Modelling of internal energy exchanges in sprays

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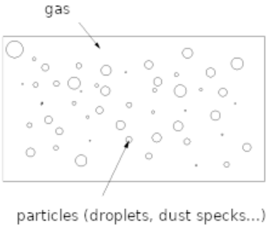
Introduction

Sprays

- Non-gaseous dispersed phase of small volume fraction (e.g. droplets or dust grains) in an underlying gas.
- Examples : clouds, diesel engine, medical aerosol, cosmic dust, dispersion of pollutants, impurities in a Vacuum Vessel (ITER)...
- Their study is a sub-field of the study of multiphase flows.



Models for gaz-particle flows

Hypothesis

- Number density in particles $\ll$ compared to number density in molecules.
- Radius of dust particle $\gg$ radius of gas molecule

$\Rightarrow$ various time and length scales...

Differents possible description

Dust / Molecules	microscopic	mesoscopic	macroscopic
microscopic	mixture of particles		
mesoscopic	kinetic equations with particles	fully kinetic	
macroscopic	fluid equations with particles	fluid-kinetic models	two phase fluid

Models for gaz-particle flows

Fluid-kinetic modelling

- Gas described by $\rho_g(t,x)$, $u_g(t,x)$, $p(t,x)$
- Kinetic equation for the particles
  $F(t,x,v,r)$: number of particles of position x, velocity v, radius r
- **Classification of sprays** [P.J. O'Rourke]
  Volume fraction of particles : $1-\alpha(t,x) = \iint \frac{4}{3}\pi r^3 F(t,x,v,r)dvdr$
  - $1-\alpha(t,x) \ll 10^{-3}$: very thin spray. Coupling from fluid to particles but no retroaction from the particles to the fluid
  - $1-\alpha(t,x) \ll 1$: thin spray. We take into account retroaction of particles on the fluid
  - $1-\alpha(t,c) \sim 0.1$: thick sprays

Models for gas-particle flows

Fluid-kinetic modelling

- Forces exerced on particles
  - Drag force : Stokes drag force on a sphere on a viscous laminar ($R_e < 1$) fluid

$$\mathcal{F}_d(t,x,v,r) = 6\pi\mu r(u_g(t,x) - v)$$

or more generally

$$\mathcal{F}_d(t,x,v,r) = D(u_g(t,x) - v) \text{ or } \mathcal{F}_d(t,x,v,r) = D|u_g(t,x) - v|(u_g(t,x) - v)$$

  - Pressure force on a spherical particles

$$\mathcal{F}_p(r) = -\frac{4}{3}\pi r^3 \nabla_x p, \quad p : \text{ gas pressure}$$

- Vlasov equation for particles

$$\partial_t F + v \cdot \nabla_x F + \frac{1}{m(r)} \nabla_v \left((\mathcal{F}_d + \underbrace{\mathcal{F}_p}_{\text{often neglected}}) F \right) = \underbrace{Q(F,F)}_{\text{often neglected}}$$

Models for gas-particle flows

Fluid-kinetic modelling

- Fluid equation for the gas, for example :
  - Navier-Stokes equation for a viscous incompressible gas

$$\partial_t u_g + (u_g \cdot \nabla_x) u_g + \rho_g^{-1} \nabla_x p - \nu \Delta_x u_g = - \iint \frac{\mathcal{F}_d(t,x,v,r)}{m(r)\rho_g} F(t,x,v,r) dv dr$$

with $\nabla_x \cdot u_g = 0$.

  - Euler equations for a compressible non-viscous barotropic fluid, for very thin or thin sprays

$$\partial_t \rho_g + \nabla_x \cdot (\rho_g u_g) = 0$$

$$\partial \partial_t (\rho_g u_g) + \nabla_x \cdot (\rho_g u_g \otimes u_g) + \nabla_x p(\rho_g) = - \iint \frac{\mathcal{F}_d(t,x,v,r)}{m(r)\rho_g} F(t,x,v,r) dv dr$$

Models for gas-particle flows

Fluid-kinetic modelling

- Fluid equation for the gas, for example :
  - Case of thick sprays

$$\partial_t(\alpha\rho_g) + \nabla_x \cdot (\alpha\rho_g u_g) = 0$$

$$\partial\partial_t(\alpha\rho_g u_g) + \nabla_x \cdot (\alpha\rho_g u_g \otimes u_g) + \alpha\nabla_x p(\rho_g) = -\iint \frac{\mathcal{F}_d(t,x,v,r)}{m(r)\rho_g} F(t,x,v,r)$$

$$1 - \alpha(t,x) = \iint \frac{4}{3}\pi r^3 F(t,x,v,r) dv dr$$

Models for gas-particle flows

Exchange of internal energy in fluid-kinetic models

(cf code KIVA of Los Alamos)

- $F = F(t, x, v, r, e_p)$, with e_p internal energy
- We assume that particles have a temperature given by a law $T_p(t, x, e_p) = \tau(p(t, x), e_p)$
- Vlasov equation for particles

$$\partial_t F + v \cdot \nabla_x F + \nabla_x \left(\frac{D}{m(r)}(u_g(t,x) - v) - \frac{1}{\varrho_p} \nabla_x p(t,x) F \right) + \partial_{e_p} \left(C(T_g - T_p) + \ldots\ldots \right) F) = Q(F),$$

- Equation of energy in compressible Euler equations

$$\partial_t \left(\alpha \rho_g (e_g + \frac{1}{2}|u_g|^2) \right) + \nabla_x \cdot \left(\alpha \rho_g (e_g + p) u_g + \alpha \rho_g \frac{1}{2} |u_g|^2 u_g \right) + \rho_g p \partial_t \alpha = - \iiint \left(C(T_g - T_p) + D(u_p - u_g) \cdot u_p \right) F(t, x, v, e_p, r) dv de_p dr$$

Outline

Objectives

Derivation of the terms corresponding to internal energy exchanges in a Vlasov-Euler model, starting from a kinetic model.

Summary

Collisional model

$f(t, x, w)$: density function of the gas,
$F(t, x, v)$: density function of particles (no dependance on r to simplify)

$$\begin{cases} \dfrac{\partial F}{\partial t} + v \cdot \nabla_x F = \mathcal{D}(F, f) + \overbrace{\cancel{\mathcal{C}(F)}}^{neglected}, \\ \dfrac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}(F, f) + \mathcal{Q}(f), \end{cases}$$

$\mathcal{D}(F, f)$ and $\mathcal{R}(F, f)$ describe molecule-particles interactions

Collision operator $\mathcal{Q}(f)$ for molecules

Collisions between molecules : binary, elastic. $\mathcal{Q}(f)$ is the classical Boltzmann operator for monoatomic gases :

$$\mathcal{Q}(f)(w) = \int_{\mathbb{R}^3}\int_{S^2} \left[f(w'')f(w''_*) - f(w)f(w_*)\right] c(|w-w_*|, \cos(\chi))d\omega d\sigma$$

with

$$(w'', w''_*) = (\frac{w+w_*}{2} + \frac{|w-w_*|}{2}\sigma, \frac{w+w_*}{2} - \frac{|w-w_*|}{2}\sigma)$$

Properties of $\mathcal{Q}(f)$

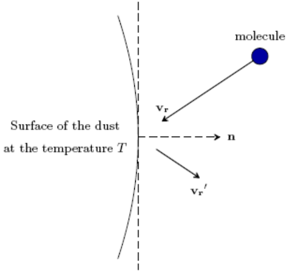
$$\int_{\mathbb{R}^3} \mathcal{Q}(f)(w) \begin{pmatrix} 1 \\ w \\ |w|^2 \end{pmatrix} dw = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Equilibrium

$$\mathcal{Q}(f) = 0 \Leftrightarrow f(w) = \mathcal{M}[\rho_g, u_g, \theta_g](w) = \frac{\rho_g m_g^{3/2}}{(2\pi k_B \theta_g)^{3/2}} e^{-\frac{m_g|w-u_g|^2}{2k_B\theta_g}}$$

Collisional operators $\mathcal{D}(F, f)$ and $\mathcal{R}(F, f)$

- First possibility : elastic collisions (specular reflexion)
- Second possibility : diffuse reflexion
  Hypothesis : dust particles have the same constant temperature of surface T_p.



Density of probability of the post-collisional relative velocity :

$$h_n(v) = \frac{1}{2\pi} \frac{m_g^2}{k_B^2 T_p^2} (n \cdot v)\, e^{-\frac{m_g |v|^2}{2 k_B T_p}} \mathbb{1}_{\{n \cdot v \geq 0\}},$$

Consequences :

- Kinetic energy not conserved,
- Non planar, non microreversible collisions.

Collisional operators $\mathcal{D}(F,f)$ and $\mathcal{R}(F,f)$

$$\mathcal{D}^1(F,f)(v) = \sigma_{gp} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \left[F(v')f(w')e^{\frac{m_g|v'-w'|^2}{2k_BT_p}} - F(v)f(w)e^{\frac{m_g|v-w|^2}{2k_BT_p}} \right] \times e^{-\frac{m_g|v-w|^2}{2k_BT_p}} \varsigma(v-w,n) h_n(z) \mathrm{d}n\, \mathrm{d}z\, \mathrm{d}w$$

and

$$\mathcal{R}^1(F,f)(w) = \sigma_{gp} \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\int_{\mathbb{S}^2} \left[F(v')f(w')e^{\frac{m_g|v'-w'|^2}{2k_BT_p}} - F(v)f(w)e^{\frac{m_g|v-w|^2}{2k_BT_p}} \right] \times e^{-\frac{m_g|v-w|^2}{2k_BT_p}} \varsigma(v-w,n) h_n(z) \mathrm{d}n\, \mathrm{d}z\, \mathrm{d}v$$

- hard sphere collision cross section : $\varsigma(v-w,n) := [n\cdot(v-w)]\mathbb{1}_{\{n\cdot(v-w)\geq 0\}}$
- post-collisional velocities : $\begin{cases} v' := \dfrac{m_p v + m_g w}{m_p+m_g} - \dfrac{m_g}{m_g+m_p} z, \\ w' := \dfrac{m_p v + m_g w}{m_g+m_p} + \dfrac{m_p}{m_g+m_p} z. \end{cases}$

Collisional operators $\mathcal{D}(F,f)$ and $\mathcal{R}(F,f)$

Conservation of momentum

$$m_p \int_{\mathbb{R}^3} \mathcal{D}^1(F,f)(v) \begin{pmatrix} 1 \\ v \end{pmatrix} dv + m_g \int_{\mathbb{R}^3} \mathcal{R}^1(F,f)(w) \begin{pmatrix} 1 \\ w \end{pmatrix} dw = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix},$$

but

$$m_p \int_{\mathbb{R}^3} \mathcal{D}^1(F,f)(v)|v|^2 dv + m_g \int_{\mathbb{R}^3} \mathcal{R}^1(F,f)(w)|w|^2 dw \neq 0,$$

Entropy dissipation

$$H^d(F,f)(t) = \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} f(w) \ln\left(f(w) e^{\frac{(m_g+m_p)}{m_p} \frac{m_g|w|^2}{2k_B T_p}} \right) \mathrm{d}w\mathrm{d}x + \int_{\mathbb{R}^3}\int_{\mathbb{R}^3} F(v) \ln\left(F(v) e^{\frac{(m_g+m_p)}{m_p} \frac{m_p|v|^2}{2k_B T_p}} \right) \mathrm{d}v\mathrm{d}x,$$

$$\frac{d}{dt} H^d(F,f) \leq 0$$

Asymptotic to a Vlasov-Boltzman model

Collisions, for the point of view of a particle

The post-collisional velocity v' of the particle after a dust-molecule collision verifies

$$v' - v = \frac{\eta}{1+\eta}(w - z - v), \qquad \eta := \frac{m_g}{m_p} \ll 1$$

$\Rightarrow$ **small change of velocity, analogous to grazing collisions !**

Hypothesis for the dimensionless system

- the thermal speeds of gas molecules and particles are of the same order of magnitude
- the ratio of density between particles and molecules is identical to the mass ratio between molecules and particle : $\mathcal{N}_p/\mathcal{N}_g = \eta$

Asymptotic to a Vlasov-Boltzman model

Dimensionless system

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

with $\delta = \frac{\lambda_{gg}}{L}$ is the Knudsen number K_n.

Weak form of the operator $\mathcal{D}_\eta(F,f)$

$$\int_{\mathbb{R}^3} \mathcal{D}_\eta(F,f)(v)\varphi(v)\mathrm{d}v$$
$$= \iiiint \left[\varphi(v') - \varphi(v)\right] F(v) f(w) \varsigma(v-w,n) h_n(z) \mathrm{d}z\, \mathrm{d}n\, \mathrm{d}w\, \mathrm{d}v\,,$$

Asymptotic to a Vlasov-Boltzman model

Formal asymptotic expansion of $\mathcal{D}_\eta(F,f)$

We have

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

with, in the case of diffuse reflexion

$$a(F,f)(v) = \pi \nabla_v \cdot \left(F(v) \int_{\mathbb{R}^3} \left(|w-v| + \frac{\sqrt{2\pi T_p}}{3\beta} \right) (v-w) f(w) dw \right)$$

Vlasov-Boltzmann system

$$\begin{cases} \dfrac{\partial F}{\partial t} + v \cdot \nabla_x F + \nabla_v \cdot (F(v,T)\Gamma(F,f)(v)) = 0 \\ \dfrac{\partial f}{\partial t} + w \cdot \nabla_x f = \mathcal{R}^l(F,f) + \dfrac{1}{\delta} C(f), \end{cases}$$

with

$$\int_{\mathbb{R}^3} \mathcal{R}^l(F,f)(w)\psi(w)\mathrm{d}w = \int [\psi(v+z) - \psi(w)]\, F(v) f(w) \varsigma(v-w,n) h_n(z) \mathrm{d}z \mathrm{d}n \mathrm{d}v$$

Summary

Internal energy in the function F

with Laurent Desvillettes : *From collisional kinetic models to sprays : internal energy exchanges*, accepté pour publication dans Communications in Mathematical Sciences, 2024

With the previous model : no conservation of kinetic energy during a dust-molecule collision

$$m_p|v'|^2 + m_g|w'|^2 \neq m_g|v|^2 + m_p|w|^2$$

We introduce a variable T in the density of particles :

$$F(t, x, v, T)$$

Post-collisional temperature : T' is given by the relation of conservation of energy

$$\frac{1}{2}m_p|v'|^2 + \frac{1}{2}m_g|w'|^2 + c_p m_p T' = \frac{1}{2}m_p|v|^2 + \frac{1}{2}m_g|w|^2 + c_p m_p T$$

Modified density

Previously : $z = w' - v'$ given with the density of probability :

$$h_{n,T}(v) = \frac{1}{2\pi} \frac{m_g^2}{k_B^2 T^2} (n \cdot v) \, e^{-\frac{m_g |v|^2}{2k_B T}} \mathbb{1}_{\{n \cdot v \geq 0\}}$$

Post-collisional velocity $T' = T + \frac{1}{2c_p} \frac{\eta}{1+\eta} [|v-w|^2 - |v'-w'|^2]$, (with $\eta = m_g/m_p$).

Modified density function of post-collisional relative velocity :

$$\tilde{h}_{n,v,w,\eta,T}(z) := \frac{1}{\mathcal{H}_{v,w,\eta,T}} h_{n,T}(z) \mathbb{1}_{\{|z|^2 \leq |v-w|^2 + 2c_p \frac{1+\eta}{\eta} T\}}(z),$$

where

$$\mathcal{H}_{v,w,\eta,T} := \int_{\mathbb{R}^3} h_{n,T}(z) \mathbb{1}_{\{|z|^2 \leq |v-w|^2 + 2c_p \frac{1+\eta}{\eta} T\}}(z) dz.$$

Collision operators

$$\mathcal{D}(F,f)(v,T) = \frac{m_g^2 \sigma_{gp}}{2\pi k_B^2} \int_{\mathbb{S}^2\times\mathbb{R}^3\times\mathbb{R}^3} \Big[\frac{F(v',T')f(w')}{\mathcal{H}_{v',w',\eta,T'}} \frac{1}{T'^2} e^{-\frac{m_g}{2k_B T'}|v-w|^2} - \frac{F(v,T)f(w)}{\mathcal{H}_{v,w,\eta,T}} \frac{1}{T^2} e^{-\frac{m_g}{2k_B T}|z|^2} \Big] \mathbb{1}_{\{T'>0\}} \varsigma(z,n)\varsigma(v-w,n)\mathrm{d}n\,\mathrm{d}z\,\mathrm{d}w,$$

(similar expression for $\mathcal{R}(F,f)$), with

$$v' = \frac{v+\eta w}{1+\eta} - \frac{\eta}{1+\eta} z, \qquad w' = \frac{v+\eta w}{1+\eta} + \frac{1}{1+\eta} z.$$

and

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

Conservation of mass, momentum and total energy

$$\int \mathcal{D}(F,f)(v,T) \begin{pmatrix} 1 \\ m_p v \\ m_p \frac{|v|^2}{2} + c_p m_p T \end{pmatrix} \mathrm{d}v\,\mathrm{d}T + \int \mathcal{R}(F,f)(w) \begin{pmatrix} 1 \\ m_g w \\ m_g \frac{|w|^2}{2} \end{pmatrix} \mathrm{d}w = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Asymptotic when $\eta \to 0$

Same assumptions as previously, and we assume that the ratio between the kinetic temperature of the gas and the temperature of surface of dust particles does not depend of δ or η.

Dimensionless weak form of $\mathcal{D}(F, f)$

$$\int \int_{\mathbb{R}^3} \mathcal{D}_\eta(F, f)(v, T)\varphi(v, T)\mathrm{d}v\,\mathrm{d}T$$
$$= \int \iiiint \left[\varphi(v', T') - \varphi(v, T)\right] F(v, T) f(w) \varsigma(v - w, n) \tilde{h}_{n,v,w,\eta,T}(z)\mathrm{d}z\,\mathrm{d}n\,\mathrm{d}w\,\mathrm{d}v$$

Proposition

The following asymptotic expansion holds :

$$\tilde{h}_{n,v,w,\eta,T}(z) = h_{n,T}(z) + o(\eta^\infty).$$

More precisely, the o holds in $L^1(\mathbb{R}^3)$, uniformly with respect to the parameters n, v, w, T.

Asymptotic when $\eta \to 0$

Asymptotic expansion of $\mathcal{D}(F, f)$

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

with

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

where we denote

$$I_{f,1}(t, x, v) := \int_{\mathbb{R}^3} |w - v| f(t, x, w) \mathrm{d}w \qquad I_{f,3}(t, x, v) := \int_{\mathbb{R}^3} |w - v|^3 f(t, x, w) \mathrm{d}w.$$

Asymptotic when $\eta \to 0$ and $\delta \to 0$

If (f^δ, F^δ) is a solution of the previous system, then (at a formal level) $f^\delta \to \mathcal{M}[n_g, u_g, \theta]$ when $\delta \to 0$.
We introduce, 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 $q(a) = a\,\tilde{q}(|a|)$.
Moreover, we observe that it is possible to write, for some smooth functions $\tilde{q}_0$, $\tilde{q}_3$,

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

with

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

Asymptotic when $\eta \to 0$ and $\delta \to 0$

Vlasov equation for particles

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

with

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

and

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

where

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

Asymptotic when $\eta \to 0$ and $\delta \to 0$

Full Vlasov-Euler system

$$\begin{cases} \dfrac{\partial F}{\partial t} + v \cdot \nabla_x F - \nabla_v \cdot (bF) + \dfrac{\partial}{\partial T}(\gamma F) = 0, \\ \partial_t n_g + \nabla_x \cdot_x (n_g u_g) = 0, \\ \partial_t (n_g u_g) + \nabla_x \cdot_x \left(n_g u_g \otimes u_g + n_g \dfrac{\theta_g}{\beta^2} I \right) = \displaystyle\iint b(v,T) F(v,T) \mathrm{d}v \mathrm{d}T, \\ \partial_t \left(\dfrac{n_g |u_g|^2}{2} + \dfrac{3 n_g}{2\beta^2} \theta_g \right) + \nabla_x \cdot_x \left(\left(\dfrac{n_g |u_g|^2}{2} + \dfrac{5 n_g}{2\beta^2} \theta_g \right) u_g \right) \\ \qquad = \displaystyle\iint \Big[b(v,T) \cdot v - c_p \, \gamma(v,T) \Big] F(v,T) \mathrm{d}v \mathrm{d}T \end{cases}$$