Deriving Models for Thin Sprays

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Aerosol/Spray Flows

Aerosol/Spray=dispersed phase (solid particles, droplets) in a gas (sometimes referred to as the propellant)

A class of models for aerosols/sprays consists of

(a) a kinetic equation for the dispersed phase

(b) a fluid equation for the gas/propellant

The kinetic equation for the dispersed phase and the fluid equation for the propellant are coupled by the friction force

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...

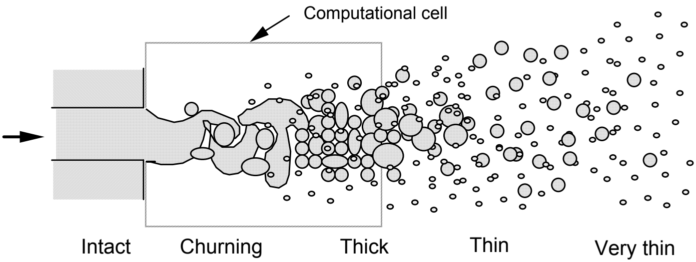


Figure: Schematic representation of spray regimes for liquid injection from a single hole nozzle [R.D. Reitz "Computer Modeling of Sprays" 1996]. Terminology taken from [P.J. O'Rourke's PhD Princeton University, 1981]

Thin regime: volume fraction of dispersed phase $\ll 0.1$, feedback force i.e. friction on propellant not neglected

Unknowns

$F \equiv F(t,x,v) \geq 0$	velocity distribution function of dispersed phase
$u \equiv u(t,x) \in \mathbf{R}^3$	velocity field in the gas
$p \equiv p(t,x) \in \mathbf{R}$	gas pressure

VNS system

$$\begin{cases} \partial_t F + v \cdot \nabla_x F - \kappa \operatorname{div}_v((v-u)F) = 0 \\ \partial_t u + u \cdot \nabla_x u = -\nabla_x p + \nu \Delta_x u + \kappa \int (v-u) F dv \\ \operatorname{div}_x u = 0 \end{cases}$$

Parameters $\kappa =$ drag coefficient, $\nu =$ gas viscosity; gas density $= 1$

DERIVING NAVIER-STOKES + BRINKMAN FORCE

THE HOMOGENIZATION APPROACH

L. Desvillettes, F.G., V. Ricci
J. Stat. Phys. **131** (2008), 941–967

Spherical Particles in a Navier-Stokes Fluid

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

Time-dependent domain filled by the propellant

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

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

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

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

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

Scaling of the fluid dynamical quantities

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

Inserting this in the Navier Stokes equation, one finds

$$\begin{cases} \tau(\partial_{\hat{t}} + \hat{u} \cdot \nabla_x)\hat{u} = -\nabla_x \hat{p} + \nu \Delta_x \hat{u} + \hat{\mathbf{f}}, \quad \operatorname{div}_x \hat{u} = 0 \\ \hat{u}(\hat{t}, \cdot)\big|_{\partial B(\hat{X}_k(\hat{t}),r)} = \hat{V}_k(\hat{t}) \end{cases}$$

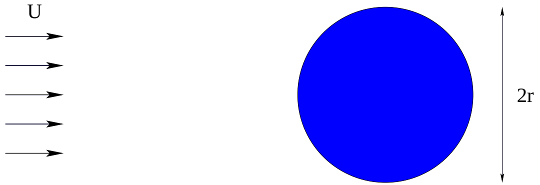
Drag Force: Stokes Formula

Stokes formula (1851) for the drag force exerted on a sphere of radius r by a viscous fluid of viscosity μ with velocity U at infinity

$$6\pi\mu rU$$

Total friction exerted by N noninteracting spheres of radius r

$$6\pi\mu NrU$$



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 $\partial\mathcal{O}$

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

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

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

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

$$\text{div}_x \mathbf{f} = 0\,, \qquad \int_{\mathcal{O}} |\mathbf{f}(x)|^2 dx < \infty$$

Theorem 1 (Derivation of the Brinkman Force)

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

$$\begin{cases} \nabla_x p_r = \nu \Delta_x u_r + \mathbf{f}\,, & \operatorname{div}_x u_r = 0\,, \quad x \in \mathcal{O}_r \\ u_r\big|_{\partial B(x_k,r)} = v_k\,, & u_r\big|_{\partial\mathcal{O}} = 0 \end{cases}$$

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

$$\int_{\mathcal{O}_r} |\nabla u_r(x) - \nabla u(x)|^2 dx \to 0$$

where u is the solution to the Stokes equation with friction force

$$\begin{cases} \nabla_x p = \nu \Delta_x u + \mathbf{f} + 6\pi\nu \displaystyle\int (v-u) F dv\,, \quad x \in \mathcal{O} \\ \operatorname{div}_x u = 0\,, \quad u\big|_{\partial\mathcal{O}} = 0 \end{cases}$$

Extensions/Open Pbms

(1) Argument extends without difficulty to steady Navier-Stokes, provided that $\nu \geq \nu_0[\mathbf{f}, F, \mathcal{O}] > 0$

See also [Allaire: Arch. Rational Mech. Anal. 1990] (periodic case, based on earlier work by Cioranescu-Murat, and Khruslov's group)

(2) Recent improvement by [Hillairet: Arch. Rational Mech. Anal. 2018] 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
Comm. Math. Sci. **15** (2017), 1703–1741
(Kinetic and Related Models **11** (2018), 43–69)

Table of Parameters

Parameter	Definition
L	size of the container
$\mathcal{N}_p$	number of dust particles$/L^3$
$\mathcal{N}_g$	number of gas molecules$/L^3$
V_p	thermal speed of dust particles
V_g	thermal speed of gas molecules
S_{pg}	particle/gas cross-section
S_{gg}	molecular cross-section
$\eta = m_g/m_p$	mass ratio (gas molecules/particles)
$\epsilon = V_p/V_g$	thermal speed ratio (particles/gas)

Dimensionless Quantities

Dimensionless variables

$$\hat{x} = x/L\,, \quad \hat{t} = tV_p/L\,, \quad \underbrace{\hat{v} = v/V_p}_{\text{particles}}\,, \quad \underbrace{\hat{w} = w/V_g}_{\text{molecules}}$$

Dimensionless velocity distribution functions

$$\hat{F}(\hat{t},\hat{x},\hat{v}) = V_p^3 F(t,x,v)/\mathcal{N}_p \quad \text{dispersed phase}$$

$$\hat{f}(\hat{t},\hat{x},\hat{w}) = V_g^3 f(t,x,w)/\mathcal{N}_g \quad \text{propellant gas}$$

Dimensionless Boltzmann system

$$\partial_{\hat{t}}\hat{F} + \hat{v}\cdot\nabla_{\hat{x}}\hat{F} = \overbrace{\mathcal{N}_g S_{pg} L \tfrac{V_g}{V_p}\hat{\mathcal{D}}(\hat{F},\hat{f})}^{\text{deflection of particles/droplets}}$$

$$\partial_{\hat{t}}\hat{f} + \tfrac{V_g}{V_p}\hat{w}\cdot\nabla_{\hat{x}}\hat{f} = \underbrace{\mathcal{N}_p S_{pg} L \tfrac{V_g}{V_p}\hat{\mathcal{R}}(\hat{f},\hat{F})}_{\text{friction on gas molecules}} + \underbrace{\mathcal{N}_g S_{gg} L \tfrac{V_g}{V_p}\hat{\mathcal{C}}(\hat{f})}_{\text{Boltzmann collision } \int}$$

Scaling assumptions

$$\begin{cases}\epsilon := V_p/V_g = \mathcal{N}_p S_{pg} L = (\mathcal{N}_g S_{gg} L)^{-1} \ll 1\\ \eta := \mathcal{N}_p/\mathcal{N}_g \ll \epsilon^2\end{cases}$$

Scaled Boltzmann system — dropping hats on scaled quantities

$$\begin{cases}\partial_t F + v\cdot\nabla_x F = \frac{1}{\eta}\mathcal{D}(F,f)\\ \partial_t f + \frac{1}{\epsilon} w\cdot\nabla_x f = \mathcal{R}(f,F) + \frac{1}{\epsilon^2}\mathcal{C}(f)\end{cases}$$

Gas distribution function

$$f(t,x,w) = M(w)(1+\underbrace{\epsilon g(t,x,w)}_{\text{fluctuation}})\,,\quad \underbrace{M(w) := \tfrac{1}{(2\pi)^{3/2}} e^{-|w|^2/2}}_{\text{centered Maxwellian}}$$

Scaled Boltzmann Collision Integral

(Maxwell-)Boltzmann collision integral given by

$$\mathcal{C}(f)(w) = \iint_{\mathbf{R}^3 \times \mathbf{S}^2} (f(w')f(w'_*) - f(w)f(w_*))c(|\tfrac{w-w_*}{|w-w_*|} \cdot \omega|) dw_* d\omega$$

where

$$\begin{cases} w' = w \ - (w - w_*) \cdot \omega\omega \\ w'_* = w_* + (w - w_*) \cdot \omega\omega \end{cases}$$

Pseudo-Maxwellian collision kernel for gas molecules satisfying

$$4\pi \int_0^1 c(\mu) d\mu = 1$$

Geometry of Molecular Collisions

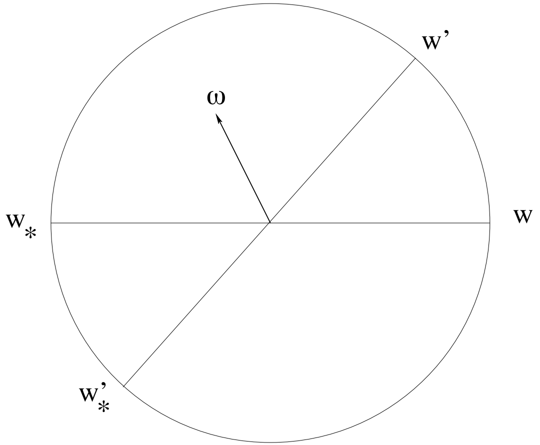


Figure: Unit vector $\omega =$ exterior angle bissector of $(w - \widehat{w_*, w'} - w'_*)$

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

$$\begin{cases}\mathcal{D}(F,f)(v)=\iint_{\mathbf{R}^3\times\mathbf{S}^2}(F(v'')f(w'')-F(v)f(w))b(\epsilon v-w,\omega)dwd\omega\\ \mathcal{R}(f,F)(w)=\iint_{\mathbf{R}^3\times\mathbf{S}^2}(f(w'')F(v'')-f(w)F(v))b(\epsilon v-w,\omega)dvd\omega\end{cases}$$

where

$$v''=v-\tfrac{2\eta}{1+\eta}\left(v-\tfrac{1}{\epsilon}w\right)\cdot\omega\omega\,,\qquad w''=w-\tfrac{2}{1+\eta}\,(w-\epsilon v)\cdot\omega\omega$$

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

$$0<b(z,\omega)\le B_*(1+|z|)\,,\quad\int_{\mathbf{S}^2}b(z,\omega)d\omega\ge\tfrac{1}{B_*}\tfrac{|z|}{1+|z|}\qquad\text{a.e.}$$

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

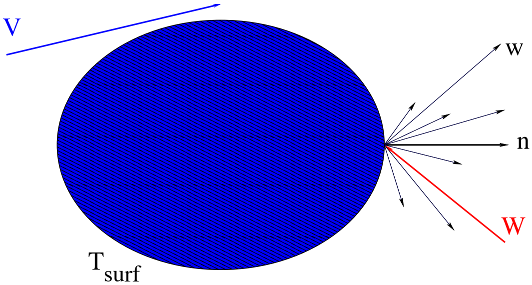


Figure: Diffuse reflection of gas molecules at the surface of a particle or of a droplet with surface temperature T_{surf}; velocity of particle/droplet denoted V; molecular velocity denoted w, W

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

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

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

where

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

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 $F_n \to F$ and $g_n \to g$ with

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

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

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

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

satisfy the VNS system with friction rate κ defined below and

$$\frac{1}{\nu} := 6\pi \int_0^1 c(\mu)(\tfrac{5}{3} - \mu^2)\mu^2 d\mu$$

Lemma A (Drag force)

Under the assumptions of Theorem 2

$$\frac{1}{\eta_n}\mathcal{D}(F_n, f_n)(t,x,v) \to \kappa\,\mathrm{div}_v((v-u(t,x))F(t,x,v))$$

with

$$\kappa := \begin{cases} \frac{8\pi}{3}\int |z|^2 M(z)\left(\int_0^1 B(|z|,\mu)\mu^2 d\mu\right) dz & \text{elastic} \\ \frac{1}{3}\int (\frac{\sqrt{2\pi}}{3\beta} + |z|)|z|^2 M(z) dz & \text{inelastic} \end{cases}$$

Lemma B (Brinkman (friction) force)

Under the assumptions of Theorem 2

$$\frac{1}{\epsilon_n}\int \mathcal{R}(f_n, F_n)(t,x,w) w dw \to \kappa \int (v-u(t,x))F(t,x)dv$$

• Let $\phi \equiv \phi(v)$ be a smooth test function; due to collision symmetries

$$\left.\begin{array}{r} v'' = v - \frac{2\eta}{1+\eta}\left(v - \frac{1}{\epsilon}w\right)\cdot\omega\omega \\ \text{with } \eta \ll \epsilon^2 \ll 1 \end{array}\right\} \implies J := \frac{1}{\eta}\int \phi(v)\mathcal{D}(F,f)(v)dv$$

$$= \iint F(v)f(w)\left(\int \frac{1}{\eta}\underbrace{(\phi(v)-\phi(v''))}_{\text{Taylor expand at } v} b(\epsilon v - w,\omega)d\omega\right)dvdw$$

$$\simeq -\iint F(v)f(w)\nabla\phi(v)\cdot\left(\int (v - \tfrac{1}{\epsilon}w)\cdot\omega\omega b(\epsilon v - w,\omega)d\omega\right)dvdw$$

$$\simeq -\kappa \int F(v)(v-u)\cdot\nabla\phi(v)dv \quad \text{and integrate by parts}$$

• Lemma A implies Lemma B by momentum conservation

Proof of Theorem 2

•Write the equation for $g_n = (f_n - M)/\epsilon_n M$ in the form

$$\partial_t g_n + \frac{1}{\epsilon_n} w \cdot \nabla_x g_n + \frac{1}{\epsilon_n^2} \mathcal{L} g_n = \frac{\mathcal{C}(M g_n) + \mathcal{R}(M(1 + \epsilon_n g_n), F_n)}{\epsilon_n M}$$

where $\mathcal{L} g_n := -M^{-1} D\mathcal{C}(M) \cdot (M g_n)$

•Follow the same argument as in Bardos-FG-Levermore (JSP1991), or use a Hilbert or Chapman-Enskog expansion, to find the equations satisfied by the velocity field u

(a) Multiplying both sides of this equation by $\epsilon_n M$ and integrating in w leads to the incompressibility equation $\text{div}_x\, u = 0$

(b) Applying the operator $Mw - \epsilon_n M \mathcal{L}^{-1} A \cdot \nabla_x$ componentwise to each side of this equation, with $A := w \otimes w - \frac{1}{3}|w|^2 I$, and integrating in w leads to the motion equation for the velocity field u

Conclusion/Extensions/Open Problems

The kinetic model can be easily extended
(a) to derive the Vlasov-Stokes system
(b) to take into account compressibility in the propellant
(c) to take into account dispersed phase collisions, polydispersion

Richer description of the drag force than the Stokes formula
(a) inelastic collision model with temperature of the dispersed phase
(b) detailed description of rarefied flow past a sphere
[Sone-Aoki Rarefied Gas Dyn. 1977, J. Méc. Th. Appl. 1983, Sone-Aoki-Takata Phys. Fluids 1993, Taguchi J. Fluid Mech. 2015]

Formal derivations Boltzmann → Navier-Stokes [Sone: RGD1969, Bardos-G.-Levermore: C.R. Acad. Sci. 1989 & J. Stat. Phys. 1991]

Rigorous derivations more difficult [Bardos-Ukai: Math. Models Meth. Appl. Sci. 1993 (small data), G.-Saint-Raymond: Invent. Math. 2004 & J. Math. Pures Appl. 2009 (all data)]