From the Kinetic Theory of Gases to Models for Aerosol Flows

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Works in collaboration with E. Bernard, L. Desvillettes, V. Ricci
Aerosol/Spray flows arise in different contexts (from diesel engines to medical aerosols in the trachea and the upper part of the lungs)

**Problem**: How to justify these models?
In the Context of Diesel Engines...

2. GOVERNING EQUATIONS

2.1 Two-phase Flow Regimes

The dynamics and evaporation of drops in a spray is influenced by the spray regime. Important regimes are summarized in Fig. 2.1. In a region where the spray drops occupy a significant fraction of the total volume of the two-phase mixture, the spray is termed "thick" or dense. This regime is typically found in the region near the injector nozzle exit. At the other extreme, because practical sprays often diverge away from the nozzle, and the size of the drops is reduced due to evaporation and breakup, the spray drops far from the nozzle become isolated and have negligible mass and volume compared to that of the gas that has been set in motion by the spraying process. In this case, the spray is termed "very thin" or dilute and, although the drops continue to exchange mass, momentum and energy with the gas, the state of the gas is not altered appreciably by the exchange. The term "thin" spray has been used to describe the intermediate spray regime between the "very thin" and the "thick" regimes (O'Rourke, 1981).

Figure: Schematic representation of spray regimes for liquid injection from a single hole nozzle [R.D. Reitz “Computer Modeling of Sprays” 1996]

Local volume fraction of the dispersed phase denoted $\phi(t, x)$

- **Very thin spray regime (typically $\phi(t, x) \ll 10^{-3}$)**
  Volume fraction of the dispersed phase negligible; particles in the dispersed phase accelerated by the friction force exerted by the propellant; no feedback from the dispersed phase on the propellant

  **Typical model** Vlasov equation for the dispersed phase, driven by the fluid (e.g. Navier-Stokes) equation

- **Thin spray regime (typically $\phi(t, x) \ll 10^{-1}$)**
  Same as in the very thin spray regime, except that the feedback interaction of the dispersed phase on the propellant is taken into account

  **Typical model** Vlasov-Navier-Stokes or Vlasov-Stokes systems
The Vlasov-Navier-Stokes System

Unkowns:

\( F \equiv F(t, x, v) \) particle distribution function (in the dispersed phase)
\( u \equiv u(t, x) \) and \( p \equiv p(t, x) \) velocity and pressure fields (propellant)

Vlasov eqn for \( F \ldots \)

\[
\partial_t F + v \cdot \nabla_x F - \kappa \text{div}_v ((v - u)nF) = 0
\]

... coupled to the Navier-Stokes eqn for \( (u, p) \) (here \( \text{Ma} \ll 1 \))

\[
\begin{align*}
\text{div}_x u &= 0 \\
\partial_t u + u \cdot \nabla_x u &= -\frac{1}{n} \nabla_x p + \nu \Delta_x u + \kappa \int (v - u)Fdv \\
&\quad \underbrace{0 \text{ for very thin sprays}}
\end{align*}
\]

Parameters:
\( \kappa = \) friction coefficient, \( n = \) gas density, and \( \nu = \) viscosity of the gas
DERIVING NAVIER-STOKES + BRINKMAN FORCE

THE HOMOGENIZATION APPROACH

L. Desvillettes, F.G., V. Ricci
Spherical Particles in a Navier-Stokes Fluid

Dispersed phase = moving system of $N$ identical rigid spheres centered at $X_k(t) \in \mathbb{R}^3$ for $k = 1, \ldots, N$, with radius $r > 0$

Time-dependent domain filled by the propellant

$$\Omega_g(t) := \{ x \in \mathbb{R}^3 \text{ s.t. } \text{dist}(x, X_k(t)) > r \text{ for } k = 1, \ldots, N \}$$

Fluid equation for the propellant: Navier-Stokes + external force

$$\begin{cases} (\partial_t + u \cdot \nabla_x)u = -\nabla_x p + \nu \Delta_x u + f , & \text{div}_x u = 0 , & x \in \Omega_g(t) \\ u(t, \cdot)\big|_{\partial B(X_k(t), r)} = \dot{X}_k(t) , & k = 1, \ldots, N \end{cases}$$

Solid rotation/Torque of each particle around its center neglected (one is interested in a limit where $r \to 0$)
Quasi-Static Approximation

Small parameter $0 < \tau \ll 1$; dispersed phase assumed to be slow

Slow time variable

$$\hat{t} = \tau t$$

Scaling of the particle/droplets dynamical quantities

$$X_k(t) = \hat{X}_k(\hat{t}), \quad \dot{X}_k(t) = \tau \hat{V}_k(\hat{t}) \quad \text{with} \quad \hat{V}_k = \frac{d\hat{X}_k}{d\hat{t}}$$

Scaling of the fluid dynamical quantities

$$u(t, x) = \tau \hat{u}(\hat{t}, x), \quad p(t, x) = \tau \hat{p}(\hat{t}, x), \quad f(t, x) = \tau \hat{f}(\hat{t}, x)$$

Inserting this in the Navier Stokes equation, one finds

$$\begin{cases} \tau (\partial_{\hat{t}} + \hat{u} \cdot \nabla_x) \hat{u} = -\nabla_x \hat{p} + \nu \Delta_x \hat{u} + \hat{f}, \quad \text{div}_x \hat{u} = 0 \\ \hat{u}(\hat{t}, \cdot) \bigg|_{\partial B(\hat{X}_k(\hat{t}), r)} = \hat{V}_k(\hat{t}) \end{cases}$$
Stokes formula (1851) for the drag force exerted on a sphere of radius $r$ by a viscous fluid of viscosity $\mu$ with velocity $U$ at infinity

$$6\pi \mu r U$$

Total friction exerted by $N$ noninteracting spheres of radius $r$

$$6\pi \mu N r U$$
Homogenization Assumptions

**Scaling assumption** on particle radius $r$ and particle number $N$:

$$N \to \infty, \quad r \to 0, \quad Nr \to 1$$

**Spacing condition**: bounded domain $\mathcal{O}$ with smooth boundary $\partial\mathcal{O}$

$$\text{dist}(X_k, X_l) > 2r^{1/3} \quad \text{and} \quad \text{dist}(X_k, \partial\mathcal{O}) > r^{1/3}, \quad 1 \leq k \neq l \leq N$$

**Particle distribution function** $F$ continuous on $\bar{\mathcal{O}} \times \mathbb{R}^3$ s.t.

$$F_N := \frac{1}{N} \sum_{k=1}^{N} \delta_{x_k, v_k} \to F, \quad \sup_{N \geq 1} \iint_{\mathcal{O} \times \mathbb{R}^3} |v|^2 F_N < \infty$$

**External force** $f \equiv f(x) \in \mathbb{R}^3$ s.t.

$$\text{div}_x f = 0, \quad \int_{\mathcal{O}} |f(x)|^2 dx < \infty$$
Theorem 1 (Derivation of the Brinkman Force)

Let \( \mathcal{O}_r := \{ x \in \mathcal{O} \text{ s.t. } \text{dist}(x, X_k) > r \text{ for all } 1 \leq k \leq N \} \), and for each \( 0 < r \ll 1 \), let \( u_r \) be the solution to the Stokes equation

\[
\begin{align*}
\nabla x p_r &= \nu \Delta_x u_r + f, \\
\text{div}_x u_r &= 0, \quad x \in \mathcal{O}_r \\
u_r \big|_{\partial B(x_k, r)} &= v_k, \quad u_r \big|_{\partial \mathcal{O}} = 0
\end{align*}
\]

Then, in the limit as \( r \to 0 \), one has

\[
\int_{\mathcal{O}_r} |\nabla u_r(x) - \nabla u(x)|^2 dx
\]

where \( u \) is the solution to the Stokes equation with friction force

\[
\begin{align*}
\nabla x p &= \nu \Delta_x u + f + 6\pi \nu \int (v - u) F dv, \quad x \in \mathcal{O} \\
\text{div}_x u &= 0, \quad u \big|_{\partial \mathcal{O}} = 0
\end{align*}
\]
(1) Argument extends without difficulty to steady Navier-Stokes, provided that $\nu \geq \nu_0[f, F, \mathcal{O}] > 0$


(2) Recent improvement by Hillairet (arXiv:1604.04379v2 [math.AP]) relaxing the spacing condition

(3) In order to derive the coupled VNS system, one could try to propagate the spacing condition by the dynamics. Some ideas (on a different pbm) in [Jabin-Otto: Commun Math. Phys. 2004]?

(4) But even if one can propagate the spacing condition, such configurations are of negligible statistical weight...
DERIVING VLASOV-NAVIER-STOKES FROM
THE KINETIC THEORY OF A BINARY GAS MIXTURE

E. Bernard, L. Desvillettes, F.G., V. Ricci
(Kinetic and Related Models 11 (2018), 43–69)
A Multiphase Boltzmann System

Unkowns:
\[ F(t, x, v) = \text{distribution function of dust particles/droplets} \]
\[ f(t, x, w) = \text{distribution function of gas molecules} \]

Multiphase Boltzmann equation

\[ (\partial_t + v \cdot \nabla_x)F = D(F, f) \]
\[ (\partial_t + w \cdot \nabla_x)f = R(f, F) + C(f) \]

Collision integrals:

- \( D(F, f) \) deflection of particles by collisions with gas molecules
- \( R(f, F) \) friction of gas molecules due to collisions with particles
- \( C(f) \) Boltzmann collision integral for gas molecules

Dispersed phase collisions possible, but neglected here for simplicity
<table>
<thead>
<tr>
<th>Parameter</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>$L$</td>
<td>size of the container</td>
</tr>
<tr>
<td>$N_p$</td>
<td>number of dust particles/$L^3$</td>
</tr>
<tr>
<td>$N_g$</td>
<td>number of gas molecules/$L^3$</td>
</tr>
<tr>
<td>$V_p$</td>
<td>thermal speed of dust particles</td>
</tr>
<tr>
<td>$V_g$</td>
<td>thermal speed of gas molecules</td>
</tr>
<tr>
<td>$S_{pg}$</td>
<td>particle/gas cross-section</td>
</tr>
<tr>
<td>$S_{gg}$</td>
<td>molecular cross-section</td>
</tr>
<tr>
<td>$\eta = m_g/m_p$</td>
<td>mass ratio (gas molecules/particles)</td>
</tr>
<tr>
<td>$\epsilon = V_p/V_g$</td>
<td>thermal speed ratio (particles/gas)</td>
</tr>
</tbody>
</table>
Dimensionless Quantities

Dimensionless variables

\[ \hat{x} = x/L, \quad \hat{t} = tV_p/L, \quad \hat{v} = v/V_p, \quad \hat{w} = w/V_g \]

Dimensionless distribution functions

\[ \hat{F} = V_p^3 F/N_p, \quad \hat{f} = V_g^3 f/N_g \]

Dimensionless Boltzmann system

\[
\partial_{\hat{t}} \hat{F} + \hat{v} \cdot \nabla_{\hat{x}} \hat{F} = N_g S_{pg} L \frac{V_g}{V_p} \hat{D}(\hat{F}, \hat{f}) \\
\partial_{\hat{t}} \hat{f} + \frac{V_g}{V_p} \hat{w} \cdot \nabla_{\hat{x}} \hat{f} = N_p S_{pg} L \frac{V_g}{V_p} \hat{R}(\hat{f}, \hat{F}) + N_g S_{gg} L \frac{V_g}{V_p} \hat{C}(\hat{f})
\]
Scaling assumptions

\[
\begin{align*}
\epsilon &:= \frac{V_p}{V_g} = N_p S_{pg} L = (N_g S_{gg} L)^{-1} \ll 1 \\
\eta &:= \frac{N_p}{N_g} \ll \epsilon^2
\end{align*}
\]

Scaled Boltzmann system — dropping hats on scaled quantities

\[
\begin{align*}
\partial_t F + v \cdot \nabla_x F &= \frac{1}{\eta} D(F, f) \\
\partial_t f + \frac{1}{\epsilon} w \cdot \nabla_x f &= R(f, F) + \frac{1}{\epsilon^2} C(f)
\end{align*}
\]

Assumption on the gas distribution function

\[
f(t, x, w) = M(w)(1 + \epsilon g(t, x, w)), \quad M(w) := \frac{1}{(2\pi)^{3/2}} e^{-|w|^2/2}
\]

centered Maxwellian
(Maxwell-)Boltzmann collision integral given by

\[ C(f)(w) = \int_{\mathbb{R}^3} \int_{S^2} (f(w')f(w'_*) - f(w)f(w_*))c\left(\frac{w-w_*}{|w-w_*|} \cdot \omega\right)d\omega_* d\omega \]

where

\[
\begin{align*}
    w' &= w - (w - w_*) \cdot \omega \\
    w'_* &= w_* + (w - w_*) \cdot \omega
\end{align*}
\]

Pseudo-Maxwellian collision kernel for the gas molecules with

\[ 4\pi \int_0^1 c(\mu) d\mu = 1 \]
Figure: Unit vector \( \omega = \) exterior angle bissector of \( (\mathbf{w} - \mathbf{w}_*, \mathbf{w}' - \mathbf{w}_*) \)
Deflection $\mathcal{D}$ and friction $\mathcal{R}$ integrals given by

$$
\begin{align*}
\mathcal{D}(F, f)(v) &= \int \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left( F(v'') f(w'') - F(v) f(w) \right) b(\epsilon v - w, \omega) \, dwd\omega \\
\mathcal{R}(f, F)(w) &= \int \int_{\mathbb{R}^3 \times \mathbb{S}^2} \left( f(w'') F(v'') - f(w) F(v) \right) b(\epsilon v - w, \omega) \, dvd\omega
\end{align*}
$$

where

$$
v'' = v - \frac{2\eta}{1+\eta} (v - \frac{1}{\epsilon} w) \cdot \omega \omega, \quad w'' = w - \frac{2}{1+\eta} (w - \epsilon v) \cdot \omega \omega
$$

Collision kernel of the form $b(z, \omega) = B(|z|, |\omega \cdot \frac{z}{|z|}|)$ s.t.

$$
0 < b(z, \omega) \leq B_*(1 + |z|), \quad \int_{\mathbb{S}^2} b(z, \omega) d\omega \geq \frac{1}{B_*} \frac{|z|}{1+|z|} \quad \text{a.e.}
$$
Inelastic Collision Model

Model developed by F. Charles [PhD Thesis, ENS Cachan 2009]

Figure: Diffuse reflection of gas molecules at the surface of a particle or of a droplet with surface temperature $T_{\text{surf}}$; velocity of particle/droplet denoted $V$; molecular velocity denoted $w, W$
Scaled Deflection/Friction Operators: Inelastic Case

Deflection $\mathcal{D}$ and friction $\mathcal{R}$ integrals given by

$$
\mathcal{D}(F,f)(v) = \iint f(W)(F(V)K_{pg}(v|V,W) - F(v)K_{pg}(V|v,W))dVdW
$$

$$
\mathcal{R}(f,F)(w) = \iint F(V)(f(W)K_{gp}(w|V,W) - f(w)K_{pg}(W|V,w))dVdW
$$

Inelastic kernels denoting $\beta := \sqrt{m_g/k_B T_{surf}}$, collision kernels are

$$
K_{pg}(v|V,W) := \frac{\epsilon^3}{\pi} \int_{S^2} P[\beta \frac{1+\eta}{\eta}](\frac{\epsilon V + \eta W}{1+\eta} - \epsilon v, n)((\epsilon V - W) \cdot n)_+dn
$$

$$
K_{gp}(w|V,W) := \frac{1}{\pi} \int_{S^2} P[\beta (1+\eta)](w - \frac{\epsilon V + \eta W}{1+\eta}, n)((\epsilon V - W) \cdot n)_+dn
$$

where

$$
P[\lambda](\xi, n) := \frac{\lambda^4}{2\pi} \exp(-\frac{1}{2} \lambda^2 |\xi|^2)(\xi \cdot n)_+
$$
Theorem 2 (Formal VNS limit)

Let \((F_n, f_n = M(1 + \epsilon_n g_n))\) be a sequence of solutions to the scaled Boltzmann system with \(\eta_n \ll \epsilon_n^2\). Assume \(F_n \rightarrow F\) and \(g_n \rightarrow g\) with

\[
(a) \sup_{t+|x| \leq R} \left( \sup_v |v|^7 F_n(t, x, v) + \int g_n(t, x, w)^2 M(w) \, dw \right) < \infty
\]

\[
(b) \int_{t+|x| < R} \left| \int (g - g_n) \phi M \, dv \right|^2 \, dx \, dt \rightarrow 0
\]

for all \(R > 0\) and all continuous bounded \(\phi \equiv \phi(t, x, v)\). Then

\[
F \equiv F(t, x, v) \quad \text{and} \quad u(t, x) := \int w g(t, x, w) M(w) \, dw
\]

satisfy the VNS system with friction rate \(\kappa\) defined below and

\[
\frac{1}{\nu} := 6\pi \int_0^1 c(\mu) \left( \frac{5}{3} - \mu^2 \right) \mu^2 \, d\mu
\]
The Vlasov-Navier-Stokes System

Unkowns:

\[ F \equiv F(t, x, v) \geq 0, \quad u \equiv u(t, x) \in \mathbb{R}^3, \quad \text{and} \quad p \equiv p(t, x) \in \mathbb{R} \]

\[
\begin{aligned}
\partial_t F + v \cdot \nabla_x F - \kappa \text{div}_v((v - u)F) &= 0 \\
\partial_t u + u \cdot \nabla_x u &= -\nabla_x p + \nu \Delta_x u + \kappa \int (v - u)Fdv \\
\text{div}_x u &= 0
\end{aligned}
\]
Lemma A (Drag force)

Under the assumptions of Theorem 2

\[
\frac{1}{\eta_n} \mathcal{D}(F_n, f_n)(t, x, \nu) \to \kappa \text{div}_\nu((\nu - u(t, x))F(t, x, \nu))
\]

with

\[
\kappa := \begin{cases} 
\frac{8\pi}{3} \int |z|^2 M(z) \left( \int_0^1 B(|z|, \mu) \mu^2 \, d\mu \right) \, dz & \text{elastic} \\
\frac{1}{3} \int \left( \frac{\sqrt{2\pi}}{3\beta} + |z| \right) |z|^2 M(z) \, dz & \text{inelastic}
\end{cases}
\]
Let $\phi \equiv \phi(v)$ be a smooth test function; collision symmetries imply

$$J := \frac{1}{\eta} \int \phi(v) D(F, f)(v) dv$$

$$= \int \int F(v)f(w) \left( \int \frac{1}{\eta} (\phi(v) - \phi(v'')) b(\epsilon v - w, \omega) d\omega \right) dv dw$$

since

$$v'' = v - \frac{2\eta}{1+\eta} (v - \frac{1}{\epsilon} w) \cdot \omega \omega \quad \text{with } \eta \ll \epsilon^2 \ll 1$$

Hence

$$J \approx - \int \int F(v)f(w) \nabla \phi(v) \cdot \left( \int (v - \frac{1}{\epsilon} w) \cdot \omega \omega b(\epsilon v - w, \omega) d\omega \right) dv dw$$

$$\approx - \kappa \int F(v)(v - u) \cdot \nabla \phi(v) dv \quad \text{and integrate by parts}$$
Lemma B (Brinkman (friction) force)

Under the assumptions of Theorem 2

\[ \frac{1}{\epsilon_n} \int R(f_n, F_n)(t, x, w)wdw \rightarrow \kappa \int (v - u(t, x))F(t, x)dv \]

Proof The integrals \( D(f_n, F_n) \) and \( R(F_n, f_n) \) satisfy the momentum balance identity

\[ \epsilon_n \int D(f_n, F_n)(t, x, v)vdv + \eta_n \int R(F_n, f_n)(t, x, w)wdw = 0 \]

Multiply both sides by \( 1/\epsilon_n\eta_n \), apply Lemma A and integrate by parts
Fluctuation $g_n$ of distribution function in the propellant satisfies

$$
\varepsilon_n \partial_t g_n + w \cdot \nabla_x g_n = M^{-1} \mathcal{R}(f_n, F_n) + M^{-1} \mathcal{C}(Mg_n) - \frac{1}{\varepsilon_n} \mathcal{L}g_n \quad \text{lin'd coll.} \int
$$

Asymptotic fluctuation

$$
\mathcal{L}g_n \to 0 \implies g(t, x, w) = \rho(t, x) + u(t, x) \cdot w + \theta(t, x) \frac{1}{2} (|w|^2 - 3)
$$

Continuity equation

$$
\varepsilon_n \partial_t \int g_n Mdw + \text{div}_x \int wg_n Mdw = 0 \implies \text{div}_x u = 0
$$

Momentum equation

$$
\varepsilon_n \partial_t \int wg_n Mdw + \text{div}_x \int w \otimes wg_n Mdw = \int w \mathcal{R}(f_n, F_n) dw \to 0
$$

$$
\implies \nabla_x (\rho + \theta) = 0
$$
Viscosity of a Gas of Pseudo-Maxwellian Molecules

Rescaled momentum equation, where \( A(w) := w \otimes w - \frac{1}{3} |w|^2 I \)

\[
\partial_t \int w g_n M dw + \text{div}_x \frac{1}{\epsilon_n} \int A(w) g_n M dw + \nabla_x \int \frac{|w|^2}{3 \epsilon_n} g_n M dw \rightarrow \nabla_x \text{sthg}
\]

\[
= \frac{1}{\epsilon_n} \int w R(f_n, F_n) dw \rightarrow \kappa \int (v - u) F dv
\]

Key point Observing that

\[
\frac{1}{\epsilon_n} \int A(w) g_n M dw = \frac{1}{\epsilon_n} \int (\mathcal{L}^{-1} A)(w) \frac{1}{\epsilon_n} \mathcal{L} g_n M dw
\]

and using the Boltzmann equation to express \( \frac{1}{\epsilon_n} \mathcal{L} g_n \) shows that

\[
\frac{1}{\epsilon_n} \int A(w) g_n M dw \rightarrow A(u) - \nu (\nabla_x u + (\nabla_x u)^T - \frac{2}{3} (\text{div}_x u) I)
\]
We have presented two methods for deriving the Vlasov-Navier-Stokes system for aerosols in the thin regimes, starting either from a fluid model with immersed discrete dispersed phase, or from a kinetic model for a binary mixture.

The kinetic model can be easily extended:
(a) to derive the Vlasov-Stokes system
(b) to include an equation for the fluctuations of temperature
(c) to take into account compressibility in the propellant
(d) to take into account collisions in the dispersed phase
(e) to take into account polydispersion
One advantage of the kinetic model is the possibility of a description of the **drag force richer than Stoke’s formula**
(a) inelastic collision model with **temperature of the dispersed phase**
(b) detailed description of **rarefied flow past a sphere**
