SOME REMARKS ABOUT THE SCALING OF SYSTEMS OF REACTIVE BOLTZMANN EQUATIONS

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Abstract. An asymptotics leading from the reactive Boltzmann equation towards reaction–diffusion equations has been introduced in [1] (cf. also [10], for an analogous scaling starting from reactive BGK equations). We propose here a justification of this asymptotics, at the formal level, based on a non–dimensional form of the original equations.

1. Introduction. Reaction–diffusion equations are widely used to describe the evolution of species which undergo chemical reactions and which are dispersed in an underlying fluid.

Those equations can be derived in some situations from a microscopic model (cf. [5]), but it is also possible to obtain them when one starts with a system of reactive Boltzmann equations (or from simpler kinetic models, like Fokker–Planck equations, cf. [9], reactive BGK equations, cf. [10], discrete velocity models, cf. [11]).

This is done in [1] under the assumption that the molecules of the reacting species collide between themselves, and also collide with the molecules of a “dominant” species, that is a species whose density is much larger than the density of the reactive species. As a consequence, it is assumed in this asymptotics that the density in the phase space of the “dominant” species is an absolute (that is, not depending on time and space) Maxwellian function of the velocity.

The whole procedure has then been extended to a more complicated physical situation, involving chemical irreversible processes of dissociation/recombination type, cf. [3], and mathematical properties of the final macroscopic reaction–diffusion system have been investigated by means of entropy methods, cf. [2].

The objective of this short note is to show that the asymptotics proposed in [1] can be obtained after putting the system of reactive Boltzmann equations in a non–dimensional form. It includes a proof (at the formal level) of the assumption on the density in the phase space of the “dominant” species described above.

In Section 2, notations are established, together with the system of reactive Boltzmann equations under study. Section 3 is devoted to the establishment of the
corresponding non-dimensional equations. Finally, Section 4 deals with the passage from reactive Boltzmann equations to macroscopic reaction–diffusion systems.

2. Notations and exposition of the kinetic model. We consider a mixture of an “inert” species $M$ and of four reactive species $(A_i)_{i=1,...,4}$, their density in the phase space being $\tilde{f}_M(\tilde{t},\tilde{x},\tilde{v}), \left(\tilde{f}_{A_i}(\tilde{t},\tilde{x},\tilde{v})\right)_{i=1,...,4}$. Here $\tilde{t}$, $\tilde{x}$ and $\tilde{v}$ denote the time, space and velocity variables. We assume that the four gases $A_1,\ldots,A_4$, besides all elastic collisions, are subject to the following bimolecular and reversible chemical reaction:

$$A_1 + A_2 \rightleftharpoons A_3 + A_4,$$

and, in order to avoid unessential constants, we take all particle masses equal to 1.

Then, the distribution functions satisfy the following system of Boltzmann equations:

$$\begin{cases}
\partial_t \tilde{f}_M + \tilde{v} \cdot \nabla \tilde{x} \tilde{f}_M = Q_{B,M}(\tilde{f}_M, \tilde{f}_M) + \sum_{j=1}^{4} Q_{B,Mj}(\tilde{f}_M, \tilde{f}_{A_j}), \\
\partial_t \tilde{f}_{A_i} + \tilde{v} \cdot \nabla \tilde{x} \tilde{f}_{A_i} = Q_{B,A_i}(\tilde{f}_{A_i}, \tilde{f}_M) + \sum_{j=1}^{4} Q_{B,A_ij}(\tilde{f}_{A_i}, \tilde{f}_{A_j}) + Q_{\text{chem}}(\tilde{f}_{A_i}, \tilde{f}_{A_j}, \tilde{f}_{A_k}, \tilde{f}_{A_l}),
\end{cases}$$

(1)

where $Q_B$ denotes the elastic Boltzmann operator with cross section $B$: for $f = f(\tilde{v}), g = g(\tilde{v})$,

$$Q_B(f,g)(\tilde{v}) = \int_{\tilde{v} \in \mathbb{R}^3} \int_{\tilde{\omega} \in S^2} B \left( |\tilde{v} - \tilde{v}_s|, \frac{\tilde{v} - \tilde{v}_s}{|\tilde{v} - \tilde{v}_s|} \cdot \tilde{\omega} \right) \left[ f(\tilde{v}')g(\tilde{v}_s') - f(\tilde{v})g(\tilde{v}_s) \right] d\tilde{v}_s d\tilde{\omega}. $$

(2)

Here, $(\tilde{v}, \tilde{v}_s)$ stand for the pre–collision velocities, while $(\tilde{v}', \tilde{v}_s')$ stand for the post–collision ones. Taking into account the conservations of momentum and of kinetic energy, $(\tilde{v}', \tilde{v}_s')$ can be expressed in terms of $(\tilde{v}, \tilde{v}_s)$ and of the unit vector $\tilde{\omega} \in S^2$ as

$$\begin{cases}
\tilde{v}' = \tilde{v} + (\tilde{\omega} \cdot (\tilde{v}_s - \tilde{v})) \tilde{\omega}, \\
\tilde{v}_s' = \tilde{v}_s - (\tilde{\omega} \cdot (\tilde{v}_s - \tilde{v})) \tilde{\omega}.
\end{cases}$$

(3)

Moreover, $Q_{\text{chem}}^i$ is the Boltzmann operator for reactive species, that we write here in the form proposed in [8, 7]. We assume the direct reaction $A_1 + A_2 \rightarrow A_3 + A_4$ to be endothermic, in the sense that, if $E_i$ denotes the chemical energy of species $i$, we suppose $\Delta E = E_3 + E_4 - E_1 - E_2 > 0$. Under this assumption, chemical operator for gas $A_1$ takes the form:

$$Q_{\text{chem}}^1(\tilde{f}_{A_1}, \tilde{f}_{A_2}, \tilde{f}_{A_3}, \tilde{f}_{A_4})(\tilde{v}) =$$

$$= \int_{\tilde{v}_s \in \mathbb{R}^3} \int_{\tilde{\omega} \in S^2} H \left( |\tilde{v} - \tilde{v}_s|^2 - 4 \Delta E \right) \tilde{E}_{\text{chem}} \left( |\tilde{v} - \tilde{v}_s|, \frac{\tilde{v} - \tilde{v}_s}{|\tilde{v} - \tilde{v}_s|} \cdot \tilde{\omega} \right)$$

$$\times \left[ f^3(\tilde{v}_s^{34})f^4(\tilde{v}_s^{34}) - f^1(\tilde{v})f^2(\tilde{v}_s) \right] d\tilde{v}_s d\tilde{\omega},$$

(4)

where $H$ denotes the unit step function, and represents a threshold for the endothermic reaction, that may occur only if the ingoing relative speed overcomes the
potential barrier $2\sqrt{\Delta E}$, and the velocities $\tilde{\nu}_{12}^{34}, \tilde{\nu}_{*12}^{34}$ are given by the formulas:

$$
\begin{align*}
\tilde{\nu}_{12}^{34} &= \frac{\tilde{\nu} + \tilde{\nu}_s}{2} + \frac{1}{2} \left( |\tilde{\nu} - \tilde{\nu}_s|^2 - 4 \Delta E \right)^{1/2} T_\varnothing \left( \frac{\tilde{\nu} - \tilde{\nu}_s}{|\tilde{\nu} - \tilde{\nu}_s|} \right), \\
\tilde{\nu}_{*12}^{34} &= \frac{\tilde{\nu} + \tilde{\nu}_s}{2} - \frac{1}{2} \left( |\tilde{\nu} - \tilde{\nu}_s|^2 - 4 \Delta E \right)^{1/2} T_\varnothing \left( \frac{\tilde{\nu} - \tilde{\nu}_s}{|\tilde{\nu} - \tilde{\nu}_s|} \right),
\end{align*}
$$

where

$$
T_\varnothing y = y - 2 (\tilde{\varnothing} \cdot y) \tilde{\varnothing}.
$$

Chemical operators for species 2, 3, 4 may be obtained from $Q_\text{chem}^{\beta}$ by suitable permutations of indices, bearing in mind that differential cross sections of direct and reverse reactions are related by the so-called microreversibility condition, cf. [8].

3. **Non-dimensional form of the equations.** We now denote by $T, X, \text{ and } V$ a typical time, space, and velocity of the problem under study, together with $F$ and $G$ a typical number density of the species $M$ and $(A_i)_{i=1,4}$ respectively. Finally, we consider $\beta$ and $\beta_\text{chem}$ a typical cross section for elastic and reactive collisions.

We introduce the rescaled densities

$$
f_M(t, x, v) = \frac{1}{F} \tilde{f}_M(\tilde{t}, \tilde{x}, \tilde{v}), \quad f_{A_i}(t, x, v) = \frac{1}{G} \tilde{f}_{A_i}(\tilde{t}, \tilde{x}, \tilde{v}),
$$

where

$$
\tilde{t} = T t, \quad \tilde{x} = X x, \quad \tilde{v} = V v,
$$

and

$$
\tilde{B} \left( |\tilde{v} - \tilde{v}_s|, \frac{\tilde{v} - \tilde{v}_s}{|\tilde{v} - \tilde{v}_s|} \cdot \tilde{\varnothing} \right) = \beta B \left( |v - v_s|, \frac{v - v_s}{|v - v_s|} \cdot \varnothing \right),
$$

$$
\tilde{\beta}_\text{chem} \left( |\tilde{v} - \tilde{v}_s|, \frac{\tilde{v} - \tilde{v}_s}{|\tilde{v} - \tilde{v}_s|} \cdot \tilde{\varnothing} \right) = \beta_\text{chem} \beta_\text{chem} \left( |v - v_s|, \frac{v - v_s}{|v - v_s|} \cdot \varnothing \right).
$$

Equations (1) become in non-dimensional form

$$
\begin{align*}
\frac{\partial f_M}{\partial t} + \frac{V T}{X} v \cdot \nabla_x f_M &= F \beta V^3 T Q_{B_{M,M}}(f_M, f_M) \\
&\quad + \sum_{j=1}^4 G \beta V^3 T Q_{B_{M,A_j}}(f_M, f_{A_j}), \\
\frac{\partial f_{A_i}}{\partial t} + \frac{V T}{X} v \cdot \nabla_x f_{A_i} &= F \beta V^3 T Q_{B_{A_i,M}}(f_{A_i}, f_M) \\
&\quad + \sum_{j=1}^4 G \beta V^3 T Q_{B_{A_i,A_j}}(f_{A_i}, f_{A_j}) \\
&\quad + G \beta_\text{chem} V^3 T Q_\text{chem}^{\beta_\text{chem}}(f_{A_1}, f_{A_2}, f_{A_3}, f_{A_4}).
\end{align*}
$$

The scaling that we propose can be understood in this way: first, $T, X, \text{ and } V$ are chosen in such a way that $\frac{V T}{X} = \frac{1}{2}$, then $F$ and $G$ are chosen in such a way that $F \beta V^3 T = \frac{1}{2}$, $G \beta V^3 T = \frac{1}{2}$ for some $\delta \in [0, 1]$ (this corresponds to the idea that $M$ is a dominant species in terms of concentration, i.e. $F \gg G$); finally $\beta_\text{chem}$ is chosen in such a way that $G \beta_\text{chem} V^3 T = 1$ (this corresponds to the fact that chemically reactive collisions are much rarer than elastic collisions, i.e. $\beta_\text{chem} \ll \beta$). Notice that in this scaling $T$ coincides essentially with a typical chemical relaxation time $(G \beta_\text{chem} V^3)^{-1}$, which turns out to be much larger than the macroscopic time $\frac{1}{V}$. 
\[O(\frac{1}{\varepsilon})\], and quite large \(O(\frac{1}{\varepsilon^2})\) also with respect to the elastic scattering relaxation time \((G\beta V^3)^{-1}\).

All in all, we impose
\[
\frac{VT}{\chi} = \frac{1}{\varepsilon} ; \quad F\beta V^3 T = \frac{1}{\varepsilon^2} ; \quad G\beta V^3 T = \frac{1}{\varepsilon^3} ; \quad G\beta^{\text{chem}} V^3 T = 1 . \tag{10}
\]

As a consequence, we end up with the following asymptotics (where \(f_M\) and \(f_A\) are renamed \(f_M^\varepsilon\) and \(f_A^\varepsilon\), and we recall that \(\delta \in [0,1]\)):
\[
\begin{align*}
\partial_t f_M^\varepsilon + \frac{1}{\varepsilon} \mathbf{v} \cdot \nabla_x f_M^\varepsilon &= \frac{1}{\varepsilon^2} Q_{B_M,M}(f_M^\varepsilon, f_M^\varepsilon) + \frac{1}{\varepsilon^4} \sum_{j=1}^{4} Q_{B_{M,j},j}(f_M^\varepsilon, f_M^\varepsilon), \\
\partial_t f_A^\varepsilon + \frac{1}{\varepsilon} \mathbf{v} \cdot \nabla_x f_A^\varepsilon &= \frac{1}{\varepsilon^2} Q_{B_{A,M},M}(f_A^\varepsilon, f_A^\varepsilon) + \frac{1}{\varepsilon^4} \sum_{j=1}^{4} Q_{B_{A,j},j}(f_A^\varepsilon, f_A^\varepsilon) + Q_{\text{chem}}(f_A^\varepsilon, f_A^\varepsilon). \\
\end{align*}
\tag{11}
\]

4. From reactive Boltzmann equations to reaction–diffusion. In this section, we do not try to deduce an expansion of \(f_M\) and \(f_A\) (with respect to \(\varepsilon\)) from (11), since this seems too ambitious. What we propose is rather to prove more modestly that a certain expansion satisfies (11) up to order \(o(1)\).

In order to do so, we shall suppose that the operator
\[
L_i : \{ f := f(\mathbf{v}) \} \mapsto \{ \mathbf{v} \mapsto M^{-1}(\mathbf{v}) Q_{B_{A,m}}(f M, M)(\mathbf{v}) \}, \tag{12}
\]
where
\[
M(\mathbf{v}) = \frac{1}{(2\pi T_M)^{3/2}} e^{-\frac{\mathbf{v}^2}{2 T_M}} \tag{13}
\]
for some constant \(T_M > 0\), satisfies
\[
\int_{\mathbb{R}^3} M(\mathbf{v}) g(\mathbf{v}) \, d\mathbf{v} = 0 \iff \exists \, q \text{ s.t. } \int_{\mathbb{R}^3} q(\mathbf{v}) M(\mathbf{v}) \, d\mathbf{v} = 0 \text{ and } L_i g = g. \tag{14}
\]

We denote then \(q = L_i^{-1} g\).

Note that this property is satisfied for a large class of cross sections (including hard potentials with angular cutoff) when suitable functional spaces are considered (cf. [4]).

Then, we introduce the expansion:
\[
\begin{align*}
f_M^\varepsilon(t, \mathbf{x}, \mathbf{v}) &= \rho_M M(\mathbf{v}), \\
f_A^\varepsilon(t, \mathbf{x}, \mathbf{v}) &= \left[\rho_i(t, \mathbf{x}) + \varepsilon q_i(t, \mathbf{x}, \mathbf{v}) + \varepsilon^2 r_i(t, \mathbf{x}, \mathbf{v})\right] M(\mathbf{v}), \tag{15}
\end{align*}
\]
where \(\rho_M > 0\) is an absolute constant, and
\[
q_i(t, \mathbf{x}, \mathbf{v}) = L_i^{-1}(\mathbf{v} \mapsto \nabla_\mathbf{x} \rho_i(t, \mathbf{x}) \frac{\rho_M}{\rho_M}), \tag{16}
\]
\[
r_i(t, \mathbf{x}, \mathbf{v}) = L_i^{-1} (\mathbf{v} \mapsto \partial_\mathbf{x} \rho_i(t, \mathbf{x}) + \mathbf{v} \cdot \nabla_\mathbf{x} q_i(t, \mathbf{x}, \mathbf{v}) - M^{-1}(\mathbf{v}) Q_i^{\text{chem}}(\rho_1(t, \mathbf{x}) M, \rho_2(t, \mathbf{x}) M, \rho_3(t, \mathbf{x}) M, \rho_4(t, \mathbf{x}) M) \frac{1}{\rho_M}). \tag{17}
\]

The fact that \(q_i\) and \(r_i\) are well-defined (that is, the l.h.s. of (14) is satisfied) is discussed below.
We first observe that
\[
\partial_t f_M + \frac{1}{\epsilon} \mathbf{v} \cdot \nabla_x f_M - \frac{1}{\epsilon^2} Q_{BM,M}(f_M^*, f_M) - \frac{1}{\epsilon^3} \sum_{j=1}^{4} Q_{B,A_j}(f_{A_j}^*, f_{A_j}) = O(\epsilon^{1-\delta}). \quad (18)
\]

Then,
\[
\partial_t f_{A_i}^\varepsilon + \frac{1}{\epsilon} \mathbf{v} \cdot \nabla_x f_{A_i}^\varepsilon - \frac{1}{\epsilon^2} Q_{B,A_{i\mu}}(f_{A_i}^\varepsilon, f_M^*) - \frac{1}{\epsilon^3} \sum_{j=1}^{4} Q_{B,A_j}(f_{A_j}^\varepsilon, f_{A_j})
\]
\[= (\partial_t \rho_i) M + O(\epsilon) + \frac{1}{\epsilon} (\mathbf{v} \cdot \nabla_x \rho_i) M + (\mathbf{v} \cdot \nabla_x q_i) M + O(\epsilon)
\]
\[- \frac{1}{\epsilon} Q_{B,A_{i\mu}}(q_i M, \rho_M M) - Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) + O(\epsilon^{1-\delta})
\]
\[= Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) + O(\epsilon). \quad (19)
\]

Using the form (16) of \(q_i\) (which is well defined since \(\int_{\mathbb{R}^3} v M(v) \, dv = 0\)), we get for the right hand side of (19):
\[(\partial_t \rho_i) M + (\mathbf{v} \cdot \nabla_x q_i) M - Q_{B,A_{i\mu}}(r_i M, \rho_M M) - Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) + O(\epsilon^{1-\delta}),
\]
which in turn gives
\[
\partial_t f_{A_i}^\varepsilon + \frac{1}{\epsilon} \mathbf{v} \cdot \nabla_x f_{A_i}^\varepsilon - \frac{1}{\epsilon^2} Q_{B,A_{i\mu}}(f_{A_i}^\varepsilon, f_M^*) - \frac{1}{\epsilon^3} \sum_{j=1}^{4} Q_{B,A_j}(f_{A_j}^\varepsilon, f_{A_j})
\]
\[= (\partial_t \rho_i) M + O(\epsilon) + \frac{1}{\epsilon} (\mathbf{v} \cdot \nabla_x \rho_i) M + (\mathbf{v} \cdot \nabla_x q_i) M + O(\epsilon)
\]
\[- \frac{1}{\epsilon} Q_{B,A_{i\mu}}(\rho_i M, \rho_M M) - Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) + O(\epsilon^{1-\delta})
\]
\[= Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) + O(\epsilon). \quad (20)
\]

thanks to the form (17) of \(r_i\). This form exists when
\[
\int_{\mathbb{R}^3} (M(v) \left\{ \partial_t \rho_i + \mathbf{v} \cdot \nabla_x q_i \right\} - Q_{i\mu}^{\text{chem}}(\rho_1 M, \rho_2 M, \rho_3 M, \rho_4 M) ) \, dv = 0,
\]
which is equivalent (cf. [1]) to the reaction–diffusion equation
\[
\partial_i \rho_i - d_i \Delta_x \rho_i = c \lambda_i \left( \gamma \rho_3 \rho_4 - \rho_1 \rho_2 \right), \quad (22)
\]
where \(\lambda = (1, 1, -1, -1)\) contains the stoichiometric coefficients, the \((d_i)_{i=1,...,4}\) are obtained by computing the solution of a linear Boltzmann equation (for the elastic interspecies kernel):
\[
d_i = \frac{1}{3 \rho_M} \int_{\mathbb{R}^3} M(v) \mathbf{v} \cdot L_i^{-1}(v \mapsto v) \, dv,
\]
\[
\gamma = \exp\left( \frac{\Delta E}{T_M} \right), \text{ and}
\]
\[
c = \int_{\mathbb{R}^3} \int_{\mathbb{R}^2} H R^{\text{chem}} M(v) M(v_*) \, dv \, dv_*, \, d\omega,
\]
where \(H\) denotes a suitably scaled unit step function. The same computation can be performed also for models taking into account the internal energy owned by the gases, cf. [7, 6]. Note that chemical contributions vanish only if number densities are related by the “mass action law” of chemical collision equilibrium, cf. [8].

Thanks to (18) and (20), we see that the expression (15)–(17), (22) satisfies the rescaled equations (11) up to order \(O(\epsilon^{1-\delta})\). We have therefore established at the
formal level the passage from a set of reactive Boltzmann equations to reaction diffusion equations under a suitable scaling.

The case $\delta = 1$ is of special interest: it does not seem possible to treat it with the method presented here, but it still leads to (the same) reaction-diffusion equations when the dominant species has a fixed density (cf. [1]).

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