = c_v(T) + R$ is the heat capacity at constant pressure. Moreover, the corresponding Prandtl number is

$$\mathrm{Pr} = \frac{\mu c_p(T)}{\kappa} = 1 \quad for\ BGK,\ and \quad \frac{3}{2} \quad for\ Fokker\text{-}Planck. \tag{27}$$

6 Extension of the model to different internal energies

6.1 Internal energies, distributions and entropies

We assume gas molecules have n different and independent internal energies, and we denote by $e_{int}^1, \ldots, e_{int}^n$ the corresponding specific internal energies of the gas (like rotational, vibrational, electronical energies, for instance). Each e_{int}^i is supposed to be an increasing function of the temperature. The total energy is defined as $e = e_{tr} + \sum_{i=1}^{n} e_{int}^i$, and is also an increasing function of the temperature.

Consequently, we can define the inverse functions $\mathbb{T}_{int}^i$ and $\mathbb{T}$ that map any given energy E to the corresponding temperatures. In other words, for any energy E, we define the temperatures

$$T_{int}^i = \mathbb{T}_{int}^i(E), \quad and \quad T = \mathbb{T}(E), \tag{28}$$

such that $e_{int}^i(T_{int}^i) = E$ and $e(T) = E$.

The corresponding specific heats are $c_{v,int}^i(T) = \frac{de_{int}^i(T)}{dT}$. We can also define entropies $s_{int}^1, \ldots, s_{int}^n$ associated to each energy by $\frac{ds_{int}^i(E)}{dE} = \frac{1}{\mathbb{T}_{int}^i(E)}$.

Then we define by F the kinetic mass distribution while $G^1, \ldots, G^n$ are the distributions of internal energies. The macroscopic mass density ρ, velocity u, and energy density ρE are obtained through F and $G^1, \ldots, G^n$ by

$$\rho = \langle F \rangle, \qquad \rho u = \langle vF \rangle, \qquad \rho E = \left\langle \frac{1}{2}|v - u|^2 F \right\rangle + \sum_{i=1}^{n} \langle G^i \rangle. \tag{29}$$

Now it is possible to write a reduced entropy functional as a function of F and $G^1, \ldots, G^n$, as it is shown in the following proposition.

Proposition 6.1 (Entropy). *We define for $F, G^1, \ldots, G^n$ the following reduced entropy functional*

$$\mathcal{H}(F, G^1, \ldots, G^n) = \big\langle H(F, G^1, \ldots, G^n) \big\rangle, \tag{30}$$

14

where

$$H(F, G^1, \ldots, G^n) = F \log F - \sum_{i=1}^{n} \frac{1}{R} F s_{int}^i \left(\frac{G^i}{F} \right). \tag{31}$$

1. The partial derivatives of H computed at $(F, G^1, \ldots, G^n)$ are:

$$D_F H = 1 + \log(F) + \sum_{i=1}^{n} \left(\frac{G^i}{R\mathbb{T}_{int}^i(G^i/F)F} - \frac{1}{R} s_{int}^i \left(\frac{G^i}{F} \right) \right),$$

$$D_{G^i} H = -\frac{1}{R\mathbb{T}_{int}^i(G^i/F)}.$$

2. The second order derivatives of H, computed at $(F, G^1, \ldots, G^n)$ are

$$D_{F,F} H = \frac{1}{F} + \sum_{i=1}^{n} \frac{G^{i2}}{F^3 c_{v,int}^i(G^i/F) R\mathbb{T}_{int}^i{}^2(G^i/F)},$$

$$D_{F,G^i} H = -\frac{G^i}{F^2 c_{v,int}^i(G^i/F) R\mathbb{T}_{int}^i{}^2(G^i/F)}$$

$$D_{G^i,G^j} H = \frac{1}{F c_{v,int}^i(G^i/F) R\mathbb{T}_{int}^i{}^2(G^i/F)} \delta_{ij}$$

Moreover, we have the following equalities:

$$F D_{F,F} H + \sum_{i=1}^{n} G^i D_{F,G^i} H = 1, \quad and \quad F D_{F,G^i} H + G^i D_{G^i,G^i} H = 0, \tag{32}$$

for every i.

3. The function $(F, G^1, \ldots, G^n) \mapsto H(F, G^1, \ldots, G^n)$ is convex.

4. Let F be a given mass distribution and $\boldsymbol{G} = (G^1, \ldots, G^n)$ a n-uple of n distributions of internal energies. Let ρ, ρu, and ρE their moments as defined by (29). Let $\mathcal{S}$ be the convex set of distributions that have the same moments, that is to say

$$\mathcal{S} = \left\{ (\tilde{F}, \tilde{\boldsymbol{G}}) \text{ such that } \left\langle \tilde{F} \right\rangle = \rho, \quad \left\langle v\tilde{F} \right\rangle = \rho u, \quad \left\langle \frac{1}{2}|v - u|^2 \tilde{F} + \sum_{i=1}^{n} \tilde{G}^i \right\rangle = \rho E \right\}.$$

The minimum of $\mathcal{H}$ on $\mathcal{S}$ is obtained for $(M[F, \boldsymbol{G}], e_{int}^1(T)M[F, \boldsymbol{G}], \ldots, e_{int}^n(T)M[F, \boldsymbol{G}])$ with

$$M[F, \boldsymbol{G}] = \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{|v - u|^2}{2RT} \right). \tag{33}$$

5. The following inequalities hold:

$$0 \geq H(M[F, \boldsymbol{G}], e_{int}^1(T)M[F, \boldsymbol{G}], \ldots, e_{int}^n(T)M[F, \boldsymbol{G}]) - H(F, \boldsymbol{G})$$

$$\geq D_F H(F, \boldsymbol{G})(M[F, \boldsymbol{G}] - F) + \sum_{i=1}^{n} D_{G^i} H(F, \boldsymbol{G})(e_{int}^i(T)M[F, \boldsymbol{G}] - G^i).$$

15

Proof. The proof is the same as the one with one internal energy, except for point 3, for which the proof that the Hessian matrix $\mathbb{H}$ of H is positive definite is more difficult. Note that $\mathbb{H}$ is a $(n+1) \times (n+1)$ matrix whose block $\mathbb{H}(2:n+1,2:n+1)$ is diagonal with positive coefficients. Then Sylvester criterion ensures that $\mathbb{H}$ is positive definite if its determinant is positive. This determinant can be easily computed and we find

$$\det(\mathbb{H}) = D_{F,F}H \prod_{i=1}^{n} D_{G^i,G^i}H - \sum_{i=1}^{n}(D_{F,G^i}H)^2 \prod_{i \neq j} D_{G^j,G^j}H.$$

Then we note that (32) imply

$$D_{F,G^i}H = -\frac{G^i}{F}D_{G^i,G^i}H \quad \text{and} \quad D_{F,F}H = \frac{1}{F}\left(1 + \sum_{i=1}^{n}\frac{G_i^2}{F}D_{G^i,G^i}H\right),$$

and we find

$$\det(\mathbb{H}) = \frac{1}{F}\prod_{i=1}^{n} D_{G^i,G^i}H$$

which is clearly positive, so that the Hessian is positive definite. $\qquad\square$

6.2   BGK model

The extension of our BGK model (13) to this new framework is readily obtained: we set

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{\tau}\left(M[F, G^1, .., G^n] - F\right), \tag{34}$$

$$\partial_t G^i + v \cdot \nabla_x G^i = \frac{1}{\tau}(e_{int}^i(T)M[F, G^1, .., G^n] - G^i), \quad \text{for } i = 1 \text{ to } n \tag{35}$$

where the reduced Maxwellian is

$$M[F, G^1, .., G^n] = \frac{\rho}{\sqrt{2\pi RT}^3} \exp\left(-\frac{|v - u|^2}{2RT}\right),$$

and the macroscopic quantities are defined by

$$\rho = \langle F \rangle, \qquad \rho u = \langle vF \rangle, \qquad \rho E = \left\langle \frac{1}{2}|v - u|^2 F \right\rangle + \sum_{i=1}^{n} \langle G^i \rangle, \tag{36}$$

and T is defined by (28).

System (34–35) naturally satisfies local conservation laws of mass, momentum, and energy. Moreover, the H-theorem holds, as it is stated below.

Proposition 6.2. *The BGK system (34–35) satisfies the H-theorem*

$$\partial_t \mathcal{H}(F, G^1, ..., G^n) + \nabla_x \cdot \langle vH(F, G^1, ..., G^n) \rangle \leq 0,$$

where $\mathcal{H}(F, G^1, ..., G^n)$ is the entropy functional defined in (30).

Moreover, we can prove that this BGK system has the same compressible Euler and Navier-Stokes asymptotics as that given in Propositions 5.1 and 5.2 for the model with one single internal energy. The proof is a simple extension of that given in appendix A.2.1 and is left to the reader.

16

6.3 Fokker-Planck model

By analogy, we propose the following Fokker-Planck model:

$$\partial_t F + v \cdot \nabla_x F = D_F(F, G^1, ..., G^n), \tag{37}$$

$$\partial_t G^i + v \cdot \nabla_x G^i = D_{G^i}(F, G^i, ..., G^n), \quad \text{for } i = 1 \text{ to } n \tag{38}$$

with

$$
\begin{aligned}
D_F(F, G^1, ..., G^n) &= \frac{1}{\tau} \left(\nabla_v \cdot \left((v - u)F + RT\nabla_v F \right) \right), \\
D_{G^i}(F, G^1, ..., G^n) &= \frac{1}{\tau} \left(\nabla_v \cdot \left((v - u)G^i + RT\nabla_v G^i \right) \right) + \frac{2}{\tau} \left(e^i_{int}(T)F - G^i \right),
\end{aligned}
\tag{39}
$$

where the macroscopic values are defined as in (36) and (28). Using direct calculations and dissipation properties we can prove the following proposition.

Proposition 6.3. *The collision operator conserves the mass, momentum, and energy:*

$$\left\langle (1, v) D_F(F, G^1, ..., G^n) \right\rangle = 0 \quad and \quad \left\langle \frac{1}{2}|v|^2 D_F((F, G^1, ..., G^n) + D_{G^i}(F, G^1, ..., G^n) \right\rangle = 0,$$

the entropy functional $\mathcal{H}(F, G^1, ..., G^n)$ satisfies the H-theorem:

$$\partial_t \mathcal{H}(F, G^1, ..., G^n) + \nabla_x \cdot \left\langle v H(F, G^1, ..., G^n) \right\rangle \leq 0,$$

and we have the equilibrium property

$$
\begin{aligned}
&(D_F(F, G^1, ..., G^n) = 0 \text{ and } D_{G^i}(F, G^1, ..., G^n) = 0) \quad \text{for every } i \\
\Leftrightarrow \quad &(F = M[F, G^1, ..., G^n] \text{ and } G^i = e^i_{int}(T) M[F, G^1, ..., G^n]) \quad \text{for every } i.
\end{aligned}
$$

The proof is a simple extension of the proof of Proposition 4.1 and is left to the reader.

Moreover, we can prove that this BGK system has the same compressible Euler and Navier-Stokes asymptotics as that given in Propositions 5.1 and 5.2 for the model with one single internal energy. The proof is a simple extension of that given in appendix A.2.2 and is also left to the reader.

6.4 Example: rotational and vibrational cases

We briefly explain how to apply our framework to a diatomic gas for which translational, rotational and vibrational energies are taken into account, as defined by

$$e_{tr}(T) = \frac{3}{2}RT, \quad e_{rot}(T) = RT, \quad e_{vib}(T) = \frac{RT_0}{e^{T_0/T} - 1}, \tag{40}$$

According to section 6.1 (we set $n = 2$ and we replace the index $i = 1$ by *rot* and i=2 by *vib*), the associated macroscopic entropy for the internal degrees of freedom are

$$s_{rot}(E) = R\ln(E), \quad s_{vib}(E) = \left(\frac{E}{T_0} + R \right) \ln\left(\frac{E + RT_0}{RT_0} \right) - \frac{E}{T_0} \ln\left(\frac{E}{RT_0} \right), \tag{41}$$

which leads to the following kinetic entropy functional

$$
\begin{aligned}
& \mathcal{H}(F, G^{rot}, G^{vib}) \\
= \; & \left\langle F \log(F) - F \frac{s^{rot}}{R} \left(\frac{G^{rot}}{F} \right) - F \frac{s^{vib}}{R} \left(\frac{G^{vib}}{F} \right) \right\rangle \\
= \; & \left\langle F \log(F) + F \ln \left(\frac{F}{G^{rot}} \right) + F \ln \left(\frac{RT_0 F}{RT_0 F + G^{vib}} \right) + \frac{G^{vib}}{RT_0} \ln \left(\frac{G^{vib}}{RT_0 F + G^{vib}} \right) \right\rangle .
\end{aligned}
$$

This is the same functional as that obtained in [21] for an ES-BGK model: however, in [21], the functional was obtained through the reduction of a model with velocity and internal energy variables (continuous rotational energy and discrete vibrational energy levels). Also note that in the case of rotational energy only, we also recover the entropy functional of [14], also obtained through the reduction of a fully kinetic model.

7 Conclusion and perspectives

In this paper, we have proposed to different models (BGK and Fokker-Planck) of the Boltzmann equation for thermally perfect gases. These models can be viewed as intermediate models between fully kinetic equations (with a kinetic variable for each degrees of freedom) and macroscopic equations, since they are based on distribution functions with only velocity as a kinetic variable. As opposed to already existing models obtained by reduction of kinetic equations, our models do not require any superior kinetic model. They can be obtained as soon as internal energies are known as function of the temperature. Our model has been proved to satisfy conservation laws, and we have been able to propose an entropy functional for which our models satisfy an H-theorem.

The low complexity of the reduced BGK model can make it attractive to be implemented in a deterministic code, while the Fokker-Planck model can be easily simulated with a stochastic method. Of course, since these models are based on a single time relaxation, they cannot allow for multiple relaxation times scales. However, we believe it should be possible to extend these models by using the ellipsoidal-statistical approach, like in [14, 13, 15, 20, 21].

Finally, we note that these models should be sufficiently accurate to simulate rarefied flows with usual equilibrium inflow boundary conditions and Maxwell reflection at a solid wall. For more complex boundary conditions with energy exchanges between different modes, a fully kinetic model will be required.

A Derivation of the hydrodynamic limits

A.1 Euler limit

When Kn is very small, if all the time and space derivatives of F and G are $O(1)$ with respect to Kn (we exclude any initial layer and assume that the gradients lengths are larger than the mean free path), then (18) implies $F = M[F, G] + O(\text{Kn})$ and $G = e_{int}(T)M[F, G] + O(\text{Kn})$ so that $P(F) = P(M[F, G]) + O(\text{Kn}) = pI + O(\text{Kn})$, where I is the unit tensor, and $q(F, G) = q(M[F, G], e_{int}(T)M[F, G]) + O(\text{Kn}) = O(\text{Kn})$, which gives the Euler equations (23). The same analysis can be applied for the reduced Fokker-Planck model (19). Finally, the non conservative

form is readily obtained from the conservative form. We also get the internal energy equation:

$$\partial_t e_{int}(T) + u \cdot \nabla e_{int}(T) + T \frac{c_v^{int}(T)}{c_v(T)} \nabla_x \cdot u = O(\text{Kn}).$$

A.2 Navier-Stokes asymptotics

A.2.1 BGK model

The usual Chapman-Enskog method is applied as follows. We decompose F and G as $F = M[F,G] + \text{Kn}\, F_1$ and $G = e_{int}(T)M[F,G] + \text{Kn}\, G_1$, which gives

$$P(F) = pI - \text{Kn}\, P(F_1), \qquad \text{and} \qquad q(F,G) = \text{Kn}\, q(F_1, G_1).$$

Then we have to approximate $P(F_1)$ and $q(F_1, G_1)$ up to $O(\text{Kn})$. This is done by using the previous expansions and (13) to get

$$F_1 = -\tau(\partial_t M[F,G] + v \cdot \nabla_x M[F,G]) + O(\text{Kn}),$$
$$G_1 = -\tau(\partial_t e_{int}(T)M[F,G] + v \cdot \nabla_x e_{int}(T)M[F,G]) + O(\text{Kn}).$$

This gives the following approximations

$$P(F_1) = -\tau \left\langle (v-u) \otimes (v-u)(\partial_t M[F,G] + v \cdot \nabla_x M[F,G]) \right\rangle + O(\text{Kn}), \tag{42}$$

and

$$q(F_1, G_1) = -\tau \left\langle (v-u)\frac{1}{2}|v-u|^2(\partial_t M[F,G] + v \cdot \nabla_x M[F,G]) \right\rangle$$
$$- \tau \left\langle (v-u)(\partial_t e_{int}(T)M[F,G] + v \cdot \nabla_x e_{int}(T)M[F,G]) \right\rangle + O(\text{Kn}). \tag{43}$$

Now it is standard to write $\partial_t M[F,G]$ and $\nabla_x M[F,G]$ as functions of derivatives of ρ, u, and T, and then to use Euler equations (22) to write time derivatives as functions of the space derivatives only. After some algebra, we get

$$\partial_t M[F,G] + v \cdot \nabla_x M[F,G] = \frac{\rho}{T^{\frac{3}{2}}} M_0(V) \left(A \cdot \frac{\nabla T}{\sqrt{T}} + B : \nabla u \right) + O(\text{Kn}), \tag{44}$$

where

$$V = \frac{v-u}{\sqrt{T}}, \qquad M_0(V) = \frac{1}{(2\pi)^{\frac{3}{2}}} \exp(-\frac{|V|^2}{2})$$

$$A = \left(\frac{|V|^2}{2} - \frac{5}{2} \right) V, \qquad B = V \otimes V - \left(\frac{1}{c_v(T)} \frac{1}{2}|V|^2 + \frac{e'_{int}(T)}{c_v(T)} \right) I.$$

Then we introduce (44) into (42) to get

$$P_{ij}(F_1) = -\tau \rho T \left\langle V_i V_j B_{kl} M_0 \right\rangle \partial_{x_l} u_k + O(\text{Kn}),$$

where we have used the change of variables $v \mapsto V$ in the integral (the term with A vanishes due to the parity of M_0). Then standard Gaussian integrals (see appendix B) give

$$P(F_1) = -\mu \left(\nabla u + (\nabla u)^T - \alpha \nabla \cdot u\, I \right) + O(\text{Kn}),$$

19

with $\mu = \tau\rho T$ and $\alpha = \frac{c_p(T)}{c_v(T)} - 1$, which is the announced result, in a non-dimensional form.

For the heat flux, we use the same technique. First for $e_{int}(T)M[F,G]$ we obtain

$$\partial_t\left(e_{int}M[F,G]\right) + v\cdot\nabla_x\left(e_{int}M[F,G]\right) = \frac{\rho}{T^{\frac{3}{2}}}M_0(V)\left(\tilde{A}\cdot\frac{\nabla T}{\sqrt{T}} + \tilde{B}:\nabla u\right) + O(\text{Kn}), \qquad (45)$$

where

$$\tilde{A} = e_{int}(T)A + VTe'_{int}(T), \quad \text{and} \quad \tilde{B} = e_{int}(T)B - \frac{T}{c_v(T)}e'_{int}(T)I.$$

Then $q(F_1, G_1)$ as given in (43) can be reduced to

$$q_i(F_1, G_1) = -\tau\rho\left(T\left\langle\frac{1}{2}|V|^2 V_i A_j M_0\right\rangle - \left\langle V_i\tilde{A}_j M_0\right\rangle\right)\partial_{x_j}T.$$

Using again Gaussian integrals , we get

$$q(F_1, G_1) = -\kappa\nabla T,$$

where $\kappa = \mu c_p(T)$.

A.2.2 Fokker-Planck model

Here, we rather use the decomposition $F = M(1 + \text{Kn}\, F_1)$ and $G = e_{int}M(1 + \text{Kn}\, G_1)$, which gives

$$P(F) = pI - \text{Kn}\, P(MF_1) \quad \text{and} \quad q(F, G) = \text{Kn}\, q(MF_1, e_{int}MG_1),$$

in which, for clarity, the dependence of M on F and G has been omitted, and the dependence of e_{int} on T as well. Finding F_1 and G_1 is more complex than for the BGK model: however, the computations are very close to what is done in the standard monoatomic Fokker-Planck model (see [13] for instance), so that we only give the main steps here (see appendix B for details).

First, the decomposition is injected into (19) to get

$$D_F(F, G) = \frac{1}{\tau}ML_F(F_1),$$

$$D_G(F, G) = \frac{1}{\tau}e_{int}ML_G(F_1, G_1),$$

where L_F and L_G are linear operators defined by

$$\begin{aligned} L_F(F_1) &= \frac{1}{M}\Big(\nabla_v\cdot(TM\nabla_v F_1)\Big), \\ L_G(F_1, G_1) &= \frac{1}{M}\Big(\nabla_v\cdot(TM\nabla_v G_1) + 2(F_1 - G_1)\Big). \end{aligned} \qquad (46)$$

Then Fokker-Planck equations (19) suggest to look for an approximation of F_1 and G_1 up to $O(\text{Kn})$ as solutions of

$$\partial_t M + v\cdot\nabla_x M = \frac{1}{\tau}M[F,G]L_F(F_1)$$

$$\partial_t e_{int}M + v\cdot\nabla_x e_{int}M = \frac{1}{\tau}e_{int}M[F,G]L_G(F_1, G_1).$$

By using (44)-(45), these relations are equivalent, up to another $O(Kn)$ approximation, to

$$L_F(F_1) = \tau \left(A \cdot \frac{\nabla T}{\sqrt{T}} + B : \nabla u \right), \quad \text{and} \quad L_G(F_1, G_1) = \frac{\tau}{e_{int}} \left(\tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tilde{B} : \nabla u \right), \quad (47)$$

where A, B, $\tilde{A}$, and $\tilde{B}$ are the same as for the BGK equation in the previous section. Now we have to solve (47) for F_1 and G_1.

First, we rewrite $L_F(F_1)$ and $L_G(F_1, G_1)$, defined in (46), by using the change of variables $V = \frac{v-u}{\sqrt{T}}$ to get

$$L_F(F_1) = -V \cdot \nabla_V F_1 + \nabla_V \cdot (\nabla_V F_1),$$
$$L_G(F_1, G_1) = L_F(G_1) + 2(F_1 - G_1).$$

Then simple calculation of derivatives show that A, B, $\tilde{A}$, and $\tilde{B}$ satisfy the following properties

$$L_F(A) = -3A, \qquad L_F(B) = -2B, \qquad L_F(V) = -V.$$

Consequently, we look for F_1 and G_1 as solution of (47) under the following form

$$F_1 = \tau a A \cdot \frac{\nabla T}{\sqrt{T}} + \tau b B : \nabla u \quad \text{and} \quad G_1 = \tau \frac{\tilde{a}}{e_{int}} \tilde{A} \cdot \frac{\nabla T}{\sqrt{T}} + \tau \frac{\tilde{b}}{e_{int}} \tilde{B} : \nabla u,$$

and we find $\tilde{a} = a = -1/3$ and $\tilde{b} = b = 1/2$.

Finally, using these relations into P and q and using some Gaussian integrals (see appendix B) give

$$P(MF_1) = -\mu \left(\nabla u + (\nabla u)^T - \alpha \nabla \cdot u\, I \right) \quad \text{and} \quad q(MF_1, e_{int} MG_1) = -\kappa \nabla T,$$

where $\alpha = \frac{c_p}{c_v} - 1$, $\mu = \frac{\tau}{2} \rho T$, and $\kappa = \frac{2}{3} \mu c_p(T)$, which is the announced result, in a non-dimensional form.

B   Gaussian integrals and other summation formula

In this section, we give some integrals and summation formula that are used in the paper.

First, we remind the definition of the absolute Maxwellian $M_0(V) = \frac{1}{(2\pi)^{\frac{3}{2}}} \exp(-\frac{|V|^2}{2})$. We denote by $\langle \phi \rangle = \int_{\mathbb{R}^3} \phi(V)\, dV$ for any function ϕ. It is standard to derive the following integral relations (see [1], for instance and note that some computations are redundant), written with the Einstein notation:

$$\langle M_0 \rangle_V = 1,$$
$$\langle V_i V_j M_0 \rangle_V = \delta_{ij}, \qquad \langle V_i^2 M_0 \rangle_V = 1, \qquad \langle |V|^2 M_0 \rangle_V = 3,$$
$$\langle V_i^2 V_j^2 M_0 \rangle_V = 1 + 2\, \delta_{ij}, \qquad \langle V_i V_j V_k V_l M_0 \rangle_V = \delta_{ij}\delta_{kl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}$$
$$\langle V_i V_j |V|^2 M_0 \rangle_V = 5\, \delta_{ij}, \qquad \langle |V|^4 M_0 \rangle_V = 15,$$
$$\langle V_i V_j |V|^4 M_0 \rangle_V = 35\, \delta_{ij}, \qquad \langle |V|^6 M_0 \rangle = 105,$$

while all the integrals of odd power of V are zero. From the previous Gaussian integrals, it can be shown that for any 3×3 matrix C, we have

$$\langle V_i V_j C_{kl} V_k V_l M_0 \rangle_V = C_{ij} + C_{ji} + C_{ii}\delta_{ij}.$$

21

C   Data availability statement

Data sharing is not applicable to this article as no new data were created or analyzed in this study.

References

[1] S. Chapman and T.G. Cowling. *The mathematical theory of non-uniform gases*. Cambridge University Press, 1970.

[2] V. Giovangigli. *Multicomponent Flow Modeling*. Birkhäuser Boston, Boston, MA, 1999.

[3] G. A. Bird. *Molecular Gas Dynamics and the Direct Simulation of Gas Flows*. Oxford Engineering Science Series, 2003.

[4] T. E. Schwartzentruber I. D. Boyd. *Nonequilibrium Gas Dynamics and Molecular Simulation*. Cambridge Aerospace Series. Cambridge University Press, 2017.

[5] M. Pfeiffer, P. Nizenkov, A. Mirza, and S. Fasoulas. Direct simulation Monte Carlo modeling of relaxation processes in polyatomic gases. *Physics of Fluids*, 28(2):027103, feb 2016.

[6] M. Pfeiffer. Extending the particle ellipsoidal statistical Bhatnagar-Gross-Krook method to diatomic molecules including quantized vibrational energies. *Physics of Fluids*, 30:116103, 11 2018.

[7] G. Dimarco and L. Pareschi. Numerical methods for kinetic equations. *Acta Numerica*, 23:369–520, 2014.

[8] E.P. Gross, P.L. Bhatnagar, and M. Krook. A model for collision processes in gases. *Physical review*, 94(3):511–525, 1954.

[9] C. Cercignani. *The Boltzmann Equation and Its Applications*, volume 68. Springer-Verlag, Lectures Series in Mathematics, 1988.

[10] Jr. Lowell H. Holway. New statistical models for kinetic theory: Methods of construction. *Physics of Fluids*, 9(9):1658–1673, 1966.

[11] E. M. Shakhov. Generalization of the Krook relaxation kinetic equation. *Izv. Akad. Nauk SSSR. Mekh. Zhidk. Gaza*, 1(5):142–145, 1968.

[12] M.H. Gorji, M. Torrilhon, and P. Jenny. Fokker-Planck model for computational studies of monatomic rarefied gas flows. *Journal of fluid mechanics*, 680:574–601, August 2011.

[13] J. Mathiaud and L. Mieussens. A Fokker–Planck model of the Boltzmann equation with correct Prandtl number. *Journal of Statistical Physics*, 162(2):397–414, Jan 2016.

[14] P. Andriès, P. Le Tallec, J.-F. Perlat, and B. Perthame. The Gaussian-BGK model of Boltzmann equation with small Prandtl number. *Eur. J. Mech. B/Fluids*, 2000.

[15] J. Mathiaud and L. Mieussens. A Fokker–Planck model of the Boltzmann equation with correct Prandtl number for polyatomic gases. *Journal of Statistical Physics*, 168(5):1031–1055, Sep 2017.

[16] M. Bisi and M.J. Cáceres. A BGK relaxation model for polyatomic gas mixtures. *Commun. Math. Sci.*, 14(2):297–325, October 2016.

[17] Z. Wang, H. Yan, Q. Li, and K. Xu. Unified gas-kinetic scheme for diatomic molecular flow with translational, rotational, and vibrational modes. *Journal of Computational Physics*, 350:237 – 259, 2017.

[18] T. Arima, T. Ruggeri, and M. Sugiyama. Rational extended thermodynamics of a rarefied polyatomic gas with molecular relaxation processes. *Phys. Rev. E*, 96:042143, Oct 2017.

[19] S. Kosuge, H.-W. Kuo, and K. Aoki. A kinetic model for a polyatomic gas with temperature-dependent specific heats and its application to shock-wave structure. *Journal of Statistical Physics*, 177(2):209–251, Oct 2019.

[20] J. Mathiaud and L. Mieussens. BGK and Fokker-Planck models of the Boltzmann equation for gases with discrete levels of vibrational energy. *Journal of Statistical Physics*, Jan 2020.

[21] Y. Dauvois, J. Mathiaud, and L. Mieussens. An ES-BGK model for polyatomic gases in rotational and vibrational nonequilibrium. *European Journal of Mechanics - B/Fluids*, 88:1–16, 2021.

[22] C. K. Chu. Kinetic-theoretic description of the formation of a shock wave. *Phys. Fluids*, 8(1):12, 1965.

[23] Byung-Hoon Hwang and Seok-Bae Yun. Ellipsoidal BGK model near a global Maxwellian in the whole space. *Journal of Mathematical Physics*, 60(7):071507, 2019.

[24] L. Mieussens. A survey of deterministic solvers for rarefied flows. *AIP Conference Proceedings*, 1628(1):943–951, 2014.

[25] Marlies Pirner. A review on BGK models for gas mixtures of mono and polyatomic molecules. *Fluids*, 6(11), 2021.

[26] C. Baranger, Y. Dauvois, G. Marois, J. Mathé, J. Mathiaud, and L. Mieussens. A BGK model for high temperature rarefied gas flows. *European Journal of Mechanics - B/Fluids*, 80:1 – 12, 2020.