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

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May, 26th 2015

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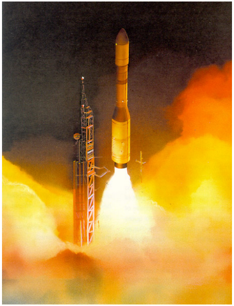
Overview

Overview

Solid Rocket Motors (SRM)

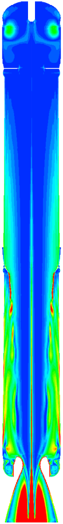


Solid Rocket Motors (SRM) : anaerobic propellers for rockets and missiles

⊕ high thrust	⊖ less **efficient**
⊕ cheap	⊖ subject to **thrust oscillations**
⊕ storable	⊖ difficult to throttle

Physics of a SRM

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



Vorticity in a P230
[Doisneau et al., 2013a, CRM

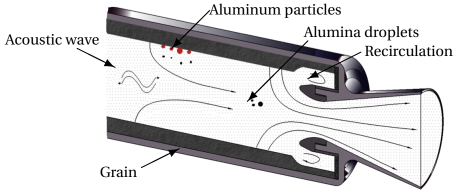
Internal flow is complex

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

Origin and impact of the condense phase

Propellant is aluminized to increase specific impulse

- combustion ⇒ liquid Al_2O_3
- **polydisperse droplets** (below 200μm)
- mass concentration 35% ⇒ **strong interaction** with flow



Condense phase impact

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

Particle sizes in a LP10
[Doisneau et al., 2011, EUC

Liquid Rocket Engines (LRE)

Vinci engine (SAFRAN)

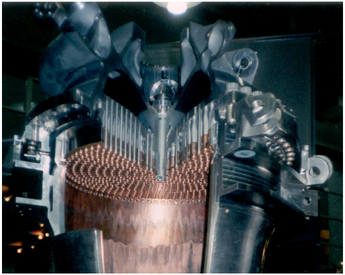
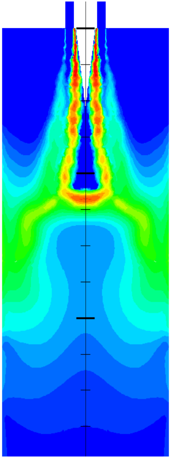


Plate of coaxial injectors
Vulcain 2 (SAFRAN)

Subcritical regime

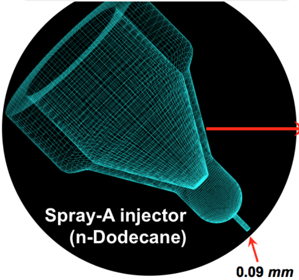
- atomization of liquid oxygen (LOx)
- combustion of dense LOx spray with gaseous fuel
- combustion and acoustics



Transient heat release rate in a coaxial GCH4/LOx inj. [Doisneau, 2013b]

Atmospheric engines

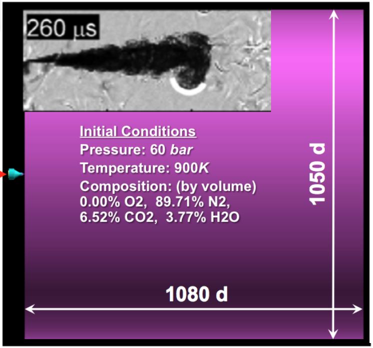
- Gasoline Direct Injection (GDI)
- Diesel injection
- Gas Turbine (GT)



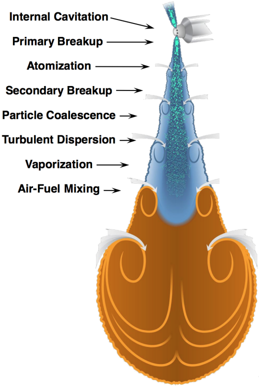
Injection Conditions

Peak Velocity:	600 *m/s*
Peak Re_d:	117,000
Density:	650 kg/m^3
Temperature:	363 *K*

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



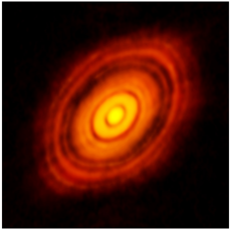
Computational Domain



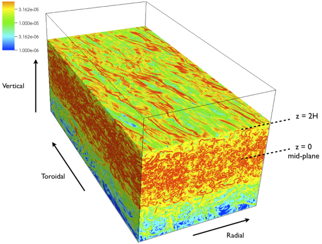
Injection modeling focuses

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

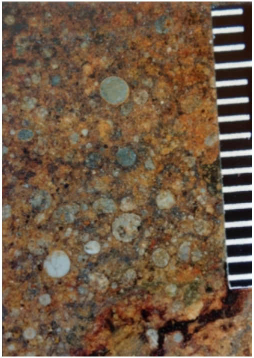
Astrophysics



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 $\lambda = 1\,\mathrm{m} \ll \eta_K = 1000\,\mathrm{m}$
- Polydisperse loading of dust from μm to km
- Agglomeration and gravitational capture $\Rightarrow$ planet formation

What two-way coupling ?

Flow regimes depend on the disperse phase

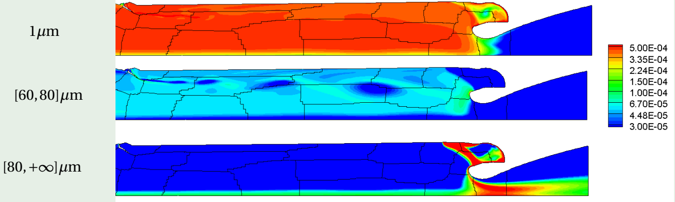
- Volume fraction : α_l
- Mass fraction : Y_l
- Inertia : St

$\Rightarrow$ **Classifications**

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

Case of the P230 SRM

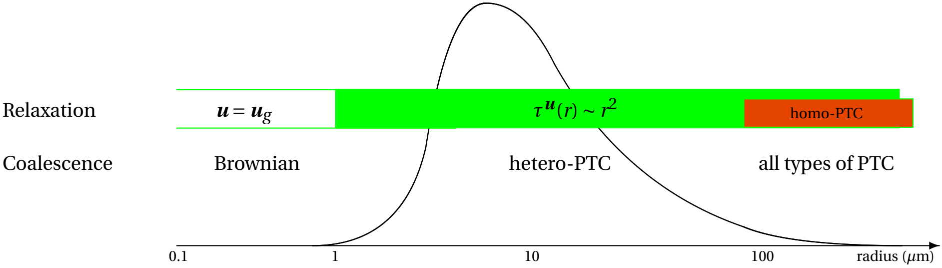
Volume fractions α_p of alumina droplets in P230 with coalescence [Doisneau et al., 2013a, CRM]



In SRMs where $\rho_l/\rho_g \sim 10^3$ → **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



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 $= \frac{\tau_c}{\tau_g}$

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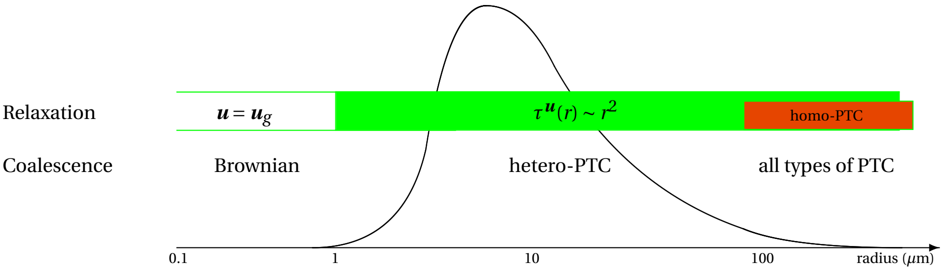

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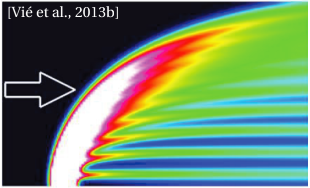
Flow times

$\tau_g^{chamber} / \tau_g^{nozzle}$

Low inertia droplets $\quad \mathrm{St} < \mathrm{St}_c$

Low inertia droplet velocities and temperatures

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



Crossings at different sizes

Hetero-PTC

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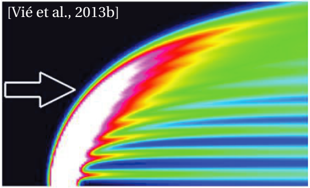


Crossings at **different** sizes

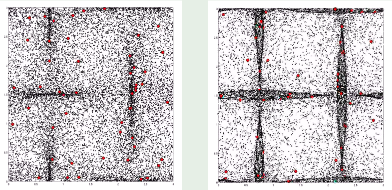
Hetero-PTC

Low inertia droplet modeling issues

- stiffness
- hetero-coalescence

Moderate inertia droplets $\mathrm{St} \sim \mathrm{St}_c$

Homo-crossings



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

Crossings at same size

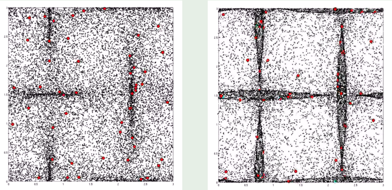
Homo-PTC

Hypercompressibility

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

Moderate inertia droplets $\quad St \sim St_c$

Homo-crossings



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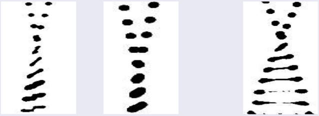
Moderate inertia droplet modeling issues

- hypercompressibility
- homo-coalescence

Coalescence induced couplings

Crossings + high volume fraction ⇒ **collisions**

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



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

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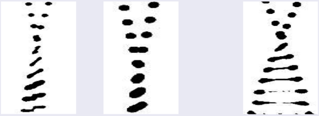
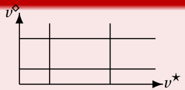


Colliding droplet regimes : reflexion, **coalescence**, and stretching [Qian and Law, 1997]

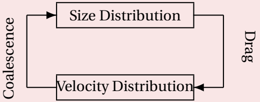
Size-Size coupling

- Collision rates
- Size distribution prediction



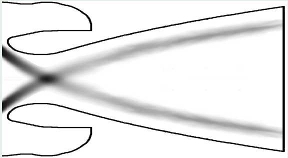
Size-velocity coupling

- Collision rates
- Induced polydispersity



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** !

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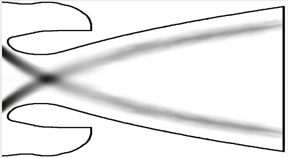

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Nozzle efficiency modeling

Inertial particle modeling
+
Size-Velocity coupling
+
Two-way coupling

Overview

Kinetic modeling for the disperse phase

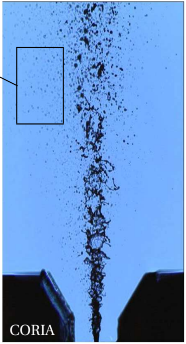
Point particles with velocity $\boldsymbol{c}$, temperature θ, surface S

Number density function **NDF** : describes the disperse phase

$$\mathrm{d}N = f(t, \boldsymbol{x}, \boldsymbol{c}, S, \theta)\mathrm{d}\boldsymbol{x}\mathrm{d}\boldsymbol{c}\mathrm{d}S\mathrm{d}\theta$$

NDF satisfies a Boltzmann-like PDE [Williams, 1958]

$$\partial_t f + \partial_{\boldsymbol{x}} \cdot (\boldsymbol{c} f) + \partial_{\boldsymbol{c}} \cdot (\boldsymbol{F} f) + \partial_\theta (\mathrm{H} f) + \partial_S (\mathrm{R} f) = \mathfrak{B} + \mathfrak{C}$$



Closures : all the physical modeling job

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

Kinetic coalescence

Inertial droplet coalescence :

$$\mathfrak{C}^{+} = \frac{1}{2}\int_{\boldsymbol{c}^\star}\int_{v^\star\in[0,v]} f(t,\boldsymbol{x},\boldsymbol{c}^\diamond,v^\diamond) f(t,\boldsymbol{x},\boldsymbol{c}^\star,v^\star)\mathfrak{K}_{\text{coal}} J \mathrm{d}v^\star \mathrm{d}\boldsymbol{c}^\star$$
$$\mathfrak{C}^{-} = \int_{\boldsymbol{c}^\star}\int_{v^\star} f(t,\boldsymbol{x},\boldsymbol{c},v) f(t,\boldsymbol{x},\boldsymbol{c}^\star,v^\star)\mathfrak{K}_{\text{coal}} \mathrm{d}v^\star \mathrm{d}\boldsymbol{c}^\star$$

Balistic coalescence kernel modeling

$$\mathfrak{K}_{\text{coal}} = \pi(r^\diamond + r^\star)^2 \, ||\boldsymbol{u}-\boldsymbol{u}^\star|| \, \mathfrak{E}(......)$$

Efficiency $\mathfrak{E}$ models

- collision efficiency [Langmuir, 1948, Beard and Grover, 1974]
- coalescence efficiency [Brazier-Smith et al., 1972, Ashgriz and Poo, 1990]

$\Rightarrow$ **closed**

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Coalescence source term

- integral
- quadratic
- multivariate kernel
- non-linear kernel

Balistic coalescence kernel modeling

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Approaches for polydisperse NDFs

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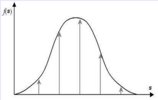
- **Direct** (finite volumes) intractable
- **Lagrangian** (NDF samples) convergence, parallelization
- **Eulerian** (fields) several approaches

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

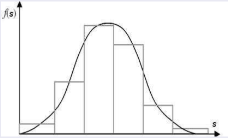
Correlation of **velocity** and temperature to **size** :

$$f(t,\boldsymbol{x},\boldsymbol{c},s,\theta) \approx n(t,\boldsymbol{x},s)\delta(\boldsymbol{c}-\overline{\boldsymbol{u}}(t,\boldsymbol{x},s))\delta(\theta - T(t,\boldsymbol{x},s))$$

Multi-Fluid level

Size discretization in **sections** $[s_{k-1}, s_k[$ ⇒ **Reconstructions**

- Velocity $\overline{\boldsymbol{u}}(t,\boldsymbol{x},s) \approx \boldsymbol{u}_k(t,\boldsymbol{x})$
- Temperature $T(t,\boldsymbol{x},s) \approx T_k(t,\boldsymbol{x})$
- **One size moment** $n(t,\boldsymbol{x},s) \approx m_k(t,\boldsymbol{x})\kappa_k(s)$



...higher order requires modeling AND numerics ! [Kah et al., 2010, Vié et al., 2013b]

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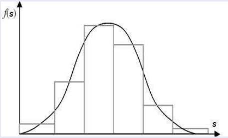

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Pros

Flexible on **polydispersity**

Captures **dynamics** for $\mathrm{St} \le \mathrm{St}_c$

Two-way coupling to Eulerian gas solver

Parallelization

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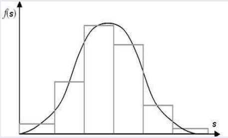

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Cons

Hypercompressibility and transport scheme

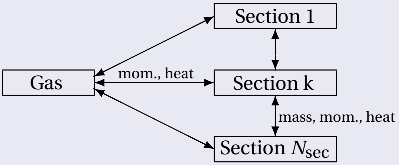
Complex algebra

Fails for **homo-PTC**

Resulting two-phase model

Superimposed fluids

- Sets of moment fields
- Coupled through source terms



A moment method

- conserve some moments $\boldsymbol{U}$
- reconstruction $f_{\boldsymbol{U}}$ to compute sources Ω
- realizability : $\boldsymbol{U} \in M$

$$\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = \Omega\left(\int \Phi \cdot f_{\boldsymbol{U}}\right)$$

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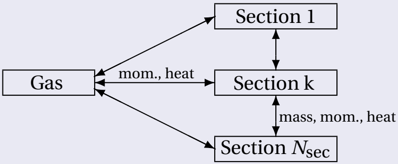

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Example : Drag term

$$\frac{\mathrm{d}m_k\boldsymbol{u}_k}{\mathrm{d}t} = \int_{S_{k-1}}^{S_k} F(\boldsymbol{u}_k, \boldsymbol{u}_g; S)\kappa(S)\mathrm{d}S$$

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

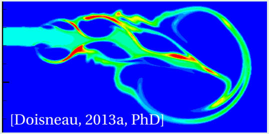
Structured grids (research codes)

Kinetic schemes

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

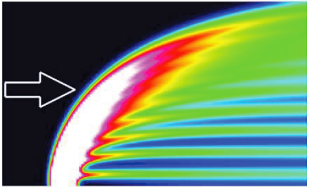
Unstructured grids (industrial codes)

- 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]

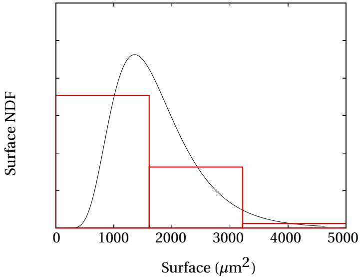


Overview

LOW INERTIA droplets

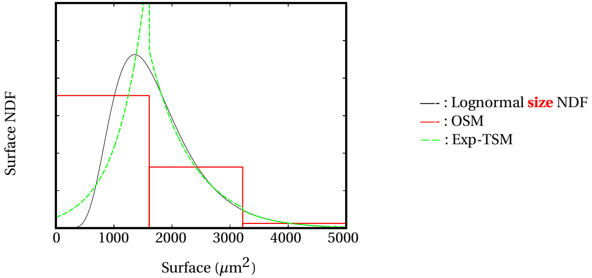


1) Size reconstruction



—- : Lognormal **size** NDF
—- : OSM

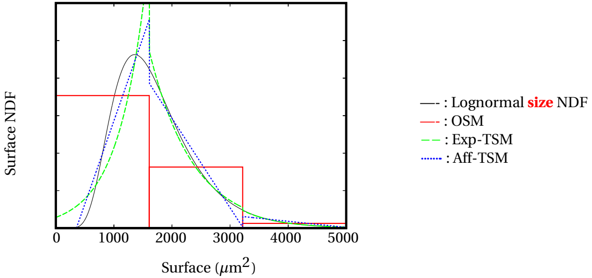
1) Size reconstruction



Two-Size moment Multi-Fluid approaches

- **Exp-TSM** method in CEDRE [Dufour et al., 2003]

1) Size reconstruction



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- **Exp-TSM** method in CEDRE [Dufour et al., 2003]
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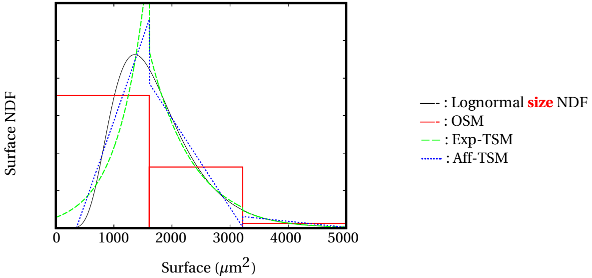


Two-Size moment Multi-Fluid approaches

- **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**

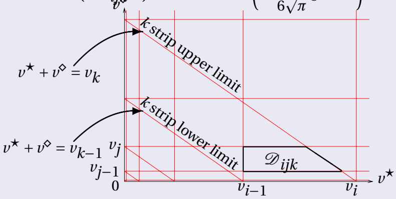
2) Coalescence sources

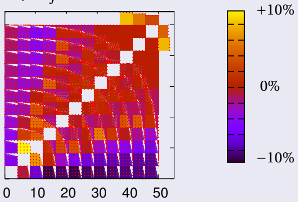
Coalescence terms : quadratic sums of 2D elementary integrals

$$
\begin{aligned}
{}^2\mathcal{C}_k^{n+} &= \sum_{i=1}^{k}\sum_{j=1}^{i-1} Q^n_{ijk} &\qquad {}^2\mathcal{C}_k^{n-} &= \sum_{i=1}^{N}\sum_{j=1}^{N} Q^n_{kji}\\
{}^2\mathcal{C}_k^{m+} &= \sum_{i=1}^{k}\sum_{j=1}^{i-1} (Q^\star_{ijk}+Q^\diamond_{ijk}) &\qquad {}^2\mathcal{C}_k^{m-} &= \sum_{i=1}^{N}\sum_{j=1}^{N} (Q^\star_{kji}+Q^\diamond_{kji})\\
{}^2\boldsymbol{\mathcal{C}}_k^{u+} &= \sum_{i=1}^{k}\sum_{j=1}^{i-1} (\boldsymbol{u}_i Q^\star_{ijk}+\boldsymbol{u}_j Q^\diamond_{ijk}) &\qquad {}^2\boldsymbol{\mathcal{C}}_k^{u-} &= \boldsymbol{u}_k \cdot {}^2\mathcal{C}_k^{m-}
\end{aligned}
$$

Elementary integrals

$$
\begin{pmatrix} Q^n_{ijk}\\ Q^\star_{ijk}\\ Q^\diamond_{ijk}\end{pmatrix}(t,\boldsymbol{x}) = \iint_{\mathcal{D}_{ijk}} \begin{pmatrix} 1\\ \frac{\rho_l}{6\sqrt{\pi}} S^{\star\frac{3}{2}}\\ \frac{\rho_l}{6\sqrt{\pi}} S^{\diamond\frac{3}{2}}\end{pmatrix} {}^2\kappa_i(t,\boldsymbol{x},S^\star)\,{}^2\kappa_j(t,\boldsymbol{x},S^\diamond)\,|\,\boldsymbol{u}_i-\boldsymbol{u}_j\,|\,\mathfrak{E}(\ldots)\pi(r^\star+r^\diamond)^2\,\mathrm{d}S^\star\,\mathrm{d}S^\diamond
$$





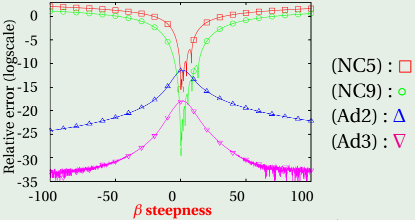
Relative error of integrals for Exp-TSM with (NC5)
13 sections, sizes in radius (μm) ; + quadrature nodes.

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

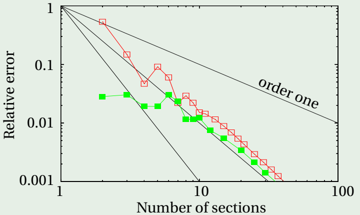
Comparison of quadrature error of Exp-TSM



Test integral $I(\beta)$ with $S_1 = 1$, $S_2 = 2$ and $S^\star = 0.75$

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 2×2 points !
Aff-TSM : Polynomial quadrature allows more points

2) Coalescence sources : Validation

New phase space strategy

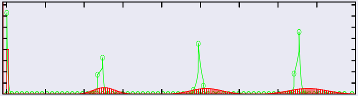
Doisneau, F., Laurent, F., Murrone, A., Dupays, J., and Massot, M. (2013b). Eulerian Multi-Fluid models for the simulation of dynamics and coalescence of particles in solid propellant combustion.
, 234 :230–262

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



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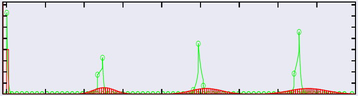


Achievements : accuracy and efficiency

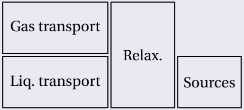
- for complex source terms
- for stiff cases (e.g. bimodal)

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

$$
\begin{cases}
\partial_t \rho_g + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g) = 0 \\
\partial_t (\rho_g \boldsymbol{u}_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g \otimes \boldsymbol{u}_g + p\boldsymbol{I}) = -\sum_{k=1}^{N_{\mathrm{sec}}} m_k \boldsymbol{F}_k \\
\partial_t (\rho_g \boldsymbol{c}_g T_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{c}_g T_g \boldsymbol{u}_g) = -\sum_{k=1}^{N_{\mathrm{sec}}} m_k \mathrm{H}_k - \sum_{k=1}^{N_{\mathrm{sec}}} m_k \boldsymbol{F}_k (\boldsymbol{u}_g - \boldsymbol{u}_k) \\
\left.\begin{array}{l}
\partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^{n+} - {}^2\mathrm{C}_k^{n-} \\
\partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^{m+} - {}^2\mathrm{C}_k^{m-} \\
\partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k + {}^2\boldsymbol{\mathrm{C}}_k^{u+} - {}^2\boldsymbol{\mathrm{C}}_k^{u-} \\
\partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k + {}^2\boldsymbol{\mathrm{C}}_k^{u+} - {}^2\boldsymbol{\mathrm{C}}_k^{u-}
\end{array}\right\} \quad k = 1, N_{\mathrm{sec}}
\end{cases}
$$

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

Gas transport	Relax.	
Liq. transport		Sources

The $\mathscr{T}_g$ operator τ_g

$$\begin{cases} \partial_t \rho_g + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g) \\ \partial_t (\rho_g \boldsymbol{u}_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g \otimes \boldsymbol{u}_g + p\boldsymbol{I}) = 0 \\ \partial_t (\rho_g \boldsymbol{c}_g T_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{c}_g T_g \boldsymbol{u}_g) = 0 \end{cases}$$

3) Strategy for two-way coupling

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

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Gas transport	Relax.	
Liq. transport		Sources

The $\mathscr{T}_k$ operators $\quad \overline{\tau}_k \quad \forall k$

$$\left\{ \begin{aligned} &\partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = 0 \\ &\partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = 0 \\ &\partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = 0 \\ &\partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = 0 \end{aligned} \right\} \quad k = 1, N_{\text{sec}}$$

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- to capture strong gas-liquid coupling

Gas transport	Relax.	
Liq. transport		Sources

The $\mathscr{R}$ operator $\tau_{\mathbf{min}}$

$$\begin{cases} \partial_t \rho_g = 0 \\ \partial_t(\rho_g \boldsymbol{u}_g) = -\sum_{k=1}^{N_{\text{sec}}} m_k \boldsymbol{F}_k \\ \partial_t(\rho_g \boldsymbol{c}_g T_g) = -\sum_{k=1}^{N_{\text{sec}}} m_k \mathrm{H}_k - \sum_{k=1}^{N_{\text{sec}}} m_k \boldsymbol{F}_k(\boldsymbol{u}_g - \boldsymbol{u}_k) \\ \left.\begin{array}{l} \partial_t n_k = 0 \\ \partial_t m_k = 0 \\ \partial_t(m_k \boldsymbol{u}_k) = m_k \boldsymbol{F}_k \\ \partial_t(m_k h_k) = m_k \mathrm{H}_k \end{array}\right\} \quad k = 1, N_{\text{sec}} \end{cases}$$

3) Strategy for two-way coupling

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

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- to capture strong gas-liquid coupling

Gas transport	Relax.	Sources
Liq. transport		

The $\mathscr{C}$ operator $\tau^{\mathbf{coal}}_{\mathbf{min}}$

$$
\left\{
\begin{aligned}
\partial_t n_k &= {}^2\mathrm{C}_k^{n+} - {}^2\mathrm{C}_k^{n-} \\
\partial_t m_k &= {}^2\mathrm{C}_k^{m+} - {}^2\mathrm{C}_k^{m-} \\
\partial_t (m_k \boldsymbol{u}_k) &= {}^2\boldsymbol{C}_k^{u+} - {}^2\boldsymbol{C}_k^{u-} \\
\partial_t (m_k h_k) &= {}^2\boldsymbol{C}_k^{u+} - {}^2\boldsymbol{C}_k^{u-}
\end{aligned}
\right\}
\quad k = 1, N_{\mathrm{sec}}
$$

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Gas transport
Liq. transport
Relax.
Sources

$$
\begin{cases}
\partial_t \rho_g + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g) = 0 \\
\partial_t (\rho_g \boldsymbol{u}_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{u}_g \otimes \boldsymbol{u}_g + p\boldsymbol{I}) = -\displaystyle\sum_{k=1}^{N_{\mathrm{sec}}} m_k \boldsymbol{F}_k \\
\partial_t (\rho_g \boldsymbol{c}_g T_g) + \partial_{\boldsymbol{x}} \cdot (\rho_g \boldsymbol{c}_g T_g \boldsymbol{u}_g) = -\displaystyle\sum_{k=1}^{N_{\mathrm{sec}}} m_k \mathrm{H}_k - \displaystyle\sum_{k=1}^{N_{\mathrm{sec}}} m_k \boldsymbol{F}_k (\boldsymbol{u}_g - \boldsymbol{u}_k) \\
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\end{array}\right\} \quad k = 1, N_{\mathrm{sec}}
\end{cases}
$$

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- to allow optimal time steps (reaction-diffusion-convection systems [Duarte, 2011])
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Gas transport	Relax.	
Liq. transport		Sources

Time stepping of a **splitting** method :

$$\boldsymbol{U}(t+\Delta t_{\mathrm{a}}) = \mathscr{R}\,\mathscr{T}_{\mathrm{g}}\mathscr{R}\left(\sum_k \mathscr{T}_k\right)\mathscr{C}\,\boldsymbol{U}(t)$$

3) Strategy for two-way coupling

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Gas transport
Liq. transport
Relax.
Sources

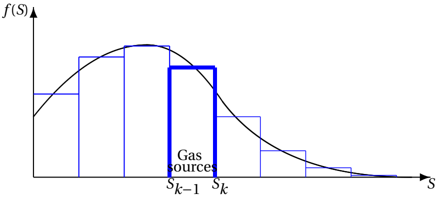
Time stepping of a **splitting** method :

$$\boldsymbol{U}(t+\Delta t_{\mathrm{a}}) = \mathscr{R}\,\mathscr{T}_{\mathbf{g}}\,\mathscr{R}\left(\sum_k \mathscr{T}_k\right)\mathscr{C}\,\boldsymbol{U}(t)$$

Capturing dissipation of acoustics

$$\boxed{\Delta t_{\mathrm{a}} = \max\{K_p \tau_{\mathrm{min}}; K_g \tau_{\mathbf{g}}\}} \qquad K_p, K_g \lesssim 1$$

Overall strategy for low inertia droplets



MF needs

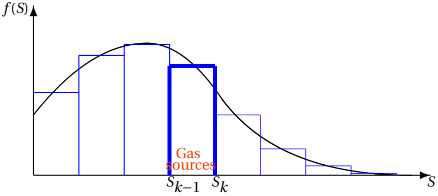
- Two-way coupling : time integration
- Polydispersity : reconstruction
- Sources : quadratures and integration

N_{sec} systems

$$\begin{cases} \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = 0 \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k \end{cases}$$

$\longleftarrow$ Navier-Stokes

Overall strategy for low inertia droplets



MF needs

- **Two-way coupling**
- Polydispersity
- Sources

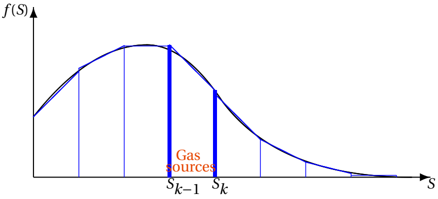
$$N_{\text{sec}} \text{ systems} \quad \begin{cases} \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = 0 \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k \end{cases}$$

$\rightleftharpoons$ Navier-Stokes with **sources**

Improvements

1. **Acoustic-convection splitting** [Doisneau et al., 2014, JPP]
2. **Two size moments** Exp-TSM [Dufour, 2005] Aff-TSM [Laurent, 2006, Laurent, 2013]
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



$$N_{\text{sec}} \text{ systems} \quad \begin{cases} \partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = 0 \\ \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = 0 \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k \end{cases}$$

$\rightleftharpoons$ Navier-Stokes with **sources**

MF needs

- Two-way coupling
- **Polydispersity**
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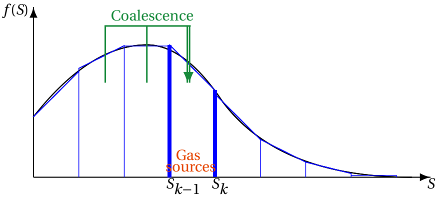

MF needs

- Two-way coupling
- Polydispersity
- **Sources**

N_{sec} systems

$$\begin{cases} \partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^n \\ \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^m \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k + {}^2\boldsymbol{C}_k^u \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k + {}^2\mathrm{C}_k^h \end{cases}$$

$\rightleftharpoons$ Navier-Stokes with **sources**

Improvements

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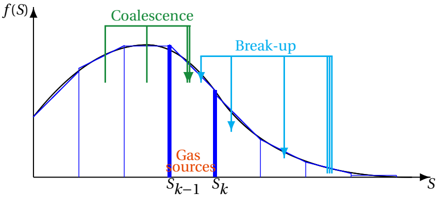
Overall strategy for low inertia droplets



MF needs

- Two-way coupling
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N_{sec} systems

$$\begin{cases} \partial_t n_k + \partial_{\boldsymbol{x}} \cdot (n_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^n + {}^2\mathrm{B}_k^n \\ \partial_t m_k + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k) = {}^2\mathrm{C}_k^m + {}^2\mathrm{B}_k^m \\ \partial_t (m_k \boldsymbol{u}_k) + \partial_{\boldsymbol{x}} \cdot (m_k \boldsymbol{u}_k \otimes \boldsymbol{u}_k) = m_k \boldsymbol{F}_k + {}^2\boldsymbol{C}_k^u + {}^2\boldsymbol{B}_k^u \\ \partial_t (m_k h_k) + \partial_{\boldsymbol{x}} \cdot (m_k h_k \boldsymbol{u}_k) = m_k \mathrm{H}_k + {}^2\mathrm{C}_k^h + {}^2\mathrm{B}_k^h \end{cases}$$

$\rightleftharpoons$ Navier-Stokes with **sources**

Improvements

1. **Acoustic-convection splitting** [Doisneau et al., 2014, JPP]
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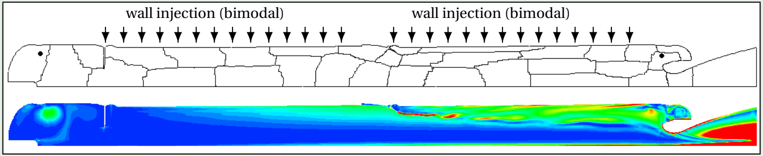
Applicative computations (1)

P230 realistic case



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

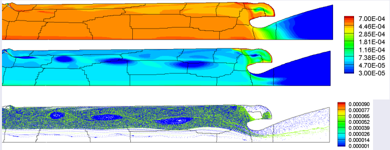
- Bimodal injection with $d_2 \approx 60 d_1$: **stiff**
- Vortex Shedding instabilities **VSO** and **VSP** : **unsteady**

Purpose

Feasibility of the **time integration/coalescence** strategy [Doisneau et al., 2013a, CRM]

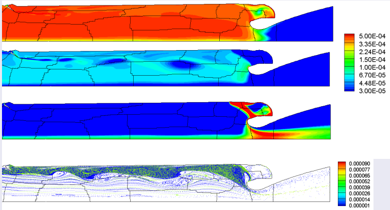
Applicative computations (1)

No coalescence



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

Coalescence



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

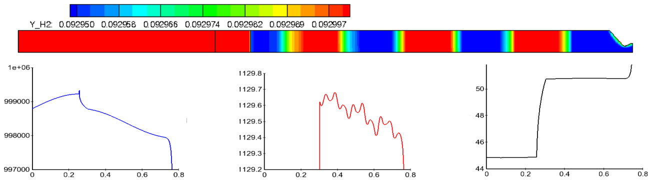
Eulerian/Lagrangian comparison

- both depend on particle distribution at boundary
- limited homo-PTC
- good agreement

Applicative computations (2)

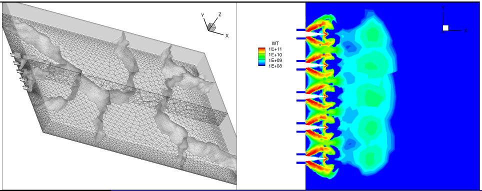
Simulation of LRE subcritical flames

Doisneau, F. (2013b). High frequency combustion instability activities – Report on the thermoacoustic evaluation of a compact flame in a cavity – Preliminary studies for the computation of cryogenic flames under acoustic modulation.
Technical Report RT 2/16530 DEFA, ONERA, Chatillon



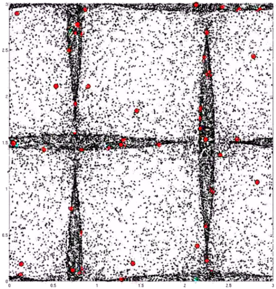
Model cryogenic spray, flame, and chamber under free regime (Y_{H_2}, pressure, temperature, velocity)

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



Overview

MODERATE INERTIA droplets



Moderately dense + inertial model ?

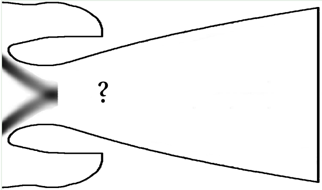
Homo-PTC in SRM

[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

Need for a moderately dense/inertial model

Homo-PTC in SRM

[Simoes, 2006] for one-way coupling

Homo-collisions

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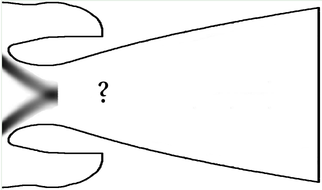
Predicting nozzle flow



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

Anisotropic Gaussian model

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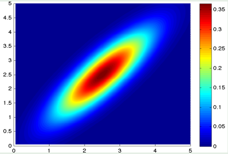
Mulitvariate gaussian [Vié et al., 2013a, CICP]

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

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



Velocity PDF for $\sigma_{11} = 1$, $\sigma_{22} = 0.8$ and $\sigma_{12} = 0.75$.

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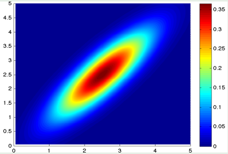


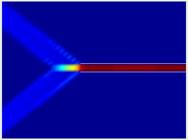
Velocity PDF for $\sigma_{11} = 1$, $\sigma_{22} = 0.8$ and $\sigma_{12} = 0.75$.

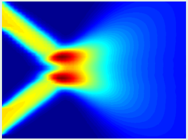
Mathematical properties

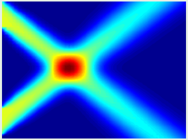
- hyperbolic equations and entropic structure
- still hypercompressible
- but less singularities

Model behavior analysis

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


Monokinetic : **singularity**


Anisotropic Gaussian


Multi-velocities : **"exact"**

Potential of AG : variance of repartition after the crossing

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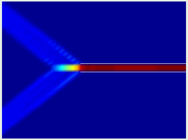
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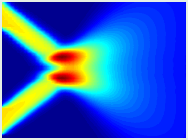
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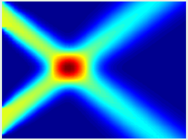
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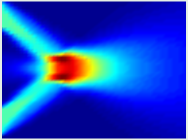
Remarks on isotropy



Isotropic Gaussian

- fails on variance
- spurious "backscattering"

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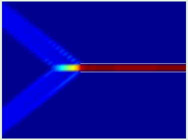

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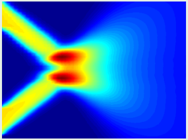

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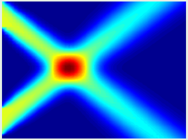

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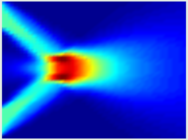

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Second order moments : “Energies”

- macroscopic energy $u_i u_j$: **mean velocities**
- ”microscopic” energy σ_{ij} : **agitation**

$$\partial_t(n\sigma_{ij}) + \partial_{\boldsymbol{x}} \cdot (n\sigma_{ij}\boldsymbol{u}) = -\frac{1}{3} n\sigma_{ij}\partial_{\boldsymbol{x}}^{Sym} \cdot \boldsymbol{u} - \frac{n\sigma_{ij}}{\tau_{\boldsymbol{u}}}$$

Transport scheme

AG hypercompressibility

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

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

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

$\Rightarrow$ 3D structured grids

AG2D (Research 2D code developed at EM2C)

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

Tested configurations

- unique crossing
- crossing with a potential force
- Taylor-Green vortices
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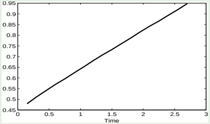
Results on transport

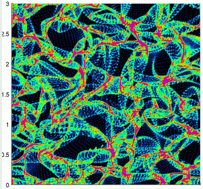
HIT test case [Vié et al., 2013a, CICP]

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

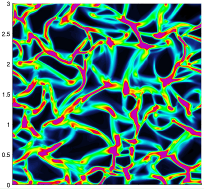


Time evolution of the Kolmogorov time scale

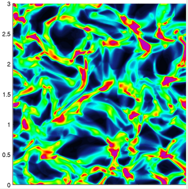
Number density fields ($\mathrm{St} = 7.5\mathrm{St}_c$, $t = 3.6\,\mathrm{s}$)



Lagrangian tracking



Eulerian isotropic (IG)



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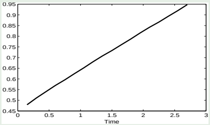

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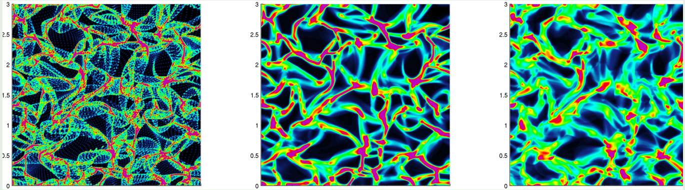


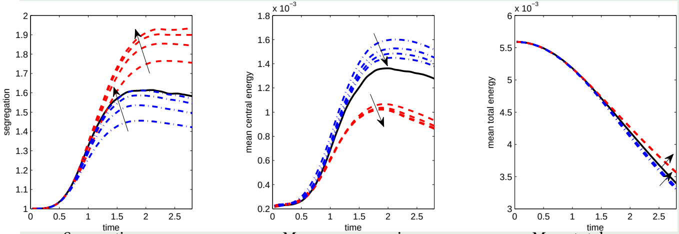
Lagrangian tracking | Eulerian isotropic (IG) | Eulerian anisotropic (AG)

Space repartition

- satisfactory (vacuum, spatial structures)
- visible differences on small scales

Results on transport (cont'd)

Second order statistics (St = $7.5 St_c$)



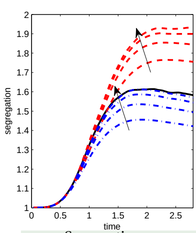
Segregation | Mean macroscopic energy | Mean total energy

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

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

Results on transport (cont'd)

Second order statistics ($St = 7.5St_c$)



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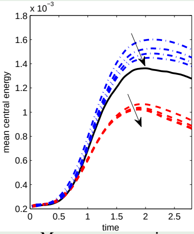
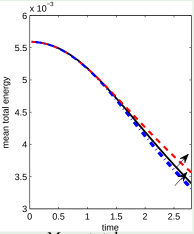


Mean macroscopic energy



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- AG behaves well : captures segregation and enrages
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Conclusion on transport

- AG closure : sensitive on statistics
- needed for the physics of sources (drag, two-way, reactive, radiative)
- 2^{nd} 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

$$\int |\boldsymbol{c}^\star - \boldsymbol{c}^\diamond| \mathcal{N}^\star \mathcal{N}^\diamond \mathrm{d}\boldsymbol{c}^\star \mathrm{d}\boldsymbol{c}^\star$$

up to 6D !
⇒ mass, mean and agitation sources

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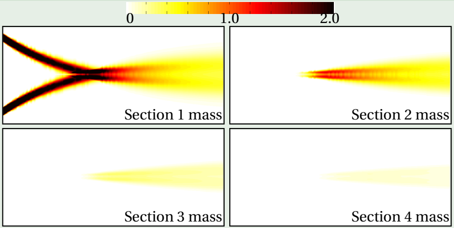
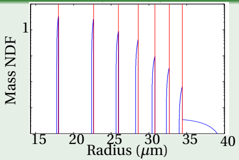
Homo-PTC with drag (Kn ∼ 1, St ∼ St_c) [Doisneau et al., 2014, CTR-COAL]





Size distribution (log-scale) at the output

Homo-coalescence dynamics

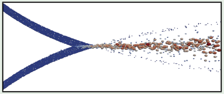
- expected polydispersity
- angle reduction observed

Reference validation

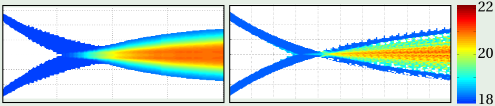
Lagrangian DPS cross comparison [Doisneau et al., 2014, CTR-COAL]

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}

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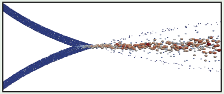

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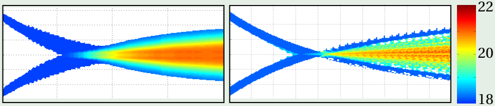

Inst. Eulerian r_{30} Time average DPS r_{30}

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]

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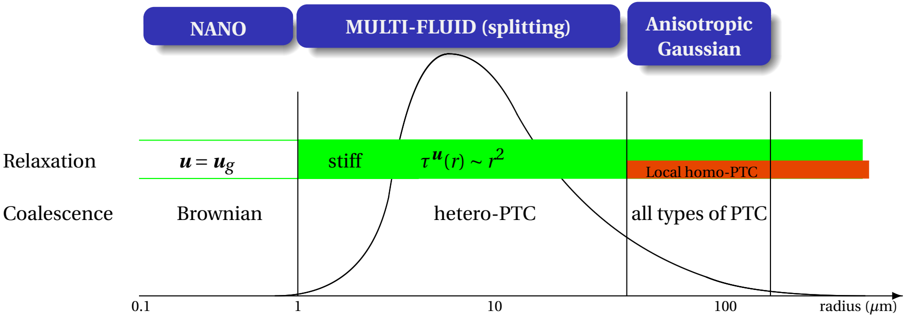
SRM prospects

- 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

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

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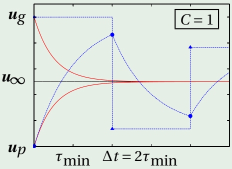
Liability of a multi-solver approach : CEDRE [Errera et al., 2011]

- time integration per phase
- with conservative coupling strategy

⚠ high loadings C or time steps Δt

[Doisneau et al., 2014, JPP]



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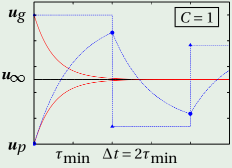

Splitting methods [Strang, 1968, Descombes and Massot, 2004]

- Many possibilities !

$\Rightarrow$

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)

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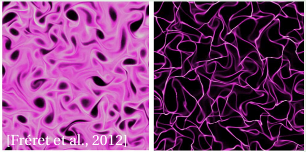
Structured grids (research codes)

Kinetic schemes

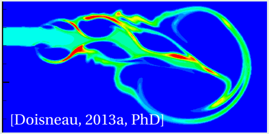
- pressureless : 2^{nd} order Bouchut/dimensional splitting [de Chaisemartin, 2009]
- weak pressure : open topic



[Fréret et al., 2012]

Unstructured grids (industrial codes)

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



[Doisneau, 2013a, PhD]

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)

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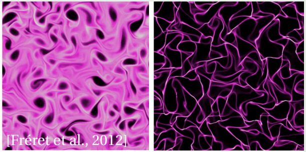

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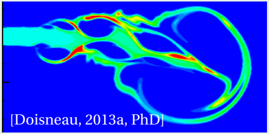

Phase space evolution

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

$$\boxed{\frac{\mathrm{d}\boldsymbol{U}}{\mathrm{d}t} = \Omega\left(\int \Phi \cdot f_{\boldsymbol{U}}\right)}$$

Quadratures [Abramowitz and Stegun, 1964, Gautschi, 1996]

- Many possibilities !

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$$\tilde{f}_{\boldsymbol{U}} \xrightarrow{(2)} \sum_i \omega_i \Phi(\boldsymbol{M}_i) \tilde{f}_{\boldsymbol{U}}(M_i) \xrightarrow{(3)} \tilde{\Omega}(\cdot)$$

$$\boldsymbol{U} \xrightarrow{(1)} \tilde{f}_{\boldsymbol{U}}$$

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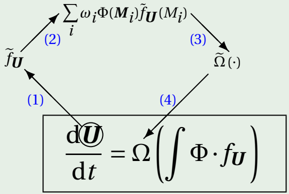

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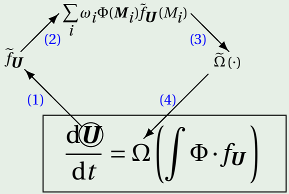

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- Many possibilities !

$\Rightarrow$

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
- 2^{nd} order MUSCL
- upcoming 4^{th} 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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$\Rightarrow$

Present work

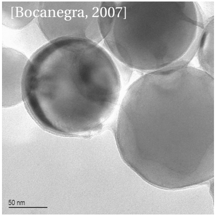
- **feasibility** of the developed strategies
- **cross-comparisons** with Lagrangian
- **applicative** computations

Extra slides

Towards "Nanopropellants"

Aluminum nanoparticle synthesis

Path	Average Size (nm)	Surface state	Quantities	Reference
Wire explosion	150 nm	uncoated	100 g/h/machine	[Gromov et al., 2006]
Precipitation	40 nm	coated	0.5 g/bath	[Aït Atmane, 2012]
Plasma condensation	40 to 200 nm	coated or uncoated		[DeLuca et al., 2010]
Pneumatic milling	2500 nm	uncoated		[DeLuca et al., 2010]



Nano-fuel properties

- ⊕ combustion rate
- ⊖ oxide layer
- **?** residual size

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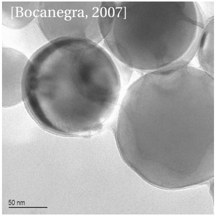


Nano-fuel properties

- ⊕ combustion rate
- ⊖ oxide layer
- **?** residual size

Need for preliminary studies on nano-residual flows

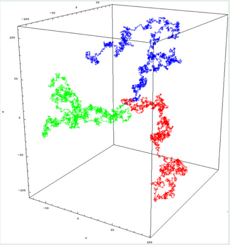
- reduction of I_{sp} loss ?
- reduction of slag ?
- what impact on instabilities ?

Nanometric droplets $\quad St \ll St_c$

Ensemble transport

negligible inertia

Brownian motion



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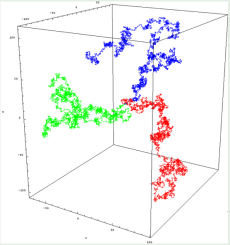

Nanometric droplet modeling issues

- nanoparticle combustion, nanoresidual formation
- transport : **diffusion**, **out-of-equilibrium** forces (thermophoresis)
- **Brownian coalescence**

1) Kinetic model for dense nanoparticle flows

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
(coexisting and coupled through sources)

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Nano Fluid-Kinetic
Fluid and Williams-Boltzmann
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Achievements : model unification

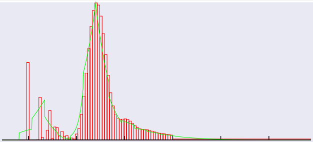
- of transport
- of coalescence

2) Nano-micro mixture modeling

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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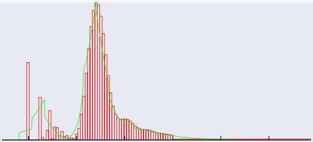


Achievements : application

- 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

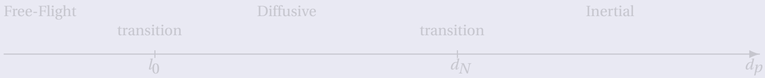
- **negligible inertia**
- **transport** properties ?
- origin of **coalescence** ?

Aerosol theory [Fuchs, 1964, Friedlander, 2000] and Fokker-Planck equation [Pottier, 2007]

- **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**
- **transport** properties ?
- origin of **coalescence** ?

Aerosol theory [Fuchs, 1964, Friedlander, 2000] and Fokker-Planck equation [Pottier, 2007]

- **transport** properties of diffusion and thermophoresis
- **coalescence** rates

but

- in a **one-way coupling** frame
- for **limited size intervals**

A comprehensive approach

Fully kinetic model

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

$\downarrow$

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

- two kinetic equations **coupled by collisions**
- **scale separation** $\varepsilon = \sqrt{\dfrac{m_g^0}{m_p^0}}$
- Chapman-Enskog expansion [Chapman and Cowling, 1939]
- $\Rightarrow$ **Fluid-Kinetic frame**

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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

$$\partial_t n + \partial_{\boldsymbol{x}} \cdot (n\boldsymbol{u}_g) = \partial_{\boldsymbol{x}} \cdot D \partial_{\boldsymbol{x}} n + \mathscr{C}(n, n)$$

Frame : macroscopic

Fokker-Planck equation [Pottier, 2007]

$$\partial_t f + \boldsymbol{c} \cdot \partial_{\boldsymbol{x}} f + \partial_{\boldsymbol{c}} \left(\frac{\boldsymbol{u}_g - \boldsymbol{c}}{\tau^{\boldsymbol{u}}(S)} f \right) = \partial_{\boldsymbol{c}} \cdot (D \partial_{\boldsymbol{c}} f)$$

Frame : kinetic

Collision kernel (integrated)

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

NA

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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

NA

Identifying the scales

Characteristic lengths

- $d_{pp} = d_p \sqrt{\frac{\rho_l \frac{4}{3}\pi}{\rho_g C}}$
- a_{drift} (inertia or diffusion)

A scale separation for nano-collisions

Nanoparticle collisions after a significant drift

$$a_{drift} \ll d_{pp}$$

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Particle-particle correlations

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

$$\begin{aligned}\mathfrak{C} = \frac{1}{2} \iint_{\boldsymbol{x}^\star, \boldsymbol{c}^\star} \int_{v^\star \in [0,v]} & f^{(2)}(t, \boldsymbol{x}, \boldsymbol{c}^\diamond, v^\diamond, \boldsymbol{x}^\star, \boldsymbol{c}^\star, v^\star)\, |\boldsymbol{c}^\diamond - \boldsymbol{c}^\star|\, \beta(v^\diamond, v^\star) J \mathrm{d}v^\star \mathrm{d}\boldsymbol{x}^\star \mathrm{d}\boldsymbol{c}^\star \\ + \iint_{\boldsymbol{x}^\star, \boldsymbol{c}^\star} \int_{v^\star} & f^{(2)}(t, \boldsymbol{x}, \boldsymbol{c}, v, \boldsymbol{x}^\star, \boldsymbol{c}^\star, v^\star)\, |\boldsymbol{c} - \boldsymbol{c}^\star|\, \beta(v, v^\star) \mathrm{d}v^\star \mathrm{d}\boldsymbol{x}^\star \mathrm{d}\boldsymbol{c}^\star\end{aligned}$$

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

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Diffusive kernel [Fuchs, 1964]

$$\mathfrak{K}_{\text{coal}}^{\text{bro}}(r^{\star}, r^{\diamond}) = \frac{2kT_g}{3\mu_g}\left(\frac{1}{r^{\star}} + \frac{1}{r^{\diamond}}\right)\left(r^{\star} + r^{\diamond}\right)$$

no slip

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Additive Kernel

$$\mathfrak{K}_{\text{coal}}^{\text{bro+bal}} = \mathfrak{K}_{\text{coal}}^{\text{bro}} + \mathfrak{K}_{\text{coal}}^{\text{bal}}$$

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

FMR-balistic

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FMR-balistic

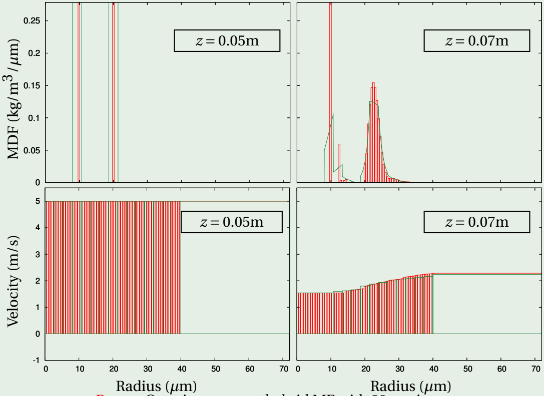
Hybrid Kernel : analogy with mass transfer convective correction

$$\mathfrak{K}^{\text{D-B}}_{\text{coal}} = 4\pi(D^\star + D^\diamond)(r^\star + r^\diamond)\left(1 + \frac{0.3\sqrt{2(r^\star + r^\diamond)\,|\boldsymbol{u}^\star - \boldsymbol{u}^\diamond|}}{\nu_g^{\frac{1}{6}}\,(D^\star + D^\diamond)^{\frac{1}{3}}}\right)$$

Diffusive-balistic

Phenomenology of nano-micro mixtures

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



Boxes : One size moment hybrid MF with 80 sections

Lines : Two size moment hybrid MF with 16 sections.

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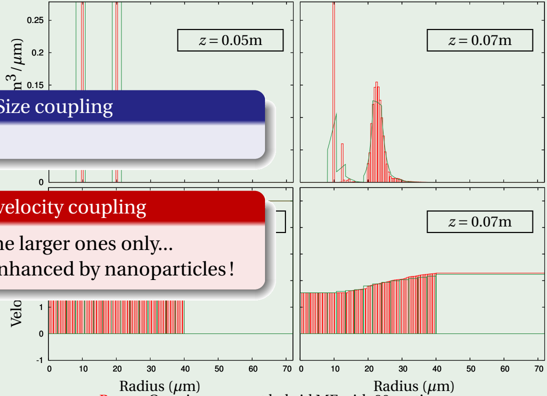


Size-Size coupling

Total

Size-velocity coupling

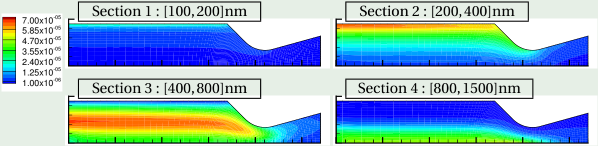
For the larger ones only...
but enhanced by nanoparticles !

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

The TEP test case

A small motor

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



Dispersed phase volume fractions per section

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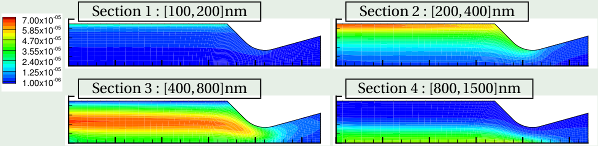

Dispersed phase volume fractions per section

Achievements

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

Extra slides

Break-up source terms

$$
\begin{aligned}
{}^2\mathrm{B}_k^{n+} &= \sum_{i=k}^{N} Q_{ik}^{n} & \qquad {}^2\mathrm{B}_k^{n-} &= \sum_{i=1}^{N} L_k^{n} \\
{}^2\mathrm{B}_k^{m+} &= \sum_{i=k}^{N} Q_{ik}^{m} & \qquad {}^2\mathrm{B}_k^{m-} &= \sum_{i=1}^{N} Q_{ki}^{m} \\
{}^2\boldsymbol{B}_k^{u+} &= \sum_{i=1}^{k} Q_{ik}^{mu} & \qquad {}^2\boldsymbol{B}_k^{u-} &= \boldsymbol{u}_k \,.\, {}^2\mathrm{B}_k^{m-}
\end{aligned}
$$

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

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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]

$\boldsymbol{u}_{\mathrm{bu}}$ [Hsiang and Faeth, 1993]

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$$ L_k^n = \iint_{S_{k-1}}^{S_k} {}^2\kappa_k(t, \boldsymbol{x}, S) \nu_{\mathrm{bu}}(\mathrm{We}(S)) \mathrm{d}S $$

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