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THE MAXWELL-STEFAN DIFFUSION LIMIT FOR A KINETIC MODEL OF MIXTURES

LAURENT BOUDIN, BÉRÉNICE GREC, AND FRANCESCO SALVARANI

ABSTRACT. We consider the non-reactive fully elastic Boltzmann equation for mixtures. We deduce that, under the standard diffusive scaling, its limit for vanishing Mach and Knudsen numbers is the Maxwell-Stefan model for a multicomponent gaseous mixture.

1. INTRODUCTION

The derivation of macroscopic equations starting from kinetic theory is a very active research field. The interest on such a question has a long history, being even pointed out by Hilbert in the famous lecture [9] delivered at the International Congress of Mathematicians, in Paris in 1900. The problem, known as *Hilbert's sixth problem*, has been translated in a rigorous mathematical language in a series of pioneering papers [1, 2, 3]. That led to significant articles, such as [8], where the authors established a Navier-Stokes limit for the Boltzmann equation considered over \mathbb{R}^3 .

All the aforementioned papers deal with a mono-species, monoatomic and ideal gas. However, many common physical situations are far more intricate: multi-species mixtures, possibility of chemical reactions... The mathematical analysis of the Boltzmann-like equations describing the mixture is much harder, due to the presence of multi-species kernels, with cross interactions between the different densities describing each component of the mixture. Nevertheless, in that situation, the derivation, even formal, of the macroscopic equations from kinetic models is crucial. Indeed, it allows to show a link between different modelling levels and to specify the range of validity of the target equations.

The origin of our work is the study of diffusive phenomena in the lower airways. As pointed out in [4], standard Fickian diffusion may not be appropriate to model the biological flow of a mixture of helium and oxygen, and another set of equations should be adopted instead: the Maxwell-Stefan equations, see [10, 7, 5] for instance. It is therefore crucial to determine if and how Boltzmann-like equations for mixtures can lead to the Maxwell-Stefan system in the diffusive regime.

Our study generalizes the kinetic model for gas mixtures from [11], which can be seen as the non-reactive fully elastic version of the model proposed in [6]. We first briefly recall the Maxwell-Stefan model, and then consider our kinetic model and its diffusive limit, studied, at a formal level, in the Maxwellian case. We asymptotically recover the Maxwell-Stefan equations.

2. THE MAXWELL-STEFAN MODEL

Consider a bounded domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$, with a smooth boundary. We deal with an ideal gas mixture constituted with $I \geq 2$ species. For each species of the mixture \mathcal{A}_i , $1 \leq i \leq I$, we define its macroscopic number density function n_i and its concentration c_i , only depending on time t and position $x \in \Omega$, which are directly proportional to each other through the Avogadro constant

$\mathcal{N}_A \simeq 6.022 \times 10^{23} \text{ mol}^{-1}$. More precisely, we have $n_i = \mathcal{N}_A c_i$. Hence we shall only focus on the macroscopic density functions. We can also define the molecular flux N_i of species \mathcal{A}_i , which is involved in the continuity equation, holding for any i ,

$$(1) \quad \partial_t n_i + \nabla_x \cdot N_i = 0.$$

For any i , the Maxwell-Stefan law is then written

$$(2) \quad -\nabla_x n_i = \sum_{j \neq i} \frac{n_j N_i - n_i N_j}{D_{ij}},$$

where the D_{ij} are the so-called effective diffusion coefficients. We only need an initial datum n_i^{in} , and we assume that $\sum n_i^{\text{in}}(x) = n_{\text{tot}}$ does not depend on x : the molecules of the mixture are initially uniformly distributed. Then, by summing (2) over all i , we observe that the Maxwell-Stefan laws are linearly dependent: we need a closure equation. We choose to impose $\sum N_i = 0$ almost everywhere. It is natural, because it ensures that the model is purely diffusive. Consequently, by summing (1) over all i , and since n_{tot} does not depend on x , $\sum n_i$ remains constant with respect to both t and x . Note that it prevents vacuum in the mixture.

3. A KINETIC MODEL FOR GASEOUS MIXTURES

For each species of the mixture \mathcal{A}_i , we introduce a mesoscopic number density function f_i , which depends on time t , space position $x \in \mathbb{R}^d$ and velocity $v \in \mathbb{R}^d$. For any i , the quantity $f_i(t, x, v) dx dv$ is the number of molecules of species \mathcal{A}_i at time t in an elementary volume of the space phase, of size $dx dv$, centered at (x, v) . The mesoscopic number density function is then related to f_i thanks to

$$(3) \quad n_i(t, x) = \int_{\mathbb{R}^d} f_i(t, x, v) dv.$$

We assume that the mixture only involves mechanical collisions between molecules. More precisely, let us consider two molecules of species \mathcal{A}_i and \mathcal{A}_j , $1 \leq i, j \leq I$, with respective masses m_i, m_j , and respective pre-collisional velocities v', v'_* . After a collision, the particles belong to the same species, so they still have the same masses, but their velocities have changed, now denoted by v and v_* . The collisions are supposed to be elastic, meaning that both momentum and kinetic energy are conserved:

$$(4) \quad m_i v' + m_j v'_* = m_i v + m_j v_*, \quad \frac{1}{2} m_i |v'|^2 + \frac{1}{2} m_j |v'_*|^2 = \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2.$$

From (4), it is possible to write v' and v'_* with respect to v and v_* :

$$(5) \quad v' = \frac{1}{m_i + m_j} (m_i v + m_j v_* + m_j |v - v_*| \omega), \quad v'_* = \frac{1}{m_i + m_j} (m_i v + m_j v_* - m_i |v - v_*| \omega),$$

where ω is an arbitrary element of S^{d-1} , which takes into account that (4) allows $d - 1$ degrees of freedom.

We now introduce the collisional operators.

3.1. Mono-species collisions. Let i , $1 \leq i \leq I$. The collisional operator associated to species \mathcal{A}_i is defined by

$$(6) \quad Q_i^m(f, f)(v) = \int_{v_* \in \mathbb{R}^d} \int_{\omega \in S^{d-1}} B_i(v, v_*, \omega) [f(v')f(v'_*) - f(v)f(v_*)] \, d\omega \, dv_*,$$

where v', v'_* are defined by (4), and the cross section B_i satisfies the microreversibility assumptions: $B_i(v, v_*, \omega) = B_i(v_*, v, \omega)$ and $B_i(v, v_*, \omega) = B_i(v', v'_*, \omega)$. It can also be written under a weak form, obtained from (6) using the changes of variables $(v, v_*) \mapsto (v_*, v)$ and $(v, v_*) \mapsto (v', v'_*)$, $\omega \in S^{d-1}$ remaining fixed. This weak form allows to get the conservation, for species \mathcal{A}_i , of the total number of molecules, the total momentum and kinetic energy.

3.2. Bi-species collisions. Let i, j such that $1 \leq i, j \leq I$ and $i \neq j$. The collisional operator associated to species \mathcal{A}_i and \mathcal{A}_j is defined by

$$(7) \quad Q_{ij}^b(f, g)(v) = \int_{v_* \in \mathbb{R}^d} \int_{\omega \in S^{d-1}} B_{ij}(v, v_*, \omega) [f(v')g(v'_*) - f(v)g(v_*)] \, d\omega \, dv_*,$$

where v' and v'_* are again defined thanks to (4), and the cross section B_{ij} satisfies the microreversibility assumptions $B_{ij}(v, v_*, \omega) = B_{ji}(v_*, v, \omega)$ and $B_{ij}(v, v_*, \omega) = B_{ij}(v', v'_*, \omega)$. In the same way as in the mono-species case, there are several weak formulations involving Q_{ij}^b , for instance,

$$(8) \quad \int_{v \in \mathbb{R}^d} Q_{ij}^b(f, g)(v) \psi_i(v) \, dv \\ = \iint_{v, v_* \in \mathbb{R}^d} \int_{\omega \in S^{d-1}} B_{ij}(v, v_*, \omega) f(v)g(v_*) [\psi_i(v') - \psi_i(v)] \, d\omega \, dv \, dv_*,$$

obtained from (7) using the same changes of variables as in the mono-species case. Here, ψ_i is a suitable test function. Those weak forms allow to recover the conservation of the total number of molecules of species \mathcal{A}_i , and the conservation of the momentum and kinetic energy when all the species are simultaneously considered.

3.3. H-theorems. We conclude this section by writing down the H-theorems corresponding to the collisional operators we defined and by discussing the mechanical equilibrium. More precisely, the following result holds.

Proposition 1. *We assume that the cross sections $(B_i)_{1 \leq i \leq I}$ and $(B_{ij})_{i \neq j}$ are nonnegative a.e.*

(a) *For all $f_i \equiv f_i(v) \geq 0$, $1 \leq i \leq I$, such that the following quantities are defined, one has*

$$\sum_{i=1}^I \int_{v \in \mathbb{R}^d} Q_i^m(f_i, f_i)(v) \log \left(\frac{f_i(v)}{m_i^d} \right) \, dv + \sum_{i=1}^I \sum_{j \neq i} \int_{v \in \mathbb{R}^d} Q_{ij}^b(f_i, f_j)(v) \log \left(\frac{f_i(v)}{m_i^d} \right) \, dv \leq 0.$$

(b) *Moreover, the three following properties are equivalent.*

i. *For any $1 \leq i, j \leq I$, $j \neq i$ and $v \in \mathbb{R}^d$,*

$$Q_i^m(f_i, f_i)(v) = 0, \quad Q_{ij}^b(f_i, f_j)(v) = 0.$$

ii. *The previous inequality is an equality:*

$$\sum_{i=1}^I \int_{v \in \mathbb{R}^d} Q_i^m(f_i, f_i)(v) \log \left(\frac{f_i(v)}{m_i^d} \right) \, dv + \sum_{i=1}^I \sum_{j \neq i} \int_{v \in \mathbb{R}^d} Q_{ij}^b(f_i, f_j)(v) \log \left(\frac{f_i(v)}{m_i^d} \right) \, dv = 0.$$

iii. *There exist $T > 0$ and $u \in \mathbb{R}^d$ such that, for any i ,*

$$(9) \quad f_i(v) = n_i \left(\frac{m_i}{2\pi T} \right)^{d/2} \exp\left(-\frac{m_i}{2T}|v-u|^2\right).$$

The proof follows the same strategy as in [6], Proposition 1, mainly using the symmetrized weak forms of the collisional operators and properties of the logarithm.

4. THE MAXWELL-STEFAN DIFFUSION LIMIT

The Maxwell-Stefan limit is obtained in the framework of the classical diffusive scaling. The physical situation we study only allows diffusion. This means that we suppose that the initial situation is in complete mechanical equilibrium, from the velocity point of view. But we assume that the mixture may be initially nonhomogeneous in space, i.e. that the system is far from macroscopic equilibrium.

4.1. The scaled equation. We assume that we are in the Maxwellian case: each cross section B only depends on ω and lies in $L^1(S^{d-1})$. For symmetry reasons, we also assume that $B(\omega) = B(-\omega)$ for any $\omega \in S^{d-1}$. In the classical diffusive case, the scaling is held by the mean free path, which we denote $\varepsilon > 0$.

For any i , each number density function f_i^ε solves the scaled Boltzmann equation, that is

$$(10) \quad \varepsilon \partial_t f_i^\varepsilon + v \cdot \nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} Q_i^m(f_i^\varepsilon, f_i^\varepsilon) + \frac{1}{\varepsilon} \sum_{j \neq i} Q_{ij}^b(f_i^\varepsilon, f_j^\varepsilon), \quad t > 0, \quad x \in \Omega, \quad v \in \mathbb{R}^d.$$

The number density functions satisfy the specular boundary conditions, that are, for any i ,

$$f_i^\varepsilon(t, x, v) = f_i^\varepsilon(t, x, v - 2(v \cdot \nu_x)\nu_x), \quad v \in \mathbb{R}^d, \quad x \in \partial\Omega, \quad t > 0,$$

where ν_x is the outgoing normal vector to $\partial\Omega$ at $x \in \partial\Omega$. Eventually, we define the macroscopic number density function n_i^ε thanks to (3) with f_i^ε .

4.2. Initial conditions. We can suppose that the initial data for the number density functions are local Maxwellians, with the same temperature T^{in} which does not depend on x , and a nil macroscopic velocity (since we are interested in a purely diffusive setting). Hence, we can write

$$(11) \quad f_i^{\text{in}}(x, v) = n_i^{\text{in}}(x) \left(\frac{m_i}{2\pi T^{\text{in}}} \right)^{d/2} e^{-m_i|v|^2/2T^{\text{in}}}.$$

Since each f_i^{in} has the form given in (11), we immediately have, for any i ,

$$\int_{v \in \mathbb{R}^d} v f_i^{\text{in}}(x, v) dv = 0.$$

4.3. Asymptotics. In the following, let us set

$$N_i^\varepsilon(t, x) = \frac{1}{\varepsilon} \int_{v \in \mathbb{R}^d} v f_i^\varepsilon(t, x, v) dv,$$

and denote, as usual when dealing with formal diffusive limits,

$$n_i(t, x) = \lim_{\varepsilon \rightarrow 0^+} n_i^\varepsilon(t, x), \quad N_i(t, x) = \lim_{\varepsilon \rightarrow 0^+} N_i^\varepsilon(t, x).$$

Since the initial flux is zero, and the boundary conditions are of specular type, we immediately deduce that $N_i^\varepsilon(0, x) = 0$ for a.e. $x \in \Omega$, and that $N_i^\varepsilon(t, x) = 0$ for all $t > 0$ and a.e. $x \in \partial\Omega$.

Moreover, $f_i^\varepsilon(t, x, v)$ converges at a formal level towards the mechanical equilibrium $f_i(t, x, v)$ described by (9) in the H-theorem, where both T and u may depend on t and x . More precisely, we have

$$\lim_{\varepsilon \rightarrow 0^+} f_i^\varepsilon(t, x, v) := f_i(t, x, v) = n_i(t, x) \left(\frac{m_i}{2\pi T(t, x)} \right)^{d/2} e^{-m_i|v-u(t,x)|^2/2T(t,x)}.$$

Since we assume that each $(\varepsilon N_i^\varepsilon)_{\varepsilon > 0}$, for any i , goes to 0 when ε goes to 0, that implies that $u \equiv 0$. Then, asymptotically, the number of molecules of species \mathcal{A}_i , their momentum and their energy are given by

$$\int_{\mathbb{R}^d} f_i(t, x, v) \begin{pmatrix} 1 \\ v \\ \frac{1}{2}|v|^2 \end{pmatrix} dv = \begin{pmatrix} n_i(t, x) \\ 0 \\ \frac{d}{2}n_i(t, x)T(t, x) \end{pmatrix}.$$

Since the mixture is constituted of ideal gases and since n_{tot} is constant, that ensures that T is also constant (in fact, equal to T^{in}). We can now obtain the Maxwell-Stefan equations by studying the moments of orders zero and one of the distribution functions governed by the Hilbert expansion (10), and by letting ε go to 0.

4.3.1. *Conservation of the number of molecules of species \mathcal{A}_i .* We first consider the moments of order 0 of the number density functions. More precisely, for any i , we integrate (10) with respect to v in \mathbb{R}^d , and obtain, thanks to the conservation properties of the collisional operators,

$$\frac{\partial}{\partial t} \int_{\mathbb{R}^d} f_i^\varepsilon(t, x, v) dv + \frac{1}{\varepsilon} \nabla_x \cdot \left(\int_{\mathbb{R}^d} f_i^\varepsilon(t, x, v) v dv \right) = 0,$$

Letting ε go to 0, we immediately get the continuity equation (1) for species \mathcal{A}_i .

4.3.2. *Balance of momentum.* Let $\ell = 1, \dots, d$, and denote v_ℓ the ℓ -th component of any v in \mathbb{R}^d . The balance law of momentum for a given species \mathcal{A}_i is obtained by multiplying (10) by v_ℓ and integrating with respect to v in \mathbb{R}^d . We obtain, for any i ,

$$(12) \quad \varepsilon \frac{\partial}{\partial t} \int_{\mathbb{R}^d} v_\ell f_i^\varepsilon(v) dv + \nabla_x \cdot \left(\int_{\mathbb{R}^d} v_\ell f_i^\varepsilon(v) v dv \right) = \frac{1}{\varepsilon} \sum_{j \neq i} \int_{\mathbb{R}^d} v_\ell Q_{ij}^b(f_i^\varepsilon, f_j^\varepsilon)(v) dv := \Theta_\ell^\varepsilon,$$

because the term involving Q_i^m vanishes. Let us first focus on Θ_ℓ^ε , which depends on (t, x) . Thanks to (5) and (8) with $\psi_i(v) = v$, we can write

$$\Theta_\ell^\varepsilon = \frac{1}{\varepsilon} \sum_{j \neq i} \frac{m_j}{m_i + m_j} \iint_{\mathbb{R}^{2d}} \int_{S^{d-1}} B_{ij}(\omega) f_i^\varepsilon(v) f_j^\varepsilon(v_*) (v_{*\ell} - v_\ell + |v - v_*| \omega_\ell) d\omega dv_* dv.$$

In the previous equality, the term where ω_ℓ appears is in fact nil, because of the properties of B_{ij} with respect to ω . The rest of the equality can be written in terms of macroscopic quantities:

$$\Theta_\ell^\varepsilon = \sum_{j \neq i} \frac{m_j}{m_i + m_j} \|B_{ij}\|_{L^1(S^{d-1})} (n_i^\varepsilon N_j^\varepsilon - n_j^\varepsilon N_i^\varepsilon).$$

We can now perform the limit $\varepsilon \rightarrow 0$ in (12). The time derivative formally vanishes, so that (12) eventually becomes, for any ℓ ,

$$(13) \quad \nabla_x \cdot \left(\int_{\mathbb{R}^d} v_\ell f_i(v) v dv \right) = \sum_{j \neq i} \frac{m_j}{m_i + m_j} \|B_{ij}\|_{L^1(S^{d-1})} (n_i(N_j)_\ell - n_j(t, x)(N_i)_\ell).$$

Let us now focus on the left-hand side of (13). We successively write

$$\begin{aligned} \nabla_x \cdot \left(\int_{\mathbb{R}^d} v_\ell f_i(v) v \, dv \right) &= \sum_{k=1}^d \frac{\partial}{\partial x_k} \int_{\mathbb{R}^d} v_\ell v_k f_i(v) \, dv = \sum_{k=1}^d \frac{\partial n_i}{\partial x_k} \int_{\mathbb{R}^d} v_\ell v_k \left(\frac{m_i}{2\pi T} \right)^{d/2} e^{-m_i|v|^2/2T} \, dv \\ &= \frac{\partial n_i}{\partial x_\ell} \int_{\mathbb{R}^d} v_\ell^2 \left(\frac{m_i}{2\pi T} \right)^{d/2} e^{-m_i|v|^2/2T} \, dv = \frac{T}{m_i} \frac{\partial n_i}{\partial x_\ell}. \end{aligned}$$

From (13) for any ℓ , we recover, for any i , the Maxwell-Stefan law (2), in which we set

$$D_{ij}^{-1} = \frac{m_i m_j \|B_{ij}\|_{L^1(S^{d-1})}}{(m_i + m_j)T},$$

and check that $D_{ij} = D_{ji}$.

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