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The Maxwell-Stefan Diffusion Limit for a Kinetic Model of Mixtures

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Abstract We consider the non-reactive elastic Boltzmann equation for multicomponent gaseous mixtures. We deduce, under the standard diffusive scaling, that well prepared initial conditions lead to solutions satisfying the Maxwell-Stefan diffusion equations in the vanishing Mach and Knudsen numbers limit.

Keywords Diffusion limit · Maxwell-Stefan equations · Boltzmann equations · 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 his famous lecture [18] 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 [2–4]. That led to significant articles, such as [16, 17], where the authors established a Navier-Stokes limit for the Boltzmann equation considered over $\mathbb{R}^3$.

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All the aforementioned papers deal with a mono-species, monatomic and ideal gas. However, many common physical situations are more intricate: multi-species mixtures, polyatomic gas, chemical reactions, *etc*. In this work, we focus on a multi-species mixture of monatomic ideal gases with no chemical reactions.

The mathematical study of Boltzmann-like equations describing such a mixture is far more complex, mainly because of the presence of multi-species kernels, with cross interactions between the different densities describing each component of the mixture. The readers can refer, for example, to [22, 24] as founding works on kinetic models for mixtures, to [1, 10, 14] with a focus on BGK models, to [12] for Boltzmann equations with chemical reactions, and to [8] for a Boltzmann model very similar to the one studied here.

However, the relationship (even at a formal level) between the kinetic level and the macroscopic description is crucial and specifies the range of validity of the target equations.

On the macroscopic point of view, the time evolution of diffusive phenomena for mixtures is well described by the Maxwell-Stefan equations [21, 25] (see [20] for a fairly complete review on the main aspects of multicomponent diffusive phenomena). However, its mathematical study is very recent and solid results on the subject only appeared in the last few years [6, 9, 15, 19]. Let us emphasize that this problem has not a mere academical interest, since it has applications to the respiration mechanism [7, 11, 26], in particular when dealing with a Helium/Oxygen/Carbon dioxide mixture in the lung. Note that the Maxwell-Stefan equations lie in the class of cross diffusion models, which are commonly introduced in population dynamics, see [23] for instance.

The relationship between the kinetic description of a phenomena and its macroscopic picture governed by the Maxwell-Stefan equations is still an open question. In this article, we shall show that well prepared initial conditions formally generate, in the classical diffusive scaling, solutions of the Boltzmann equation for monatomic gas mixtures satisfying the Maxwell-Stefan equations in the asymptotic regime, see [5] for other results in the same scaling. Note that the relationship between those equations and some kinetic equations for mixtures were already investigated, in a more general setting, in [27]. Our work is in fact, up to our knowledge, the first attempt to recover the Maxwell-Stefan equations as a hydrodynamic limit of a kinetic system. The rigorous proof of this limit remains an open problem, as well as extensions to polyatomic gas mixtures.

The article is organized as follows. First, we briefly recall the Maxwell-Stefan model. Then we propose a Boltzmann-type model of multi-species mixtures and detail the mono and bi-species collision kernels involved in the kinetic equations. Finally, we formally discuss the diffusive asymptotics of our kinetic model towards the Maxwell-Stefan equations.

2 The Maxwell-Stefan Model

Consider a bounded domain $\Omega \subset \mathbb{R}^3$, with a smooth boundary. We deal with an ideal gas mixture constituted with $I \geq 2$ species with molecular masses m_i, in a purely diffusive setting (*i.e.* without any convective effect).

For each species of the mixture $\mathcal{A}_i$, $1 \leq i \leq I$, we define its concentration c_i, only depending on the macroscopic variables of time $t \in \mathbb{R}^+$ and position $x \in \Omega$. We can also define the (diffusive) concentration flux F_i of species $\mathcal{A}_i$. Both quantities are involved in the continuity equation, holding for any i,

$$\partial_t c_i + \nabla_x \cdot F_i = 0 \quad \text{on } \mathbb{R}_+^* \times \Omega. \tag{1}$$

Let $c = \sum c_i$ be the total concentration of the mixture and set $n_i = c_i/c$ the mole fraction of species $\mathcal{A}_i$. The Maxwell-Stefan equations give relationships between the fluxes and the concentrations. They can be written, for any i, as

$$-c\nabla_x n_i = \frac{1}{c}\sum_{j\neq i}\frac{c_j F_i - c_i F_j}{D_{ij}} \quad \text{on } \mathbb{R}_+^* \times \Omega, \tag{2}$$

where D_{ij} are the so-called effective diffusion coefficients between the species $\mathcal{A}_i$ and $\mathcal{A}_j$. For obvious physical reasons, the diffusion coefficients are symmetric with respect to the particles exchange, *i.e.* $D_{ij} = D_{ji}$.

By summing (2) over all $1 \leq i \leq I$, we observe that the Maxwell-Stefan laws are linearly dependent. More precisely, there are exactly $(I-1)$ independent equalities of type (2).

Hence, we need one closure (vectorial) relationship. If one works in a closed system with global constant and uniform temperature and pressure, as in Duncan and Toor's experiment [13], it is natural to assume that there is a transient equimolar diffusion in the mixture before reaching the stationary state. That means that the total diffusive flux satisfies

$$\sum_{i=1}^{I} F_i = 0 \quad \text{on } \mathbb{R}_+^* \times \Omega. \tag{3}$$

In the whole paper, we focus on an equimolar diffusion process in a closed system and study Eqs. (1)–(3). Of course, in some other realistic situations, the systems may be not closed, so that the equimolar diffusion assumption does not hold any more (see for instance [11]).

Summing (1) over i, one can observe that c does not depend on t, and equals its initial value. It is then clear that, if we assume that the molecules of the mixture are initially uniformly distributed, the quantity c does not depend on x either. Note that this assumption prevents vacuum in the mixture.

We still need a set of boundary conditions to ensure that the system is closed, that is for any i,

$$\nu \cdot F_i = 0 \quad \text{on } \mathbb{R}_+ \times \partial\Omega, \tag{4}$$

where $\nu(x)$ is the outward normal vector at $x \in \partial\Omega$.

3 A Kinetic Model for Gaseous Mixtures

From now on, we consider a mixture of monatomic ideal gases.

3.1 Framework

For each species of the mixture $\mathcal{A}_i$, we introduce the corresponding distribution function f_i, which depends on time $t \in \mathbb{R}^+$, space position $x \in \Omega$ and velocity $v \in \mathbb{R}^3$. For any i, $f_i(t,x,v)\,\mathrm{d}x\,\mathrm{d}v$ denotes the quantity of matter, expressed in moles, of species $\mathcal{A}_i$ in the mixture, at time t in an elementary volume of the space phase of size $\mathrm{d}x\,\mathrm{d}v$ centred at (x,v). The distribution function is then related to c_i thanks to

$$c_i(t,x) = \int_{\mathbb{R}^3} f_i(t,x,v)\,\mathrm{d}v, \quad t \geq 0, \quad x \in \Omega. \tag{5}$$

Since the mixture is non reactive, only mechanical collisions between molecules are allowed. More precisely, let us consider two molecules of species $\mathcal{A}_i$ and $\mathcal{A}_j$, $1 \le i, j \le I$, 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 and are now denoted by v and v_*. The collisions are supposed to be elastic. Therefore, both momentum and kinetic energy are conserved:

$$m_i v' + m_j v'_* = m_i v + m_j v_*, \qquad \frac{1}{2} m_i |v'|^2 + \frac{1}{2} m_j |v'_*|^2 = \frac{1}{2} m_i |v|^2 + \frac{1}{2} m_j |v_*|^2. \tag{6}$$

From (6), it is possible to write v' and v'_* with respect to v and v_*:

$$v' = \frac{1}{m_i + m_j}\big(m_i v + m_j v_* + m_j |v - v_*| \sigma\big), \qquad v'_* = \frac{1}{m_i + m_j}\big(m_i v + m_j v_* - m_i |v - v_*| \sigma\big), \tag{7}$$

where σ is an arbitrary element of $\mathbb{S}^2$, which takes into account that (6) allows two degrees of freedom. Note that, if $m_i = m_j$, we recover the standard collision rules in the Boltzmann equation.

Let us now introduce the collision operators.

3.2 Mono-species Collision Operators

They are the standard Boltzmann collision operators. Let $1 \le i \le I$. If $f := f(v)$ is a nonnegative function, the collision operator describing the interactions between molecules of species $\mathcal{A}_i$ is defined by

$$Q_i^{\mathrm{m}}(f, f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B_i(v, v_*, \sigma) \big[f\big(v'\big) f\big(v'_*\big) - f(v) f(v_*)\big] \,\mathrm{d}\sigma \,\mathrm{d}v_*, \tag{8}$$

where v', v'_* are defined by (7) with $m_i = m_j$, and the cross section B_i satisfies the microreversibility assumptions: $B_i(v, v_*, \sigma) = B_i(v_*, v, \sigma)$ and $B_i(v, v_*, \sigma) = B_i(v', v'_*, \sigma)$. It can also be written in weak form, for instance,

$$\begin{aligned} \int_{\mathbb{R}^3} Q_i^{\mathrm{m}}(f, f)(v) \psi(v) \,\mathrm{d}v = -\frac{1}{4} \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \int_{\mathbb{S}^2} B_i(v, v_*, \sigma) \big[f\big(v'\big) f\big(v'_*\big) - f(v) f(v_*)\big] \\ \times \big[\psi\big(v'\big) + \psi\big(v'_*\big) - \psi(v) - \psi(v_*)\big] \,\mathrm{d}\sigma \,\mathrm{d}v_* \,\mathrm{d}v, \end{aligned} \tag{9}$$

for any $\psi : \mathbb{R}^3 \to \mathbb{R}$ such that the first integral in (9) is well defined. Equation (9) is obtained from (8) by using the changes of variables $(v, v_*) \mapsto (v_*, v)$ and $(v, v_*) \mapsto (v', v'_*)$, $\sigma \in \mathbb{S}^2$ remaining fixed.

These weak forms classically allow to get the conservation, for each species $\mathcal{A}_i$, of the total number of molecules, the total momentum and the kinetic energy by successively choosing $\psi(v) = 1$, v and $|v|^2/2$.

3.3 Bi-species Collision Operators

Let i, j such that $1 \le i, j \le I$ and $i \ne j$. If $f := f(v)$ and $g := g(v_*)$ are nonnegative functions, let us define the operator describing the collisions of molecules of species $\mathcal{A}_i$ with molecules of species $\mathcal{A}_j$ by

$$Q_{ij}^{\mathrm{b}}(f, g)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B_{ij}(v, v_*, \sigma) \big[f\big(v'\big) g\big(v'_*\big) - f(v) g(v_*)\big] \,\mathrm{d}\sigma \,\mathrm{d}v_*, \tag{10}$$

where v' and v'_*, are defined thanks to (7), and the cross section B_{ij} satisfies the microreversibility assumptions $B_{ij}(v, v_*, \sigma) = B_{ji}(v_*, v, \sigma)$ and $B_{ij}(v, v_*, \sigma) = B_{ij}(v', v'_*, \sigma)$. We also need the operator describing the collisions of molecules of species $\mathcal{A}_j$ with molecules of species $\mathcal{A}_i$. It is given by

$$Q^{\mathrm{b}}_{ji}(g, f)(v) = \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B_{ji}(v, v_*, \sigma)\big[g\big(w'\big) f\big(w'_*\big) - g(v) f(v_*)\big] \,\mathrm{d}\sigma \,\mathrm{d}v_*,$$

where w' and w'_* are defined similarly to (7), that is

$$w' = \frac{1}{m_i + m_j}\big(m_j v + m_i v_* + m_i |v - v_*|\sigma\big),$$
$$w'_* = \frac{1}{m_i + m_j}\big(m_j v + m_i v_* - m_j |v - v_*|\sigma\big).$$

In the same way as in the mono-species case, there are several weak formulations involving Q^{b}_{ij}, for instance,

$$\begin{aligned}
&\int_{\mathbb{R}^3} Q^{\mathrm{b}}_{ij}(f, g)(v)\psi(v) \,\mathrm{d}v \\
&\quad = -\frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \int_{\mathbb{S}^2} B_{ij}(v, v_*, \sigma)\big[f\big(v'\big)g\big(v'_*\big) - f(v)g(v_*)\big]\big[\psi\big(v'\big) - \psi(v)\big] \,\mathrm{d}\sigma \,\mathrm{d}v \,\mathrm{d}v_* \\
&\quad = \iint_{\mathbb{R}^3\times\mathbb{R}^3} \int_{\mathbb{S}^2} B_{ij}(v, v_*, \sigma) f(v)g(v_*)\big[\psi\big(v'\big) - \psi(v)\big] \,\mathrm{d}\sigma \,\mathrm{d}v \,\mathrm{d}v_*, \qquad (11)
\end{aligned}$$

or

$$\begin{aligned}
&\int_{\mathbb{R}^3} Q^{\mathrm{b}}_{ij}(f, g)(v)\psi(v) \,\mathrm{d}v + \int_{\mathbb{R}^3} Q^{\mathrm{b}}_{ji}(g, f)(v)\phi(v) \,\mathrm{d}v \\
&\quad = -\frac{1}{2} \iint_{\mathbb{R}^3\times\mathbb{R}^3} \int_{\mathbb{S}^2} B_{ij}(v, v_*, \sigma)\big[f\big(v'\big)g\big(v'_*\big) - f(v)g(v_*)\big] \\
&\qquad \times \big[\psi\big(v'\big) + \phi\big(v'_*\big) - \psi(v) - \phi(v_*)\big] \,\mathrm{d}\sigma \,\mathrm{d}v \,\mathrm{d}v_*, \qquad (12)
\end{aligned}$$

for any $\psi, \phi : \mathbb{R}^3 \to \mathbb{R}$ such that the first integrals in (11)–(12) are well defined. Let us emphasize that (v, v') and (v_*, v'_*) are respectively associated to species $\mathcal{A}_i$ and $\mathcal{A}_j$. Equations (11)–(12) are obtained from (10) by using the same changes of variables $(v, v_*) \mapsto (v_*, v)$ and $(v, v_*) \mapsto (v', v'_*)$, as in the mono-species case.

The choice $\psi(v) = 1$ in (11) allows to recover the conservation of the total number of molecules of species $\mathcal{A}_i$. Moreover, if we set $\psi(v) = m_i v$ and $\phi(v_*) = m_j v_*$, and then $\psi(v) = m_i |v|^2/2$ and $\phi(v) = m_j |v_*|^2/2$, and plug those values in (12), we recover the conservation of the momentum and kinetic energy when species $\mathcal{A}_i$ and $\mathcal{A}_j$ are simultaneously considered, *i.e.*

$$\int_{\mathbb{R}^3} Q^{\mathrm{b}}_{ij}(f, g)(v) \begin{pmatrix} m_i v \\ m_i |v|^2/2 \end{pmatrix} \mathrm{d}v + \int_{\mathbb{R}^3} Q^{\mathrm{b}}_{ji}(g, f)(v) \begin{pmatrix} m_j v \\ m_j |v|^2/2 \end{pmatrix} \mathrm{d}v = 0. \qquad (13)$$

3.4 Boltzmann's Equations

The system of coupled equations satisfied by the set of unknowns $(f_i)_{1\le i\le I}$ is hence

$$\partial_t f_i + v\cdot\nabla_x f_i = Q_i^{\mathrm{m}}(f_i, f_i) + \sum_{j\neq i} Q_{ij}^{\mathrm{b}}(f_i, f_j) \quad \text{on } \mathbb{R}_+^* \times \Omega \times \mathbb{R}^3. \tag{14}$$

The conservation laws of mass, momentum and kinetic energy are guaranteed by the weak forms (9) and (12). The boundary conditions are not detailed here but they are chosen as specular reflections on $\partial\Omega$ to fit the macroscopic boundary conditions (4).

4 The Maxwell-Stefan Diffusion Limit

The Maxwell-Stefan equations describe a purely diffusive behaviour. Therefore, we cannot hope to deduce them only by scaling a kinetic model that, in principle, can describe also convection phenomena, without making any additional assumptions on the time evolution of the system and on the initial conditions.

In order to study the relationships between the kinetic system and the Maxwell-Stefan equations, we need to clearly identify the physical situation that leads to the Maxwell-Stefan cross diffusion phenomenon and impose to the kinetic system the same physical properties. We hence assume that the scaling on the kinetic equation allows the description of diffusion phenomena, *i.e.* we suppose that the Knudsen and the Mach numbers are of the same order of magnitude and that they can be considered very small. Moreover, we assume that

- there exists a uniform (in space) and constant (in time) temperature $T > 0$;
- for any time, the bulk velocity of the mixture is small and goes to zero in the vanishing Knudsen and Mach numbers limit.

4.1 Scaled Equation

From now on, let us focus on the Maxwell molecules case. It means that each cross section B_{ij} depends on v, v_* and σ only through the deviation angle $\theta \in [0,\pi]$ between $v - v_*$ and σ, and more precisely through its cosine. For each (i, j) with $i \neq j$, there exists a function $b_{ij} : [-1, 1] \to \mathbb{R}_+$ such that

$$B_{ij}(v, v_*, \sigma) = b_{ij}\left(\frac{v - v_*}{|v - v_*|}\cdot\sigma\right) = b_{ij}(\cos\theta).$$

We moreover assume that b_{ij} is even and that $b_{ij} \in L^1(-1, 1)$, following Grad's angular cutoff assumption. Thanks to the microreversibility assumption and because of the parity of b_{ji}, we note that

$$\begin{aligned} b_{ij}(\cos\theta) &= b_{ij}\left(\frac{v - v_*}{|v - v_*|}\cdot\sigma\right) = B_{ij}(v, v_*, \sigma) = B_{ji}(v_*, v, \sigma) \\ &= b_{ji}\left(\frac{v_* - v}{|v - v_*|}\cdot\sigma\right) = b_{ji}\left(\frac{v - v_*}{|v - v_*|}\cdot\sigma\right) = b_{ji}(\cos\theta), \end{aligned}$$

which ensures $b_{ij} = b_{ji}$.

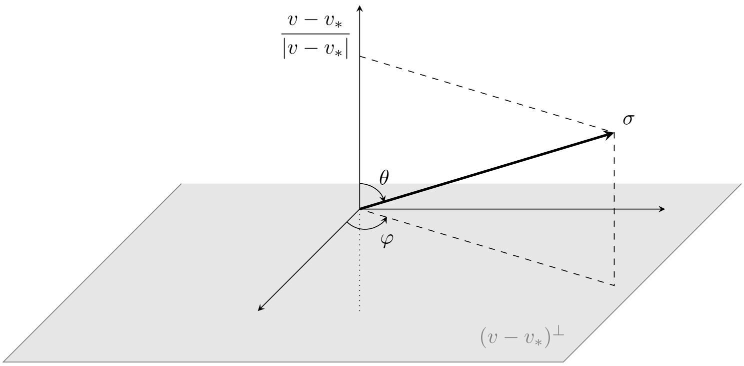

Fig. 1 Angular variables to describe $\sigma \in \mathbb{S}^2$

We here make no formal assumption about the mono-species cross section B_i, but it seems logical that each B_i satisfies the same properties as the bi-species cross sections.

For the readers' sake, let us introduce in Fig. 1 the other angular variable $\varphi \in [0, 2\pi]$, so that we can write the Euclidean coordinates of σ with respect to θ and φ, *i.e.*

$$\sigma_{(1)} = \sin\theta \cos\varphi, \qquad \sigma_{(2)} = \sin\theta \sin\varphi, \qquad \sigma_{(3)} = \cos\theta.$$

In the classical diffusive limit, the scaling is held by the mean free path $\varepsilon > 0$ and the corresponding unknowns in this regime are denoted $(f_i^\varepsilon)_{1\leq i\leq I}$. Each distribution function f_i^ε hence solves the scaled version of (14), that is

$$\varepsilon\partial_t f_i^\varepsilon + v\cdot\nabla_x f_i^\varepsilon = \frac{1}{\varepsilon} Q_i^{\mathrm{m}}\big(f_i^\varepsilon, f_i^\varepsilon\big) + \frac{1}{\varepsilon}\sum_{j\neq i} Q_{ij}^{\mathrm{b}}\big(f_i^\varepsilon, f_j^\varepsilon\big), \quad \text{on } \mathbb{R}_+^* \times \Omega \times \mathbb{R}^3. \tag{15}$$

Finally, we define $(c_i^\varepsilon)_{1\leq i\leq I}$ through (5), for each distribution function f_i^ε:

$$c_i^\varepsilon(t,x) = \int_{\mathbb{R}^3} f_i^\varepsilon(t,x,v)\,\mathrm{d}v, \quad t\geq 0, \quad x\in\Omega.$$

4.2 Ansatz

We assume that the initial conditions of the system of Boltzmann equations (15) are local Maxwellian functions, with small macroscopic velocity (since we are interested in a purely diffusive setting), *i.e.* the initial conditions have the form

$$\big(f_i^{\mathrm{in}}\big)^\varepsilon(x,v) = c_i^{\mathrm{in}}(x)\left(\frac{m_i}{2\pi kT}\right)^{3/2} e^{-m_i|v-\varepsilon u_i^{\mathrm{in}}(x)|^2/2kT}, \quad x\in\Omega, \quad v\in\mathbb{R}^3, \tag{16}$$

where $T>0$ is a fixed constant, and

$$c_i^{\mathrm{in}}:\Omega\to\mathbb{R}_+, \qquad u_i^{\mathrm{in}}:\Omega\to\mathbb{R}^3, \quad 1\leq i\leq I,$$

do not depend on ε. We moreover suppose that

$$\sum_{i=1}^I c_i^{\mathrm{in}} = 1 \quad \text{on } \Omega,$$

which of course implies that each c_i^{in} lies in [0, 1]. Since each $(f_i^{\mathrm{in}})^\varepsilon$ has the form (16), we immediately have, for any i,

$$\frac{1}{\varepsilon}\int_{\mathbb{R}^3} v\big(f_i^{\mathrm{in}}\big)^\varepsilon(x,v)\mathrm{d}v = c_i^{\mathrm{in}}(x)u_i^{\mathrm{in}}(x), \quad x\in\Omega.$$

We assume that the system evolution leaves the distribution functions in the local Maxwellian state, with the same constant and homogeneous temperature T. We hence suppose that there exist

$$c_i^\varepsilon : \mathbb{R}_+\times\Omega\to\mathbb{R}_+, \qquad u_i^\varepsilon : \mathbb{R}_+\times\Omega\to\mathbb{R}^3, \quad 1\le i\le I,$$

such that

$$f_i^\varepsilon(t,x,v) = c_i^\varepsilon(t,x)\left(\frac{m_i}{2\pi kT}\right)^{3/2} e^{-m_i|v-\varepsilon u_i^\varepsilon(t,x)|^2/2kT}, \quad t>0, \quad x\in\Omega, \quad v\in\mathbb{R}^3. \tag{17}$$

Since T is constant, the macroscopic equations should be obtained only through the conservation laws of mass and momentum. The moments of order 0 and 1 of each distribution function can be computed thanks to Ansatz (17):

$$\int_{\mathbb{R}^3} f_i^\varepsilon(t,x,v)\begin{pmatrix}1\\ v\end{pmatrix}\mathrm{d}v = \begin{pmatrix} c_i^\varepsilon(t,x)\\ \varepsilon c_i^\varepsilon(t,x)u_i^\varepsilon(t,x)\end{pmatrix}, \quad t>0, \quad x\in\Omega. \tag{18}$$

Note that the first moment of f_i^ε is of order 1 in ε since we focus on the diffusive asymptotics.

4.2.1 Matter Conservation

We first consider the moment of order 0 of the distribution functions. More precisely, for any i, we integrate (15) with respect to v in $\mathbb{R}^3$, and obtain, thanks to the conservation properties of the collisional operators,

$$\varepsilon\partial_t\left(\int_{\mathbb{R}^3} f_i^\varepsilon(t,x,v)\,\mathrm{d}v\right) + \nabla_x\cdot\left(\int_{\mathbb{R}^3} f_i^\varepsilon(t,x,v)v\,\mathrm{d}v\right) = 0.$$

Using (18), we get, for all $1\le i\le I$,

$$\partial_t c_i^\varepsilon + \nabla_x\cdot\big(c_i^\varepsilon u_i^\varepsilon\big) = 0. \tag{19}$$

4.2.2 Balance of Momentum

For $\ell\in\{1,2,3\}$, denote $w_{(\ell)}$ the ℓ-th component of any vector $w\in\mathbb{R}^3$. The balance law of momentum for a given species $\mathcal{A}_i$ is obtained by multiplying (15) by $v_{(\ell)}$ and integrating with respect to v in $\mathbb{R}^3$. We obtain, for any i and ℓ,

$$\begin{aligned}\varepsilon\partial_t\left(\int_{\mathbb{R}^3} v_{(\ell)} f_i^\varepsilon(v)\mathrm{d}v\right) + \nabla_x\cdot\left(\int_{\mathbb{R}^3} v_{(\ell)} f_i^\varepsilon(v)v\,\mathrm{d}v\right) &= \frac{1}{\varepsilon}\sum_{j\neq i}\int_{\mathbb{R}^3} v_{(\ell)} Q_{ij}^{\mathrm{b}}\big(f_i^\varepsilon, f_j^\varepsilon\big)(v)\,\mathrm{d}v\\ &:= \Theta_{(\ell)}^\varepsilon,\end{aligned} \tag{20}$$

because the term involving Q_i^{m} vanishes. Let us first focus on $\Theta^{\varepsilon}_{(\ell)}$, which depends on the set of independent variables (t,x). Thanks to (7) and (11) with $\psi(v)=v$, we can write

$$\Theta^{\varepsilon}_{(\ell)} = \frac{1}{\varepsilon}\sum_{j\neq i}\iint_{\mathbb{R}^6}\int_{\mathbb{S}^2} b_{ij}\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right) f_i^{\varepsilon}(v) f_j^{\varepsilon}(v_*)\big(v'_{(\ell)}-v_{(\ell)}\big)\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v$$

$$= \frac{1}{\varepsilon}\sum_{j\neq i}\frac{m_j}{m_i+m_j}\iint_{\mathbb{R}^6}\int_{\mathbb{S}^2} b_{ij}\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right) f_i^{\varepsilon}(v)$$

$$\times f_j^{\varepsilon}(v_*)(v_{*(\ell)}-v_{(\ell)}+|v-v_*|\sigma_{(\ell)})\,\mathrm{d}\sigma\,\mathrm{d}v_*\,\mathrm{d}v.$$

In the previous equality, the term containing $\sigma_{(\ell)}$ vanishes, because of the symmetry properties of B_{ij} with respect to σ. Indeed, both terms for $\ell=1$ or 2 are zero because

$$\int_0^{2\pi}\sin\varphi\,\mathrm{d}\varphi = \int_0^{2\pi}\cos\varphi\,\mathrm{d}\varphi = 0,$$

and the third one writes

$$\int_{\mathbb{S}^2} b_{ij}\left(\frac{v-v_*}{|v-v_*|}\cdot\sigma\right)\sigma_{(3)}\,\mathrm{d}\sigma = 2\pi\int_0^{\pi}\sin\theta\cos\theta\, b_{ij}(\cos\theta)\,\mathrm{d}\theta = 2\pi\int_{-1}^{1}\eta\, b_{ij}(\eta)\,\mathrm{d}\eta = 0,$$

because b_{ij} is even.

The remaining part of the expression of Θ^{ε} can then be written in terms of macroscopic quantities:

$$\Theta^{\varepsilon} = \varepsilon\sum_{j\neq i}\frac{2\pi m_j\|b_{ij}\|_{L^1}}{m_i+m_j}\big(c_i^{\varepsilon}c_j^{\varepsilon}u_j^{\varepsilon} - c_j^{\varepsilon}c_i^{\varepsilon}u_i^{\varepsilon}\big).$$

The time derivative in (20) can be evaluated by means of (18), so that (20) eventually becomes, for any $\ell\in\{1,2,3\}$ and any i,

$$\varepsilon^2\partial_t\big(c_i^{\varepsilon}(u_i^{\varepsilon})_{(\ell)}\big) + \nabla_x\cdot\left(\int_{\mathbb{R}^3} v_{(\ell)} f_i^{\varepsilon}(v) v\,\mathrm{d}v\right) = \sum_{j\neq i}\frac{2\pi m_j\|b_{ij}\|_{L^1}}{m_i+m_j}\big(c_i^{\varepsilon}c_j^{\varepsilon}(u_j^{\varepsilon})_{(\ell)} - c_j^{\varepsilon}c_i^{\varepsilon}(u_i^{\varepsilon})_{(\ell)}\big). \tag{21}$$

Let us now focus on the divergence term in (21). We successively write

$$\nabla_x\cdot\left(\int_{\mathbb{R}^3} v_{(\ell)} f_i^{\varepsilon}(v) v\,\mathrm{d}v\right) = \sum_{k=1}^{3}\frac{\partial}{\partial x_{(k)}}\int_{\mathbb{R}^3} v_{(\ell)}v_{(k)} f_i^{\varepsilon}(v)\,\mathrm{d}v$$

$$= \sum_{k=1}^{3}\frac{\partial}{\partial x_{(k)}}\int_{\mathbb{R}^3} c_i^{\varepsilon}\big(v_{(\ell)}+\varepsilon(u_i)^{\varepsilon}_{(\ell)}\big)\big(v_{(k)}+\varepsilon(u_i)^{\varepsilon}_{(k)}\big)$$

$$\times\left(\frac{m_i}{2\pi kT}\right)^{3/2} e^{-m_i|v|^2/2kT}\,\mathrm{d}v$$

$$= \sum_{k=1}^{3}\frac{\partial}{\partial x_{(k)}}\int_{\mathbb{R}^3} c_i^{\varepsilon}\big[\varepsilon^2(u_i^{\varepsilon})_{(\ell)}(u_i^{\varepsilon})_{(k)} + v_{(\ell)}{}^2\delta_{k\ell}\big]$$

$$\times \left(\frac{m_i}{2\pi kT}\right)^{3/2} e^{-m_i|v|^2/2kT}\, \mathrm{d}v$$

$$= \varepsilon^2 \sum_{k=1}^{3} \frac{\partial}{\partial x_{(k)}} \left[c_i^\varepsilon \left(u_i^\varepsilon\right)_{(\ell)} \left(u_i^\varepsilon\right)_{(k)}\right] + \frac{kT}{m_i} \frac{\partial c_i^\varepsilon}{\partial x_{(\ell)}}.$$

We finally obtain, from (21) and the previous equality,

$$\varepsilon^2\left[\partial_t\left(c_i^\varepsilon u_i^\varepsilon\right) + \nabla_x \cdot \left(c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon\right)\right] + \frac{kT}{m_i}\nabla_x c_i^\varepsilon = \sum_{j\neq i} \frac{2\pi m_j \|b_{ij}\|_{L^1}}{m_i + m_j}\left(c_i^\varepsilon c_j^\varepsilon u_j^\varepsilon - c_j^\varepsilon c_i^\varepsilon u_i^\varepsilon\right). \quad (22)$$

4.2.3 Macroscopic Equations and Formal Asymptotics

By putting together (19) and (22), we deduce that the Maxwellian functions (17) are solution of the initial-boundary value problem for the system of scaled Boltzmann equations (15) if $(c_i^\varepsilon, u_i^\varepsilon)$ solves

$$\partial_t c_i^\varepsilon + \nabla_x \cdot \left(c_i^\varepsilon u_i^\varepsilon\right) = 0, \quad (23)$$

$$\varepsilon^2 \frac{m_i}{kT}\left[\partial_t\left(c_i^\varepsilon u_i^\varepsilon\right) + \nabla_x \cdot \left(c_i^\varepsilon u_i^\varepsilon \otimes u_i^\varepsilon\right)\right] + \nabla_x c_i^\varepsilon = \sum_{j\neq i} \frac{c_i^\varepsilon c_j^\varepsilon u_j^\varepsilon - c_j^\varepsilon c_i^\varepsilon u_i^\varepsilon}{\Delta_{ij}}, \quad (24)$$

where

$$\Delta_{ij} = \frac{(m_i + m_j)kT}{2\pi\ m_i m_j \|b_{ij}\|_{L^1}}.$$

Note that the previous coefficients are symmetric with respect to each pair of species since $b_{ij} = b_{ji}$.

In the following, let us set

$$F_i^\varepsilon(t,x) = \frac{1}{\varepsilon}\int_{\mathbb{R}^3} v f_i^\varepsilon(t,x,v)\,\mathrm{d}v = c_i^\varepsilon(t,x) u_i^\varepsilon(t,x), \quad t \geq 0, \quad x \in \Omega,$$

and denote, as usual when dealing with formal diffusive limits, for any $t \geq 0$ and $x \in \Omega$,

$$c_i(t,x) = \lim_{\varepsilon\to 0^+} c_i^\varepsilon(t,x), \qquad F_i(t,x) = \lim_{\varepsilon\to 0^+} F_i^\varepsilon(t,x).$$

Hence, in the limit, Eqs. (19)–(22) give a system of equations, which has the following form for the density-flux set of unknown (c_i, F_i):

$$\partial_t c_i + \nabla_x \cdot F_i = 0,$$
$$-\nabla_x c_i = \sum_{j\neq i} \frac{c_j F_i - c_i F_j}{\Delta_{ij}}. \quad (25)$$

In order to recover the Maxwell-Stefan system, we still have to prove that c is constant in the limit.

Let us now write the kinetic energy conservation of the whole system before the asymptotics, at the kinetic level. We first observe that

$$\int_{\mathbb{R}^3} |v|^2 f_i^\varepsilon(v)\,\mathrm{d}v = 3\frac{kT}{m_i}c_i^\varepsilon + o(\varepsilon), \qquad \int_{\mathbb{R}^3} |v|^2 v f_i^\varepsilon(v)\,\mathrm{d}v = 5\varepsilon\frac{kT}{m_i}c_i^\varepsilon u_i^\varepsilon + o(\varepsilon). \quad (26)$$

Then we multiply (15) by $m_i|v|^2/2$, integrate with respect to $v \in \mathbb{R}^3$ and sum over i, to obtain, thanks to (9), (13) and (26),

$$3\partial_t\left(\sum_{i=1}^{I} c_i^\varepsilon\right) + 5\nabla_x \cdot \left(\sum_{i=1}^{I} c_i^\varepsilon u_i^\varepsilon\right) = o(1), \tag{27}$$

by keeping the lowest order term in ε. We formally perform the asymptotics $\varepsilon \to 0$ in (27) to simultaneously obtain, thanks to (19),

$$\partial_t c = 0 \quad \text{and} \quad \nabla_x \cdot \left(\sum_{i=1}^{I} F_i\right) = 0.$$

The second equality is obviously consistent with the boundary conditions (4) and the closure relationship (3). The first one ensures that $c = \sum c_i^{\text{in}} = 1$, which allows to recover (2) from (25):

$$\begin{cases} \partial_t c_i + \nabla_x \cdot F_i = 0 & \text{on } \mathbb{R}_+^* \times \Omega, \\ -c\nabla_x n_i = \dfrac{1}{c}\displaystyle\sum_{j\neq i} \dfrac{c_j F_i - c_i F_j}{D_{ij}} & \text{on } \mathbb{R}_+^* \times \Omega, \end{cases}$$

where $D_{ij} = \Delta_{ij}/c$ and has the physical dimension of a drag coefficient ($\text{m}^2\,\text{s}^{-1}$).

Remark The Euler system for mixtures (23)–(24) is composed of $4I$ independent scalar equations governing $4I$ unknown scalar functions. The limiting procedure implies that both first terms in (24) vanishes when ε goes to 0. That induces a singular perturbation in the limit: the Maxwell-Stefan system consists only of $(4I-3)$ scalar independent equations, as discussed in Sect. 2, and needs a closure relationship.

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