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From collisional kinetic models to sprays: internal energy exchanges

Frédérique Charles, Laurent Desvillettes

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Abstract

In this paper, we present an improvement of the modeling of collisional operators introduced in [6] and [5], which are devoted to the modeling of the interaction between macroscopic dust particles and molecules of a rarefied gas. The model developed in [6] is based on the hypothesis that collisions between dust particles and gas molecules are inelastic and are given by a diffuse reflexion mechanism on the surface of dust particles. In the present work, we propose a model which preserves the total energy by introducing a new variable in the density function of macroscopic particles. We then write the equations in non-dimensional form, and establish, like in [10], a formal asymptotics to the Vlasov-Euler equation of compressible fluid when two small parameters tend to zero, namely the ratio of masses between gas molecules and dust particles on the one hand, and the Knudsen number of the gas on the other hand.

1 Introduction

Sprays are complex flows consisting of droplets or dust specks in suspension in a surrounding gas. They can be modeled by different types of equations (cf. [7]), including coupled systems of Euler-like equations (Eulerian-Eulerian modeling, cf. [12]), and fluid-kinetic couplings (Eulerian-Lagrangian modeling, cf. [14], [11] for early works on the subject). This work is devoted to this last type of modeling. It belongs to a series of papers aiming at linking fluid-kinetic models (more precisely, models displaying a coupling between a Vlasov equation and an Euler or Navier-Stokes system through a drag force) with fully kinetic systems (more precisely, couplings of equations of Boltzmann type). We refer to [8], [9] and [10] for the cases in which the fluid-kinetic model is respectively the incompressible Vlasov-Navier-Stokes system, the incompressible Vlasov-Stokes system, and the compressible Euler system. However, in all those papers, the temperature of the droplets/dust specks and its evolution (through exchanges with the temperature of the fluid) is not considered, whereas it constitutes a significant feature of the fluid-kinetic couplings appearing in engineering issues (cf. [1, 13] for example). Our intent is to present here a derivation of a typical fluid-kinetic system (that is, a compressible Vlasov-Euler system) in which the gas and the disperse phase are coupled not only by the drag force, but also by the exchange of temperature between the gas and the droplets/dust specks. This requires the establishment of nonstandard Boltzmann type equations, in

which collisions between molecules and macroscopic objects have an effect on the internal energy of the objects.

In section 2, we recall the model defined in [6], and propose a modification of this model in which the evolution of the temperature of the particles is taken into account. The unknowns of this modified model are the density function $f := f(t, x, w) \geq 0$ of gas molecules which at time t and point x possess the velocity w , and the density function $F(t, x, v, T) \geq 0$ of dust particles which at time t and point x possess the velocity v and the temperature T . The set of Boltzmann equations for F and f writes

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F = \mathcal{D}(F, f), \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}(F, f) + \mathcal{C}(f), \end{cases} \quad (1)$$

where \mathcal{C} is a collision operator for the molecules, and \mathcal{R}, \mathcal{D} are operators corresponding to collisions between molecules and dust particles.

In subsection 3.1, we present a non-dimensional version of those equations, which leads to the system

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F = \frac{1}{\eta} \mathcal{D}_\eta(F, f), \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}_\eta(F, f) + \frac{1}{\delta} \mathcal{C}(f), \end{cases} \quad (2)$$

where η is a ratio of mass, δ is a Knudsen number related to the molecules, and $\mathcal{R}_\eta, \mathcal{D}_\eta$ are non-dimensional versions of the operators \mathcal{R}, \mathcal{D} . Then we compute in subsections 3.2 and 3.3 the formal limit of this system when $\eta \rightarrow 0$ and $\delta \rightarrow 0$.

This limit leads to the following fluid-kinetic (compressible) Vlasov-Euler system:

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F - \nabla_v \cdot (bF) + \frac{\partial}{\partial T} (\gamma F) = 0, \\ \partial_t n_g + \operatorname{div}_x (n_g u_g) = 0, \\ \partial_t (n_g u_g) + \operatorname{div}_x \left(n_g u_g \otimes u_g + n_g \frac{\theta_g}{\beta^2} I \right) = \iint b(v, T) F(v, T) \, dv \, dT, \\ \partial_t \left(\frac{n_g |u_g|^2}{2} + \frac{3}{2} \frac{n_g \theta_g}{\beta^2} \right) + \operatorname{div}_x \left(\left(\frac{n_g |u_g|^2}{2} + \frac{5}{2} \frac{n_g \theta_g}{\beta^2} \right) u_g \right) \\ = \iint [b(v, T) \cdot v - c_p \gamma(v, T)] F(v, T) \, dv \, dT, \end{cases}$$

with b and γ representing the drag and the thermodynamical exchanges between the disperse phase and the gas.

2 A Boltzmann-type model for macroscopic particles in a gas

In this section, more precisely in subsection 2.2, we introduce a new fully kinetic model of Boltzmann type, in which the total energy is conserved, thanks to a

modification of the internal energy of the particles at each collision. This model is a modification of an older model which is briefly presented in subsection 2.1.

2.1 Model without evolution of the temperature of macroscopic particles

We recall that a Boltzmann-type model describing the evolution of aerosols was proposed in [6]. One assumes there that the particles are solid and spherical, of identical radius, and that the gas is monoatomic. One denotes by $F := F(t, x, v) \geq 0$ and $f := f(t, x, w) \geq 0$ the density functions of dust particles and of gas molecules at time $t \in \mathbb{R}^+$, at point $x \in \mathbb{R}^3$, and possessing the velocity $v \in \mathbb{R}^3$ or $w \in \mathbb{R}^3$. The model is obtained by coupling two Boltzmann-type equations :

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F = \mathcal{D}^1(F, f), & \text{(a)} \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}^1(F, f) + \mathcal{C}^1(f). & \text{(b)} \end{cases} \quad (3)$$

In (3), $\mathcal{C}^1(f)$ is the classical Boltzmann operator for monoatomic gases, describing interactions between molecules [4]:

$$\mathcal{C}^1(f)(w) = \int_{\mathbb{R}^3} \int_{S^2} [f(w'')f(w_*'') - f(w)f(w_*)] c \left(|w - w_*|, \frac{w - w_*}{|w - w_*|} \cdot \sigma \right) dw_* d\sigma,$$

with

$$(w'', w_*'') = \left(\frac{w + w_*}{2} + \frac{|w - w_*|}{2} \sigma, \frac{w + w_*}{2} - \frac{|w - w_*|}{2} \sigma \right). \quad (4)$$

The nonnegative function c describes the interactions between molecules and can be written as

$$c \left(|w - w_*|, \frac{w - w_*}{|w - w_*|} \cdot \omega \right) = \sigma_{gg} |w - w_*| b \left(|w - w_*|, \frac{w - w_*}{|w - w_*|} \cdot \sigma \right),$$

where $\sigma_{gg} = 4r_g^2$, r_g is the radius of a molecule, and b is a dimensionless function. We recall the properties of $\mathcal{C}^1(f)$ relative to the conservation of mass, momentum and kinetic energy (see [4]):

$$\int_{\mathbb{R}^3} \mathcal{C}^1(f)(w) \begin{pmatrix} 1 \\ w \\ |w|^2/2 \end{pmatrix} dw = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad (5)$$

and the case of equality in Boltzmann's H-theorem:

$$\mathcal{C}^1(f) = 0 \Leftrightarrow f = \mathcal{M}[n_g, u_g, \theta_g], \quad (6)$$

where

$$\mathcal{M}[n_g, u_g, \theta_g](w) := \frac{n_g \bar{\beta}^3}{(2\pi\theta_g)^{3/2}} e^{-\frac{\bar{\beta}^2 |w - u_g|^2}{2\theta_g}}, \quad (7)$$

with

$$n_g(t, x) := \int_{\mathbb{R}^3} f(t, x, w) dw, \quad u_g(t, x) := \frac{1}{n_g(t, x)} \int_{\mathbb{R}^3} f(t, x, w) w dw,$$

$$\theta_g(t, x) := \frac{\bar{\beta}^2}{3n_g(t, x)} \int_{\mathbb{R}^3} f(t, x, w) |w - u_g(t, x)|^2 dw.$$

In (7), the constant $\bar{\beta}$ is defined by

$$\bar{\beta} := \sqrt{\frac{m_g}{k_B}}, \quad (8)$$

where m_g is the mass of a molecule, and k_B is the Boltzmann constant.

In gas mixtures, the collision mechanism between two molecules of different masses can be described, when there is no internal energy or chemical reactions involved, by elastic collisions (see [3] and [5] for instance). In [6], a novel model was proposed, where collisions between dust particles and gas molecules are supposed to be inelastic and given by a diffuse reflexion mechanism on the surface of dust particles. This collision mechanism allows to take into account the macroscopic character of dust particles compared to gas molecules. This model is based on the following assumptions:

Hypothesis 2.1. *The total momentum is conserved during collisions between particles and molecules.*

Hypothesis 2.2. *In a collision between a particle and a molecule, the post-collisional relative velocity is picked from a half-Maxwellian distribution at the temperature of surface of the particle.*

This amounts to assume that a molecule touching a particle thermalizes with the molecules constituting the surface of the particle within a negligible time with respect to the other characteristic time scales. Then the post-collisional relative velocity is in the half space delimited by the tangent plane to the surface of the particle.

Hypothesis 2.3. *All dust particles have the same surface temperature, denoted T_{surf} , which is supposed to be a constant.*

Hypothesis 2.2 leads to the introduction, for $n \in \mathbb{S}^2$, of the density of probability h_n of the post-collisional relative velocities, given by

$$h_n(v) = \frac{1}{2\pi} \frac{\bar{\beta}^4}{T_{\text{surf}}^2} (n \cdot v) e^{-\frac{\bar{\beta}^2 |v|^2}{2T_{\text{surf}}}} \mathbf{1}_{\{n \cdot v \geq 0\}}, \quad (9)$$

where $\bar{\beta}$ has been defined in (8). One can check that

$$\forall n \in \mathbb{S}^2 \quad \int_{\mathbb{R}^3} h_n(v) dv = 1. \quad (10)$$

Hypothesis 2.1 allows to express the post-collisional velocities of a particle v' and a molecule w' , in terms of $z := w' - v'$. Indeed,

$$(v', w') = \Gamma_d(v, w, z), \quad (11)$$

with

$$\begin{cases} \Gamma_d(v, w, z)_1 := \frac{v + \eta w}{1 + \eta} - \frac{\eta}{1 + \eta} z, \\ \Gamma_d(v, w, z)_2 := \frac{v + \eta w}{1 + \eta} + \frac{1}{1 + \eta} z, \end{cases} \quad (12)$$

where $\eta = \frac{m_g}{m_p}$ is the ratio of mass between a molecule and a particle. Then the post-collisional velocities can be seen as random variables \mathbf{v}' and \mathbf{w}' given by $(\mathbf{v}', \mathbf{w}') = \Gamma_d(v, w, \mathbf{z})$, where \mathbf{z} has the density of probability h_n . Moreover, we made the following assumptions on the collision cross section.

Hypothesis 2.4. *The collision cross section between a particle and a molecule is the hard sphere cross-section.*

Under these assumptions, the expressions of these operators \mathcal{D}^1 and \mathcal{R}^1 were established in [6]. They can be written in the following form (for the sake of readability, we thereafter omit the t and x variables) :

$$\begin{aligned} \mathcal{D}^1(F, f)(v) &= \sigma_{gp} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left[F(v')f(w')e^{\frac{\beta^2|v'-w'|^2}{2T_{\text{surf}}}} - F(v)f(w)e^{\frac{\beta^2|v-w|^2}{2T_{\text{surf}}}} \right] \\ &\quad \times e^{-\frac{\beta^2|v-w|^2}{2T_{\text{surf}}}} \zeta(v-w, n)h_n(z)dn \, dz \, dw, \end{aligned} \quad (13)$$

and

$$\begin{aligned} \mathcal{R}^1(F, f)(w) &= \sigma_{gp} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} \left[F(v')f(w')e^{\frac{\beta^2|v'-w'|^2}{2T_{\text{surf}}}} - F(v)f(w)e^{\frac{\beta^2|v-w|^2}{2T_{\text{surf}}}} \right] \\ &\quad \times e^{-\frac{\beta^2|v-w|^2}{2T_{\text{surf}}}} \zeta(v-w, n)h_n(z)dn \, dz \, dv, \end{aligned} \quad (14)$$

where the term

$$\zeta(v-w, n) := [n \cdot (v-w)] \mathbb{1}_{\{n \cdot (v-w) \geq 0\}} \quad (15)$$

comes from Hypothesis 2.4, and $(v', w') = \Gamma_d(v, w, z)$. The constant $\sigma_{gp} = (r_g + r_p)^2$, where r_p is the radius of a particle and r_g the radius of a molecule, comes from the collision cross section.

We can introduce the transformation

$$\tilde{\Gamma}_d : \begin{pmatrix} v \\ w \\ z \end{pmatrix} \rightarrow \begin{pmatrix} v' \\ w' \\ w-v \end{pmatrix} = \begin{pmatrix} \frac{1}{1+\eta}[v + \eta w - \eta z] \\ \frac{1}{1+\eta}[v + \eta w + z] \\ w-v \end{pmatrix} \quad (16)$$

which is an involution. Then we can obtain the following expressions of the weak forms of $\mathcal{D}^1(F, f)$ and $\mathcal{R}^1(F, f)$:

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathcal{D}^1(F, f)(v)\varphi(v)dv \\ &= \sigma_{gp} \iiint [\varphi(v') - \varphi(v)] F(v)f(w)\zeta(v-w, n)h_n(z)dz \, dn \, dw \, dv, \end{aligned} \quad (17)$$

and

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathcal{R}^1(F, f)(w)\psi(w)dw \\ &= \sigma_{gp} \iiint [\psi(w') - \psi(w)] F(v)f(w)\zeta(v-w, n)h_n(z)dz \, dn \, dv \, dw, \end{aligned} \quad (18)$$

for all test functions φ and ψ ($\varphi, \psi \in \mathcal{C}_c(\mathbb{R}^3)$).

Remark 1. In [6], the model is slightly more general since it corresponds to a mixture of gases and a collection of particles of various radiuses. The density function of particles writes therefore $F := F(t, x, v, r)$, where the variable $r \in [r_{\min}, r_{\max}]$ corresponds to the radius of particles. We assume here, for the sake of simplicity, that all particles have the same radius (this is called monodispersion in the vocabulary of sprays). However, the model proposed in Section 2.2 can easily be extended to the case of a density function F depending on the radius r .

2.2 Model with evolution of the temperature of macroscopic particles

We propose here an improvement of the modeling, based on the modification of Hypothesis 2.3. We introduce the temperature of surface T of dust particles as a variable in the density function F . Then $F(t, x, v, T)$ represents at time $t \in \mathbb{R}^+$ the number density of dust particles at point $x \in \mathbb{R}^3$, possessing the velocity $v \in \mathbb{R}^3$, and whose surface temperature is T . We consider that a dust particle of temperature of surface T has an internal energy, given by

$$e := \bar{c}_p m_p T = \frac{m_g}{\eta} \bar{c}_p T,$$

where \bar{c}_p corresponds to the thermal capacity of the material constituting the particles, and m_p is the mass of a given particle (this amounts to identifying the temperature of surface of the particles with their mean temperature).

2.2.1 The collisional mechanism

We assume that, during a collision between a dust particle of velocity v and surface temperature T and a molecule of velocity w , Hypothesis 2.1, 2.2 are still verified, but Hypothesis 2.3 is replaced by the following Assumption:

Hypothesis 2.5. *We assume that the temperature of surface of the dust particle is modified (within a negligible time with respect to the other characteristic time scales) in such way that the total energy (sum of the kinetic energy of the system particle-molecule and the internal energy of the particle) is conserved.*

Then if we consider a collision between a particle of velocity v , temperature T , and a molecule of velocity w , we call the postcollisional values v' , T' , and w' respectively. Hypothesis 2.5 leads to the following relation of conservation of energy:

$$|v'|^2 + \eta|w'|^2 + 2\bar{c}_p T' = |v|^2 + \eta|w|^2 + 2\bar{c}_p T. \quad (19)$$

Proposition 1. *Assuming Hypothesis 2.1 and Hypothesis 2.2, the post-collisional temperature of surface of a particle is given by*

$$T' = T + \frac{1}{2\bar{c}_p} \frac{\eta}{1 + \eta} \left[|v - w|^2 - |v' - w'|^2 \right]. \quad (20)$$

Proof. The equation of conservation of momentum

$$v' + \eta w' = v + \eta w \quad (21)$$

implies that

$$\begin{cases} v' = \frac{v + \eta w}{1 + \eta} - \frac{\eta}{1 + \eta}(w' - v'), \\ w' = \frac{v + \eta w}{1 + \eta} + \frac{1}{1 + \eta}(w' - v'), \end{cases}$$

and then

$$\begin{aligned} v'^2 + \eta w'^2 &= \frac{(v + \eta w)^2}{1 + \eta} + \frac{\eta^2 + \eta}{(1 + \eta)^2} |w' - v'|^2 \\ &= \frac{1}{1 + \eta} \left[|v|^2 + \eta^2 |w|^2 - \eta (|v - w|^2 - |v|^2 - |w|^2) + \eta |w' - v'|^2 \right] \\ &= |v|^2 + \eta |w|^2 + \frac{\eta}{1 + \eta} \left[|w' - v'|^2 - |v - w|^2 \right]. \end{aligned}$$

Finally equation (19) implies

$$2\bar{c}_p(T' - T) = v^2 + \eta w^2 - v'^2 - \eta w'^2 = \frac{\eta}{1 + \eta} \left[|v - w|^2 - |w' - v'|^2 \right].$$

□

Moreover, we still assume that the collisional mechanism follows Hypothesis 2.2. We now denote, for $T > 0$,

$$h_{n,T}(v) = \frac{\bar{\beta}^4 (n \cdot v)}{2\pi T^2} \exp\left(-\frac{\bar{\beta}^2 |v|^2}{2T}\right) \mathbb{1}_{\{n \cdot v \geq 0\}}, \quad (22)$$

where $\bar{\beta}$ is defined by (8), the density of probability of the random variable \mathbf{z} corresponding to the post-collisional relative velocity. Thanks to the conservation of momentum (21), the post-collisional velocities v' and w' are still given by the expressions (11), (12). Moreover, thanks to Proposition 1, the post-collisional temperature of the particle is a random variable linked to \mathbf{z} by

$$\mathbf{T}' = T + \frac{1}{2\bar{c}_p} \frac{\eta}{1 + \eta} [|v - w|^2 - |\mathbf{z}|^2]. \quad (23)$$

Note that relation (23) allows in principle to get zero or sub-zero post-collisional temperatures, which is not acceptable from a physical point of view. The probability for a particle to have a temperature which becomes negative is however small, indeed when the temperature of surface of a particle approaches zero, the probability that the temperature will decrease further is close to zero, as shown by the following Proposition:

Proposition 2. *Let $\Delta \mathbf{T} = \mathbf{T}' - T$ be the difference between the post and pre-collisional temperatures of surface of the particle during a collision. We assume that $v \neq w$. Then we have*

$$\lim_{T \rightarrow 0^+} \mathbb{P}(\Delta \mathbf{T} < 0) = 0.$$

Proof. Thanks to expression (23), we have

$$\mathbb{P}(\Delta \mathbf{T} < 0) = \mathbb{P}(|\mathbf{z}|^2 > |v - w|^2),$$

and the Markov inequality implies that

$$\mathbb{P}(|\mathbf{z}|^2 > |v - w|^2) \leq \frac{\mathbb{E}(|\mathbf{z}|^2)}{|v - w|^2}.$$

Moreover, we have (see [5] for details, or (51))

$$\mathbb{E}(|\mathbf{z}|^2) = \int_{\mathbb{R}^3} |z|^2 h_{n,T}(z) dz = \frac{4T}{\beta^2},$$

which proves the claim. \square

Remark 2. *The Hypothesis $v \neq w$ in Proposition 2 is reasonable since $\zeta(v - w, n) = 0$ when $v = w$, so that the probability of collision between a particle and a molecule of same velocity is equal to zero.*

2.2.2 Construction of the operators

We now construct the collisional operators $\mathcal{D}(F, f)$ and $\mathcal{R}(F, f)$ associated to this collisional mechanism. We first establish the weak form of those operators.

Proposition 3. *Let φ and ψ be test functions. Then*

$$\begin{aligned} & \iint \mathcal{D}(F, f)(v, T) \varphi(v, T) dv dT \\ &= \sigma_{gp} \iiint \int [\varphi(v', T') - \varphi(v, T)] F(v, T) f(w) \zeta(v - w, n) h_{n,T}(z) dz dn dw dv dT, \end{aligned} \quad (24)$$

and

$$\begin{aligned} & \int \mathcal{R}(F, f)(w) \psi(w) dw \\ &= \sigma_{gp} \iiint \int [\psi(w') - \psi(w)] F(v, T) f(w) \zeta(v - w, n) h_{n,T}(z) dz dn dv dw dT, \end{aligned} \quad (25)$$

where ζ is defined by (15), $(v', w') = \Gamma_d(v, w, z)$, and

$$T' = T + \frac{1}{2\bar{c}_p} \frac{\eta}{1 + \eta} (|v - w|^2 - |z|^2). \quad (26)$$

Proof. Since $\int_{\mathbb{R}^3} h_{n,T}(v) dv = 1$ for all $n \in \mathbb{S}^2$, the loss term $\mathcal{D}^-(F, f)(v, T)$ can be expressed, like in [6], as

$$\mathcal{D}^-(F, f)(v, T) = \sigma_{gp} \iiint F(v, T) f(w) \zeta(v - w, n) h_{n,T}(z) dz dn dw.$$

The gain term can be expressed as

$$\begin{aligned} & \mathcal{D}^+(F, f)(v, T) \\ &= \sigma_{gp} \iiint F(v^\circ, T^\circ) f(w^\circ) \zeta(v^\circ - w^\circ, n) g_{v^\circ, w^\circ, n, T^\circ}(v, T) dn dw^\circ dv^\circ dT^\circ \end{aligned}$$

where $g_{v^\circ, w^\circ, n, T^\circ}$ is the density of the couple of random variables (\mathbf{v}, \mathbf{T}) which corresponds to the velocity and the temperature of surface of a particle after a

collision between a particle of velocity v° and temperature T° and a molecule of velocity w° . The expressions of \mathbf{v} and \mathbf{T} are

$$\begin{cases} \mathbf{v} = (\Gamma_d(v^\circ, w^\circ, \mathbf{z}))_1 = \frac{v^\circ + \eta w^\circ}{1 + \eta} - \frac{\eta}{1 + \eta} \mathbf{z}, \\ \mathbf{T} = T^\circ + \frac{1}{2\bar{c}_p} \frac{\eta}{1 + \eta} (|v^\circ - w^\circ|^2 - |\mathbf{z}|^2), \end{cases} \quad (27)$$

where Γ_d is defined in (12) and where \mathbf{z} is a random variable of \mathbb{R}^3 which has a density of probability h_{n, T° . Let v°, w°, n and T° be fixed and let's determine $g_{v^\circ, w^\circ, n, T^\circ}$. We can write $(\mathbf{v}, \mathbf{T}) = \lambda_{v^\circ, w^\circ}(\mathbf{z}, T^\circ)$, with

$$\lambda_{v^\circ, w^\circ} : (z, s) \mapsto \left((\Gamma_d(v^\circ, w^\circ, z))_1, s + \frac{1}{2\bar{c}_p} \frac{\eta}{1 + \eta} (|v^\circ - w^\circ|^2 - |z|^2) \right),$$

and where the density of \mathbf{z} is h_{n, T° . The mapping $\lambda_{v^\circ, w^\circ}$ is a \mathcal{C}^1 -diffeomorphism, and the Jacobian of $\lambda_{v^\circ, w^\circ}^{-1}$ is equal to $\left(\frac{1+\eta}{\eta}\right)^3$. Then

$$g_{v^\circ, w^\circ, n, T^\circ}(v, T) = \left(\frac{1+\eta}{\eta}\right)^3 h_{n, T^\circ}(z) \delta_{T^\circ}(s), \quad \text{with } (z, s) = \lambda_{v^\circ, w^\circ}^{-1}(v, T).$$

Then, using in

$$\iint \mathcal{D}^+(F, f)(v, T) \varphi(v, T) dv dT$$

the change of variables

$$(v, T, v^\circ, T^\circ, w^\circ) \rightarrow (z, s, v^\circ, T^\circ, w^\circ), \quad \text{with } (z, s) = \lambda_{v^\circ, w^\circ}^{-1}(v, T),$$

of Jacobian equal to $\left(\frac{\eta}{1+\eta}\right)^3$, we get

$$\begin{aligned} & \iint \mathcal{D}^+(F, f)(v, T) \varphi(v, T) dv dT \\ &= \sigma_{gp} \iiint F(v^\circ, T^\circ) f(w^\circ) \zeta(v^\circ - w^\circ, n) h_{n, T^\circ}(z) \delta_{T^\circ}(s) \\ & \quad \times \varphi(\lambda_{v^\circ, w^\circ}(z, s)) dw^\circ dv^\circ dn dT^\circ dz ds \\ &= \sigma_{gp} \iiint F(v, T) f(w) \zeta(v - w, n) h_{n, T}(z) \varphi(\lambda_{v, w}(z, T)) dn dw dv dz dT, \end{aligned}$$

which proves the claim.

The establishment of the weak form of $\mathcal{R}(F, f)$ is very similar to the case of the operator $\mathcal{R}^1(F, f)$ introduced in Section 1. We have

$$\mathcal{R}^+(F, f)(w) = \sigma_{gp} \iiint F(v^\circ, T^\circ) f(w^\circ) \zeta(v^\circ - w^\circ, n) m_{v^\circ, w^\circ, n}(z) dw^\circ dv^\circ dn dT^\circ,$$

where $m_{v^\circ, T^\circ, w^\circ, n}$ corresponds to the density of probability of the post-collisional velocity \mathbf{w} of a molecule of velocity w° after a collision with a particle of velocity v° and temperature of surface T° . Since $\mathbf{w} = (\Gamma_d(v^\circ, w^\circ, \mathbf{z}))_2 = \frac{1}{1+\eta}(v^\circ + \eta w^\circ +$

\mathbf{z}) (Γ_d has been defined in (12)), where \mathbf{z} is a random variable of \mathbb{R}^3 which has a density of probability h_{n,T° , we have

$$m_{v^\circ, T^\circ, w^\circ, n}(w) = (1 + \eta)^3 h_{n, T^\circ}((1 + \eta)w - v^\circ - \eta w^\circ),$$

and thus the change of variable

$$(w, v^\circ, T^\circ, w^\circ) \rightarrow (z, v^\circ, T^\circ, w^\circ), \quad \text{with } z = (1 + \eta)w - v^\circ - \eta w^\circ$$

in

$$\int_{\mathbb{R}^3} \mathcal{R}^+(F, f)(w) \psi(w) dw,$$

leads to

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}^+(F, f)(w) \psi(w) dw \\ &= \sigma_{gp} \iiint F(v^\circ, T^\circ) f(w^\circ) \varsigma(v^\circ - w^\circ, n) h_{n, T^\circ}(z) \psi(w') dz dn dw^\circ dv^\circ dT^\circ, \end{aligned}$$

which allows to obtain expression (25). \square

Corollary 1. *We have the following conservation of mass, momentum and total energy:*

$$\iint \mathcal{D}(F, f)(v, T) \begin{pmatrix} 1 \\ v \\ |v|^2/2 + \bar{c}_p T \end{pmatrix} dv dT + \int \mathcal{R}(F, f)(w) \begin{pmatrix} 1 \\ \eta w \\ \eta |w|^2/2 \end{pmatrix} dw = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}. \quad (28)$$

Proof. It is a direct consequence of the relation of conservation of mass, momentum (21), and energy (19), and the weak forms (24) and (25) of the operators \mathcal{D} and \mathcal{R} . \square

We now express the operators in strong form.

Proposition 4. *Let $\mathcal{D}(F, f)$ and $\mathcal{R}(F, f)$ be the collision operators given in weak form by (24) and (25). They can be expressed as*

$$\begin{aligned} \mathcal{D}(F, f)(v, T) &= \frac{\bar{\beta}^4 \sigma_{gp}}{2\pi} \iiint \varsigma(z, n) \varsigma(v - w, n) \\ &\times \left[F(v', T') f(w') \frac{1}{T'^2} e^{-\frac{\bar{\beta}^2}{2T'} |v-w|^2} - F(v, T) f(w) \frac{1}{T^2} e^{-\frac{\bar{\beta}^2}{2T} |v'-w'|^2} \right] dz dn dw, \end{aligned} \quad (29)$$

and

$$\begin{aligned} \mathcal{R}(F, f)(w) &= \frac{\bar{\beta}^4 \sigma_{gp}}{2\pi} \iiint \varsigma(z, n) \varsigma(v - w, n) \\ &\times \left[F(v', T') f(w') \frac{1}{T'^2} e^{-\frac{\bar{\beta}^2}{2T'} |v-w|^2} - F(v, T) f(w) \frac{1}{T^2} e^{-\frac{\bar{\beta}^2}{2T} |v'-w'|^2} \right] dz dn dv dT, \end{aligned} \quad (30)$$

where v' , w' , and T' are given by (11), (12), and (26) respectively.

Proof. We consider in the weak expression of $\mathcal{D}^+(F, f)$ the following change of variables:

$$(v, w, z, T) \rightarrow (v', w', u, T'),$$

where $(v', w', u) = \tilde{\Gamma}_d(v, w, z)$ given by (16), and T' is given by (26). This transformation is involutive and its Jacobian is equal to 1. Then

$$\begin{aligned} & \iint \mathcal{D}^+(F, f)(v, T) \varphi(v, T) dv dT \\ &= \sigma_{gp} \iiint F(v, T) f(w) \zeta(v - w, n) h_{n, T}(z) \varphi(v', T') dn dz dw dv dT, \\ &= \sigma_{gp} \iiint F(v, T) f(w) \zeta(v - w, n) h_{n, T}(w' - v') \varphi(v', T') dn du dw' dv' dT', \\ &= \sigma_{gp} \iiint F(v', T') f(w') \zeta(v' - w', n) h_{n, T'}(w - v) \varphi(v, T) dn dz dw dv dT, \\ &= \sigma_{gp} \iiint F(v', T') f(w') \zeta(w' - v', -n) h_{-n, T'}(v - w) \varphi(v, T) dn dz dw dv dT, \end{aligned}$$

and we obtain, since $z = w' - v'$ and with the change of variable $n \mapsto -n$,

$$\mathcal{D}^+(F, f)(v, T) = \sigma_{gp} \iiint F(v', T') f(w') \zeta(z, n) h_{n, T'}(v - w) dn dz dw,$$

and finally we get (29). Computations are similar for (30). \square

3 Asymptotic expansion

3.1 Dimensionless Boltzmann system

In order to perform the asymptotic analysis of system (3), we first introduce a dimensionless version of it. As in [10], we assume here that the aerosol is associated to a length scale L . Moreover, following the approach of [5], we first make the following scaling hypothesis.

Hypothesis 3.1. *We assume that the thermal speed of gas molecules and particles are of the same order of magnitude, denoted by V .*

We define \mathcal{N}_g and \mathcal{N}_p , the typical density number per volume unit of gas molecules and particles respectively (in m^{-3}), and we recall that we denote $\sigma_{gg} = 4r_g^2$, $\sigma_{gp} = (r_g + r_p)^2$, $\sigma_{pp} = 4r_p^2$ the collisional cross sections (up to the constant π) between species (in m^2).

We define a dimensionless position variable $\hat{x} = x/L$, dimensionless velocity variables $\hat{w} = w/V$ and $\hat{v} = v/V$ for molecules and particles, a dimensionless time variable $\hat{t} = tV/L$, and a dimensionless temperature variable $\hat{T} = T/T_{\text{ref}}$. We then define a dimensionless density function for each species :

$$\hat{F}(\hat{t}, \hat{x}, \hat{v}, \hat{T}) = \frac{1}{F^\circ} F(t, x, v, T), \quad \text{and} \quad \hat{f}(\hat{t}, \hat{x}, \hat{w}) = \frac{1}{f^\circ} f(t, x, w),$$

with

$$F^\circ = \frac{\mathcal{N}_p}{V^3 T_{\text{ref}}}, \quad \text{and} \quad f^\circ = \frac{\mathcal{N}_g}{V^3}.$$

Then the left-hand side terms of system (3) become

$$\begin{aligned}\frac{\partial F}{\partial t} + v \cdot \nabla_x F &= \frac{F^\circ V}{L} \left(\frac{\partial \hat{F}}{\partial \hat{t}} + \hat{v} \cdot \nabla_{\hat{x}} \hat{F} \right), \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f &= \frac{f^\circ V}{L} \left(\frac{\partial \hat{f}}{\partial \hat{t}} + \hat{w} \cdot \nabla_{\hat{x}} \hat{f} \right).\end{aligned}$$

The collision operators $\mathcal{D}(F, f)$, $\mathcal{R}(F, f)$ and $\mathcal{C}(f)$ are scaled in the following way

$$\begin{aligned}\mathcal{D}(F, f) &= F^\circ f^\circ \sigma_{gp} V^4 \hat{\mathcal{D}}(\hat{F}, \hat{f}), \\ \mathcal{R}(F, f) &= F^\circ f^\circ \sigma_{gp} V^4 T_{\text{ref}} \hat{\mathcal{R}}(\hat{F}, \hat{f}), \\ \mathcal{C}(f) &= (f^\circ)^2 \sigma_{gg} V^4 \hat{\mathcal{C}}(\hat{f}),\end{aligned}\tag{31}$$

where $\hat{\mathcal{D}}(\hat{F}, \hat{f})$, $\hat{\mathcal{R}}(\hat{F}, \hat{f})$, $\hat{\mathcal{C}}(\hat{f})$ are the dimensionless versions of $\mathcal{D}(F, f)$, $\mathcal{R}(F, f)$ and $\mathcal{C}(f)$ (note that $\bar{\beta}^2 V^2 / T_{\text{ref}}$ is a dimensionless constant) :

$$\begin{aligned}\hat{\mathcal{D}}(\hat{F}, \hat{f})(\hat{v}, \hat{T}) &= \frac{1}{2\pi} \frac{\bar{\beta}^4 V^4}{T_{\text{ref}}^2} \iiint \varsigma(\hat{z}, n) \varsigma(\hat{v} - \hat{w}, n) \\ &\times \left[\hat{F}(\hat{v}', \hat{T}') \hat{f}(\hat{w}') \frac{1}{\hat{T}'^2} e^{-\frac{\bar{\beta}^2 V^2}{T_{\text{ref}}} \frac{|\hat{v} - \hat{w}|^2}{2\hat{T}'}} - \hat{F}(\hat{v}, \hat{T}) \hat{f}(\hat{w}) \frac{1}{\hat{T}^2} e^{-\frac{\bar{\beta}^2 V^2}{T_{\text{ref}}} \frac{|\hat{v}' - \hat{w}'|^2}{2\hat{T}}} \right] d\hat{z} dn d\hat{w},\end{aligned}$$

where

$$\hat{T}' = \hat{T} + \frac{1}{2\hat{c}_p} \frac{\eta}{1 + \eta} (|\hat{v} - \hat{w}|^2 - |\hat{z}|^2)\tag{32}$$

with $\hat{c}_p = \bar{c}_p \frac{T_{\text{ref}}}{V^2}$,

$$\begin{aligned}\hat{\mathcal{R}}(\hat{F}, \hat{f})(\hat{w}) &= \frac{1}{2\pi} \frac{\bar{\beta}^4 V^4}{T_{\text{ref}}^2} \iiint \varsigma(\hat{z}, n) \varsigma(\hat{v} - \hat{w}, n) \\ &\times \left[\hat{F}(\hat{v}', \hat{T}') \hat{f}(\hat{w}') \frac{1}{\hat{T}'^2} e^{-\frac{\bar{\beta}^2 V^2}{T_{\text{ref}}} \frac{|\hat{v} - \hat{w}|^2}{2\hat{T}'}} - \hat{F}(\hat{v}, \hat{T}) \hat{f}(\hat{w}) \frac{1}{\hat{T}^2} e^{-\frac{\bar{\beta}^2 V^2}{T_{\text{ref}}} \frac{|\hat{v}' - \hat{w}'|^2}{2\hat{T}}} \right] d\hat{z} dn d\hat{v} d\hat{T}, \\ \hat{\mathcal{C}}(\hat{f})(\hat{w}) &= \int_{\mathbb{R}^3} \int_{S^2} \left[\hat{f}(\hat{w}'') \hat{f}(\hat{w}_*') - \hat{f}(\hat{w}) \hat{f}(\hat{w}_*) \right] |\hat{w} - \hat{w}_*| b \left(|\hat{w} - \hat{w}_*|, \frac{\hat{w} - \hat{w}_*}{|\hat{w} - \hat{w}_*|} \right) d\hat{w}_* d\sigma.\end{aligned}$$

We don't express here the collision operator $\hat{\mathcal{B}}(\hat{F})$ but as in (31), we can write

$$\mathcal{B}(F) = (F^\circ)^2 \sigma_{pp} V^4 T_{\text{ref}} \hat{\mathcal{B}}(\hat{F})$$

where $\hat{\mathcal{B}}(\hat{F})$ is the dimensionless version of $\mathcal{B}(F)$.

We finally obtain the following dimensionless system

$$\begin{cases} \frac{\partial \hat{F}}{\partial \hat{t}} + \hat{v} \cdot \nabla_{\hat{x}} \hat{F} = \sigma_{gp} L \mathcal{N}_g \hat{\mathcal{D}}(\hat{F}, \hat{f}) + \sigma_{pp} L \mathcal{N}_p \hat{\mathcal{B}}(\hat{F}), \\ \frac{\partial \hat{f}}{\partial \hat{t}} + \hat{w} \cdot \nabla_{\hat{x}} \hat{f} = \sigma_{gp} L \mathcal{N}_p \hat{\mathcal{R}}(\hat{F}, \hat{f}) + \sigma_{gg} L \mathcal{N}_g \hat{\mathcal{C}}(\hat{f}). \end{cases}\tag{33}$$

We study the system in the limit of small mass ratio (that is, $\eta \rightarrow 0$) and in the fluid limit for the gas. We therefore introduce

$$\delta := \frac{1}{L \mathcal{N}_g \sigma_{gg}},\tag{34}$$

which is a dimensionless number corresponding to the ratio between the characteristic length L and the mean free path (up to a constant) of the gas (taking into account only the collisions between molecules of the gas). Following [10], we first make the following assumption:

Hypothesis 3.2. *The frequency of collisions between particles is such that*

$$\sigma_{pp} L \mathcal{N}_p \ll 1,$$

so that we can formally neglect the term $\sigma_{pp} L \mathcal{N}_p \hat{\mathcal{B}}(\hat{F})$ in system (33).

As in [5], we set $\sigma_{gp} L \mathcal{N}_p = 1$, which corresponds to studying the asymptotic of the system at the time scale of the collisions between gas molecules and particles, seen from the point of view of molecules. To express the frequency of collisions between particles and gas molecules, from the point of view of particles, we make, like in [10], the following assumption:

Hypothesis 3.3. *The ratio of density between particles and molecules is identical to the mass ratio between molecules and particles, that is*

$$\frac{\mathcal{N}_p}{\mathcal{N}_g} = \eta.$$

Moreover, we need to make an assumption on the order of magnitude of the temperature of surface of the dust particles:

Hypothesis 3.4. *We assume that the ratio between the kinetic temperature of the gas and the temperature of surface of dust particles is of order 1. We denote*

$$\hat{\beta} := \bar{\beta} \frac{V}{\sqrt{T_{\text{ref}}}} = \sqrt{\frac{m_g V^2}{k_B T_{\text{ref}}}}, \quad (35)$$

the square root of the ratio between these two temperatures, which corresponds to a dimensionless version of the constant $\bar{\beta}$.

Defining

$$h_{n,T}(v) := \frac{\hat{\beta}^4}{2\pi} \frac{(n \cdot v)}{T^2} \exp\left(-\frac{\hat{\beta}^2 |v|^2}{2T}\right) \mathbf{1}_{\{n \cdot v \geq 0\}}, \quad (36)$$

we can rewrite

$$\begin{aligned} \hat{\mathcal{D}}(\hat{F}, \hat{f})(\hat{v}, \hat{T}) &= \iiint \left[\varsigma(\hat{z}, n) h_{n, \hat{T}'}(\hat{v} - \hat{w}) \hat{F}(\hat{v}', \hat{T}') \hat{f}(\hat{w}') \right. \\ &\quad \left. - \varsigma(\hat{v} - \hat{w}, n) h_{n, \hat{T}}(\hat{z}) \hat{F}(\hat{v}, \hat{T}) \hat{f}(\hat{w}) \right] d\hat{z} dn d\hat{w}, \end{aligned} \quad (37)$$

where

$$\hat{T}' = \hat{T} + \frac{1}{2\hat{c}_p} \frac{\eta}{1 + \eta} (|\hat{v} - \hat{w}|^2 - |\hat{z}|^2), \quad (38)$$

$$\begin{aligned} \hat{\mathcal{R}}(\hat{F}, \hat{f})(\hat{w}) &= \iiint \left[\varsigma(\hat{z}, n) h_{n, \hat{T}'}(\hat{v} - \hat{w}) \hat{F}(\hat{v}', \hat{T}') \hat{f}(\hat{w}') \right. \\ &\quad \left. - \varsigma(\hat{v} - \hat{w}, n) h_{n, \hat{T}}(\hat{z}) \hat{F}(\hat{v}, \hat{T}) \hat{f}(\hat{w}) \right] d\hat{z} dn d\hat{v} d\hat{T}'. \end{aligned} \quad (39)$$

We thus study the asymptotic regime of the following system (where we drop hats on all dimensionless variables, functions, operators, on \hat{c}_p and $\hat{\beta}$) when $\eta \rightarrow 0$ and $\delta \rightarrow 0$:

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F = \frac{1}{\eta} \mathcal{D}_\eta(F, f), & \text{(a)} \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}_\eta(F, f) + \frac{1}{\delta} C(f), & \text{(b)} \end{cases} \quad (40)$$

where $\mathcal{D}_\eta(F, f)$ and $\mathcal{R}_\eta(F, f)$ are the dimensionless versions of (29) and (30) given by formulas (37) and (39), which write after all hats are dropped in the following way:

$$\begin{aligned} \mathcal{D}(F, f)(v, T) = & \iiint \left[\varsigma(z, n) h_{n, T'}(v - w) F(v', T') f(w') \right. \\ & \left. - \varsigma(v - w, n) h_{n, T}(z) F(v, T) f(w) \right] dz dn dw, \end{aligned} \quad (41)$$

$$\begin{aligned} \mathcal{R}(F, f)(w) = & \iiint \left[\varsigma(z, n) h_{n, T'}(v - w) F(v', T') f(w') \right. \\ & \left. - \varsigma(v - w, n) h_{n, T}(z) F(v, T) f(w) \right] dz dn dv dT, \end{aligned} \quad (42)$$

where ς is defined by (15), $(v', w') = \Gamma_d(v, w, z)$ is defined in (12) , T' is given by

$$T' = T + \frac{1}{2c_p} \frac{\eta}{1 + \eta} (|v - w|^2 - |z|^2), \quad (43)$$

and h_n is redefined (dropping hats on β) as

$$h_{n, T}(v) = \frac{\beta^4}{2\pi} \frac{(n \cdot v)}{T^2} \exp\left(-\frac{\beta^2 |v|^2}{2T}\right) \mathbf{1}_{\{n \cdot v \geq 0\}}. \quad (44)$$

Note also that the weak forms of $\mathcal{D}_\eta(F, f)$, $\mathcal{R}_\eta(F, f)$ write, for φ and ψ test functions,

$$\begin{aligned} & \int_0^{+\infty} \int_{\mathbb{R}^3} \mathcal{D}_\eta(F, f)(v, T) \varphi(v, T) dv dT \\ &= \iiint \left[\varphi(v', T') - \varphi(v, T) \right] F(v, T) f(w) \varsigma(v - w, n) h_{n, T}(z) dz dn dw dv dT, \end{aligned} \quad (45)$$

and

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}_\eta(F, f)(w) \psi(w) dw \\ &= \iiint \left[\psi(w') - \psi(w) \right] F(v, T) f(w) \varsigma(v - w, n) h_{n, T}(z) dz dn dv dw dT. \end{aligned} \quad (46)$$

3.2 Limit $\eta \rightarrow 0$

We first perform an asymptotic expansion of $\mathcal{D}_\eta(F, f)$ according to the mass ratio η .

Proposition 5. *We have*

$$\mathcal{D}_\eta(F, f) = \eta a(F, f) + O(\eta^2),$$

with

$$\begin{aligned} a(F, f)(v, T) := & \pi \nabla_v \cdot \left(F(v, T) \int_{\mathbb{R}^3} \left(|w - v| + \frac{\sqrt{2\pi T}}{3\beta} \right) (v - w) f(w) dw \right) \\ & + \frac{\pi}{2c_p} \frac{\partial}{\partial T} \left[\left(\frac{4T}{\beta^2} I_{f,1}(v) - I_{f,3}(v) \right) F(v, T) \right], \end{aligned}$$

where we denote

$$I_{f,1}(t, x, v) := \int_{\mathbb{R}^3} |w - v| f(t, x, w) dw \quad (47)$$

and

$$I_{f,3}(t, x, v) := \int_{\mathbb{R}^3} |w - v|^3 f(t, x, w) dw. \quad (48)$$

Proof. Let $\varphi(v, T)$ be a test function. Thanks to the weak form (45) of $\mathcal{D}(F, f)$ and to the asymptotic expansion of φ ,

$$\varphi(v', T') - \varphi(v, T) = (v' - v) \cdot \nabla_v \varphi(v, T) + (T' - T) \partial_T \varphi(v, T) + o(|v' - v| + |T' - T|).$$

We split the weak form of \mathcal{D}_η into two parts :

$$\iint \mathcal{D}_\eta(F, f)(v, T) \varphi(v, T) dv dT = A + B,$$

where A includes the gradient w.r.t. v , and B includes the derivative w.r.t. T .

Computations for the term A are similar to the asymptotic expansion made in [6] for the model with a constant temperature of surface of particles. Using (11) and the following results (see [5]):

$$\int_{\mathbb{R}^3} h_{n,T}(z) dz = 1, \quad \int_{\mathbb{R}^3} z h_{n,T}(z) dz = \frac{\sqrt{\pi T}}{\sqrt{2}\beta} n, \quad (49)$$

$$\int_{\mathbb{S}^2} \varsigma(s, n) dn = \pi |s|, \quad \int_{\mathbb{S}^2} n \varsigma(s, n) dn = \frac{2\pi}{3} s, \quad (50)$$

we get

$$\begin{aligned} A &= \iiint \iiint (v' - v) \cdot \nabla_v \varphi(v, T) F(v, T) f(w) \varsigma(v - w, n) h_{n,T}(z) dv dw dz dn dT \\ &= \frac{\eta}{1 + \eta} \iiint \iiint (w - v) \cdot \nabla_v \varphi(v, T) F(v, T) f(w) \varsigma(v - w, n) dv dw dn dT \\ &\quad - \frac{\eta}{1 + \eta} \iiint \iiint \cdot \nabla_v \varphi(v, T) F(v, T) f(w) \varsigma(v - w, n) h_{n,T}(z) dv dw dz dn dT \\ &= \eta \pi \iint \nabla_v \cdot \left[\int \left(|w - v| + \frac{\sqrt{2\pi T}}{3\beta} \right) (v - w) f(w) dw F(v, T) \right] \varphi(v, T) dv dT \\ &\quad + O(\eta^2). \end{aligned}$$

For the computation of the term B , we use (26), (49), (50) and

$$\int_{\mathbb{R}^3} |z|^2 h_{n,T}(z) dz = \frac{4T}{\beta^2}, \quad (51)$$

and we get

$$\begin{aligned} B &= \iiint (T' - T) \frac{\partial \varphi}{\partial T}(v, T) \zeta(v - w, n) h_{n,T}(z) F(v, T) f(w) dv dw dz dn dT \\ &= B_1 + B_2, \end{aligned}$$

with

$$\begin{aligned} B_1 &:= \frac{1}{2c_p} \frac{\eta}{1 + \eta} \iiint |v - w|^2 \zeta(v - w, n) h_{n,T}(z) \frac{\partial \varphi}{\partial T}(v, T) F(v, T) f(w) dv dw dz dn dT \\ &= \frac{\pi}{2c_p} \frac{\eta}{1 + \eta} \iint |v - w|^3 \frac{\partial \varphi}{\partial T}(v, T) F(v, T) f(w) dv dw dT \\ &= \frac{-\pi\eta}{2c_p} \iint \frac{\partial F}{\partial T}(v, T) \left(\int |v - w|^3 f(w) dw \right) \varphi(v, T) dv dT + O(\eta^2), \end{aligned}$$

and

$$\begin{aligned} B_2 &:= \frac{-1}{2c_p} \frac{\eta}{1 + \eta} \iiint |z|^2 \zeta(v - w, n) h_{n,T}(z) \frac{\partial \varphi}{\partial T}(v, T) F(v, T) f(w) dv dw dz dn dT \\ &= \frac{-\pi}{c_p} \frac{\eta}{1 + \eta} \iint \frac{2T}{\beta^2} |v - w| \frac{\partial \varphi}{\partial T}(v, T) F(v, T) f(w) dv dw dT \\ &= \frac{2\pi\eta}{c_p \beta^2} \iint \frac{\partial}{\partial T} (TF(v, T)) \left(\int |v - w| f(w) dw \right) \varphi(v, T) dv dT + O(\eta^2). \end{aligned}$$

□

We then obtain a formal limit when $\eta \rightarrow 0$ of equations of (40). If we denote $(f^{\delta, \eta}, F^{\delta, \eta})$ a solution of (40), then (formally) $(f^{\delta, \eta}, F^{\delta, \eta}) \rightarrow (f^\delta, F^\delta)$, solution of

$$\begin{cases} \frac{\partial F}{\partial t} + v \cdot \nabla_x F - \pi \nabla_v \cdot \left(F(v, T) \int \left(|v - w| + \frac{\sqrt{2\pi T}}{3\beta} \right) (v - w) f(w) dw \right) \\ \quad - \frac{\pi}{2c_p} \frac{\partial}{\partial T} \left[\left(\frac{4T}{\beta^2} I_{f,1}(v) - I_{f,3}(v) \right) F(v, T) \right] = 0, & (a) \\ \frac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}^l(F, f) + \frac{1}{\delta} C(f), & (b) \end{cases} \quad (52)$$

with $I_{f,1}$ and $I_{f,3}$ defined by (47) and (48). Moreover, \mathcal{R}^l writes in weak form as

$$\begin{aligned} &\int_{\mathbb{R}^3} \mathcal{R}^l(F, f)(w) \psi(w) dw \\ &= \iiint [\psi(w'^l) - \psi(w)] F(v, T) f(w) \zeta(v - w, n) h_{n,T}(z) dz dn dv dw, \end{aligned} \quad (53)$$

with $w'^l = \lim_{\eta \rightarrow 0} \Gamma_d(v, w, z)_2 = v + z$ (remember that Γ_d is defined in (12)).

3.3 Limit $\delta \rightarrow 0$

We now pass to the limit when $\delta \rightarrow 0$ in (52) in order to obtain a fluid-kinetic model (Vlasov-Euler equation) which includes exchanges of internal energy between the phases. Thanks to property (6), we see that if (f^δ, F^δ) is a solution of (52), then (at a formal level) $f^\delta \rightarrow \mathcal{M}[n_g, u_g, \theta_g]$ defined by (7). Like in [10], we introduce the following notations, for $a \in \mathbb{R}^3$:

$$q(a) := \int_{\mathbb{R}^3} (a - y)|a - y|e^{-\frac{|y|^2}{2}} \frac{dy}{(2\pi)^{3/2}},$$

$$q_0(a) := \int_{\mathbb{R}^3} |a - y|e^{-\frac{|y|^2}{2}} \frac{dy}{(2\pi)^{3/2}},$$

and

$$q_3(a) := \int_{\mathbb{R}^3} |a - y|^3 e^{-\frac{|y|^2}{2}} \frac{dy}{(2\pi)^{3/2}}.$$

The function q can be expressed under the following form (see [10]):

$$q(a) = a \tilde{q}(|a|). \quad (54)$$

Moreover, we observe that it is possible to write, for some smooth functions \tilde{q}_0, \tilde{q}_3 ,

$$q_0(a) = q_0(0) + |a|^2 \tilde{q}_0(|a|), \quad q_3(a) = q_3(0) + |a|^2 \tilde{q}_3(|a|), \quad (55)$$

with

$$q_0(0) = 2\sqrt{\frac{2}{\pi}}, \quad q_3(0) = 4q_0(0). \quad (56)$$

3.3.1 Equation for the particles

We first establish the limit of equation (52)-(a). Straightforward computations allow to express the terms involved in (52)-(a) according to the quantities q_0 , and q . On one hand, we have

$$\int |v - w|(v - w) \mathcal{M}[n_g, u_g, \theta_g](w) dw = n_g \frac{\theta_g}{\beta^2} q \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right), \quad (57)$$

and

$$\int (v - w) \mathcal{M}[n_g, u_g, \theta_g](w) dw = n_g(v - u_g), \quad (58)$$

which allow to express the term “in ∇_v .” in the limit of eq. (52) - (a), thanks to (54) :

$$\begin{aligned} & \pi \int \left(|v - w| + \frac{\sqrt{2\pi T}}{3\beta} \right) (v - w) \mathcal{M}[n_g, u_g, \theta_g](w) dw \\ &= \pi n_g \frac{\theta_g}{\beta^2} q \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right) + \pi n_g \frac{\sqrt{2\pi T}}{3\beta} (v - u_g) \\ &= \pi n_g (v - u_g) \left(\sqrt{\frac{\theta_g}{\beta^2}} \tilde{q} \left(\left| \frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right| \right) + \frac{\sqrt{2\pi T}}{3\beta} \right). \end{aligned}$$

Then, we compute the limit of the term “in $\frac{\partial}{\partial T}$ ” in the limit of eq. (52) - (a). We first observe that

$$I_{\mathcal{M}[n_g, u_g, \theta_g], 1}(v) = n_g \sqrt{\frac{\theta_g}{\beta^2}} q_0 \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right), \quad (59)$$

$$I_{\mathcal{M}[n_g, u_g, \theta_g], 3}(v) = n_g \left(\frac{\theta_g}{\beta^2} \right)^{3/2} q_3 \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right), \quad (60)$$

and then, thanks to (55) and (56) :

$$\begin{aligned} & - \frac{\pi}{2c_p} \left(\frac{4T}{\beta^2} I_{\mathcal{M}[n_g, u_g, \theta_g], 1}(v) - I_{\mathcal{M}[n_g, u_g, \theta_g], 3}(v) \right) \\ &= - \frac{\pi}{2c_p} n_g \sqrt{\frac{\theta_g}{\beta^2}} \left[\frac{4T}{\beta^2} q_0 \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right) - \frac{\theta_g}{\beta^2} q_3 \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right) \right] \\ &= - \frac{\pi}{2c_p} n_g \sqrt{\frac{\theta_g}{\beta^2}} \left[8\sqrt{\frac{2}{\pi}} \frac{(T - \theta_g)}{\beta^2} + |v - u_g|^2 \left(\frac{4T}{\theta_g} \tilde{q}_0 \left(\frac{|v - u_g|}{\sqrt{\theta_g/\beta^2}} \right) - \tilde{q}_3 \left(\frac{|v - u_g|}{\sqrt{\theta_g/\beta^2}} \right) \right) \right] \end{aligned}$$

As a consequence, we can express the limit of (52)-(a) when $\delta \rightarrow 0$. It writes

$$\frac{\partial F}{\partial t} + v \cdot \nabla_x F - \nabla_v \cdot (bF) + \frac{\partial}{\partial T} (\gamma F) = 0, \quad (61)$$

with

$$b(v, T) := \pi n_g (v - u_g) \left(\sqrt{\frac{\theta_g}{\beta^2}} \tilde{q} \left(\left| \frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right| \right) + \frac{\sqrt{2\pi T}}{3\beta} \right), \quad (62)$$

and

$$\gamma(v, T) := \frac{\pi}{2c_p} n_g \sqrt{\frac{\theta_g}{\beta^2}} \left[8\sqrt{\frac{2}{\pi}} \frac{(\theta_g - T)}{\beta^2} + |v - u_g|^2 S \left(\frac{|v - u_g|}{\sqrt{\theta_g/\beta^2}} \right) \right], \quad (63)$$

where

$$S(r) := \tilde{q}_3(r) - 4 \frac{T}{\theta_g} \tilde{q}_0(r).$$

Expression (62) corresponds to the drag force between the two phases of the mixture, while expression (63) highlights the energy exchange between those two phases. We further comment those expressions (and compare them with a typical macroscopic model) at the end of the paper.

3.3.2 Equations for the gas

By integrating equation (52)-(b) against 1, w and $|w|^2/2$ and taking the limit $\eta \rightarrow 0$, we obtain the local (in time and space) conservation laws for the mass, momentum and kinetic energy :

$$\begin{aligned} & \partial_t \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ w \\ |w|^2/2 \end{pmatrix} \mathcal{M}[n_g, u_g, \theta_g](w) dw + \operatorname{div}_x \left(\int_{\mathbb{R}^3} w \begin{pmatrix} 1 \\ w \\ |w|^2/2 \end{pmatrix} \mathcal{M}[n_g, u_g, \theta_g](w) dw \right) \\ &= \int_{\mathbb{R}^3} \begin{pmatrix} 1 \\ w \\ |w|^2/2 \end{pmatrix} \mathcal{R}^l(F, \mathcal{M}[n_g, u_g, \theta_g])(w) dw. \end{aligned} \quad (64)$$

First equation Thanks to the weak form (53) of \mathcal{R}^l , we first see that

$$\int_{\mathbb{R}^3} \mathcal{R}^l(F, \mathcal{M}[n_g, u_g, \theta_g])(w) dw = 0,$$

which leads to the equation of conservation of mass for the gas

$$\partial_t n_g + \operatorname{div}_x(n_g u_g) = 0. \quad (65)$$

Second equation We can compute, thanks to (50) and (49), the other integrals :

$$\begin{aligned} & \int_{\mathbb{R}^3} \mathcal{R}^l(F, \mathcal{M}[n_g, u_g, \theta_g])(w) w dw \\ &= \iiint \int (v + z - w) F(v, T) \mathcal{M}[n_g, u_g, \theta_g](w) \varsigma(v - w, n) h_{n, T}(z) dz dn dv dT dw \\ &= \pi \iint F(v, T) \int (v - w) |v - w| \mathcal{M}[n_g, u_g, \theta_g](w) dw dv dT \\ &\quad + \frac{\pi \sqrt{2\pi T}}{3\beta} \iiint F(v, T) \mathcal{M}[n_g, u_g, \theta_g](w) (v - w) dv dT dw \\ &= \pi n_g \frac{\theta_g}{\beta^2} \iint F(v, T) q \left(\frac{v - u_g}{\sqrt{\theta_g/\beta^2}} \right) dv dT + n_g \frac{\pi \sqrt{2\pi T}}{3\beta} \iint F(v, T) (v - u_g) dv dT \\ &= \iint b(v, T) F(v, T) dv dT, \end{aligned}$$

with b given by (62). We get thus the equation for the evolution of momentum for the gas:

$$\partial_t(n_g u_g) + \operatorname{div}_x(n_g u_g \otimes u_g + n_g \frac{\theta_g}{\beta^2} I) = \iint b(v, T) F(v, T) dv dT. \quad (66)$$

Note that this equation can be easily recovered by using the conservation of momentum and eq. (61) - (62).

Third equation In order to avoid tedious computations, we start from the conservation of total energy before passing to the limit when $\eta, \delta \rightarrow 0$, that is

$$\iint \mathcal{D}_\eta(F, f)(v, T) \left(\frac{|v|^2}{2} + c_p T \right) dv dT + \eta \int \mathcal{R}_\eta(F, f)(w) \frac{|w|^2}{2} dw = 0.$$

After passing to the limit $\eta, \delta \rightarrow 0$, we see that

$$\iint a(F, \mathcal{M}[n_g, u_g, \theta_g])(v, T) \left(\frac{|v|^2}{2} + c_p T \right) dv dT + \int \mathcal{R}^l(F, \mathcal{M}[n_g, u_g, \theta_g])(w) \frac{|w|^2}{2} dw = 0.$$

Noticing that

$$a(F, \mathcal{M}[n_g, u_g, \theta_g])(v, T) = \nabla_v \cdot (b F) - \frac{\partial}{\partial T}(\gamma F),$$

we see that

$$\begin{aligned}
& \int \mathcal{R}^l(F, \mathcal{M}[n_g, u_g, \theta_g])(w) \frac{|w|^2}{2} dw \\
&= - \iint a(F, \mathcal{M}[n_g, u_g, \theta_g])(v, T) \left(\frac{|v|^2}{2} + c_p T \right) dv dT \\
&= \iint \left[b(v, T) \cdot v - c_p \gamma(v, T) \right] F(v, T) dv dT.
\end{aligned}$$

We thus obtain the equation for the evolution of the total energy of the gas:

$$\begin{aligned}
& \partial_t \left(\frac{n_g |u_g|^2}{2} + \frac{3}{2} \frac{n_g}{\beta^2} \theta_g \right) + \operatorname{div}_x \left(\left(\frac{n_g |u_g|^2}{2} + \frac{5}{2} \frac{n_g}{\beta^2} \theta_g \right) u_g \right) \\
&= \iint \left[b(v, T) \cdot v - c_p \gamma(v, T) \right] F(v, T) dv dT.
\end{aligned} \tag{67}$$

Finally, by collecting (61), (65), (66) and (67), we end up with an Euler-Vlasov system, which writes

$$\begin{cases}
\frac{\partial F}{\partial t} + v \cdot \nabla_x F - \nabla_v \cdot (bF) + \frac{\partial}{\partial T} (\gamma F) = 0 & \text{(a),} \\
\partial_t n_g + \operatorname{div}_x (n_g u_g) = 0 & \text{(b),} \\
\partial_t (n_g u_g) + \operatorname{div}_x \left(n_g u_g \otimes u_g + n_g \frac{\theta_g}{\beta^2} I \right) = \iint b(v, T) F(v, T) dv dT & \text{(c),} \\
\partial_t \left(\frac{n_g |u_g|^2}{2} + \frac{3}{2} \frac{n_g}{\beta^2} \theta_g \right) + \operatorname{div}_x \left(\left(\frac{n_g |u_g|^2}{2} + \frac{5}{2} \frac{n_g}{\beta^2} \theta_g \right) u_g \right) \\
= \iint \left[b(v, T) \cdot v - c_p \gamma(v, T) \right] F(v, T) dv dT & \text{(d),}
\end{cases} \tag{68}$$

where b and γ are given by (62) and (63) respectively.

3.4 Comparison with a typical thin spray model

In this last subsection of the paper, we propose to compare system (68), obtained by a formal limit from a microscopic model, with a typical thin (that is, when the volume fraction of the droplets is negligible) spray system used in the modeling of engines, namely the system used for the Kiva-II numerical code (cf. [1]).

In order to do so, we first provide a version of the energy equation in which the unknown is the internal energy. We thus replace eq. (68)-(d) by the following equation (in which we use (68)-(b) and (68)-(c) in order to transform (68) - (d))

$$\begin{aligned}
& \partial_t \left(\frac{3}{2} n_g \frac{\theta_g}{\beta^2} \right) + \nabla_x \cdot \left(\frac{3}{2} n_g \frac{\theta_g}{\beta^2} u_g \right) \\
&= -n_g \frac{\theta_g}{\beta^2} \operatorname{div}_x (u_g) + \iint \left[b(v, T) \cdot (v - u_g) - c_p \gamma(v, T) \right] F(v, T) dv dT.
\end{aligned} \tag{69}$$

We first observe that system (68)-(a)-(b)-(c), (69) has the same global structure as the system (25), (2), (3), (5) p. 8 and p.13 of [1], the main difference

being the extra variables r , y , \dot{y} used in [1], which model extra physical effects (vaporization and distortion of droplets) and extra terms which also model extra physical effects ($\dot{\rho}^s$ and \dot{Q}^c for vaporization and chemical reactions, $A_0 \nabla(2/3\rho k)$ and $A_0 \rho \epsilon$ for turbulence, $\nabla \cdot \sigma$ and $\nabla \cdot J$ for dissipative effects, ρg for gravity, \dot{f}^{coll} and \dot{f}^{bu} for collision and breakup of droplets).

We then compare the term of transfer of momentum between the phases ($-b$ given by (62) in our notations and F in the notations of [1], described in eq. (24) p.16 of this reference). We observe that in both cases, the terms are proportional to $n_g(u_g - v)$ (in [1], the same quantity, up to a mass factor, is denoted by $\rho(u + u' - v)$, where u' is related to turbulence). The coefficient of proportionality is however not identical: the drag coefficient is given by a complex formula in [1], which uses measured coefficients, while in our case, it is deduced from the microscopic model of collisions between molecules and droplets that we considered.

Finally, we compare the term of transfer of energy between the phases (γ given by (63) in our notations and \tilde{T}_d in the notations of [1], described in eq. (41), (42) p.18 of this reference). Here also, in both cases, there is a term proportional to the difference of temperature $\theta_g - T$ (in [1], the same quantity is denoted by $T - T_d$). Once again, the coefficient of proportionality is not identical. We notice however that in our model, because of the specific microscopic model of collisions between molecules and droplets that we use, an extra term proportional to $|u_g - v|^2$ appears, which has no equivalent in [1] (the term $\rho_d 4\pi r^2 R L(T_d)$ appearing in eq. (41) p.18 of this reference is related to a different physical effect, namely vaporization).

Note that, as can be expected, the terms appearing in the right-hand side of the equations of conservation of momentum for the gas (68)-(c), (69), that is $\int \int b F$ and $\int \int [b \cdot (v - u_g) - c_p \gamma] F$; exactly correspond to the terms F^s and \dot{Q}^s of (46) p.19 in [1], once one discards the extra variables r , y , \dot{y} , and the terms $f \rho_d 4\pi r^2 R v$ and $f \rho_d 4\pi r^2 R [I_l(T_d) + \frac{1}{2}(v - u)^2]$ which are related to vaporization.

References

- [1] Anthony A. Amsden, Peter J. O'Rourke, and Daniel T. Butler. Kiva-II: A computer program for chemically reactive flows with sprays. Technical report, Los Alamos National Lab.(LANL), Los Alamos, NM (United States), 1989.
- [2] Laurent Boudin, Laurent Desvillettes, Renaud Motte, et al. A modeling of compressible droplets in a fluid. *Communications in Mathematical Sciences*, 1(4):657–669, 2003.
- [3] Carlo Cercignani. *Multicomponent flow modeling*. Birkhauser, 1999.
- [4] Carlo Cercignani. *Rarefied gas dynamics: from basic concepts to actual calculations*, volume 21. Cambridge University Press, 2000.

- [5] Frédérique Charles. *Modélisation mathématique et étude numérique d'un aérosol dans un gaz raréfié. Application à la simulation du transport de particules de poussière en cas d'accident de perte de vide dans ITER*. PhD thesis, École Normale Supérieure de Cachan, 2009.
- [6] Frédérique Charles, Stéphane Dellacherie, and Jacques Segré. Kinetic modelling of the transport of dust particles in a rarefied atmosphere. *Mathematical Models and Methods in Applied Sciences*, 22(40), 2012.
- [7] Laurent Desvillettes. Some aspects of the modeling at different scales of multiphase flows. *Computer methods in applied mechanics and engineering*, 199(21-22):1265–1267, 2010.
- [8] Etienne Bernard, Laurent Desvillettes, François Golse, and Valeria Ricci. A Derivation of the Vlasov-Navier-Stokes Model for Aerosol Flows from Kinetic Theory, *Communications in Mathematical Sciences*, 15:1703–1741, 2017.
- [9] Etienne Bernard, Laurent Desvillettes, François Golse, and Valeria Ricci. A Derivation of the Vlasov-Stokes Model for Aerosol Flows from Kinetic Theory, *Kinetic and Related Models*, 11(1):43–69, 2018.
- [10] Laurent Desvillettes, François Golse, and Valeria Ricci. A formal passage from a system of boltzmann equations for mixtures towards a Vlasov-Euler system of compressible fluids. *Acta Mathematicae Applicatae Sinica, English Series*, 35:158–173, 2019.
- [11] John K Dukowicz. A particle-fluid numerical model for liquid sprays. *Journal of computational Physics*, 35(2):229–253, 1980.
- [12] Mamoru Ishii and Takashi Hibiki. *Thermo-fluid dynamics of two-phase flow*. Springer Science & Business Media, 2010.
- [13] Alaric Sibra, Joel Dupays, Angelo Murrone, Frédérique Laurent, and Marc Massot. Simulation of reactive polydisperse sprays strongly coupled to unsteady flows in solid rocket motors: Efficient strategy using eulerian multi-fluid methods. *Journal of Computational Physics*, 339:210–246, 2017.
- [14] Forman A Williams. *Combustion theory*. CRC Press, 2018.
- [15] Laurent Boudin, Céline Grandmont, Bérénice Grec, Sébastien Martin, Amina Mecherbet, and Frédérique Noël. Fluid-kinetic modelling for respiratory aerosols with variable size and temperature. *ESAIM: Proceedings and Surveys*, EDP Sciences, 67:100–119, 2020.
- [16] Laurent Boudin, Benjamin Boutin, Bruno Fornet, Thierry Goudon, Pauline Lafitte, Frédéric Lagoutière, and Benoît Merlet. Fluid-particles flows: A thin spray model with energy exchanges. *ESAIM: Proceedings and Surveys*. EDP Sciences, 28:195–210, 2009.