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Derivation of a BGK model for mixtures

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ABSTRACT

The aim of this article is to construct a BGK operator for gas mixtures starting from the true Navier–Stokes equations. That is the ones with transport coefficients given by the hydrodynamic limit of the Boltzmann equation(s). Here the same hydrodynamic limit is obtained by introducing relaxation coefficients on certain moments of the distribution functions. Next the whole model is set by using entropy minimization under moment constraints as in Brull and Schneider (2008, 2009) [23,24]. In our case the BGK operator allows to recover the exact Fick and Newton laws and satisfy the classical properties of the Boltzmann equations for inert gas mixtures.

1. Introduction

The BGK equation [1] is a seminal simplified model of the nonlinear Boltzmann equation of gas dynamics. While keeping physical and mathematical properties of the Boltzmann equation (conservation laws, H-theorem, equilibrium states, etc.) it is often used for numerical purposes. Nevertheless solutions of the BGK equation are very different from those of the Boltzmann equation far from equilibrium. In the Navier–Stokes limit things are much different and a modified version of this model – the Ellipsoidal Statistical Model [2] – allows to recover the correct transport coefficients (Prandtl number).

The Boltzmann equation can be easily extended to the case of inert gas mixtures but things are more difficult for BGK type models. For example, momentum and energy conservations stand only for the whole set of particles. Besides phenomena such as diffusion (Fick law) or thermal diffusion (Soret law) must be considered in the hydrodynamic limit. The Boltzmann equation(s) for gas mixtures has been widely studied by Japanese researchers (see for example [3–6]). Their results feature essential differences with the usual monatomic Boltzmann equation. Its theoretical aspects such as existence theorems [7–9] or study of a binary mixture close to a local equilibrium [10] confirm the specificity of multi-component gases.

Coming back to modeling there exists a great variety of BGK models which traces back to the work of Gross and Krook [11] to the most recent model by Kosuge [12]. A first idea was to mimic the monatomic simplified models in the case of multi-species [11,13–15]. In the case of Maxwellian molecules, models were designed to give the right transfers of momentum and energies far from equilibrium [14,15]. Then Garzo et al. [16] extended the previous approximations for any kind of molecular interaction. In this vein, Kosuge [12] has designed a model that is able to approximate all transfers of moments up to the order two plus the "heat transfers". But no real mathematical considerations such as nonnegativness of the distribution functions or entropy decay were addressed. This was finally done by Andries et al. [17]. This model has later been widely used in the context of reactive gas mixtures (see e.g [18] and references therein). Besides a new property was stated by Garzo et al. [16]: the indifferentiability "principle". When all molecules are of same mass and cross sections are equal then the whole set of equations must reduce to a single one when adding all distribution functions. This property is also satisfied by the model of Andries et al. [17].

Let us remark that while numerical results are quite good for some models or mathematical (and physical) properties are satisfied for others it is quite surprising that none of them has attempted to reach the right hydrodynamic limit. That is to obtain the right transport coefficients as (for example) the Ellipsoidal Statistical Model [2] does in the case of monatomic molecule. In

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general all the authors rather study the hydrodynamic limit of their model and eventually compared it with the right one [19].

Our approach goes the other way. We consider the Navier–Stokes equation with transport coefficients either computed with the hydrodynamic limit of the Boltzmann equation or given by some experiments. Then the aim of the paper is to construct a BGK model that allows to recover those coefficients — in the present case the Fick law. Our main result is in Theorem 2 where we prove that our operator enjoys that property in addition to the classical properties of the Boltzmann equations. Remark that the Fick relaxation operator is not just an abstract model since the Fick matrix coefficients can be obtained using algorithms by Ern and Giovangigli [20]. The paper is organized as follows. In Section 2 we firstly recall Boltzmann equations for gas mixtures and relevant macroscopic quantities. Secondly we introduce spaces and notations that will used in the sequel. Finally we define a class of operators (so-called properly defined) basing on the properties of the Boltzmann collision operators (Section 2.4). In Section 3 we recall in a concise and clear way the link between the thermodynamic of irreversible processes (see for example [21]) and the hydrodynamic limit of the Boltzmann equation. The computation and properties of the transport coefficients obtained from the Boltzmann equations are given in Section 3.2. Such computations easily extend to the case of properly defined operators. Section 4 is devoted to the construction of our operator. We consider linear perturbations or fluctuations around thermodynamical equilibrium. Those are classical assumptions of the thermodynamic of irreversible processes [21] and of statistical physics [22]. This is also the basis of the "theory" of relaxation coefficients introduced by two of the authors [23,24]. Our model is constructed in two step. Firstly we compute those coefficients and related moments of the distribution functions basing only on the Fick matrix (Proposition 1). Then the whole Fick relaxation model is set by using a principle of entropy minimization under moment constraints (Theorem 1). Its definition is given in 3. The simplicity of this model relies on its construction which requires only to diagonalize a modified Fick matrix. In Section 5 we prove that this operator is properly defined (Proposition 2). As a consequence the derivation of its hydrodynamic limit as well as the properties of the transport coefficients just follow the steps that were given for the Boltzmann equation itself (Section 3.2). In particular this BGK model gives at the hydrodynamic limit the exact Fick laws (Section 5.2). We finally prove in Section 5.3 a result concerning the indifferentiability property and the correct Fick law (Proposition 4).

2. The Boltzmann equation and other general kinetic equation for gas mixtures

2.1. The Boltzmann operator for inert gas mixture

Let us consider a gas mixture with p components. The distribution function $f_i(t,x,v)$ (or for short f_i, $i \in [1,p]$ with $\mathbf{f} := (f_1,\ldots,f_p)$) of a given species i evolves according to the Boltzmann equation:

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

where

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

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 depends 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

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

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

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

2.2. Macroscopic quantities for the mixture

We denote with $n^i, \rho^i, u^i, E^i, \mathcal{E}^i$ and T^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 specie i. They are defined by the following relations:

$$n^i = \int_{\mathbb{R}^3} f_i\,d\mathbf{v}, \qquad \rho^i = m_i n^i, \qquad n^i\mathbf{u}^i = \int_{\mathbb{R}^3}\mathbf{v} f_i\,d\mathbf{v},$$
$$E^i = \frac{1}{2}\rho^i\left\|\mathbf{u}^i\right\|^2 + n^i\mathcal{E}^i,$$
$$\mathcal{E}^i = \frac{3}{2}k_B T^i = \frac{m_i}{2n^i}\int_{\mathbb{R}^3}\left\|\mathbf{v}-\mathbf{u}^i\right\|^2 f_i d\mathbf{v},$$

where k_B is the Boltzmann constant. In the same way macroscopic quantities for the mixture are defined by

$$n = \sum_{k=1}^{p} n^k, \qquad \rho = \sum_{k=1}^{p}\rho^k, \qquad \rho\mathbf{u} = \sum_{k=1}^{p}\rho^k\mathbf{u}^k,$$
$$n\mathcal{E} + \frac{\rho}{2}\|\mathbf{u}\|^2 = E = \sum_{k=1}^{p} E^k, \qquad \mathcal{E} = \frac{3}{2}k_B T. \tag{2}$$

Given a mixture of p species with macroscopic values n^i, $\mathbf{u}$, T an important list of functions are the Maxwellians of equilibrium reading as:

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

We denote by $\boldsymbol{M} := \left(\mathcal{M}_1,\ldots,\mathcal{M}_p\right)$. At last for any list of non negative functions $\mathbf{f} := \left(f_1,\ldots,f_p\right)$ we define the entropy function H as:

$$H(\mathbf{f}) := \sum_{i=1}^{i=p}\int_{\mathbb{R}^3}\left(f_i\ln(f_i) - f_i\right)d\mathbf{v}.$$

2.3. Other considerations

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

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

This space is equipped using its natural dot product:

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