Eulerian modeling and simulation of moderately dense spray flows: application to Solid Rocket Motors

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Overview

1. SRM two-phase flows
   - Two-phase flow applications
   - Two-way coupling
   - Polydispersity
   - Emerging issues

2. Disperse two-phase modeling
   - Kinetic modeling
   - Eulerian Multi-Fluid method
   - Numerical highlight

3. Low inertia droplets
   - Results for low inertia droplets
   - Description of size
   - Coalescence
   - Two-way coupling
   - Applicative computations

4. Moderate inertia droplets
   - Results for moderate inertia droplets
   - The Anisotropic Gaussian Model
   - AG Transport
   - Homo-coalescence
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Two-phase flow applications

Solid Rocket Motors (SRM)

Solid Rocket Motors (SRM) : anaerobic propellers for rockets and missiles

- high thrust
- cheap
- storable

- less efficient
- subject to thrust oscillations
- difficult to throttle
**Two-phase flow applications**

**Physics of a SRM**

**Star-shaped grain of a LP10 sub-scale test motor**

**Internal flow is complex**

- Turbulent: transition and up to $Re = 10^6$
- Compressible: up to $Ma = 3$
- Reactive
- Coupled to the structure: obstacles, casing
- **Two-phase**

ONERA

Vorticity in a P230 [Doisneau et al., 2013a, CRM]
Origin and impact of the condense phase

Propellant is aluminized to increase specific impulse

- combustion $\Rightarrow$ liquid Al$_2$O$_3$
- polydisperse droplets (below 200 $\mu$m)
- mass concentration 35% $\Rightarrow$ strong interaction with flow

Condense phase impact

- $I_{sp}$ losses (nozzle)
- role on oscillations (chamber)
- slag, erosion, signature

[Doisneau et al., 2011, EUCASS]
Liquid Rocket Engines (LRE)

- Plate of coaxial injectors
  Vulcain 2 (SAFRAN)

**Subcritical regime**
- Atomization of liquid oxygen (LOx)
- Combustion of dense LOx spray with gaseous fuel
- Combustion and acoustics

**Transient heat release rate**
- In a coaxial GCH4/LOx inj. [Doisneau, 2013b]
Two-phase flow applications

Atmospheric engines

- Gasoline Direct Injection (GDI)
- Diesel injection
- Gas Turbine (GT)

Injection modeling focuses
- atomization of liquid fuel
- combustion of dense fuel spray with hot compressed air + EGR
- auto-ignition, cycle-to-cycle variability

High pressure jet (subcritical)
[Skeen et al., 2015]

Initial Conditions
Pressure: 60 bar
Temperature: 900K
Composition: (by volume) 0.00% O2, 89.71% N2, 6.52% CO2, 3.77% H2O

Injection Conditions
Peak Velocity: 600 m/s
Peak Re_{\text{d}}: 117,000
Density: 650 kg/m³
Temperature: 363 K
**Astrophysics**

Planet formation in stellar nebula: Proto-planetary disc (photo: ALMA)

PPD simulation under shearing sheet approximation [Simon et al. 2013]

Chondrules

**PPDs: a two-phase problem**

- Gas continuum $\lambda = 1 \text{ m} \ll \eta_K = 1000 \text{ m}$
- Polydisperse loading of dust from $\mu \text{m}$ to km
- Agglomeration and gravitational capture $\Rightarrow$ planet formation
Two-way coupling

What two-way coupling?

Flow regimes depend on the disperse phase

- Volume fraction: $\alpha_l$
- Mass fraction: $Y_l$
- Inertia: $St$

$\Rightarrow$ Classifications

[O'Rourke, 1981, Elghobashi and Abou-Arab, 1983]

Case of the P230 SRM

Volume fractions $\alpha_p$ of alumina droplets in P230 with coalescence [Doisneau et al., 2013a, CRM]

In SRMs where $\rho_l/\rho_g \sim 10^3$ $\Rightarrow$ Moderately dense

- $Y_l > 1\% \Rightarrow$ Two-way coupling through drag, heating, and evaporation
- $\alpha_l > 0.01\% \Rightarrow$ weak retrocoupling through volume occupancy
Polydispersity: size as a key parameter

Polydispersity

Relaxation

\[ u = u_g \]

\[ \tau^u(r) \sim r^2 \]

Coalescence

Brownian

hetero-PTC

all types of PTC

Smallest droplet Stokes time \( \tau^u(r_1) \)

1 \( \mu s \)

Acoustic CFL time

10 \( \mu s \)

Convective CFL time (nozzle)

30 \( \mu s \)

Big droplet Stokes time \( \tau^u(r_2) \)

10,000 \( \mu s \)

First acoustic mode

50,000 \( \mu s \)

Eddy revolution time

50,000 \( \mu s \)

Convective CFL time (injection)

90,000 \( \mu s \)

Typical computation time

1,000,000 \( \mu s \)

Polydispersity

Miscellaneous time scales

Various physical regimes:

- **Stokes number** \( St = \frac{\tau_p}{\tau_g} \)
- **Knudsen number** \( Kn = \frac{\tau_C}{\tau_g} \)
Polydispersity: size as a key parameter

Relaxation

\[ u = u_g \]

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Coalescence

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<thead>
<tr>
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Polydispersity

Miscellaneous time scales

Various physical regimes:

- **Stokes number**
  \[ \text{St} = \frac{\tau_p}{\tau_g} \]

- **Knudsen number**
  \[ \text{Kn} = \frac{\tau_c}{\tau_g} \]

Flow times

\[ \tau_{\text{chamber}} / \tau_{\text{nozzle}} \]
Low inertia droplets \( \text{St} < \text{St}_c \)

Low inertia droplet velocities and temperatures

- **fully correlated** at a given size
- relaxation at \( \tau \sim r^2 \): wide **time scale spectrum**

[Vié et al., 2013b]

Crossings at **different** sizes

**Hetero-PTC**
Low inertia droplets $\text{St} < \text{St}_c$

- Low inertia droplet velocities and temperatures:
  - **fully correlated** at a given size
  - relaxation at $\tau \sim r^2$ : wide **time scale spectrum**

  [Vié et al., 2013b]

- Crossings at different sizes:
  - **Hetero-PTC**

Low inertia droplet modeling issues:
- stiffness
- hetero-coalescence
Moderate inertia droplets  \( \text{St} \sim \text{St}_c \)

**Homo-crossings**

Taylor-Green vortices at two different times for \( \text{St} = 7.5\text{St}_c \)
(Lagrangian simulations starting from a uniform concentration).

**Hypercompressibility**

- accumulations which participate to the physics/singularities
- vacuum
- gradients

Crossings at same size

Homo-PTC
Moderate inertia droplets $St \sim St_c$

### Homo-crossings

Taylor-Green vortices at two different times for $St = 7.5St_c$ (Lagrangian simulations starting from a uniform concentration).

### Hypercompressibility

- **accumulations** which participate to the physics/singularities
- **vacuum**
- gradients

### Moderate inertia droplet modeling issues

- hypercompressibility
- homo-coalescence
Coalescence induced couplings

Crossings + high volume fraction $\Rightarrow$ **collisions**

**Collision efficiency modeling** [D’Herbigny and Villedieu, 2001]

Colliding droplet regimes: reflexion, coalescence, and stretching [Qian and Law, 1997]
Coalescence induced couplings

Crossings + high volume fraction $\Rightarrow$ **collisions**

Collision efficiency modeling [D’Herbigny and Villedieu, 2001]

Colliding droplet regimes: reflexion, **coalescence**, and stretching [Qian and Law, 1997]

**Size-Size coupling**
- Collision rates
- Size distribution prediction

**Size-velocity coupling**
- Collision rates
- Induced polydispersity
Emerging issues

Two-way coupling of inertial particles

Losses occur in the nozzle

Weakly-colliding inertial moderately dense jets [Doisneau et al., 2013a, CRM]

PTC and strong coupling ⇒ emerging physical issue!
Two-way coupling of inertial particles

Losses occur in the nozzle

Weakly-colliding inertial moderately dense jets [Doisneau et al., 2013a, CRM]

PTC and strong coupling ⇒ emerging physical issue!

Nozzle efficiency modeling

Inertial particle modeling
  +
Size-Velocity coupling
  +
Two-way coupling
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Kinetic modeling for the disperse phase

Point particles with velocity $\mathbf{c}$, temperature $\theta$, surface $S$

Number density function \textbf{NDF} : describes the disperse phase

$$dN = f(t, \mathbf{x}, \mathbf{c}, S, \theta) d\mathbf{x} d\mathbf{c} dS d\theta$$

\textbf{NDF} satisfies a Boltzmann-like PDE [Williams, 1958]

$$\partial_t f + \partial_x \cdot (\mathbf{c} f) + \partial_c \cdot (\mathbf{F} f) + \partial_\theta (\mathbf{H} f) + \partial_S (\mathbf{R} f) = \mathcal{B} + \mathcal{C}$$

Closures : all the physical modeling job

- Drag force $\mathbf{F}$
- Heat transfer $\mathbf{H}$
- Mass transfer $\mathbf{R}$
- Secondary break-up $\mathcal{B}$
- Collisions/coalescence $\mathcal{C}$
Kinetic coalescence

Inertial droplet coalescence:

\[ \mathcal{C}^+ = \frac{1}{2} \int_{c^*} \int_{v^* \in [0, v]} f(t, x, c^\circ, v^\circ) f(t, x, c^*, v^*) \mathcal{K}_{\text{coal}} d v^* d c^* \]

\[ \mathcal{C}^- = \int_{c^*} \int_{v^*} f(t, x, c, v) f(t, x, c^*, v^*) \mathcal{K}_{\text{coal}} d v^* d c^* \]

Balistic coalescence kernel modeling

\[ \mathcal{K}_{\text{coal}} = \pi (r^{\circ} + r^*)^2 \| \mathbf{u} - \mathbf{u}^* \| \mathcal{E}(......) \]

Efficiency \( \mathcal{E} \) models

- coalescence efficiency [Brazier-Smith et al., 1972, Ashgriz and Poo, 1990]
Inertial droplet coalescence:

\[
\begin{align*}
\mathcal{C}^+ &= \frac{1}{2} \int \int_{v^* \in [0,v]} f(t,x,c^\delta,v^\delta) f(t,x,c^*,v^*) \mathcal{K}_{\text{coal}} d v^* d c^* \\
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Balistic coalescence kernel modeling:

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Efficiency \(\mathcal{E}\) models:

- coalescence efficiency [Brazier-Smith et al., 1972, Ashgriz and Poo, 1990]
Approaches for polydisperse NDFs

- **Direct** (finite volumes) intractable
- **Lagrangian** (NDF samples) convergence, parallelization
- **Eulerian** (fields) several approaches

Eulerian approaches: convergence, two-way coupling and parallelization

- Sampling (one system per droplet size) no coalescence
- DQMOM [Fox et al., 2008] multivariate
- Kinetic-based moment methods [Kah et al., 2010, Vié et al., 2013b] algebra

Multi-Fluid = continuous description of size
Multi-Fluid assumptions [Laurent and Massot, 2001]

Semi-kinetic level

Correlation of velocity and temperature to size:

\[ f(t, x, c, s, \theta) \approx n(t, x, s) \delta(c - \bar{u}(t, x, s)) \delta(\theta - T(t, x, s)) \]

Multi-Fluid level

Size discretization in sections \([s_{k-1}, s_k]\) ⇒ Reconstructions

- Velocity
  \[ \bar{u}(t, x, s) \approx u_k(t, x) \]
- Temperature
  \[ T(t, x, s) \approx T_k(t, x) \]
- One size moment
  \[ n(t, x, s) \approx m_k(t, x) \kappa_k(s) \]

...higher order requires modeling AND numerics! [Kah et al., 2010, Vié et al., 2013b]
Multi-Fluid assumptions [Laurent and Massot, 2001]

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Pros

- Flexible on polydispersity
- Captures dynamics for \(St \leq St_c\)
- Two-way coupling to Eulerian gas solver
- Parallelization
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Pros

- Flexible on polydispersity
- Captures dynamics for \(St \leq St_c\)
- Two-way coupling to Eulerian gas solver
- Parallelization

Cons

- Hypercompressibility and transport scheme
- Complex algebra
- Fails for homo-PTC
Resulting two-phase model

**Superimposed fluids**
- Sets of moment fields
- Coupled through source terms

**A moment method**
- Conserve some moments $U$
- Reconstruction $f_U$ to compute sources $\Omega$
- Realizability: $U \in M$

\[
\frac{dU}{dt} = \Omega \left( \int \Phi \cdot f_U \right)
\]
Eulerian Multi-Fluid method

Resulting two-phase model

Superimposed fluids

- Sets of moment fields
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A moment method

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- Reconstruction $f_U$ to compute sources $\Omega$
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\[
\frac{dU}{dt} = \Omega \left( \int \Phi \cdot f_U \right)
\]

Example: Drag term

\[
\frac{dm_k u_k}{dt} = \int_{S_{k-1}}^{S_k} F(u_k, u_g, S) \kappa(S) dS
\]
Transport in physical space

**Hypercompressibility** (gradients, singularities and vacuum)
- **accuracy issues** (structures participate to the physics)
- **stability issues** (high order near discontinuities, undershoots)

**Structured grids** (research codes)

- Kinetic schemes
  - pressureless: 2nd order Bouchut/dimensional splitting
    [de Chaisemartin, 2009]
  - weak pressure: open topic

**Unstructured grids** (industrial codes)

- Finite volume 2nd order MUSCL strategy:
  dedicated implementation [Le Touze et al., 2012]
- Cell-vertex with high order scheme/artificial viscosity:
  dedicated stabilization method [Martinez, 2009]
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Results for low inertia droplets
1) Size reconstruction

Description of size

Surface NDF

- Lognormal size NDF
- OSM

Type of reconstruction ⇔ integration method
1) Size reconstruction

Two-Size moment Multi-Fluid approaches

- **Exp-TSM method in CEDRE** [Dufour et al., 2003]
1) Size reconstruction

Two-Size moment Multi-Fluid approaches

- **Exp-TSM** method in CEDRE [Dufour et al., 2003]
- **Aff-TSM** method introduced by [Laurent, 2013]
1) Size reconstruction

Two-Size moment Multi-Fluid approaches

- **Exp-TSM** method in CEDRE [Dufour et al., 2003]
- **Aff-TSM** method introduced by [Laurent, 2013]

- **Two-Size Moment** methods are efficient to capture polydispersity
- Type of reconstruction ↔ integration method
2) Coalescence sources

Coalescence terms: quadratic sums of 2D elementary integrals

\[
\begin{align*}
2C^n_k &= \sum_{i=1}^k \sum_{j=1}^{i-1} Q^n_{ijk} \\
2C^m_k &= \sum_{i=1}^k \sum_{j=1}^{i-1} (Q^*_{ijk} + Q^\circ_{ijk}) \\
2C^u_k &= \sum_{i=1}^k \sum_{j=1}^{i-1} (u_i Q^*_{ijk} + u_j Q^\circ_{ijk}) \\
2C^n_k &= \sum_{i=1}^{N} \sum_{j=1}^{N} Q^n_{kji} \\
2C^m_k &= \sum_{i=1}^{N} \sum_{j=1}^{N} (Q^*_{kji} + Q^\circ_{kji}) \\
2C^u_k &= u_k \cdot 2C^m_k
\end{align*}
\]

Elementary integrals

\[
\left( \begin{array}{c} Q^n_{ijk} \\ Q^*_{ijk} \\ Q^\circ_{ijk} \end{array} \right) (t, x) = \int_{ij(k)} \left( \begin{array}{c} \frac{1}{6\sqrt{\pi}} S^{3/2} \\ \frac{\rho_l}{6\sqrt{\pi}} S^{3/2} \\ \frac{\rho_l}{6\sqrt{\pi}} S^{3/2} \end{array} \right)
\]

Relative error of integrals for Exp-TSM with (NC5) 13 sections, sizes in radius (µm); + quadrature nodes.
2) Coalescence sources: Quadratures

Two approaches tested for efficient integration [Doisneau et al., 2013b, JCP]

- (NCn): Polynomial quadratures (Newton-Cotes) but also Gauss-Legendre
- (Adn): Adaptive quadrature based on the exponential kernel

Comparison of quadrature error of Exp-TSM

<table>
<thead>
<tr>
<th>β steepness</th>
<th>Relative error (logscale)</th>
</tr>
</thead>
<tbody>
<tr>
<td>-100</td>
<td>-35</td>
</tr>
<tr>
<td>-50</td>
<td>-30</td>
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<tr>
<td>0</td>
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<tr>
<td>550</td>
<td>30</td>
</tr>
<tr>
<td>600</td>
<td>35</td>
</tr>
</tbody>
</table>

Test integral $I(β)$ with $S_1 = 1$, $S_2 = 2$ and $S^* = 0.75$

Convergence on a size-velocity coupling case

One size (Empty) and two size moment (Solid)

Excellent with low number of sections

Results

Exp-TSM: Adaptive quadrature accurate with $2 \times 2$ points!
Aff-TSM: Polynomial quadrature allows more points
2) Coalescence sources: Validation

New phase space strategy


**Exp-TSM (exponential reconstruction)**

- **Adaptive quadrature** for elementary integrals
- Validation versus Lagrangian
- Convergence study
- **Conception** of a dedicated test case
- Validation versus analytical
- Validation versus experiment
- **Implementation** in CEDRE
- Validation versus Lagrangian SRM

**Affine reconstruction** [Laurent et al., 2015]

- **Accurate quadrature** for elementary integrals
- Convergence study
- **Implementation** in CEDRE
2) Coalescence sources: Validation

New phase space strategy


Exp-TSM (exponential reconstruction)
- **adaptive quadrature** for elementary integrals
- validation versus Lagrangian
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- **conception** of a dedicated test case
- validation versus analytical
- validation versus experiment
- **implementation** in CEDRE
- **validation** versus Lagrangian SRM

Affine reconstruction [Laurent et al., 2015]
- **accurate quadrature** for elementary integrals
- convergence study
- **implementation** in CEDRE

Achievements: accuracy and efficiency
- for complex source terms
- for stiff cases (e.g. bimodal)
### 3) Strategy for two-way coupling

#### ACS: Acoustic/Convection Splitting [Doisneau et al., 2014, JPP]

**Operator splitting** [Strang, 1968, Descombes and Massot, 2004]
- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

#### The Two-way coupling System

\[
\begin{align*}
\partial_t \rho g + \partial_x (\rho g u_g) &= 0 \\
\partial_t (\rho g u_g) + \partial_x (\rho g u_g \otimes u_g + p I) &= - \sum_{k=1}^{N_{\text{sec}}} m_k F_k \\
\partial_t (\rho g c_g T_g) + \partial_x (\rho g c_g T_g u_g) &= - \sum_{k=1}^{N_{\text{sec}}} m_k H_k - \sum_{k=1}^{N_{\text{sec}}} m_k F_k (u_g - u_k) \\
\partial_t n_k + \partial_x (n_k u_k) &= 2 C_k^{n+} - 2 C_k^{n-} \\
\partial_t m_k + \partial_x (m_k u_k) &= 2 C_k^{m+} - 2 C_k^{m-} \\
\partial_t (m_k u_k) + \partial_x (m_k u_k \otimes u_k) &= m_k F_k + 2 C_k^{u+} - 2 C_k^{u-} \\
\partial_t (m_k h_k) + \partial_x (m_k h_k u_k) &= m_k H_k + 2 C_k^{u+} - 2 C_k^{u-}
\end{align*}
\]

\[k = 1, N_{\text{sec}}\]
Two-way coupling

3) Strategy for two-way coupling

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- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
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The $T_g$ operator

\[
\begin{align*}
\partial_t \rho_g + \partial_x (\rho_g u_g) \\
\partial_t (\rho_g u_g) + \partial_x (\rho_g u_g \otimes u_g + p I) &= 0 \\
\partial_t (\rho_g c_g T_g) + \partial_x (\rho_g c_g T_g u_g) &= 0
\end{align*}
\]
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The $\mathcal{T}_k$ operators

\[
\begin{align*}
\partial_t n_k + \partial_x \cdot (n_k u_k) &= 0 \\
\partial_t m_k + \partial_x \cdot (m_k u_k) &= 0 \\
\partial_t (m_k u_k) + \partial_x \cdot (m_k u_k \otimes u_k) &= 0 \\
\partial_t (m_k h_k) + \partial_x \cdot (m_k h_k u_k) &= 0
\end{align*}
\]

$k = 1, N_{sec}$

Gas transport
Relax.
Liq. transport
Sources
3) Strategy for two-way coupling

**ACS: Acoustic/Convection Splitting** [Doisneau et al., 2014, JPP]

**Operator splitting** [Strang, 1968, Descombes and Massot, 2004]
- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

**The \( R \) operator**

\[
\begin{align*}
\partial_t \rho_g & = 0 \\
\partial_t (\rho_g u_g) & = - \sum_{k=1}^{N_{\text{sec}}} m_k F_k \\
\partial_t (\rho_g c_g T_g) & = - \sum_{k=1}^{N_{\text{sec}}} m_k H_k - \sum_{k=1}^{N_{\text{sec}}} m_k F_k (u_g - u_k) \\
\partial_t n_k & = 0 \\
\partial_t m_k & = 0 \\
\partial_t (m_k u_k) & = m_k F_k \\
\partial_t (m_k h_k) & = m_k H_k
\end{align*}
\]

\( k = 1, N_{\text{sec}} \)
3) Strategy for two-way coupling

**ACS : Acoustic/Convection Splitting** [Doisneau et al., 2014, JPP]

Operator splitting [Strang, 1968, Descombes and Massot, 2004]

- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

\[
\begin{align*}
\partial_t n_k &= 2C_{k}^{n+} - 2C_{k}^{n-} \\
\partial_t m_k &= 2C_{k}^{m+} - 2C_{k}^{m-} \\
\partial_t (m_k u_k) &= 2C_{k}^{u+} - 2C_{k}^{u-} \\
\partial_t (m_k h_k) &= 2C_{k}^{u+} - 2C_{k}^{u-}
\end{align*}
\]

**The $\mathcal{C}$ operator**

\[\tau_{\text{coal min}}\]

\[k = 1, N_{\text{sec}}\]
### 3) Strategy for two-way coupling

**ACS : Acoustic/Convection Splitting** [Doisneau et al., 2014, JPP]

**Operator splitting** [Strang, 1968, Descombes and Massot, 2004]
- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

\[
\begin{align*}
\partial_t \rho g + \partial_x (\rho g u_g) &= 0 \\
\partial_t (\rho g u_g) + \partial_x (\rho g u_g \otimes u_g + p l) &= - \sum_{k=1}^{N_{sec}} m_k F_k \\
\partial_t (\rho g c_g T_g) + \partial_x (\rho g c_g T_g u_g) &= - \sum_{k=1}^{N_{sec}} m_k H_k - \sum_{k=1}^{N_{sec}} m_k F_k (u_g - u_k) \\
\partial_t n_k + \partial_x (n_k u_k) &= \frac{2}{C_k^{m+}} - \frac{2}{C_k^{n-}} \\
\partial_t m_k + \partial_x (m_k u_k) &= \frac{2}{C_k^{m+}} - \frac{2}{C_k^{m-}} \\
\partial_t (m_k u_k) + \partial_x (m_k u_k \otimes u_k) &= m_k F_k + \frac{2}{C_k^{u+}} - \frac{2}{C_k^{u-}} \\
\partial_t (m_k h_k) + \partial_x (m_k h_k u_k) &= m_k H_k + \frac{2}{C_k^{u+}} - \frac{2}{C_k^{u-}} \\
\end{align*}
\]

\( k = 1, N_{sec} \)
3) Strategy for two-way coupling

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**Operator splitting** [Strang, 1968, Descombes and Massot, 2004]
- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

Time stepping of a **splitting** method:

\[
U(t + \Delta t_a) = R T_g R \left( \sum_k I_k \right) C U(t)
\]
3) Strategy for two-way coupling

**ACS: Acoustic/Convection Splitting** [Doisneau et al., 2014, JPP]

**Operator splitting** [Strang, 1968, Descombes and Massot, 2004]
- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
- to capture strong gas-liquid coupling

Time stepping of a *splitting* method:

\[
U(t + \Delta t_a) = R \mathcal{T}_g R \left( \sum_k \mathcal{T}_k \right) C U(t)
\]

Capturing dissipation of acoustics

\[
\Delta t_a = \max\{K_p \tau_{\min}; K_g \tau_g\} \quad K_p, K_g \lesssim 1
\]
Overall strategy for low inertia droplets

Two-way coupling

\[ f(S) \]

Gas sources

\[ S_{k-1} \quad S_k \]

**MF needs**
- Two-way coupling: time integration
- Polydispersity: reconstruction
- Sources: quadratures and integration

Navier-Stokes

\[
\begin{align*}
N_{\text{sec}} & \quad \text{systems} \\
\partial_t m_k + \partial_x (m_k u_k) &= 0 \\
\partial_t (m_k u_k) + \partial_x (m_k u_k \otimes u_k) &= m_k F_k \\
\partial_t (m_k h_k) + \partial_x (m_k h_k u_k) &= m_k H_k
\end{align*}
\]
Overall strategy for low inertia droplets

\[ f(S) \]

\[ \begin{align*}
N_{\text{sec}} \text{ systems} &= \\
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\partial_t (m_k h_k) + \partial_x (m_k h_k u_k) &= m_k H_k
\end{align*} \]

\[ \Rightarrow \] Navier-Stokes with sources

**Improvements**

1. **Acoustic-convection splitting** [Doisneau et al., 2014, JPP]
3. **Coalescence terms** [Doisneau et al., 2013b, JCP]
4. **Break-up terms** [Dufour et al., 2003][Doisneau, 2013a, PhD]
Two-way coupling

**Overall strategy for low inertia droplets**

\[ f(S) \]

\[ S_{k-1} \quad S_k \]

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\partial_t n_k + \partial_x (n_k u_k) &= 0 \\
\partial_t m_k + \partial_x (m_k u_k) &= 0 \\
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\partial_t (m_k h_k) + \partial_x (m_k h_k u_k) &= m_k H_k
\end{align*} \]

MF needs
- Two-way coupling
- Polydispersity
- Sources

**Improvements**

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Overall strategy for low inertia droplets

\[
\begin{align*}
\frac{\partial n_k}{\partial t} + \frac{\partial}{\partial x}(n_k u_k) &= 2C^n_k \\
\frac{\partial m_k}{\partial t} + \frac{\partial}{\partial x}(m_k u_k) &= 2C^m_k \\
\frac{\partial}{\partial t}(m_k u_k) + \frac{\partial}{\partial x}(m_k u_k \otimes u_k) &= m_k F_k + 2C^u_k \\
\frac{\partial}{\partial t}(m_k h_k) + \frac{\partial}{\partial x}(m_k h_k u_k) &= m_k H_k + 2C^h_k
\end{align*}
\]

MF needs
- Two-way coupling
- Polydispersity
- Sources

Navier-Stokes with sources

Improvements
1. **Acoustic-convection splitting** [Doisneau et al., 2014, JPP]
3. **Coalescence terms** [Doisneau et al., 2013b, JCP]
4. **Break-up terms** [Dufour et al., 2003][Doisneau, 2013a, PhD]
**Overall strategy for low inertia droplets**

\[
\frac{\partial t}{\partial t} n_k + \nabla \cdot (n_k u_k) = 2C_n^k + 2B_n^k
\]
\[
\frac{\partial t}{\partial t} m_k + \nabla \cdot (m_k u_k) = 2C_m^k + 2B_m^k
\]
\[
\frac{\partial t}{\partial t} (m_k u_k) + \nabla \cdot (m_k u_k \otimes u_k) = m_k F_k + 2C_u^k + 2B_u^k
\]
\[
\frac{\partial t}{\partial t} (m_k h_k) + \nabla \cdot (m_k h_k u_k) = m_k H_k + 2C_h^k + 2B_h^k
\]

Navier-Stokes with sources

---

**MF needs**
- Two-way coupling
- Polydispersity
- Sources

---

**Improvements**

1. **Acoustic-convection splitting** [Doisneau et al., 2014, JPP]
3. **Coalescence terms** [Doisneau et al., 2013b, JCP]
4. **Break-up terms** [Dufour et al., 2003][Doisneau, 2013a, PhD]
Applicative computations (1)

P230 realistic case

Deformed-structured 45000 cell mesh of the P230 geometry and vorticity (rad/s)

- Bimodal injection with $d_2 \approx 60d_1$: **stiff**
- Vortex Shedding instabilities VSO and VSP: **unsteady**

Purpose

Feasibility of the **time integration/coalescence** strategy [Doisneau et al., 2013a, CRM]
Applicative computations (1)

No coalescence

$t = 1.09s$
Top: Eulerian volume fraction for $d_1$
Middle: Eulerian volume fraction for $d_2$
Bottom: Lagrangian parcels colored by diameter (m)

Coalescence

$t = 0.81s$
First: Eulerian volume fraction for $d_1$
Second: $d_2$ to $d_3$
Third: above $d_3$
Bottom: Lagrangian parcels colored by diameter (m)

Eulerian/Lagrangian comparison

- both depend on particle distribution at boundary
- limited homo-PTC
- good agreement
Applicative computations (2)

Simulation of LRE subcritical flames


Model cryogenic spray, flame, and chamber under free regime ($Y_{H_2}$, pressure, temperature, velocity)

Heat release rate of the VHAM test bed in the centerplane (Lox spray with MRE chemistry model)
Overview

1. SRM two-phase flows
   - Two-phase flow applications
   - Two-way coupling
   - Polydispersity
   - Emerging issues

2. Disperse two-phase modeling
   - Kinetic modeling
   - Eulerian Multi-Fluid method
   - Numerical highlight

3. Low inertia droplets
   - Results for low inertia droplets
   - Description of size
   - Coalescence
   - Two-way coupling
   - Applicative computations

4. Moderate inertia droplets
   - Results for moderate inertia droplets
   - The Anisotropic Gaussian Model
   - AG Transport
   - Homo-coalescence
Results for moderate inertia droplets
Homo-PTC in SRM

[Simoès, 2006] for one-way coupling

Homo-collisions

QMOM [Belt and Simonin, 2009] : adapt for industry

Predicting nozzle flow

Inertial moderately dense nozzle flow with coalescence/break-up
The Anisotropic Gaussian Model

Need for a moderately dense/inertial model

- **Homo-PTC in SRM**
  - [Simoes, 2006] for one-way coupling

- **Homo-collisions**
  - QMOM [Belt and Simonin, 2009] : adapt for industry

Predicting nozzle flow
- Inertial moderately dense nozzle flow with coalescence/break-up
Anisotropic Gaussian model

Velocity moment method for the kinetic level

- conserve information on relative velocities: Ten second order moments
- ...transported by third order ones: unclosed
- gaussian closure

The Anisotropic Gaussian Model
The Anisotropic Gaussian Model

Anisotropic Gaussian model

Velocity moment method for the kinetic level

- conserve information on relative velocities: Ten second order moments
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- gaussian closure

Multivariate gaussian [Vié et al., 2013a, CICP]

\[ N(c; u, \Sigma) = \frac{\det(\Sigma)^{-\frac{1}{2}}}{(2\pi)^{\frac{1}{2}}N_d} \exp\left(-\frac{1}{2}(c - u)^T \Sigma^{-1} (c - u)\right) \]

- origin: weakly collisional gases [Levermore and Morokoff, 1998]
- Ten parameters \( n, u, \Sigma = (\sigma_{ij}) \)
- closed

Velocity PDF for \( \sigma_{11} = 1, \sigma_{22} = 0.8 \) and \( \sigma_{12} = 0.75 \).
Anisotropic Gaussian model

**Velocity moment method** for the kinetic level

- conserve information on relative velocities: **Ten second order moments**
- ...transported by third order ones
- *gaussian* closure

**Multivariate gaussian** [Vié et al., 2013a, CICP]

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N(c; u, \Sigma) = \frac{\text{det}(\Sigma)^{-\frac{1}{2}}}{(2\pi)^{\frac{1}{2}} N_d} \exp\left(-\frac{1}{2} (c - u)^T \Sigma^{-1} (c - u)\right)
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- origin: weakly collisional gases [Levermore and Morokoff, 1998]
- **Ten** parameters \( n, u, \Sigma = (\sigma_{ij}) \)
- **closed**

**Mathematical properties**

- hyperbolic equations and entropic structure
- still hypercompressible
- but less singularities
Model behavior analysis

Homo-PTC case: $\text{Kn} = +\infty$, $\text{St} = +\infty$

Monokinetic: singularity  Anisotropic Gaussian  Multi-velocities: “exact”

Potential of AG: variance of repartition after the crossing
The Anisotropic Gaussian Model

Model behavior analysis

Homo-PTC case: $Kn = +\infty$, $St = +\infty$

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Monokinetic: singularity  Anisotropic Gaussian  Multi-velocities: “exact”

Remarks on isotropy

Isotropic Gaussian
- fails on variance
- spurious “backscattering”
The Anisotropic Gaussian Model

Model behavior analysis

Homo-PTC case: $Kn = +\infty$, $St = +\infty$

Potential of AG: variance of repartition after the crossing

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Remarks on isotropy

Isotropic Gaussian

- fails on variance
- spurious “backscattering”

Second order moments: “Energies”

- macroscopic energy $u_i u_j$: mean velocities
- ”microscopic” energy $\sigma_{ij}$: agitation

$$\partial_t (n\sigma_{ij}) + \partial_x \cdot (n\sigma_{ij} \mathbf{u}) = -\frac{1}{3} n\sigma_{ij} \partial_x \sigma^{Sym} \cdot \mathbf{u} - \frac{n\sigma_{ij}}{\tau} \mathbf{u}$$
Transport scheme

AG hypercompressibility

- 1st order scheme [Berthon, 2006] insufficient
- multi-dimension: anisotropy issue

A new 2nd order MUSCL scheme [Vié et al., 2013a, CICP]

- linear reconstruction and minmod type limiter
- FV conservative
- realizable (positivity of $n$, $\sigma_{ij}$ and $\det(\Sigma)$)
- HLL fluxes [Harten et al., 1983]

$\Rightarrow$ 3D structured grids

AG2D (Research 2D code developed at EM2C)

- Structured code
- 2nd order schemes
- dimensional splitting: adapted to anisotropy

Tested configurations

- unique crossing
- crossing with a potential force
- Taylor-Green vortices
- time-dependent HIT
**Transport scheme**

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- Structured code
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**Tested configurations**
- unique crossing
- crossing with a potential force
- Taylor-Green vortices
- time-dependent HIT
Results on transport

HIT test case [Vié et al., 2013a, CICP]

- Turbulent field ($\nabla \mathbf{u} = 0$)
- full spectrum of time/space structures
- decaying: sweeps different Stokes

Number density fields ($St = 7.5St_c$, $t = 3.6$ s)

- Lagrangian tracking
- Eulerian isotropic (IG)
- Eulerian anisotropic (AG)
Results on transport

HIT test case [Vié et al., 2013a, CICP]

- Turbulent field ($\nabla u = 0$)
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- decaying: sweeps different Stokes

Number density fields ($St = 7.5St_c$, $t = 3.6$ s)

- Lagrangian tracking
- Eulerian isotropic (IG)
- Eulerian anisotropic (AG)

Space repartition

- satisfactory (vacuum, spatial structures)
- visible differences on small scales
Results on transport (cont’d)

**Second order statistics (St = 7.5St_c)**

- Segregation
- Mean macroscopic energy
- Mean total energy

- AG behaves well: captures segregation and enranges
- Mesh refinement is beneficial

Lagrangian (—–)  
Eulerian IG (– –)  
Anisotropic AG (- -)  
→ mesh refinement (from \(256^2\) to \(2048^2\))
AG Transport

Results on transport (cont’d)

**Second order statistics (St = 7.5St_c)**

- Segregation
- Mean macroscopic energy
- Mean total energy

- **AG behaves well**: captures segregation and enranges
- **mesh refinement is beneficial**

**Conclusion on transport**

- **AG closure**: sensitive on statistics
- **needed for the physics of sources** (drag, two-way, reactive, radiative)
- **2nd order scheme needed**
Coalescence method with AG

**SAP2** (Research 2D code developed at EM2C)

- polydispersity: **TSM method**
- **AG** and 2nd order transport
- Hermite **velocity quadratures** qualified

Coalescence velocity integrals

\[
\int |c^* - c^\circ| N^* N^\circ dc^* dc^\circ
\]

up to 6D!

\[\Rightarrow\] mass, mean and agitation sources
Coalescence method with AG

**SAP2** (Research 2D code developed at EM2C)

- polydispersity: **TSM method**
- **AG** and 2\textsuperscript{nd} order transport
- Hermite **velocity quadratures** qualified

Coalescence velocity integrals

\[
\int |c^* - c^\circ| N^* N^\circ dc^* dc^* \\
\text{up to 6D!}
\Rightarrow \text{mass, mean and agitation sources}
\]

Homo-PTC with drag (Kn \sim 1, St \sim St_c) [Doisneau et al., 2014, CTR-COAL]

Homo-coalescence dynamics

- expected polydispersity
- angle reduction observed
Reference validation

Lagrangian DPS cross comparison [Doisneau et al., 2014, CTR-COAL]

Asphodele code [Reveillon and Demoulin, 2007]
- point-particle DNS
- deterministic collisions
- describes more detailed physics

Instantaneous particles colored by size

Inst. Eulerian $r_{30}$

Time average DPS $r_{30}$
Homo-coalescence

Reference validation

Lagrangian DPS cross comparison [Doisneau et al., 2014, CTR-COAL]

Asphodele code [Reveillon and Demoulin, 2007]
- point-particle DNS
- deterministic collisions
- describes more detailed physics

Instantaneous particles colored by size

Conclusion on homo-coalescence
- size growth predicted
- jet width estimated
## Conclusion on the AG model

**Anisotropic Gaussian**
- homo-PTC
- homo-coalescence

**Minimal model** for SRM nozzle flow

**Other studies**
- shear-mixing layer [Vié et al., 2012]
- unstructured grids [Sabat et al., 2013]
Conclusion on the AG model

Anisotropic Gaussian

- homo-PTC
- homo-coalescence

Minimal model for SRM nozzle flow

Other studies

- shear-mixing layer [Vié et al., 2012]
- unstructured grids [Sabat et al., 2013]

SRM prospects

- study of two-way coupling
- hybridation to monokinetic approach
Summary of the modeling strategy

A comprehensive **modeling** and **numerical strategy**

has been developed and validated for the unsteady simulation of **moderately dense** and **polydisperse** two-phase flows.
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Extra slides

5 Numerical methods
- Disperse two-phase flow numerical strategies
- Presentation of an industrial code

6 Models for flows with nanometric droplets
- Nanometric droplets
- Modeling issues
- Unifying the approach for all sizes
- Nano-micro computations

7 Break-up source terms
- Break-up source terms
Extra slides

5. Numerical methods
- Disperse two-phase flow numerical strategies
- Presentation of an industrial code

6. Models for flows with nanometric droplets
- Nanometric droplets
- Modeling issues
- Unifying the approach for all sizes
- Nano-micro computations

7. Break-up source terms
- Break-up source terms
Time integration

Physical constraints
- many fluids: no resolution at once
- strong coupling
- stiffness due to polydispersity

Industrial constraints
- efficiency
- legacy and liability
- flexibility

Splitting methods [Strang, 1968, Descombes and Massot, 2004]
- Many possibilities!
Time integration

**Physical constraints**
- many fluids: **no resolution at once**
- strong coupling
- stiffness due to polydispersity

**Industrial constraints**
- efficiency
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**Liability of a multi-solver approach: CEDRE** [Errera et al., 2011]
- time integration per phase
- with conservative coupling strategy
- △ high loadings $C$ or time steps $\Delta t$

**Splitting methods** [Strang, 1968, Descombes and Massot, 2004]
- Many possibilities!
Time integration

Physical constraints
- many fluids: no resolution at once
- strong coupling
- stiffness due to polydispersity

Industrial constraints
- efficiency
- legacy and liability
- flexibility

Liability of a multi-solver approach: CEDRE [Errera et al., 2011]
- time integration per phase
- with conservative coupling strategy

△ high loadings $C$ or time steps $\Delta t$

Splitting methods [Strang, 1968, Descombes and Massot, 2004]
- Many possibilities!

Splitting focal issues
- two-way coupling
- stiffness
Transport in physical space

Hypercompressibility (gradients, singularities and vacuum)

- **accuracy issues** (structures participate to the physics)
- **stability issues** (high order near discontinuities, undershoots)
Transport in physical space

**Hypercompressibility** (gradients, singularities and vacuum)

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### Structured grids (research codes)

**Kinetic schemes**
- pressureless: 2\textsuperscript{nd} order Bouchut/dimensional splitting
  
  [de Chaisemartin, 2009]
- weak pressure: open topic

### Unstructured grids (industrial codes)

- Finite volume 2\textsuperscript{nd} order MUSCL strategy:
  
  dedicated implementation [Le Touze et al., 2012]
- Cell-vertex with high order scheme/artificial viscosity:
  
  dedicated stabilization method [Martinez, 2009]
Transport in physical space

Hypercompressibility (gradients, singularities and vacuum)
- **Accuracy issues** (structures participate to the physics)
- **Stability issues** (high order near discontinuities, undershoots)

Need for dedicated methods
- An open topic
- In progress

Structured grids (research codes)
- Kinetic schemes
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Phase space evolution

Phase space constraints
- accuracy/stability (stiffness)
- realizability

Industrial constraints
- robust
- flexible

Moment method phase space dynamics

Sources: integrals with many dependencies
1. reconstruction from the moments
2. phase space integration
3. computation of the sources
4. time integration of the system

\[
\frac{dU}{dt} = \Omega \left( \int \Phi \cdot fU \right)
\]

Quadratures [Abramowitz and Stegun, 1964, Gautschi, 1996]
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Source focal issues
- reconstruction/quadratures
- time integration
The CEDRE code (ONERA)

Industrial-oriented code [Courbet et al., 2011]
- 3D unstructured (generic cells)
- Multi-physics (two-phase, radiative, wall conduction, soot)
- Solver coupling: exchange terms [Errera et al., 2011]

CHARME [Refloch et al., 2011]
- Navier-Stokes
- Compressible
- Reactive
- 2nd order MUSCL
- Upcoming 4th order [Haider et al., 2011]

SPARTE [Murrone and Villedieu, 2011]
- Statistical Lagrangian

SPIREE [Murrone and Villedieu, 2011]
- Eulerian size sampling
- Eulerian two size moment MF
- No coalescence
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Presentation of an industrial code

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⇒ Present work feasibility of the developed strategies cross-comparisons with Lagrangian applicative computations
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**Present work**
- **feasibility** of the developed strategies
- **cross-comparisons** with Lagrangian
- **applicative** computations
Extra slides

5. Numerical methods
   - Disperse two-phase flow numerical strategies
   - Presentation of an industrial code

6. Models for flows with nanometric droplets
   - Nanometric droplets
   - Modeling issues
   - Unifying the approach for all sizes
   - Nano-micro computations

7. Break-up source terms
   - Break-up source terms
Towards “Nanopropellants”

**Aluminum nanoparticle synthesis**

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<tr>
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<th>Average Size (nm)</th>
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**Nano-fuel properties**

- ⊕ combustion rate
- ⊖ oxide layer
- ❓ residual size

[Reference: [Bocanegra, 2007]]
Towards “Nanopropellants”

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### Nano-fuel properties

⊕ combustion rate
⊖ oxide layer
? residual size

### Need for preliminary studies on nano-residual flows

- reduction of $I_{sp}$ loss?
- reduction of slag?
- what impact on instabilities?
Nanometric droplets \( \text{St} \ll \text{St}_c \)

**Ensemble transport**

*negligible inertia*
Nanometric droplets

\[ \text{St} \ll \text{St}_c \]

Ensemble transport

negligible inertia

Nanometric droplet modeling issues

- nanoparticle combustion, nanoresidual formation
- transport: diffusion, out-of-equilibrium forces (thermophoresis)
- Brownian coalescence
1) Kinetic model for dense nanoparticle flows

Doisneau, F., Dupays, J., Laurent, F., and Massot, M. Derivation of a fluid-kinetic description from kinetic theory for a nanometric two-phase mixture. *In preparation*

- fully kinetic model
- exhibits [links to the literature](#) models
- foundation of a [fully coupled](#) approach
- coupled [out-of-equilibrium transport](#)

**Kinetic-Kinetic**
Boltzmann and Williams-Boltzmann
(coexisting and coupled through collision terms)

**Nano Fluid-Kinetic**
Fluid and Williams-Boltzmann
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Boltzmann and Williams-Boltzmann (coexisting and coupled through collision terms)

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Fluid and Williams-Boltzmann (coexisting and coupled through sources)

Achievements: model unification

- of transport
- of coalescence
2) Nano-micro mixture modeling

Doisneau, F., Dupays, J., Laurent, F., and Massot, M. *A unified model for nano-micro polydisperse sprays with coalescence.* *In preparation for Physics of Fluids*

- nano-micro model derived from a kinetic base
- **coalescence kernels** for Brownian-inertial transition
- **implementation** in CEDRE
- feasibility computations
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Achievements: application

- Achieves size-size coupling
- Insight on nano-micro physics
Suspensions of nanometric particles

Physical peculiarities below a micrometer

- **negligible inertia**
- **transport** properties?
- origin of **coalescence**?
Suspensions of nanometric particles

Physical peculiarities below a micrometer

- negligible inertia
- transport properties?
- origin of coalescence?


- transport properties of diffusion and thermophoresis
- coalescence rates

but

- in a one-way coupling frame
- for limited size intervals
Suspensions of nanometric particles

Physical peculiarities below a micrometer

- negligible inertia
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- transport properties of diffusion and thermophoresis
- coalescence rates

but

- in a one-way coupling frame
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Free-Flight transition  Diffusive transition  Inertial

\[ d_0 \quad d_N \quad d_p \]
A comprehensive approach

Fully kinetic model

- **Kinetic-Kinetic**
  - Boltzmann and Williams-Boltzmann
    (coexisting and coupled through collision terms)

- **Nano Fluid-Kinetic**
  - Fluid and Williams-Boltzmann
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- Two kinetic equations **coupled by collisions**

- **Scale separation** \( \varepsilon = \sqrt{\frac{m_0^g}{m_0^p}} \)

- Chapman-Enskog expansion
  [Chapman and Cowling, 1939]

- \( \Rightarrow \) **Fluid-Kinetic frame**
**A comprehensive approach**

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- Chapman-Enskog expansion
  - [Chapman and Cowling, 1939]

  $\Rightarrow$ **Fluid-Kinetic frame**

**Achievements**

- **Fokker-Planck**-like terms
- Out-of-equilibrium **transport** term
- **Two-way coupling**

**Limits**

- cross-section **modeling**
- **resolution** for industrial deployment
- **analysis** for reduced models
One-way coupling approaches

**[Smoluchowski, 1916]'s equation**

\[
\partial_t n + \partial_x \cdot (n u_g) = \partial_x \cdot D \partial_x n + C(n, n)
\]

Frame: macroscopic

**Fokker-Planck equation [Pottier, 2007]**

\[
\partial_t f + c \cdot \partial_x f + \partial_c \left( \frac{u_g - c}{\tau u(S)} f \right) = \partial_c \cdot (D \partial_c f)
\]

Frame: kinetic

**Collision kernel (integrated)**

- semi-empirical approach [Fuchs, 1964]
- incompatible with slip velocity

**NA**
One-way coupling approaches

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\]
Frame: kinetic

**Brownian diffusion**
\[
D = \frac{3kT_g}{2m_p}
\]

**Collision kernel (integrated)**
- semi-empirical approach [Fuchs, 1964]
- incompatible with slip velocity

---

**Modeling issues**

**Numerical methods**

Models for flows with nanometric droplets

Break-up source terms

---

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Identifying the scales

Characteristic lengths

- \( d_{pp} = dp \sqrt{\frac{\rho l_\frac{4}{3} \pi}{\rho g C}} \)
- \( a_{drift} \) (inertia or diffusion)

A scale separation for nano-collisions

Nanoparticle collisions after a significant drift

\[ a_{drift} \ll d_{pp} \]
Numerical methods

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Unifying the approach for all sizes

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A scale separation for nano-collisions

Nanoparticle collisions after a significant drift

\[ a_{drift} \ll d_{pp} \]

Particle-particle correlations

Two-point pdf \( f^{(2)} \) to describe collisions

\[
\mathcal{C} = \frac{1}{2} \int_{x^*, c^*} \int_{v^*} f^{(2)}(t, x, c^*, v^*, x^*, c^*, v^*) |c^* - c^*| \beta(v^*, v^*) J dv^* dx^* dc^* \\
+ \int_{x^*, c^*} \int_{v^*} f^{(2)}(t, x, c, v, x^*, c^*, v^*) |c - c^*| \beta(v, v^*) dv^* dx^* dc^*
\]

Evolution of \( f^{(2)} \)

- diffusion equation [Batchelor, 1982]
- neglected three-point correlations
Nano-micro coalescence kernels

Nano-micro particle correlations

Need to solve a convection-diffusion equation ... that of $f^{(2)}$!
Nano-micro coalescence kernels

Nano-micro particle correlations

Need to solve a convection-diffusion equation

... that of $f^{(2)}$!

Diffusive kernel [Fuchs, 1964]

$$K_{\text{coal}}^\text{bro} (r^*, r^\circ) = \frac{2kTg}{3\mu g} \left( \frac{1}{r^*} + \frac{1}{r^\circ} \right) \left( r^* + r^\circ \right)$$

no slip
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**no slip**

Additive Kernel

$$K_{\text{coal}}^{\text{bro+bal}} = K_{\text{coal}}^{\text{bro}} + K_{\text{coal}}^{\text{bal}}$$

**no correlation**
Unifying the approach for all sizes

**Nano-micro coalescence kernels**

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### Diffusive kernel [Fuchs, 1964]

\[
\mathcal{K}_{\text{coal}}^{\text{bro}}(r^*, r^\diamond) = \frac{2kTg}{3\mu g} \left( \frac{1}{r^*} + \frac{1}{r^\diamond} \right) (r^* + r^\diamond)
\]

- no slip

### Additive Kernel

\[
\mathcal{K}_{\text{coal}}^{\text{bro+bal}} = \mathcal{K}_{\text{coal}}^{\text{bro}} + \mathcal{K}_{\text{coal}}^{\text{bal}}
\]

- no correlation

### Kinetic Kernel

\[
\mathcal{K}_{\text{coal}}^{\text{K-B}} = \pi (r^* + r^\diamond)^2 \left[ |u^* - u^\diamond| \text{ erf} \left( \frac{|u^* - u^\diamond|}{\sqrt{2(\sigma^* \sigma^\diamond)}} \right) + \frac{\sqrt{2(\sigma^* \sigma^\diamond)}}{\sqrt{\pi}} \text{ exp} \left( -\frac{|u^* - u^\diamond|^2}{2(\sigma^* \sigma^\diamond)} \right) \right]
\]

- FMR-balistic
Nano-micro coalescence kernels

Nano-micro particle correlations

Need to solve a convection-diffusion equation ... that of $f^{(2)}$!

Diffusive kernel [Fuchs, 1964]

$$
\mathcal{R}_{\text{coal}}^{\text{bro}}(r^*, r^\circ) = \frac{2kTg}{3\mu g} \left( \frac{1}{r^*} + \frac{1}{r^\circ} \right) (r^* + r^\circ)
$$

Additive Kernel

$$
\mathcal{R}_{\text{coal}}^{\text{bro+bal}} = \mathcal{R}_{\text{coal}}^{\text{bro}} + \mathcal{R}_{\text{coal}}^{\text{bal}}
$$

Kinetic Kernel

$$
\mathcal{R}_{\text{coal}}^{\text{K-B}} = \pi (r^* + r^\circ)^2 \left[ |u^* - u^\circ| \operatorname{erf} \left( \frac{|u^* - u^\circ|}{\sqrt{2(\sigma^2 + \rho^2)}} \right) + \sqrt{\frac{2(\sigma^2 + \rho^2)}{\pi}} \exp \left( -\frac{|u^* - u^\circ|^2}{2(\sigma^2 + \rho^2)} \right) \right]
$$

FMR-ballistic

Hybrid Kernel: analogy with mass transfer convective correction

$$
\mathcal{R}_{\text{coal}}^{\text{D-B}} = 4\pi (D^* + D^\circ)(r^* + r^\circ) \left[ 1 + \frac{0.3\sqrt{2(r^* + r^\circ)|u^* - u^\circ|}}{\sqrt{g} \left( \frac{D^* + D^\circ}{3} \right)^{\frac{1}{3}}} \right]
$$

Diffusive-ballistic
Phenomenology of nano-micro mixtures

Decelerating nozzle test case with $\text{K-B}_{\text{coal}}$

- $z = 0.05\text{m}$
- $z = 0.07\text{m}$

**Boxes**: One size moment hybrid MF with 80 sections
**Lines**: Two size moment hybrid MF with 16 sections.

Mass density function (kg/m$^3$/microns) vs. Radius (microns)

Section average velocity (m/s) vs. Radius (microns)
### Phenomenology of nano-micro mixtures

#### Decelerating nozzle test case with $K\cdot B_{\text{coal}}$

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**Size-Size coupling**
- Total

**Size-velocity coupling**
- For the larger ones only...
- but enhanced by nanoparticles!

**Boxes**: One size moment hybrid MF with 80 sections
**Lines**: Two size moment hybrid MF with 16 sections.

---

Footnote: NASA ARC, Mountain View 2015
The TEP test case

A small motor

- Additive kernel to test: $K_{\text{coal}}^{\text{bro}+\text{bal}}$
- Splitting for stiffness: $\tau_{\text{min}} \sim 10^{-8}$ s

Dispersed phase volume fractions per section
The TEP test case

A small motor

- Additive kernel to test: $K_{\text{coal}}^{\text{bro+bal}}$
- splitting for stiffness: $\tau_{\text{min}} \sim 10^{-8}$ s

Dispersed phase volume fractions per section

Achievements

- time/source strategy efficient for nano-micro flows
- physical insight on nano-micro mixtures
- guides definition of new experiments
Extra slides

5. Numerical methods
   - Disperse two-phase flow numerical strategies
   - Presentation of an industrial code

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   - Nanometric droplets
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7. Break-up source terms
   - Break-up source terms
Break-up source terms

\[2B_{n+}^k = \sum_{i=k}^N Q_{ik}^n\]
\[2B_{m+}^k = \sum_{i=k}^N Q_{ik}^m\]
\[2B_{u+}^k = \sum_{i=1}^k Q_{ik}^{mu}\]

\[2B_{n-}^k = \sum_{i=1}^N L_{ik}^n\]
\[2B_{m-}^k = \sum_{i=1}^N Q_{ki}^m\]
\[2B_{u-}^k = u_k \cdot 2B_{m-}^k\]

No particular problem to integrate. Same algorithm than coalescence possible.
Break-up source terms

\[
\begin{align*}
2B^+_{nk} &= \sum_{i=k}^{N} Q^n_{ik} \\
2B^+_{mk} &= \sum_{i=k}^{N} Q^m_{ik} \\
2B^+_{mu} &= \sum_{i=1}^{k} Q^{mu}_{ik} \\
2B^-_{nk} &= \sum_{i=1}^{N} L^n_{ki} \\
2B^-_{mk} &= \sum_{i=1}^{N} Q^n_{ki} \\
2B^-_{mu} &= u_k \cdot 2B^-_{mk}
\end{align*}
\]

Break up modeling:
\( ν_{bu} \) depends on Weber number [Hsiang and Faeth, 1993]
\( n_{bu} \) [O’Rourke and Amsden, 1987, Dufour et al., 2003]
with Sauter radius from [Wert, 1995]
\( u_{bu} \) [Hsiang and Faeth, 1993]

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2B_{n-}^k &= \sum_{i=1}^{N} L_{ik}^n \\
2B_{m-}^k &= \sum_{i=1}^{N} Q_{ki}^m \\
2B_{u-}^k &= u_k \cdot 2B_{m-}^k
\end{align*}
\]

Break up modeling:

- \( \nu_{bu} \) depends on Weber number [Hsiang and Faeth, 1993]
- \( n_{bu} \) [O’Rourke and Amsden, 1987, Dufour et al., 2003]
- with Sauter radius from [Wert, 1995]
- \( u_{bu} \) [Hsiang and Faeth, 1993]

\[
\begin{align*}
\left( \begin{array}{c}
Q_{ik}^n \\
Q_{ik}^m \\
Q_{ik}^{mu}
\end{array} \right) &= \int_{S_{i-1}} S_i 
\left( \begin{array}{c}
1 \\
\frac{\rho_l}{6\sqrt{\pi}} S^* \frac{3}{2}
\end{array} \right)
\left( \begin{array}{c}
\frac{\rho_l}{6\sqrt{\pi}} S^* \frac{3}{2}
\end{array} \right) \left( S_{bu}(S^*, u_i) \frac{\rho_l}{6\sqrt{\pi}} S^* \frac{3}{2} \right) \\
&\cdot 2\kappa_i(t, x, S^*) \nu_{bu}(\text{We}(S^*)) n_{bu}(S^*) dS^* dS^*
\end{align*}
\]

\[
L_{k}^n = \int_{S_{k-1}}^{S_k} 2\kappa_k(t, x, S) \nu_{bu}(\text{We}(S)) dS
\]

No particular problem to integrate. Same algorithm than coalescence possible.
Break-up source terms

\[
2B_{n+}^k = \sum_{i=k}^N Q_{ik}^n \\
2B_{m+}^k = \sum_{i=k}^N Q_{ik}^m \\
2B_{u+}^k = \sum_{i=1}^k Q_{ik}^{mu}
\]

\[
2B_{n-}^k = \sum_{i=1}^N L_{ik}^n \\
2B_{m-}^k = \sum_{i=1}^N Q_{ki}^m \\
2B_{u-}^k = u_k \cdot 2B_{m-}^k
\]

Break up modeling:
\[
\nu_{bu} \text{ depends on Weber number} \quad [\text{Hsiang and Faeth, 1993}]
\]
\[
n_{bu} \quad [\text{O’Rourke and Amsden, 1987, Dufour et al., 2003}]
\]

with Sauter radius from [Wert, 1995]

\[
u_{bu} \quad [\text{Hsiang and Faeth, 1993}]
\]

\[
\left( \begin{array}{c}
Q_{ik}^n \\
Q_{ik}^m \\
Q_{ik}^{mu}
\end{array} \right) = \int_{S_{i-1}} S_i \left( \begin{array}{c}
1 \\
\frac{\rho_l}{6\sqrt{\pi}} S'^{3/2} \\
u_{bu}(S^*, u_i) \frac{\rho_l}{6\sqrt{\pi}} S^{3/2}
\end{array} \right) 2\kappa_i(t, x, S^*) \nu_{bu}(\text{We}(S^*)) n_{bu}(S^\circ) \, dS^* \, dS^\circ
\]

\[
L_{n}^k = \int_{S_{k-1}}^{S_k} 2\kappa_k(t, x, S) \nu_{bu}(\text{We}(S)) \, dS
\]

No particular problem to integrate. Same algorithm than coalescence possible.