Prise en compte des aspects polydisperses pour la modelisation d'un jet de carburant dans les moteurs à combustion interne

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IFP Energie nouvelles

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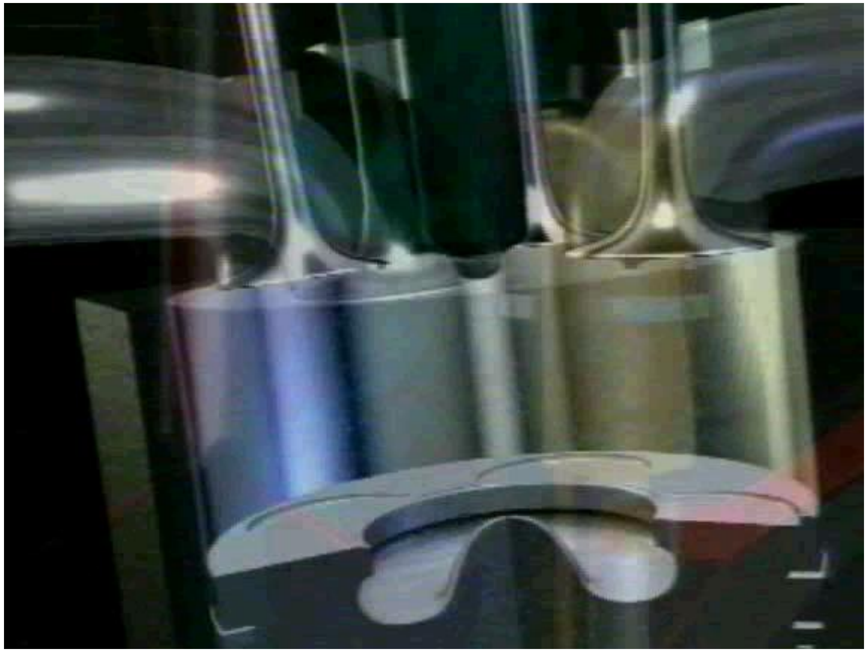
General context: Internal combustion engines

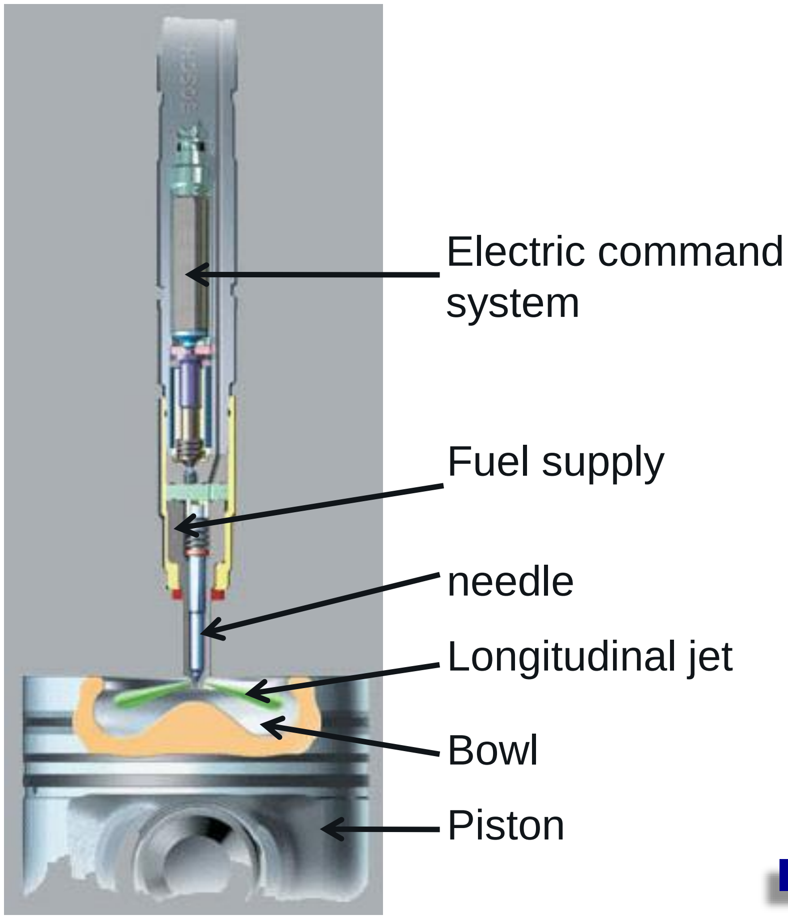
- Internal combustion engines
- Engine cycle in Diesel engines



- Compression
- Injection
- Atomisation
- Evaporation
- Auto-inflammation
- Combustion

- Critical importance to understand this cycle in order to predict:
  - Pollutants (Nox and soots) produced
  - Engine energetic yield
- Focus on the injection process

General context: Fuel injection



Multiphase flow involved

Fig: Dumouchel, Coria

Injection parameters
• Injection pressure: 2000 bar
• Injection time : 2ms
• Injection velocity: 600 m s^{-1}

Extreme conditions
Very hard to study the spray experimentally

General context:
Expertise at IFP Energies nouvelles

- Research still needs **experiments** to fully **understand** all the combined and complex physical processes occurring during injection …

Experimental expertise

- Engine test benches: Real time simulation of the engine
- Specialized laboratories: Thermodynamics and Optical diagnostic (transparent engine benches, pressurized chambers)

- … but an increasing interest is devoted to **numerical simulation** in order to **predict** these processes

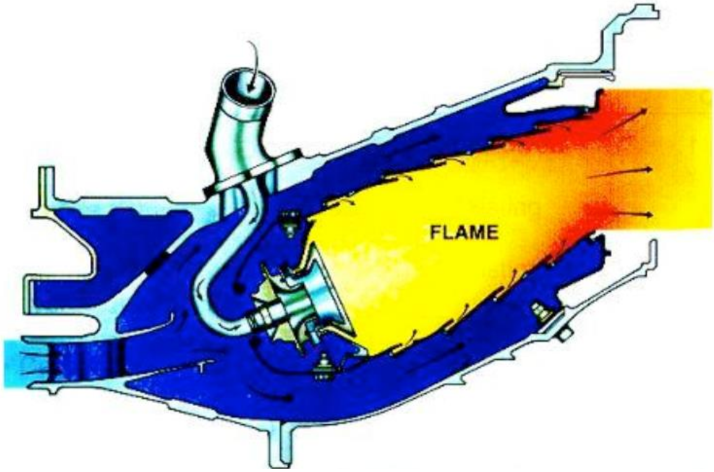
Numerical expertise

Simulation of reactive multiphase flow with spray:

- IFP-C3D: dedicated to automotive engines (RANS)
- AVBP: combustion for engines (LES), collaboration with CERFACS

General context:
More general potential application fields

Some examples:



- Turbomachines and turboreactors
- Solid propulsion
- Cryotechnic propulsion
- Soots dynamics

General context: More general potential application fields

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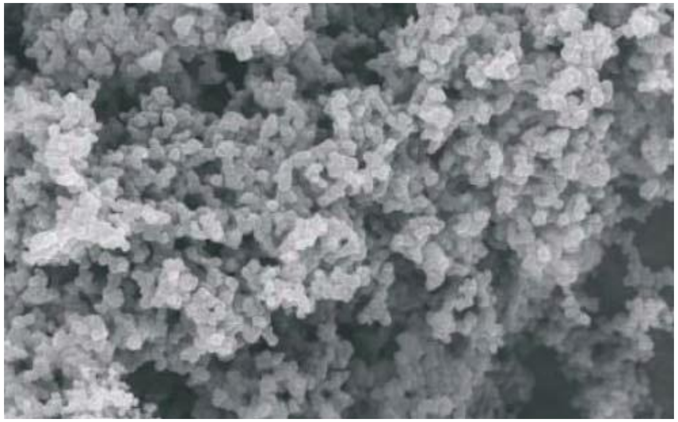

- Turbomachines and turboreactors
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General context: Physics of jet

Fig: Dumouchel, Coria

Primary break-up Secondary break-up

- Primary break-up
- Secondary break-up

General context: Physics of jet

Fig: Dumouchel, Coria

Primary break-up   Secondary break-up

- Primary break-up
- Secondary break-up
- Droplet interaction
- Turbulent dispersion
- Evaporation
- Combustion

Droplet population

Characterized by **polydispersity**

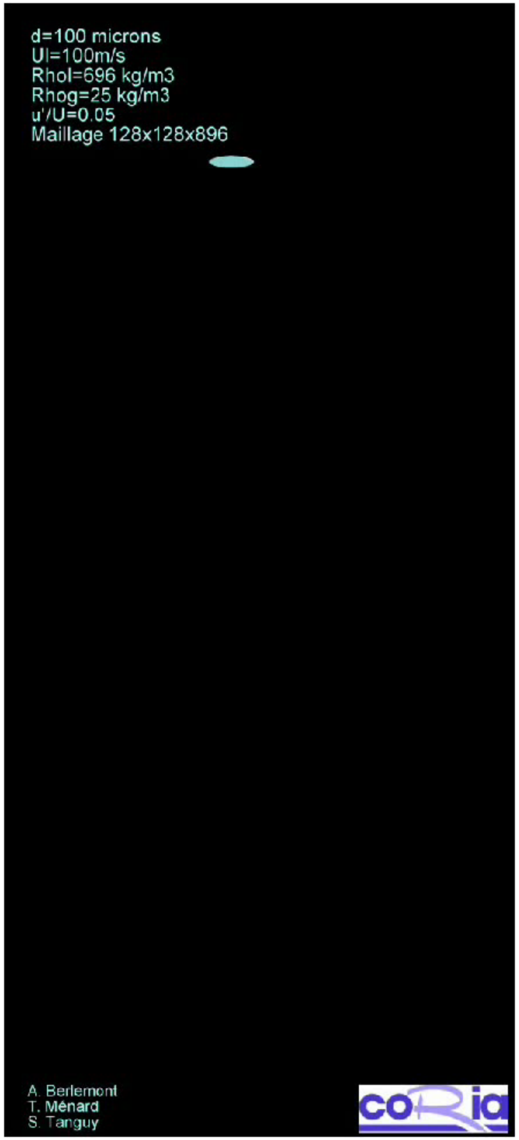
= existence of a size distribution

General context: Jet modeling

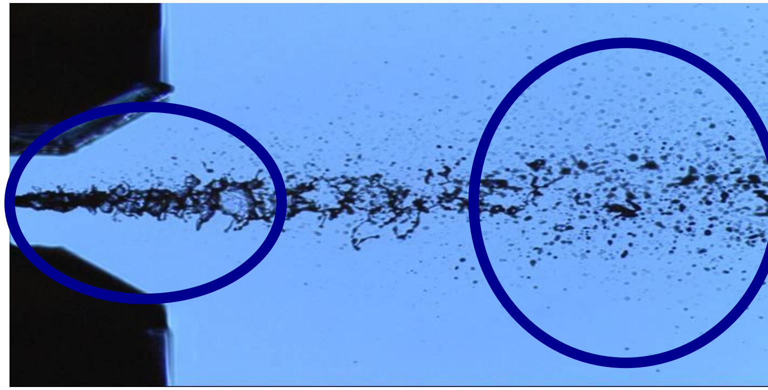
- It is possible, in terms of simulation, to solve the entire flow with a Direct Numerical simulation (DNS)

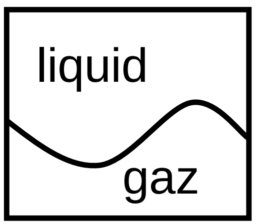
- But this resolution is too expensive in terms of computational cost in an industrial context

➡ Reduced order models

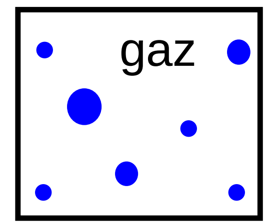


General context:
Reduced order models for jet





Separate phase



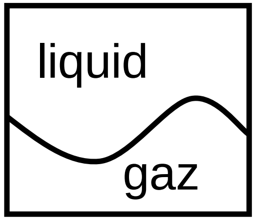
Disperse phase

Coupling ?

Two-Fluid models
• Space, time, ensemble averaging • Interface not resolved as in a DNS but liquid topology accessed through α and Σ • **No notion of polydispersity**

Spray models
• Point-particles • Spherical droplets • **Notion of polydispersity**

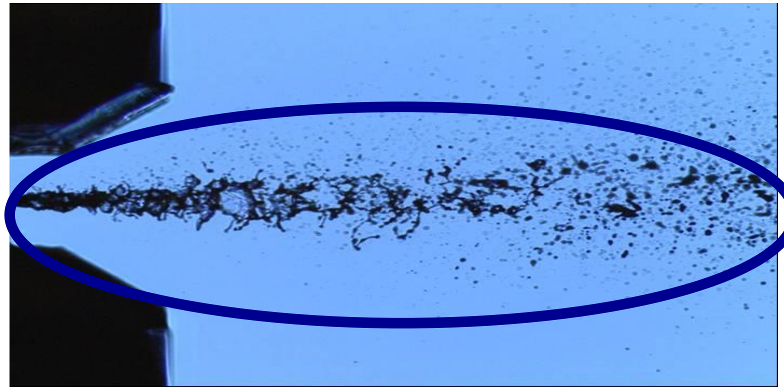
General context: Separate phase modeling



Different types of two-fluid models

- 4 equations model *(Karni 96, Abgrall 96)*
- 5 equations model *(Allaire et al. 02, Chanteperdrix et al. 02, Massoni et al. 05)*
- 6 equations model *(Ishii 75, Delhaye 76)*
- 7 equations model *(Baer and Nunziato 86, Saurel and Abgrall 00)*
- Model for surface density Σ *(Candel and Poinsot 89, Morel 97, Vallet 97)*

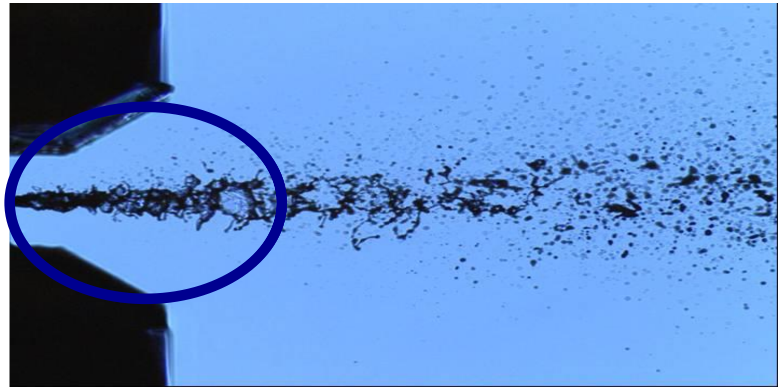
General context: Jet modeling in IFP-C3D



One single model use for the whole jet: a two-fluid model…

- B. Truchot: 7 equation model (mass, momentum, energy per phase + α) *(Truchot 05)*
- C. Vessiller: Equation on Σ *(Vessiller 07)*
- F. Bayoro: Introduction of Baer and Nunziato model *(Baer and Nunziato 86)* ideas for the equation on α and interfacial terms closure (pressure and velocity) *(Bayoro 08)*

General context:
Jet modeling in IFP-C3D



… Dedicated to the separate phase only…

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Jet modeling in IFP-C3D

… Dedicated to the separate phase only…

- B. Truchot: 7 equation model
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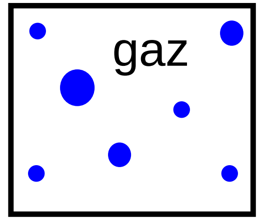
… Thus, for the disperse phase

- Access to the droplet mean diameter: $d = \frac{6\alpha}{\Sigma}$
- **Polydispersity not described**

Need for a dedicate spray model

General context: Disperse phase modeling



Deterministic approach

- Lagrangian

"Discrete particle simulation (DPS)" *(O'Rourke 81)*

Statistical approach

Kinetic model, number density function (NDF):

$$f(t, \boldsymbol{x}, S, \boldsymbol{u}, T)$$

- Lagrangian

"Discrete simulation Monte Carlo" (DSMC) *(Bird 94)*

- Eulerian

Conservation equations on moments of the NDF

General context:
Disperse phase statistical modeling

Williams-Boltzmann equation *(Williams, 58)*

$$\partial_t f + \underbrace{\nabla_{\boldsymbol{x}} \cdot (\boldsymbol{u} f)}_{\text{advection}} + \underbrace{\partial_S (K f)}_{\text{evaporation}} + \underbrace{\nabla_{\boldsymbol{u}} \cdot (\boldsymbol{F} f)}_{\text{acceleration}} + \underbrace{\partial_T (E f)}_{\text{heat exchange}} = \underbrace{\Gamma}_{\text{source}}$$

Lagrangian resolution

- Modeling
- Implementation
- Parallel computing
- Coupling
  - Gas phase (Eulerian)
  - Separate phase(Eulerian)

Eulerian resolution

- Modeling
- Implementation
- Parallel computing
- Coupling
  - Gas phase (Eulerian)
  - Separate phase(Eulerian)

We consider an Eulerian resolution

General context:
Eulerian resolution of the disperse phase

Framework kinetic equation of this PhD

$f(t, \boldsymbol{x}, S, \boldsymbol{u})$ solution of

$$\partial_t f + \underbrace{\nabla_{\boldsymbol{x}}(\boldsymbol{u} f)}_{\text{advection}} + \underbrace{\partial_S(K f)}_{\text{evaporation}} + \underbrace{\nabla_{\boldsymbol{u}}(\boldsymbol{D}_{\Gamma} f)}_{\text{drag}} = 0$$

- Resolution with Finite-Volume methods **prohibitive** (7 dimensions in 3D)

Resolution of moments of f

Definition of moments: $\mathcal{M}_{k,\boldsymbol{l}} = \int_{S_{min}}^{S_{max}} \int_{\mathbb{R}} S^k \boldsymbol{u}^{\boldsymbol{l}} f \, \mathrm{d}\boldsymbol{u} \mathrm{d}S$

Size moments: $m_k = \mathcal{M}_{k,0}$

Velocity moments: $M_{\boldsymbol{l}} = \mathcal{M}_{0,\boldsymbol{l}}$

Mean droplet velocity: $\boldsymbol{u}_p = \dfrac{\mathcal{M}_{0,1}}{\mathcal{M}_{0,0}}$

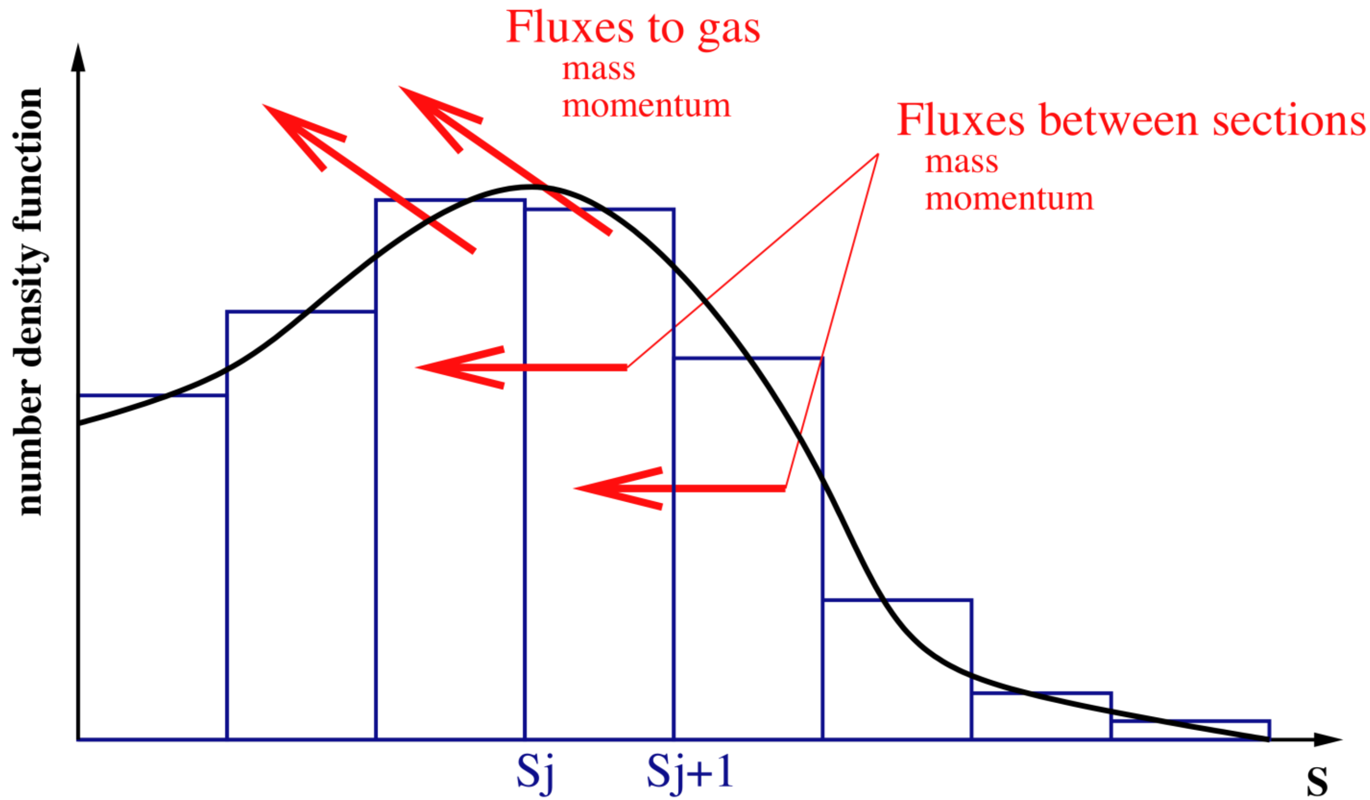
General context:
Three classes of polydisperse spray models

Sectional models: Multi-Fluid model (MF) *(de Chaisemartin, PhD09, Laurent and Massot 01)*

High order moment model with presumed NDF *(Mossa 05)*

High order moment model with Direct quadrature Method of Moments (DQMOM) *(Marchisio et al. 05, Fox et al. 08)*

Multi-Fluid model: Principle



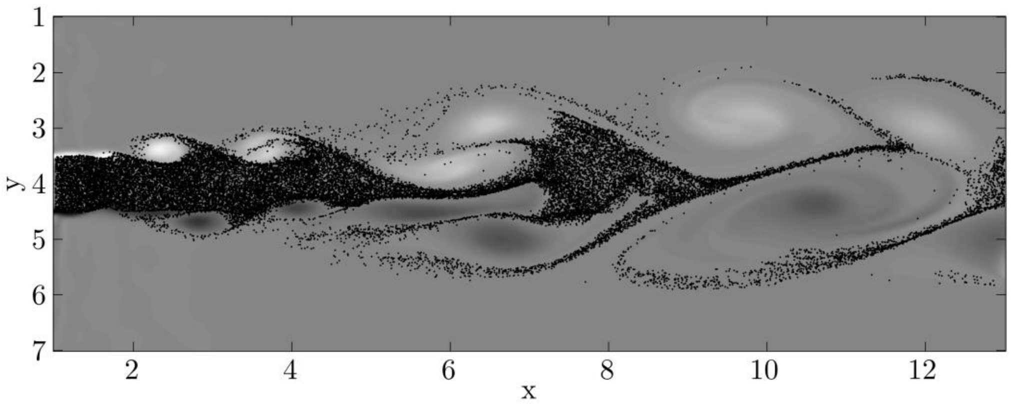
- The size phase space is discretized into sections $[S_j, S_{j+1}]$
- For each section, conservation equations are written for the mass moment $m_{3/2,j}$ and momentum $m_{3/2,j}u_{p,j}$
- For the evaporation process, the section quantities are impacted by fluxes from adajacent sections

Multi-Fluid model: Example of achievements

- Comparison MF/Lagrangian (DSMC)

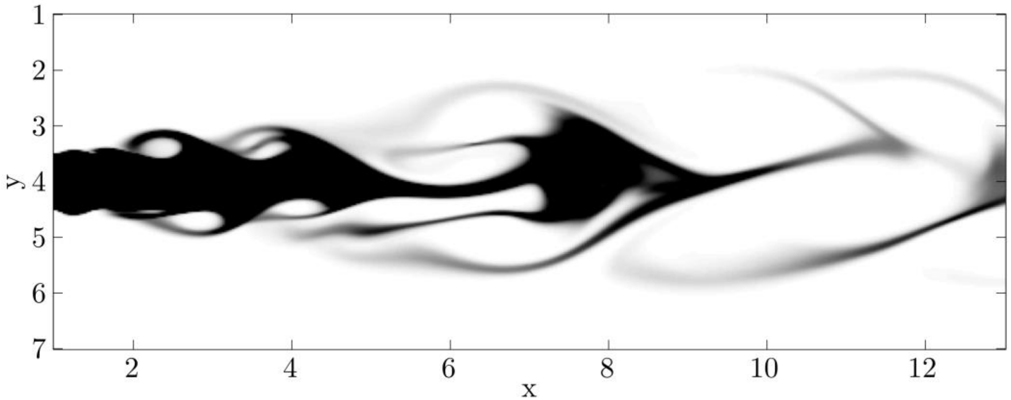
Lagrangian

Particle positions
(30000 particles)



Eulerian

Mass density
400 x 200 x 10 grid



➡ Very good level of comparison Euler/Lagrange

Multi-Fluid model: Limitations

Computational cost

Need to have a substantial number of sections

- To accurately describe polydispersity
- To limit diffusion in size phase space in the case of evaporation

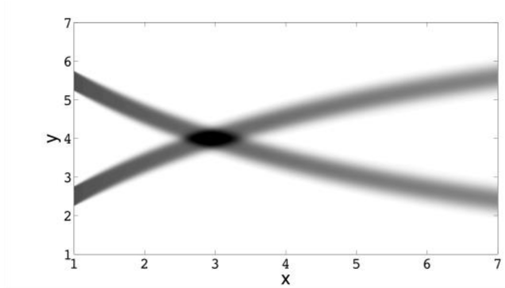
➡ Important computational cost, prohibitive for an industrial application

Particle trajectory crossing (PTC)

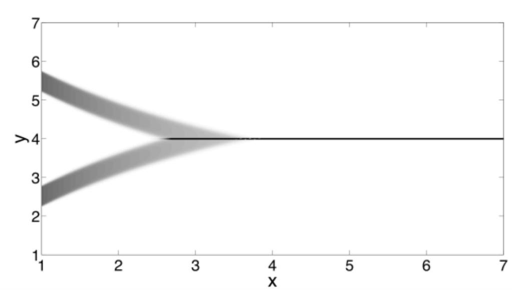
Only one velocity solved per section: $u_{p,j}$

➡ Description of droplet crossing impossible in the same section

Kinetic solution



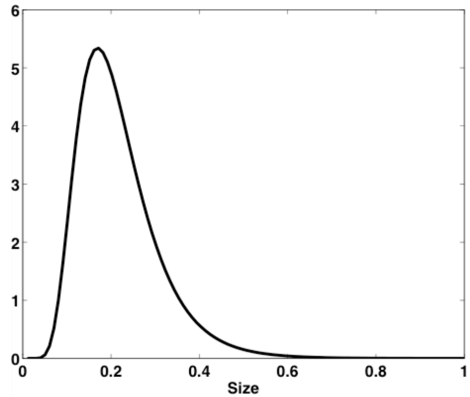
Multi-Fluid solution



High order moment model with presumed NDF

Presumed profile of the NDF

- Example: Presumed log-normal distribution function



$$f(D) = \frac{m_0}{D \ln(\sigma)\sqrt{2\pi}} \exp\left\{ -\frac{1}{2}\left[\frac{\ln(D/\bar{D})}{\ln(\sigma)}\right]^2 \right\}$$

- Evolution of the log-normal function parameters $m_0, \bar{D}, \sigma$

But, for arbitrary evaporation process, it might not be possible to reconstruct a log-normal function

The model is unstable for evaporation

High order moment model using Direct Quadrature Method of Moment (DQMOM)

Principle

- Approximation of f under the profile:

$$f(t, \boldsymbol{x}, S, \boldsymbol{u}) = \sum_{n=1}^{N} \omega_n \delta(S - S_n) \delta(\boldsymbol{u} - \boldsymbol{u}_n)$$

- Evolution of the weights and abscissas directly $\omega_n, S_n, \boldsymbol{u}_n$

- Excellent results for coalescence
- But difficulties to determine the evaporating flux of the particles
- PTC cannot be described

We distinguish three classes of models

Sectional models: Multi-Fluid model (MF) *(de Chaisemartin, PhD09, Laurent and Massot 01)*

- Size/Velocity correlation are resolved
- Several sections needed, leading to important CPU cost

High order moment model with presumed NDF *(Mossa 05)*

- Polydispersity is considered with only one section
- The model is instable through evaporation

High order moment model with Direct quadrature Method of Moments (DQMOM) *(Marchisio et al. 05, Fox et al. 08)*

- Polydispersity is considered with only one section
- There exist cases where evaporation is not accurately described

- None of these models is able to describe PTC between same size droplets

Achievements of the PhD

This PhD work has consisted in designing an **Eulerian spray** model and associated numerical tools:

- overcoming the limitations of current Eulerian models with respect to description of **polydispersity** and **particle trajectory crossing**
- in order to be extended to an **industrial context** (IFP-C3D)

Modeling work	Extension to industrial context
Polydisperse spray model: • with one section • efficient in terms of CPU cost • simulating PTC	• Adaptation to the formalism used in IFP-C3D: Arbitrary Lagrangian Eulerian (ALE) • Implementation in IFP-C3D

Achievements of the PhD

- Description of polydispersity:

  Eulerian Multi-Size Moment (EMSM) model

Development of the EMSM model and numerical tools

- Evaporation
  - design of a consistent model
  - design of an accurate and robust numerical schem

  (conf. SIAM 08, Monterey), (SIAM J. App. Math., 10)

- Advection of a moment set
  - design of a accurate and robust advection scheme

  (conf ICLASS 09, Vail)

(VKI, 09)

- Validation of the EMSM model (implemented in Muses3D) versus the MF model

  (JCP 10)

Achievements of the PhD

- Description of polydispersity:

  Eulerian Multi-Size Moment (EMSM) model

Extension to an industrial context
• Adaptation of the designed schemes to the ALE formalism
• Implementation of the EMSM model in IFP-C3D and validation
➡ *(conf. ICMF 10, Tampa Bay), (IJMF 10)*

Achievements of the PhD

- Description of particle trajectory crossing

  Eulerian Multi-Velocity Moment (EMVM) model

Development of the EMVM model and numerical tools

- 1D problem: Mathematical study of the closed system in order to prepare the design of high order advection schemes:

  ➡ *(CMS 10)*

- Multi-D problem: Study on closure of the ill-posed problem and evaluation of the EMVM model
  - Proposed closure
  - Coupling of EMVM and MF models: EMFVM model
  - Validation of EMSVM model (implemented in Muses3D) by comparison with Lagrangian results

  ➡ *(2 Proceedings of the CTR 08, Stanford), (CRAS 09), (FTC 10)*

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution
- Evaluation of the EMSM model
  - Quantitative validation
  - Comparison with the MF model
- Extension to IFP-C3D
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EMSM model: Modeling and numerical tools
General resolution strategy

Basis kinetic equation

$$\partial_t f + \underbrace{\nabla_{\boldsymbol{x}}(\boldsymbol{u} f)}_{\text{advection}} + \underbrace{\partial_S(K f)}_{\substack{\text{evaporation} \\ (d^2 \text{ law})}} + \underbrace{\nabla_{\boldsymbol{u}}(\boldsymbol{D}_{\mathrm{r}} f)}_{\text{drag}} = 0$$

Expression of the NDF

$$f(t, \boldsymbol{x}, S, \boldsymbol{u}) = \underbrace{n(t, \boldsymbol{x}, S)}_{\text{size distribution}} \underbrace{\delta(\boldsymbol{u} - \boldsymbol{u}_p(t, \boldsymbol{x}, S))}_{\text{velocity distribution}}$$

Monokinetic assumption for a given size

Quantities resolved

- $m_k = \mathcal{M}_{k,0} = \int_0^1 \int_{\mathbb{R}} S^k \boldsymbol{u}^l f \, \mathrm{d}\boldsymbol{u} \mathrm{d}S$
- $\boldsymbol{u}_p = \dfrac{\mathcal{M}_{0,1}}{\mathcal{M}_{0,0}}$

EMSM model: Modeling and numerical tools
General resolution strategy

Kinetic model
$f(t, \boldsymbol{x}, S, \boldsymbol{u})$

$\downarrow$

Velocity moments of order 0 and 1

$$\int_{\mathbb{R}} \boldsymbol{u}^l f \,\mathrm{d}\boldsymbol{u}$$

Semi-Kinetic model
$n(t, \boldsymbol{x}, S), n\boldsymbol{u}_p(t, \boldsymbol{x}, S)$

Velocity moments **conditioned by size**

$\downarrow$

Size moments of order k, k=0,…,N

$$\int_0^1 S^k n \,\mathrm{d}S$$

EMSM model
$m_k(t, \boldsymbol{x}), \boldsymbol{u}_p(t, \boldsymbol{x})$

Equations on size moments and mean velocity

EMSM model: Modeling and numerical tools
General resolution strategy

Moment equation system

We aim to solve the following system:

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = -Kn(t, \boldsymbol{x}, S = 0)$$

$$\vdots$$

$$\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) = -KN m_{N-1}$$

$$\partial_t m_1 \boldsymbol{u}_p + \underbrace{\nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p)}_{\text{advection}} = \underbrace{-K m_0 \boldsymbol{u}_p}_{\text{evaporation}} - \nabla_{\boldsymbol{x}} P + \underbrace{\boldsymbol{D}}_{\text{drag}}$$

EMSM model: Modeling and numerical tools
General resolution strategy

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Unclosed terms

- $f(t, \boldsymbol{x}, S, \boldsymbol{u}) = n(t, \boldsymbol{x}, S)\delta(\boldsymbol{u} - \boldsymbol{u}_p)$ ➔ $P = 0$ (velocity dispersion)
- $n(t, \boldsymbol{x}, S=0) = \Phi(m_0, ..., m_N)(t, \boldsymbol{x})$

EMSM model: Modeling and numerical tools
General resolution strategy

- Operator splitting strategy *(Strang 68)*
- Successive resolution of
  - **Evaporation**
  - Advection
  - Drag

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = -Kn(t, \boldsymbol{x}, S = 0)$$

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EMSM model: Modeling and numerical tools
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EMSM model: Modeling and numerical tools
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  - **Drag**

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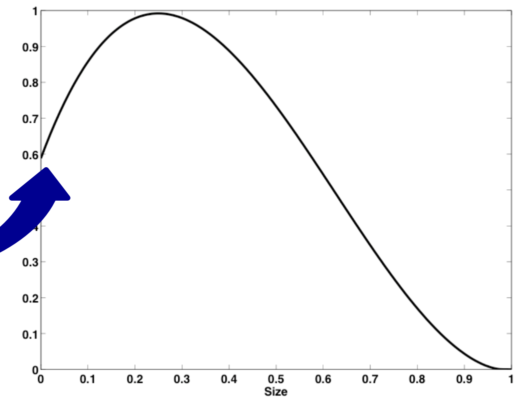
EMSM model: Modeling and numerical tools
Evaporation term resolution

Continuous problem

- Closure of $Kn(t, \boldsymbol{x}, S = 0)$ = evaporation flux
- The challenge is to reconstruct, from the data of the moments, a pointwise value of the size NDF

$$\boldsymbol{m}_N = (m_0, \dots, m_N)^t$$



- Stability condition : moment space preservation

EMSM model: Modeling and numerical tools
Evaporation term resolution

Moment space

- The vector $\boldsymbol{m}_N = (m_0, \ldots, m_N)^t$ belongs to moment space $\mathbb{M}_N$
- $\mathbb{M}_N$ has a complex geometry

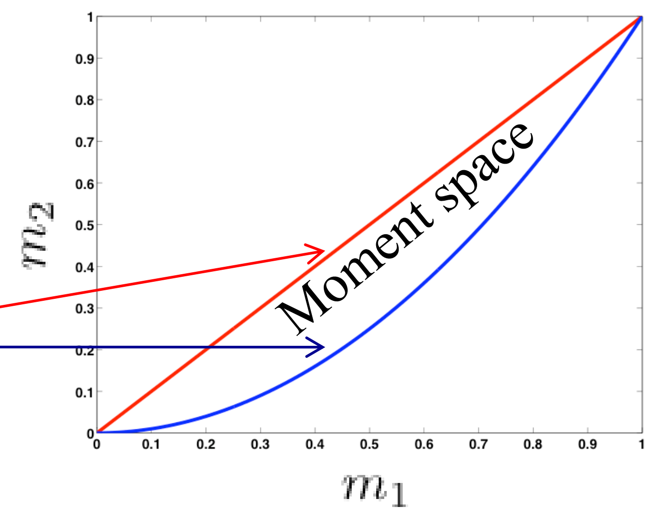
Example of moment space geometry

- Set of PDF on [0,1] such as $m_0 = 1$
- Condition on m_1 and m_2

$$m_1 = \int_0^1 S\, n\, \mathrm{d}S, \quad 0 < m_1 < 1$$

$$m_2 = \int_0^1 S^2\, n\, \mathrm{d}S, \quad \underbrace{m_1^2}_{\text{low border}} < m_2 < \underbrace{m_1}_{\text{high border}}$$

Moment space structure



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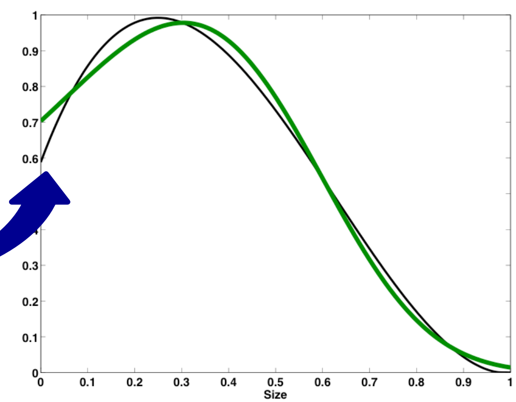


- Stability condition : moment space preservation:

Realizability condition

Solution

Approximation of the size NDF by **Maximization of Entropy** *(Mead 84)*

$$\boldsymbol{m}_N = (m_0, \ldots, m_N)^t \Rightarrow \tilde{n}_{ME}$$

EMSM model: Modeling and numerical tools
Evaporation term resolution

Challenge for the discrete problem

Evaporation system **cannot** be solved by ODE solvers

⚠ **Realizability condition**

Solution

- Finite volume scheme
- Exact temporal integration
- Flux calculation: kinetic scheme

EMSM model: Modeling and numerical tools
Evaporation term resolution

- The kinetic scheme lies on the equivalence between the two equations:
  - kinetic (or semi-kinetic): $\partial_t n - \partial_S (K\, n) = 0$
  - macroscopic: $\partial_t m_k = \ldots, \quad k = 0, \ldots, N$

Principle of a kinetic scheme

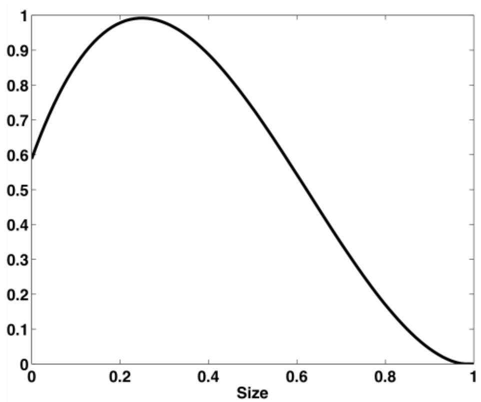
$$
\begin{tikzcd}
\boldsymbol{m}_N(0) \arrow[d] & \boldsymbol{m}_N(\Delta t) \\
\tilde{n}_{ME}(0,S) \arrow[r, "\text{exact evolution}", "\Delta t"'] & \tilde{n}_{ME}(\Delta t, S) \arrow[u]
\end{tikzcd}
$$

- $\tilde{n}_{ME}$ is reconstructed from $\boldsymbol{m}_N$
- $\tilde{n}_{ME}(\Delta t, S)$ is computed from $\tilde{n}_{ME}(0,S)$ through the kinetic equation
- Fluxes of $\boldsymbol{m}_N$ are computed using $\tilde{n}_{ME}(\Delta t, S)$

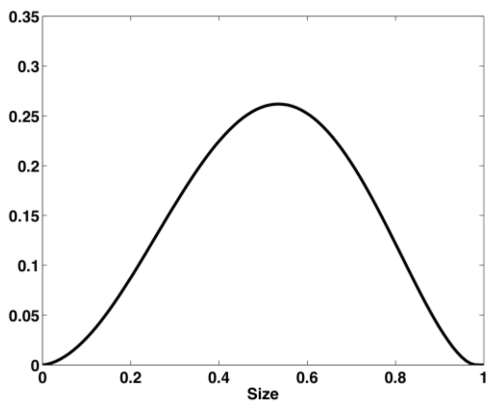
EMSM model: Modeling and numerical tools Evaporation term resolution

- Evolution of the total mass of a spray with the initial size distribution:

Number density



Mass density

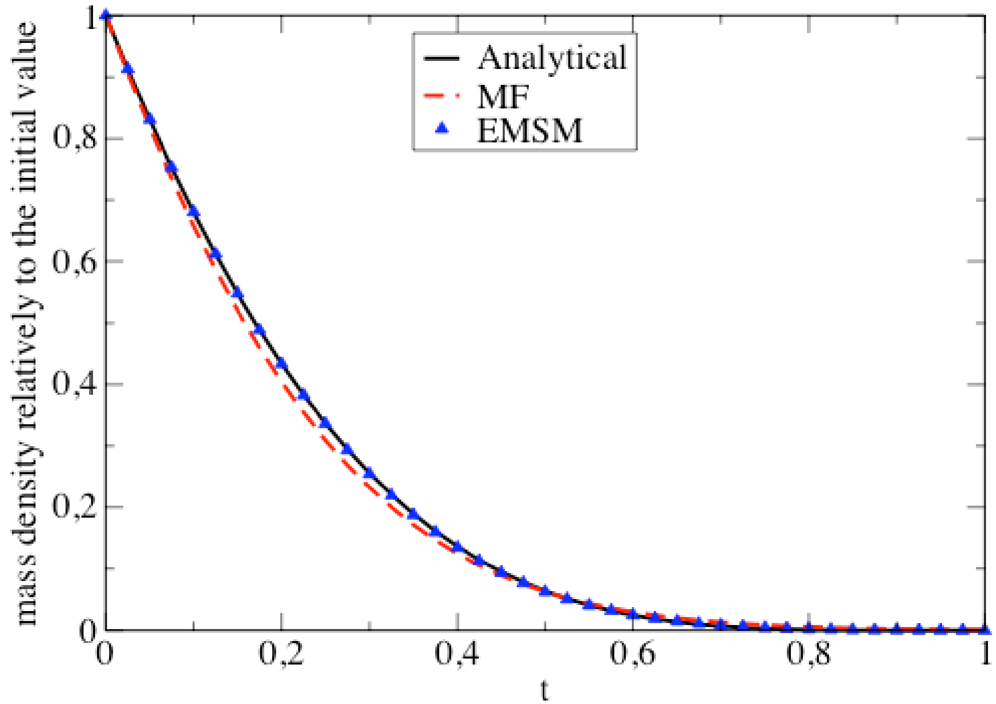


Comparison between EMSM and MF models

- MF model: $m_{3/2}$ 1 moment and 10 sections
- EMSM model: $m_k, k = 0, \dots, 3$ 4 moments and 1 section

EMSM model: Modeling and numerical tools
Evaporation term resolution

- Results



- Very good level of comparison

  Similar accuracy between EMSM with 1 section and MF with 10 sections

EMSM model: Modeling and numerical tools
Evaporation term resolution

Conclusion

- Design of theoretical (Entropy Maximization) and numerical tool (kinetic scheme)

➡ **Stable scheme for evaporation flux**
Accuracy of the EMSM model with 1 section similar to the accuracy of the MF model with 10 sections

- The designed EMSM model and numerical tools are extendable to
  - arbitrary evaporation laws
  - formalism with several sections

Perspectives

The entropy maximization can be applied to bivariate distributions

➡ Application to non spherical particles (soots)

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution
- Evaluation of the EMSM model
  - Quantitative validation
  - Comparison with the MF model
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EMSM model: Modeling and numerical tools
Advection term resolution

Purpose

Design a high order advection scheme for the system:

$$
\begin{aligned}
\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) &= 0 \\
&\vdots \\
\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) &= 0 \\
\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) &= 0
\end{aligned}
$$

EMSM model: Modeling and numerical tools
Advection term resolution

Purpose

Design a high order advection scheme for the system:

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = 0$$

$$\vdots$$

$$\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) = 0$$

$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = 0$$

Challenges

- Pressureless gas dynamics (PGD)– delta choc

EMSM model: Modeling and numerical tools
Advection term resolution

Purpose

Design a high order advection scheme for the system:

$$\begin{aligned}\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) &= 0\\ &\vdots\\ \partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) &= 0\\ \partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) &= 0\end{aligned}$$

dimensional splitting

Resolved system

1D system:

$$\begin{aligned}\partial_t m_0 + \partial_x(m_0 u_p) &= 0\\ &\vdots\\ \partial_t m_N + \partial_x(m_N u_p) &= 0\\ \partial_t m_1 u_p + \partial_x(m_1 u_p^2) &= 0\end{aligned}$$

Challenges

- Pressureless gas dynamics (PGD) – delta choc
  - Dedicated scheme designed in *(de Chaisemartin, PhD 09)* from the kinetic scheme *(Perthame 02, Bouchut 03)* and using dimensional splitting

EMSM model: Modeling and numerical tools
Advection term resolution

Purpose

Design a high order advection scheme for the system:

$$\partial_t m_0 + \nabla_{\boldsymbol{x}}(m_0 \boldsymbol{u}_p) = 0$$
$$\vdots$$
$$\partial_t m_N + \nabla_{\boldsymbol{x}}(m_N \boldsymbol{u}_p) = 0$$
$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = 0$$

dimensional splitting

Resolved system

1D system:

$$\partial_t m_0 + \partial_x(m_0 u_p) = 0$$
$$\vdots$$
$$\partial_t m_N + \partial_x(m_N u_p) = 0$$
$$\partial_t m_1 u_p + \partial_x(m_1 u_p^2) = 0$$

Challenges

- Pressureless gas dynamics (PGD)– delta choc
  - Dedicated scheme designed in *(de Chaisemartin, PhD 09)* from the kinetic scheme *(Perthame 02, Bouchut 03)* and using dimensional splitting
- **Realizability condition**

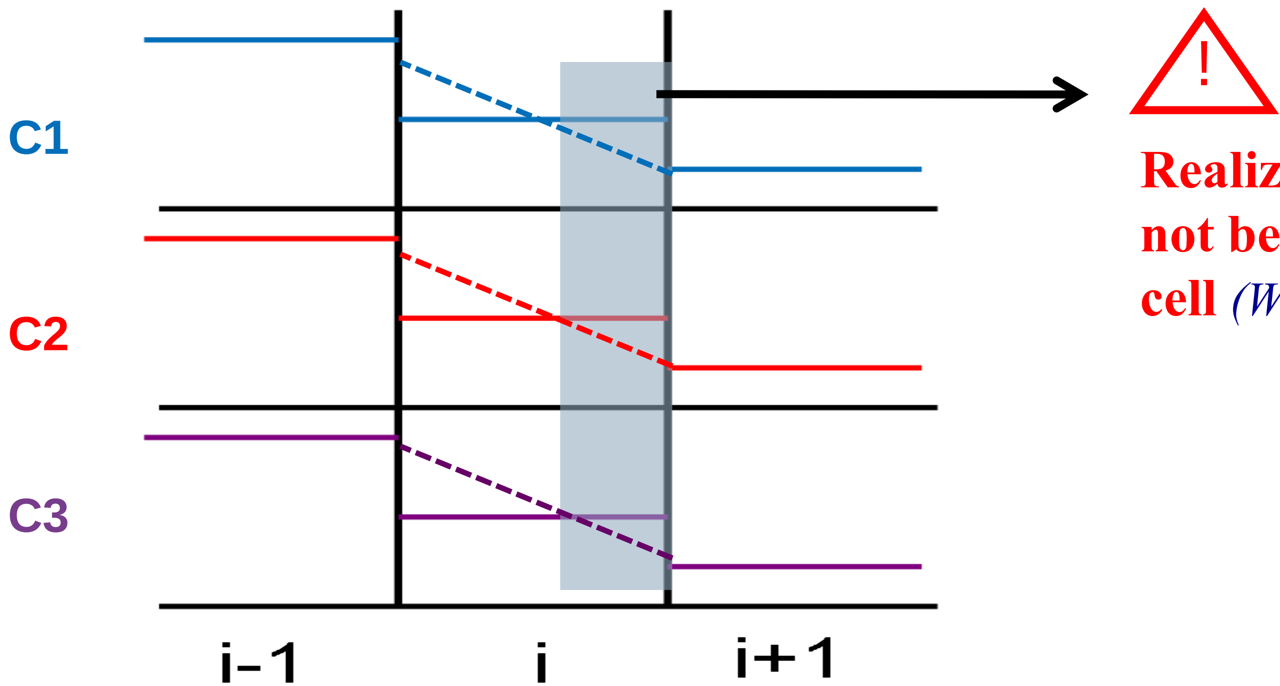
EMSM model: Modeling and numerical tools
Advection term resolution

Realizability condition

- Considering normalized moments $c_k = \frac{m_k}{m_0}, \; k = 1, \ldots, N$

  the ck are transported quantities as they verify $\partial_t c_k + u_p \partial_x c_k = 0$

- Independent reconstruction of the c_k



Realizability condition might not be satisfied in the whole cell *(Wright 07, McGraw 07)*

EMSM model: Modeling and numerical tools
Advection term resolution

Realizability condition enforcement

- From the moment space theory, we can define **canonical moments** p_k from the moment vector: $\boxed{p_k = \frac{c_k - c_k^-}{c_k^+ - c_k^-}}$ *(Dette and Studden 97)*

- Realizability condition enforced $\Longleftrightarrow$ $p_k \in [0, 1]$ **independently**

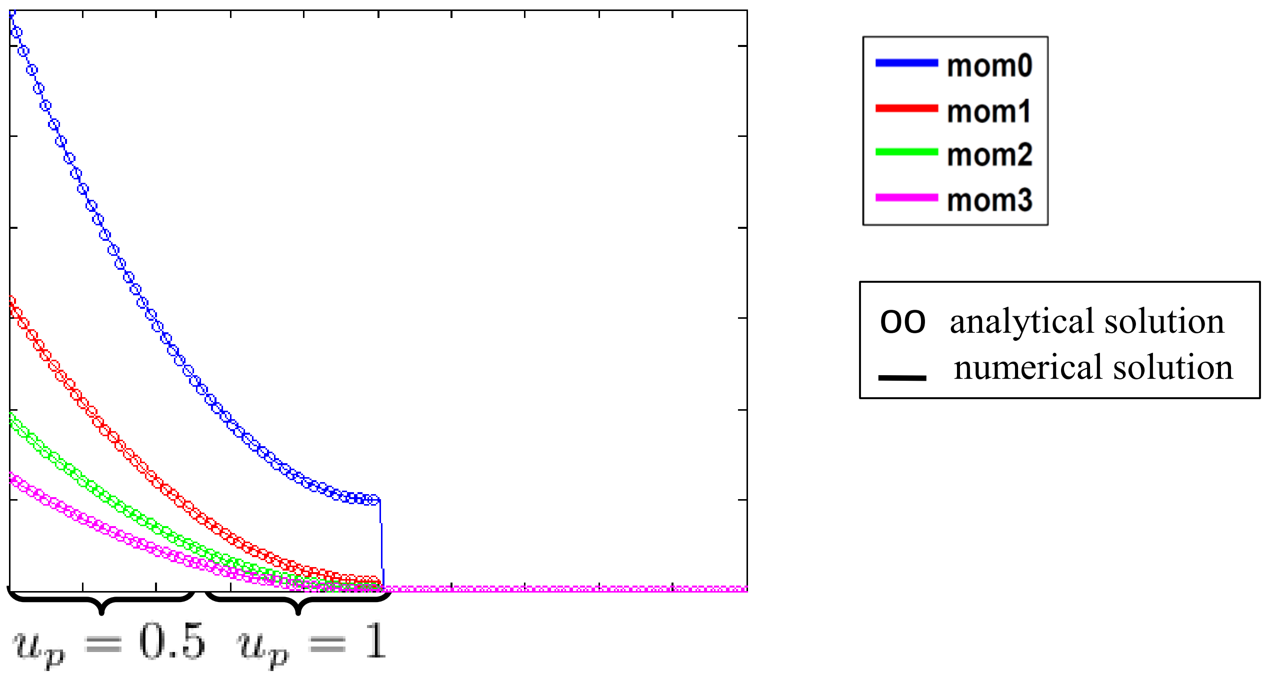
➡ **Reconstruction of canonical moments** to ensure the realizability condition everywhere in the cell

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution
- Evaluation of the EMSM model
  - Quantitative validation
  - Comparison with the MF model
- Extension to IFP-C3D
  - Adaptation to the ALE formalism
  - Implementation in IFP-C3D and validation

Evaluation of the EMVM model
Quantitative validation

Validation of the evaporation and advection operator



Interest of the test case

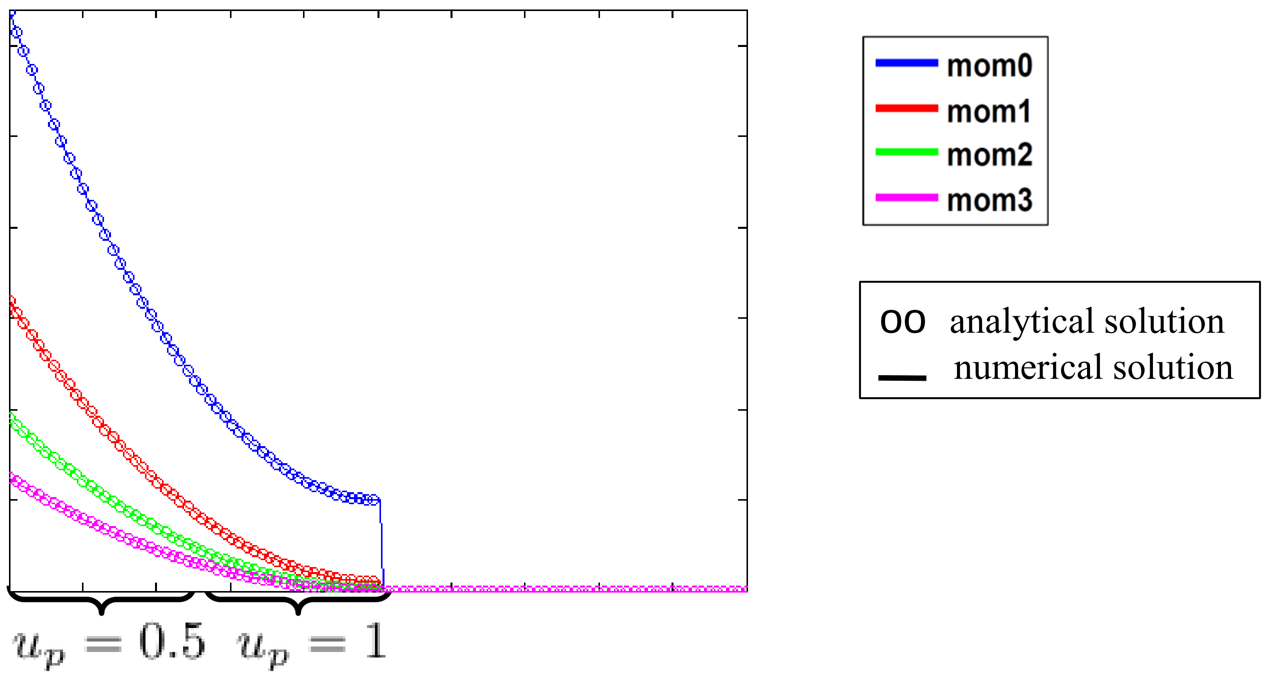
- Velocity discontinuity ➡ Creation of Vacuum zone
- Inhomogeneous size NDF profile

$$n^0(x,S) = \begin{cases} \lambda(x)\sin(\pi S) + (1-\lambda(x))\exp(-10\,S) & \text{if } x \leq 0.5 \\ 0 \text{ otherwise} \end{cases}$$

➡ Actual reconstruction of canonical moment with non null slope

Evaluation of the EMVM model
Quantitative validation

Validation of the evaporation and advection operator

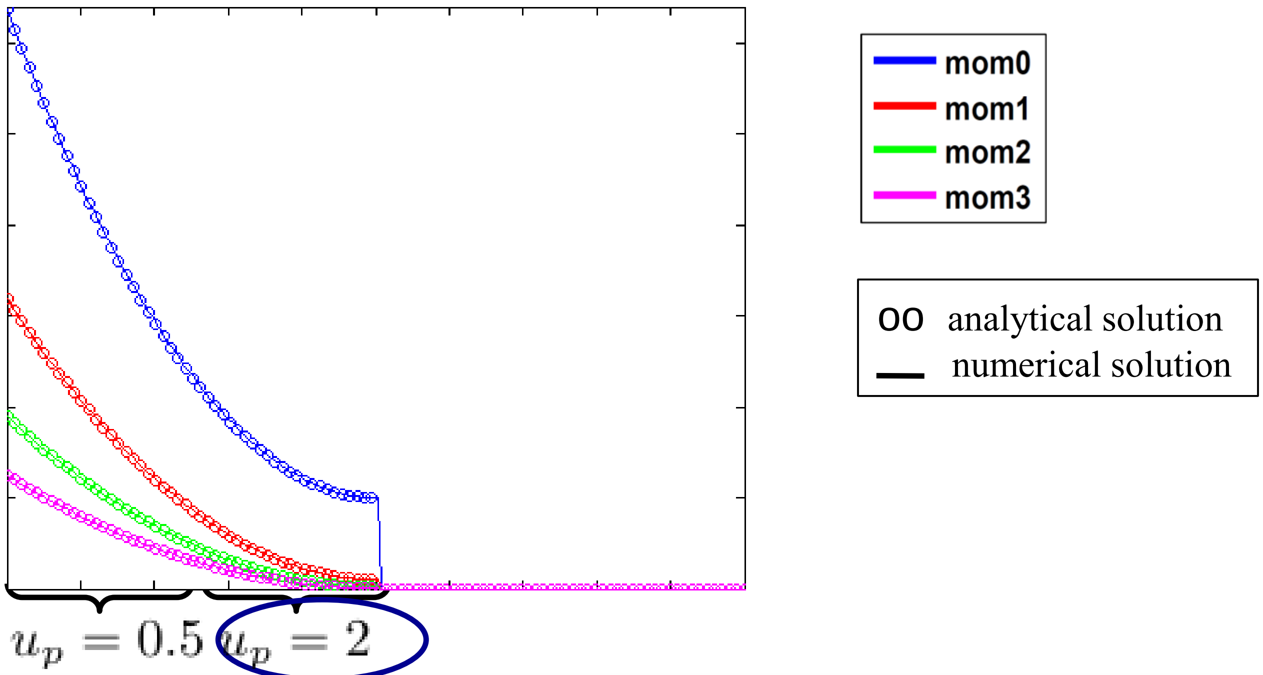


Conclusion

- **Vacuum zone well described**
- **Good level of comparison with the analytical solution**

Evaluation of the EMVM model
Quantitative validation

Validation of the evaporation and advection operator

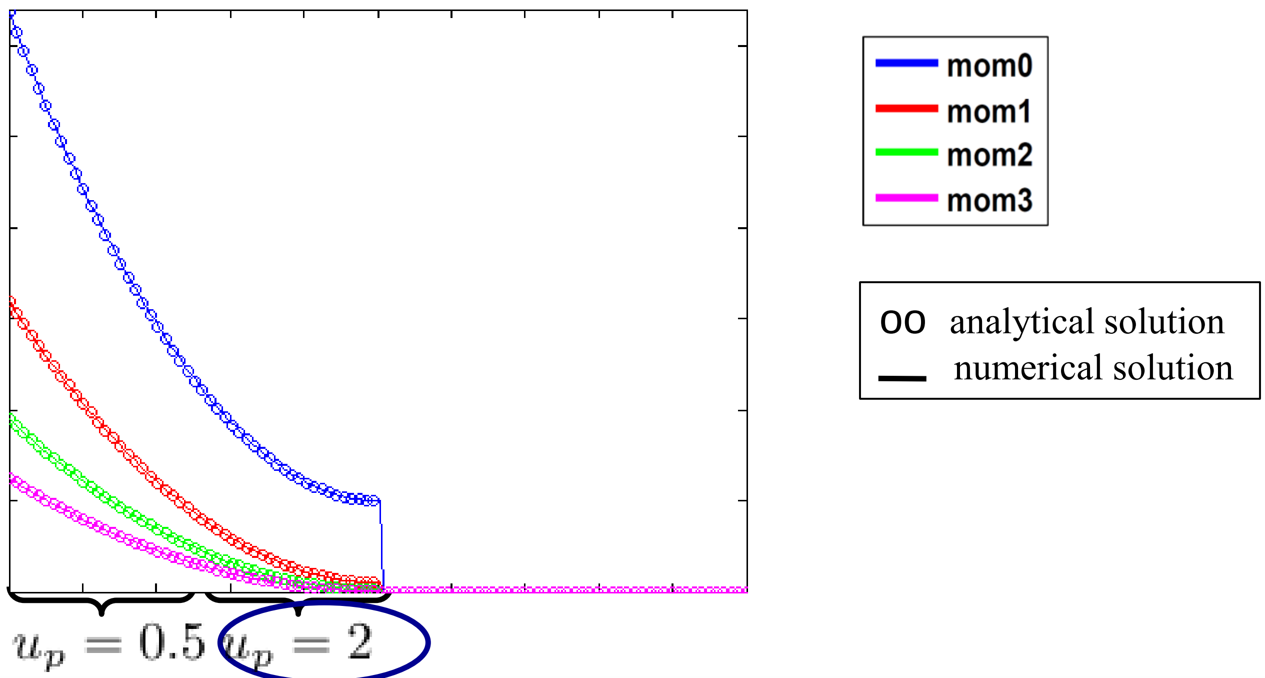


Interest of the test case

- Periodic boundary conditions
  - Cloud at $u_p = 2$ catches up the cloud at $u_p = 0.5$
    - Singularity formation

Evaluation of the EMVM model Quantitative validation

Validation of the evaporation and advection operator



Conclusion

- **Singularity (delta-shock) well captured**
- **Illustration of the monokinetic assumption limitation**

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
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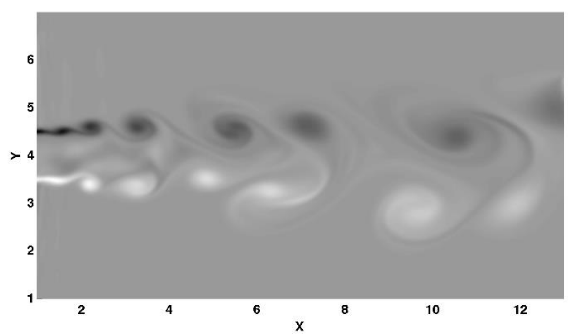
Comparison with the MF model
Free jet test case

Case run with Muses3D coupled with asphodele *(Reveillon 07)*

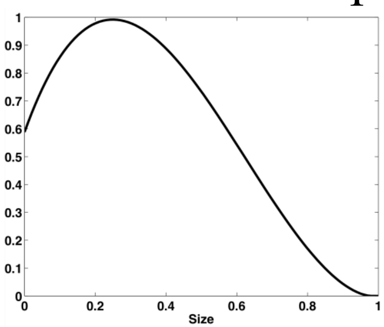
- Complex case: injected turbulence in the gas phase
- Comparison with the MF model, validated by comparison with a lagrangian model
- Time resolved dynamics
- One way coupling

Presentation of the configuration

- Gas vortices field at time t=20



- Size NDF for the droplet



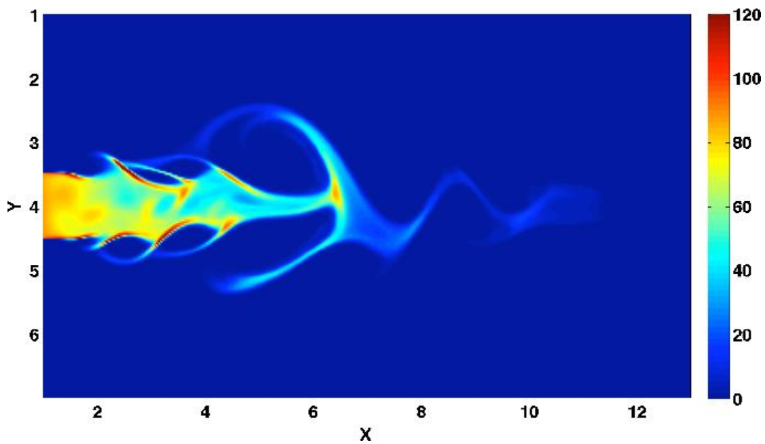
- $St_{max} = 0.75$
- Comparison of $m_{3/2}, Y_F$ (evaporated fuel mass fraction)

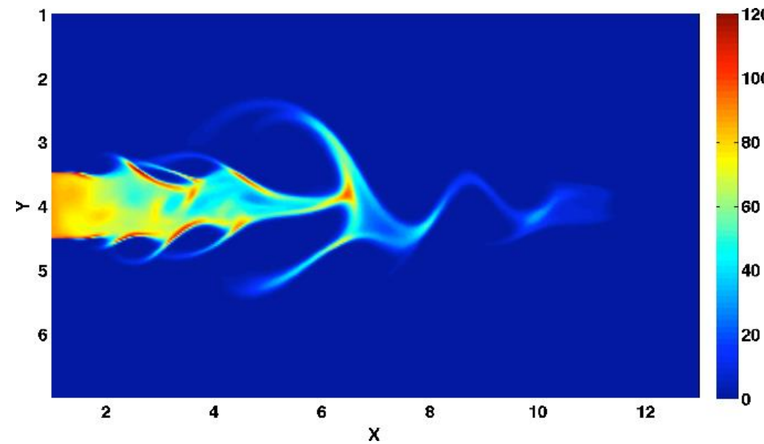
Comparison with the MF model
Free jet test case

Results at t =10

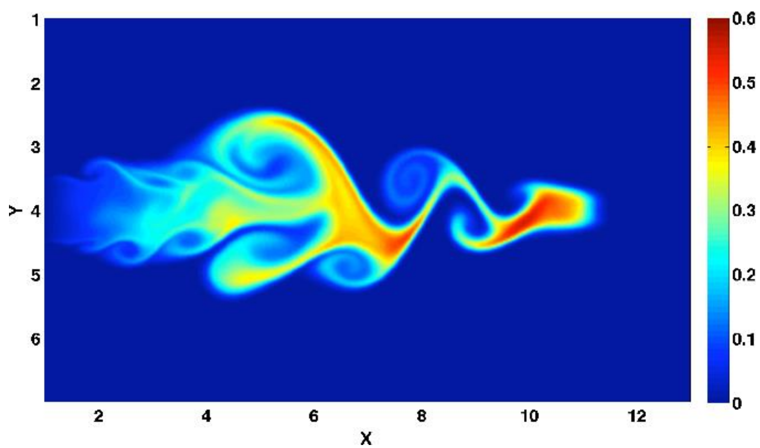
- EMSM model
- MF model

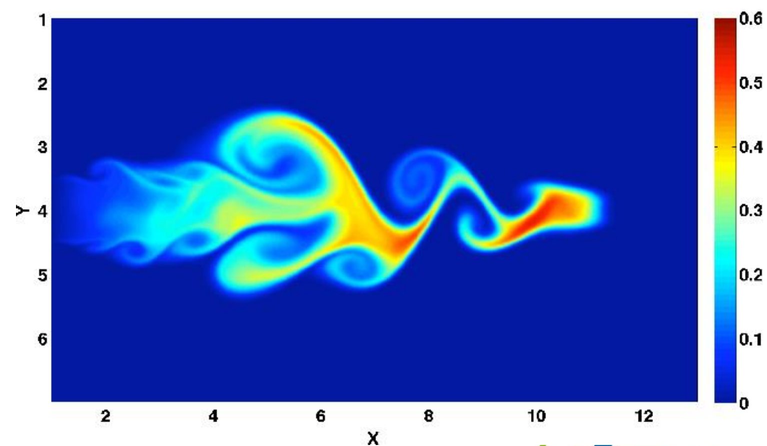
$m_{3/2}$





Y_F





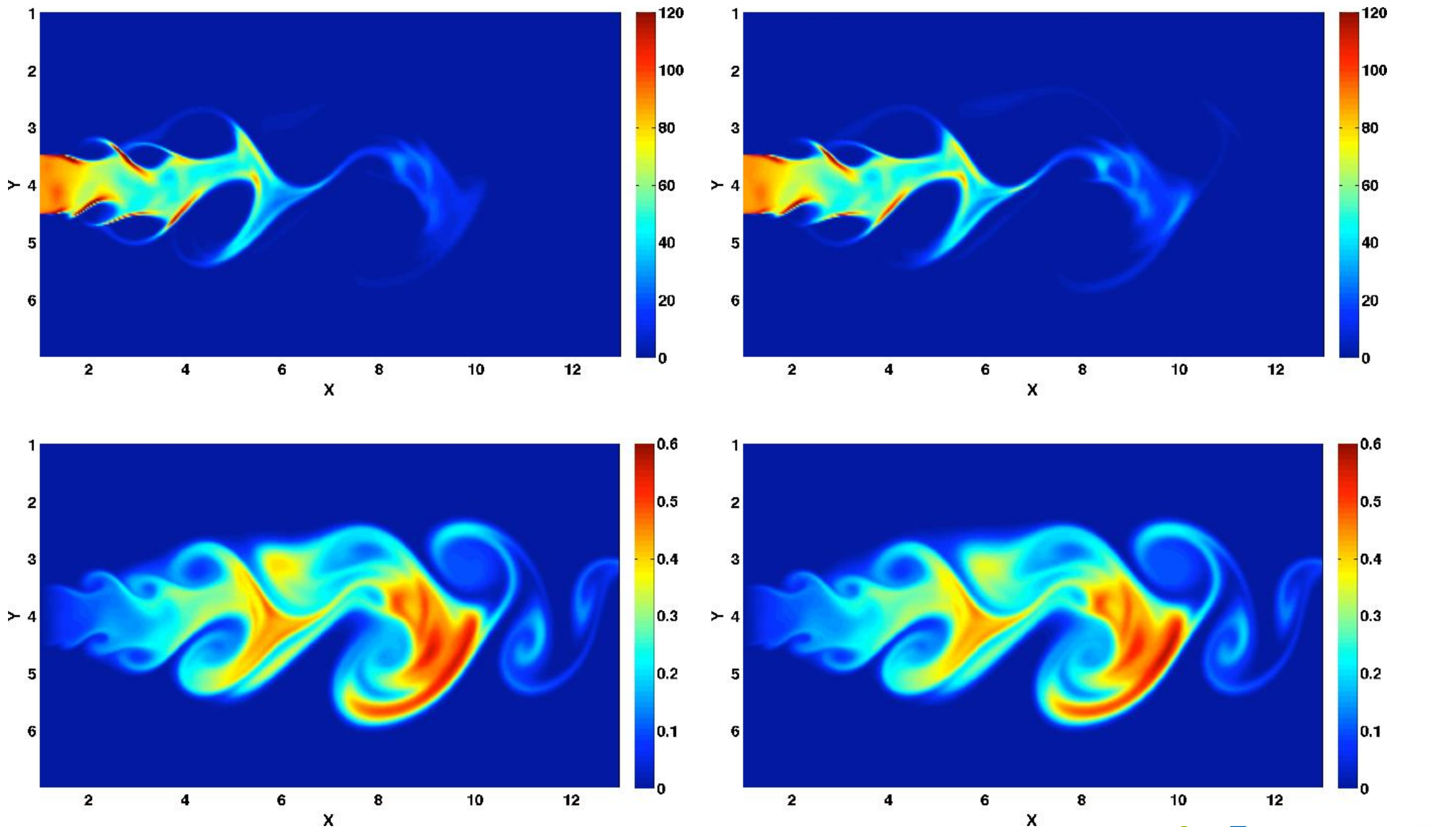
Comparison with the MF model
Free jet test case

Results at t =15

- EMSM model
- MF model

$m_{3/2}$

Y_F



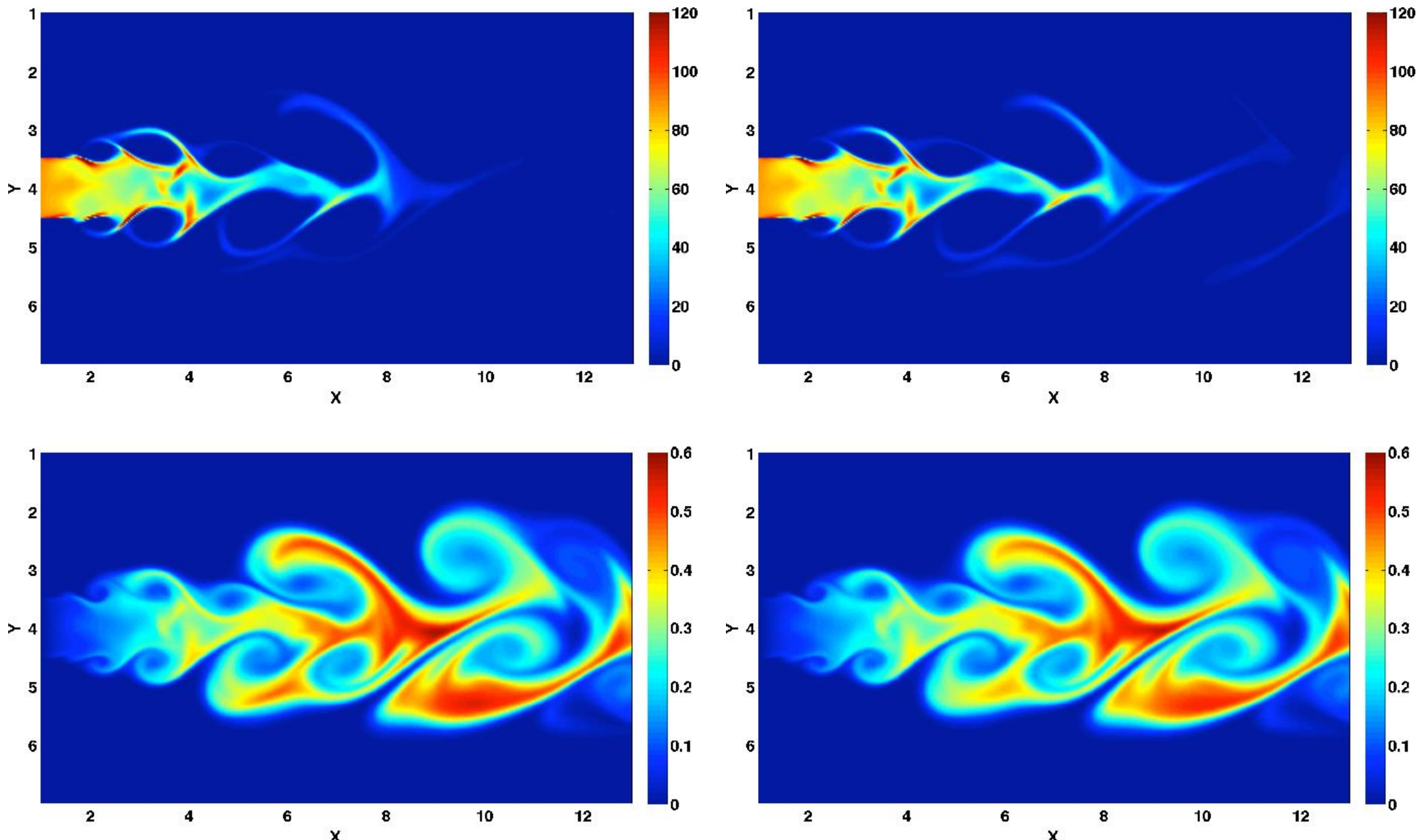
Comparison with the MF model
Free jet test case

Results at t =20

- EMSM model
- MF model

$m_{3/2}$

Y_F



Comparison with the MF model
Free jet test case

Conclusion

- Very good level of comparison
- Validates the EMSM model and numerical tools

Perspective

- Implementation in IFP-C3D

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution

- Evaluation of the EMSM model
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- Extension to IFP-C3D
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Adaptation to the ALE formalism
Presentation of the ALE formalism

Context

- IFP-C3D code: moving boundary conditions (moving piston)
- Description of motion in the context of continuum mechanics

  ⟺ Observation reference frame:
  - Eulerian formalism: fixed grid
  - Lagrangian formalism: the grid vertices follow the fluid

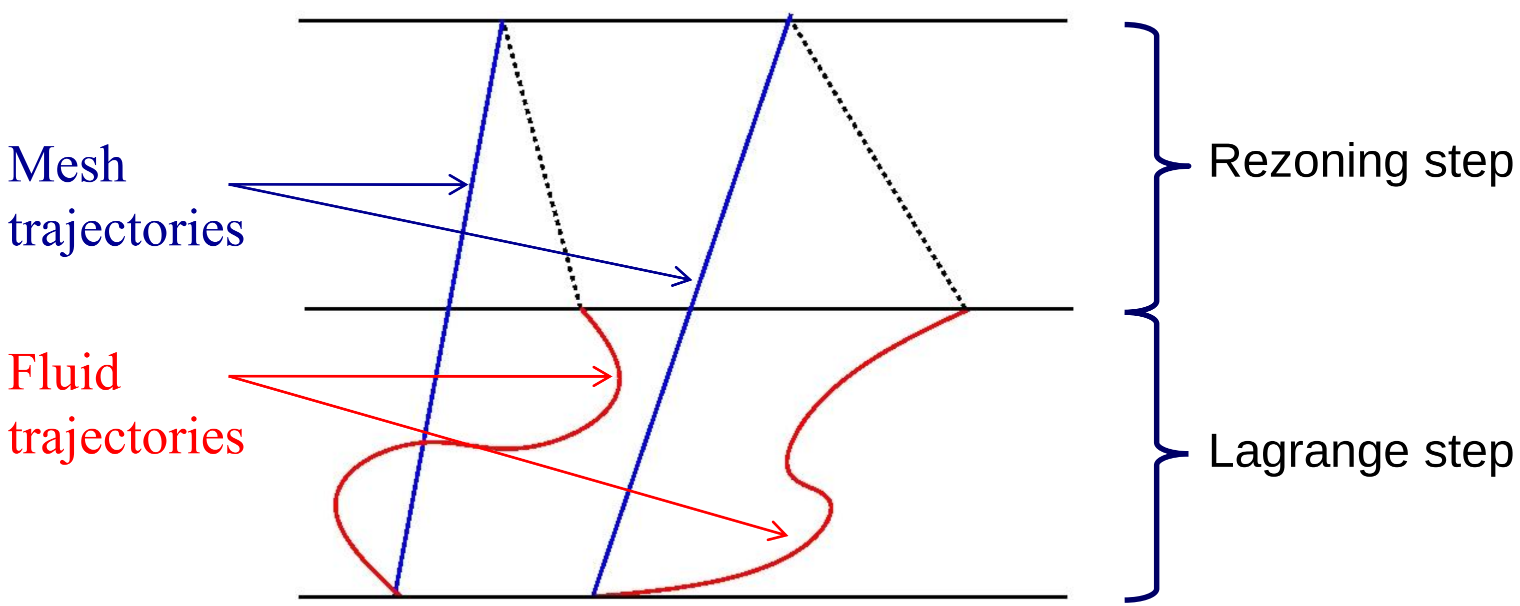
- But each of these representations has a difficulty
  - Eulerian: stable but diffusive
  - Lagrangian: accurate but unstable

Principle of the ALE formalism

- The **Arbitrary Lagrangian Eulerian (ALE)** formalism *(Hirt 71, Donea 04)* aims at combining the advantages of **stability** and **accuracy** of each of the Eulerian and Lagrangian representation, minimizing their drawback
- This formalism is used in IFP-C3D

Adaptation to the ALE formalism
General algorithm of IFP-C3D

- Operator splitting algorithm:
  - Phase A: source terms during Δt
  - Phase B: Lagrangian transport during Δt
  - Phase C: Eulerian advection “rezoning” during Δt



Adaptation to the ALE formalism Challenges and achievements

- Challenges a high order advection scheme on a 1D mesh:

  Realizability condition and Stability through PGD formalism

Realizability condition
• Adaptation of the kinetic scheme in the ALE formalism

Stability through PGD formalism

• Stability not guaranteed even for a 1st order scheme
• New advection scheme inspired from the ideas in *(Larrouturoux 04)*:
    • it ensures the conservation of the momentum
    • and the maximum principle on velocity

➡ **Second order in time and space on moving grids**

Topics discussed during this presentation

- EMSM model: Modeling and numerical tools
  - General resolution strategy
  - Evaporation term resolution
  - Advection term resolution

- Evaluation of the EMSM model
  - Quantitative validation
  - Comparison with the MF model

- Extension to IFP-C3D
  - Adaptation to the ALE formalism
  - Implementation in IFP-C3D and validation

Implementation of the EMSM model in IFP-C3D

Presentation of the IFP-C3D code

- Hexahedral unstructured solver devoted to internal CFD with spray and combustion modelling
- Conservation equations solved on moving grids
- Equations solved using a finite volume method extended with the ALE formalism. Implicit temporal integration scheme
- k-ε turbulence model (RANS)

Existing versions for multiphase flow resolution

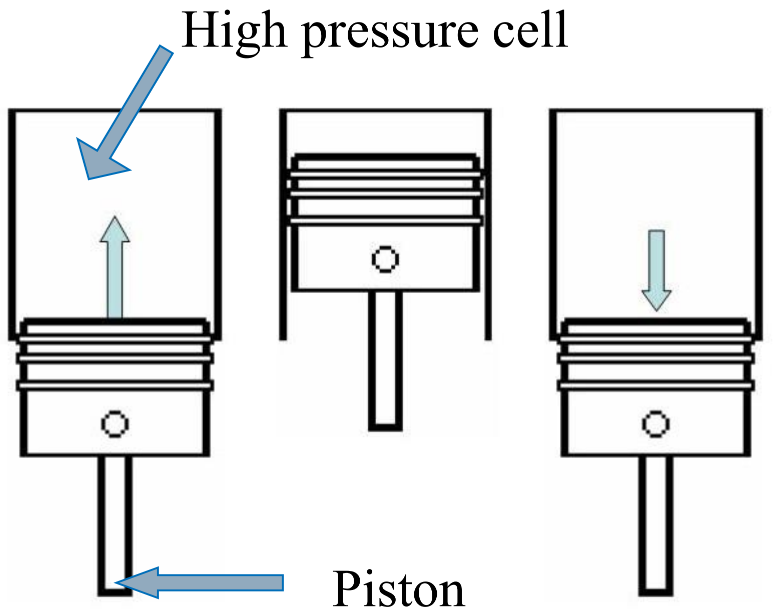
- Lagrangian solver for the spray
- Two-Fluid Eulerian solver

➡ **New code version with the EMSM model**

Implementation of the EMSM model in IFP-C3D Validations

Validation on a moving piston configuration

Piston movement



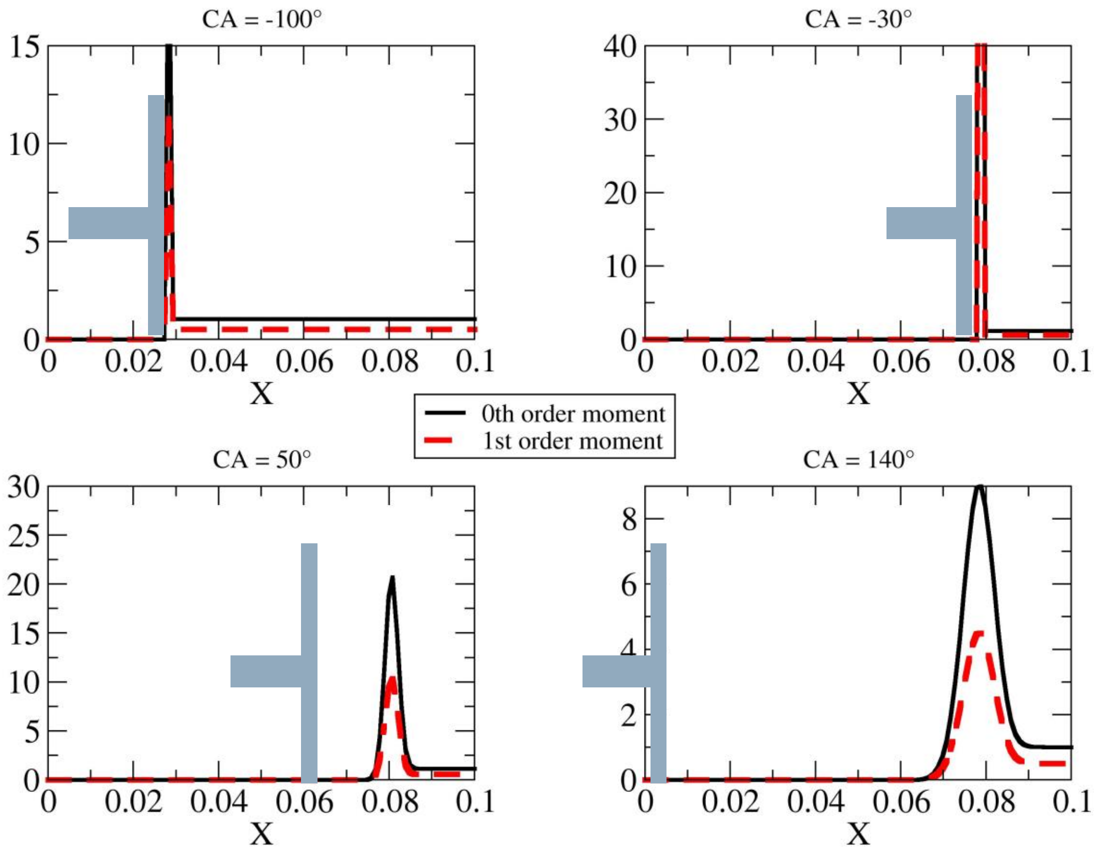
Crank Angle -180° 0° +180°

Computation parameters

- Size distribution

- Homogeneous field
- Initial velocity = 0
- Homothetic cell volume variation

Implementation of the EMSM model in IFP-C3D Validations

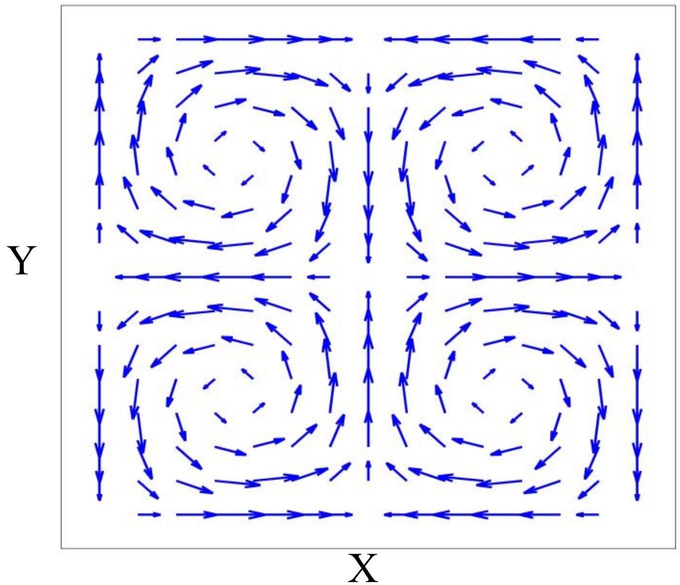


- Singularity dynamic preserved with piston boundary condition

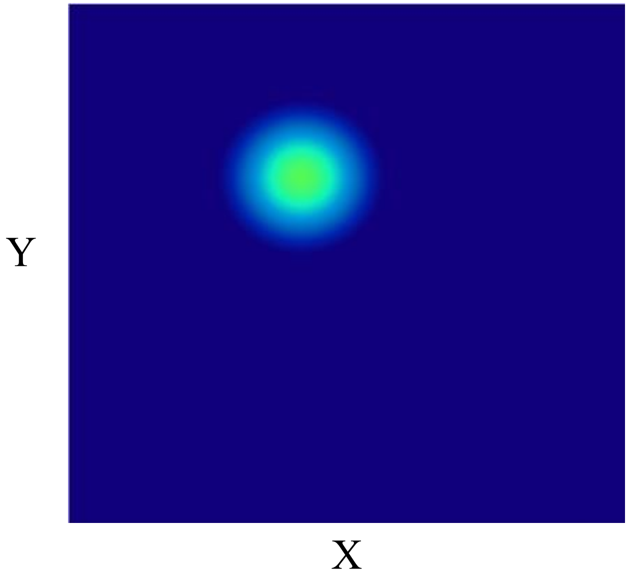
Implementation of the EMSM model in IFP-C3D Validations

2D test with evaporation and drag **compared with Muses3D**

Taylor-Green vortices for gas flow

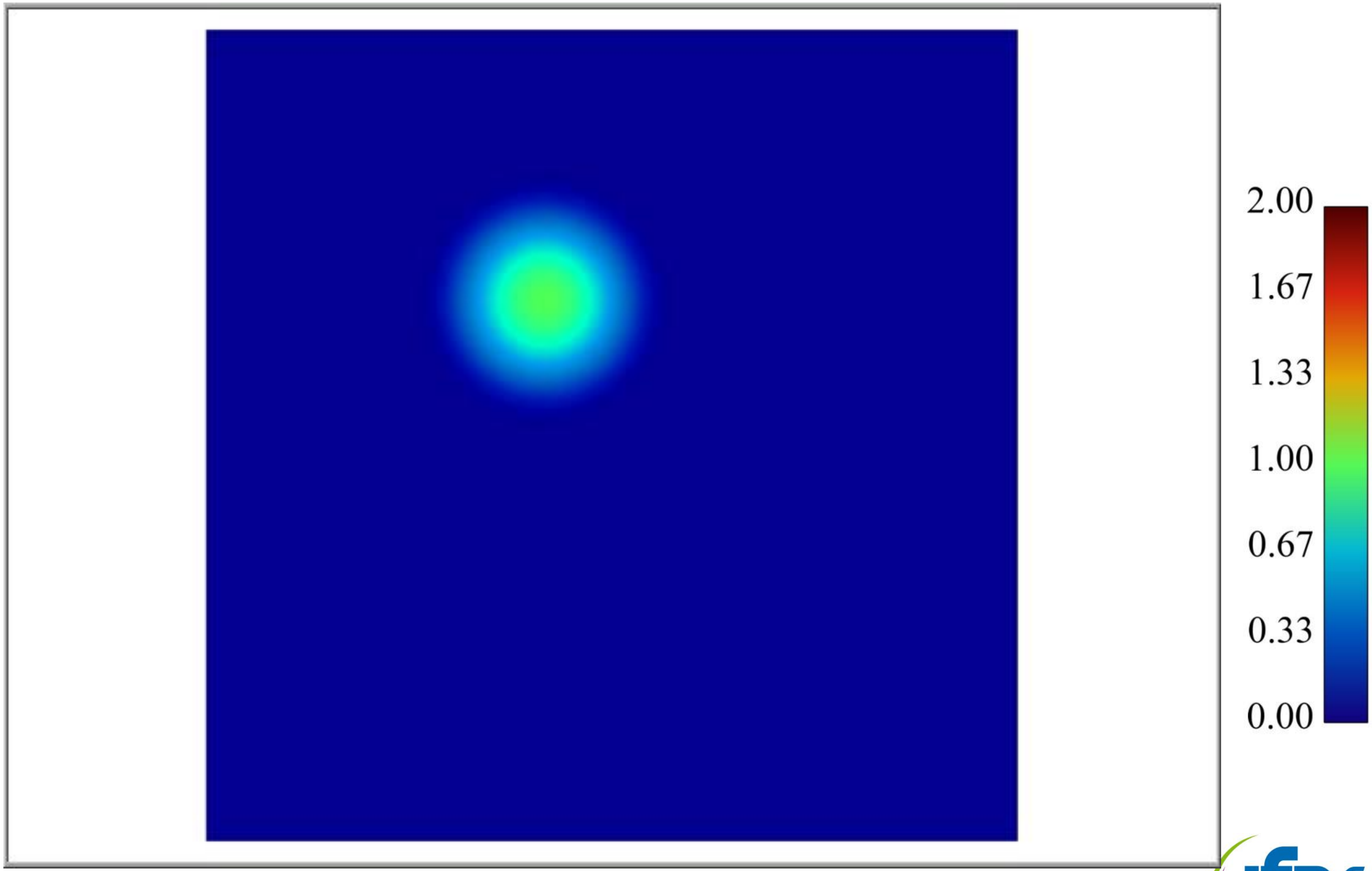


Initial condition for the spray



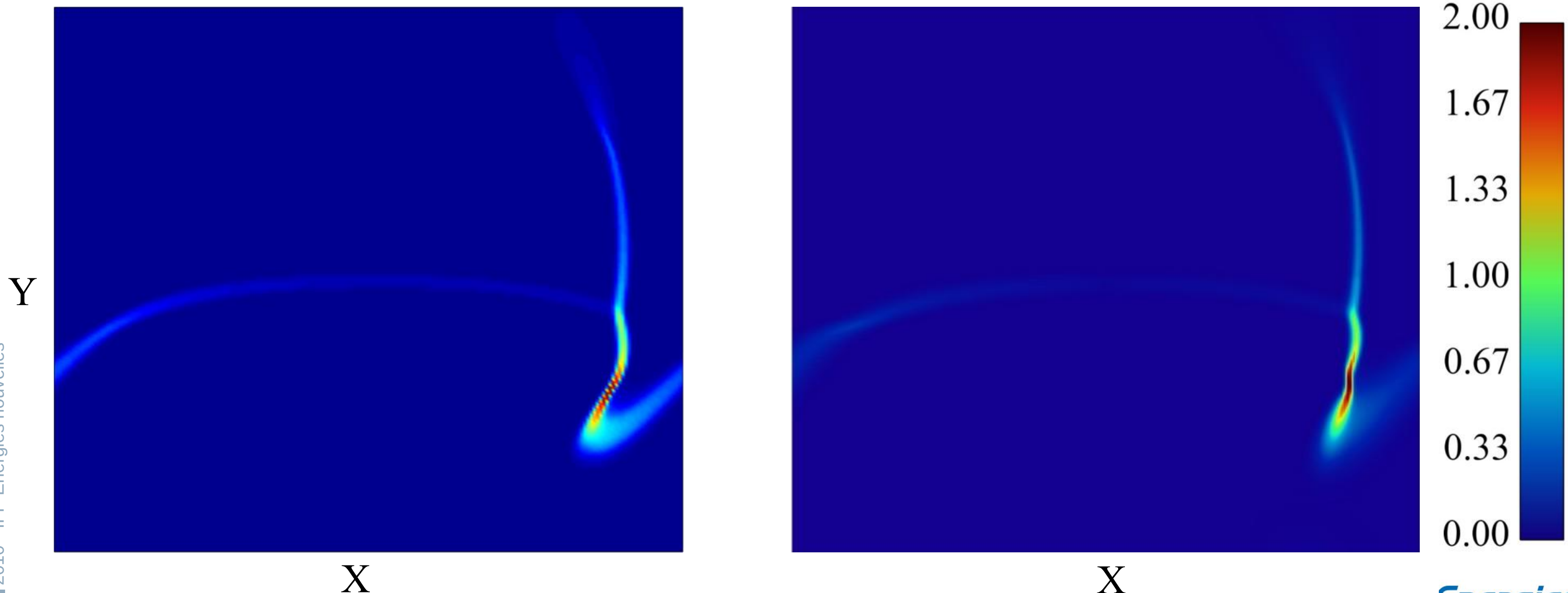
- Periodic Boundary conditions
- $\mathrm{St}_{max} = 2.81$
- Evaporation: $K = 0.21$
- Final time = 2

Implementation of the EMSM model in IFP-C3D Validations



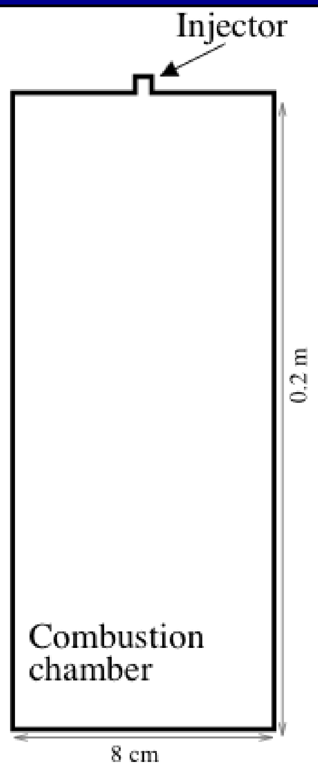
Implementation of the EMSM model in IFP-C3D Validations

- **Muses3D**
  - Structured
  - Eulerian
  - 2nd order
- **IFP-C3D**
  - Unstructured
  - ALE
  - 1st order



Implementation of the EMSM model in IFP-C3D
Injection cases

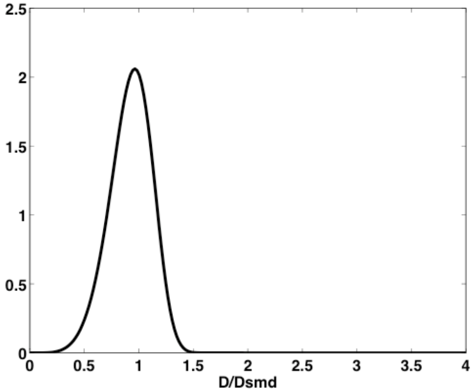
Domain



- axi-cylindric configuration
- 200×80 cells

Initial and injection conditions

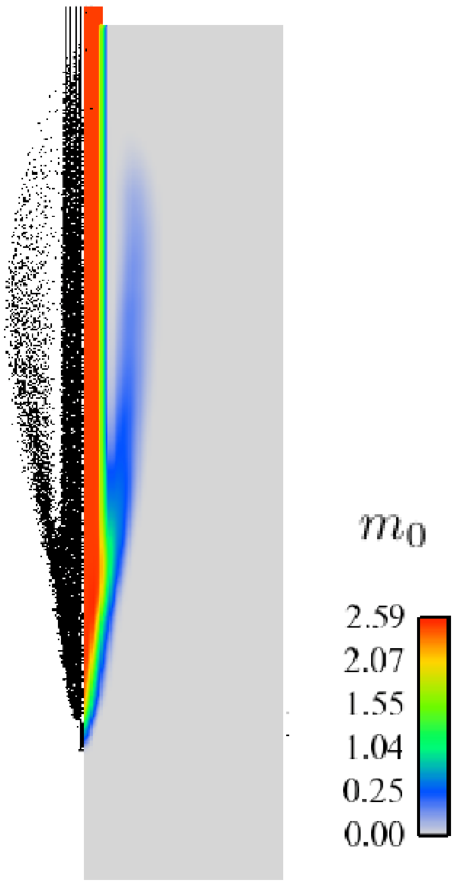
- Gas
  Initial: $P = 1bar, T = 293K, u_g = 0ms^{-1}$
  Injection: $P = 1bar, T = 293K, u_g = 18ms^{-1}$
- Spray
  Initial: vacuum
  Injection: $u_p = 18ms^{-1}, \alpha = 1.12.10^{-3}$
- Size distribution: Rosin-Rammler



Implementation of the EMSM model in IFP-C3D Injection cases

Comparison to Lagrangian results

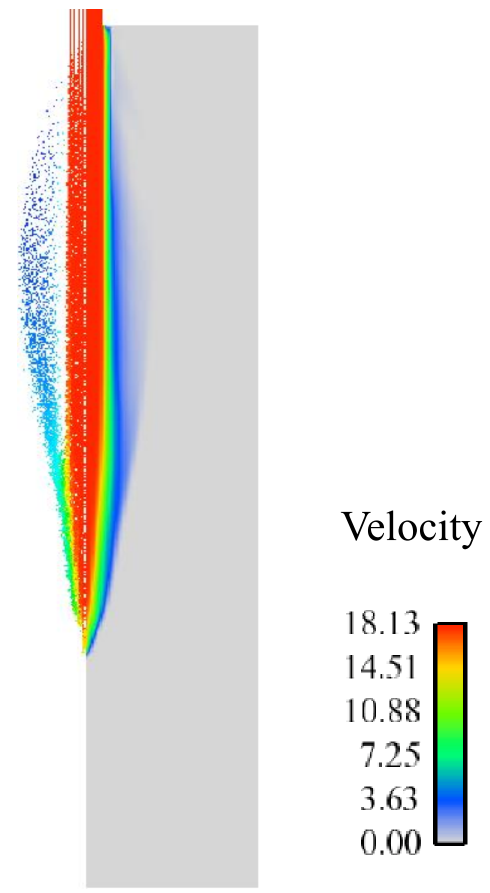
Particle number



Parameters

- Lagrangian (left)
- Eulerian (right)
- Two-way coupling (lagrangian)
- t=10^{-2} s
- $smd = 20\mu m$

Velocity field



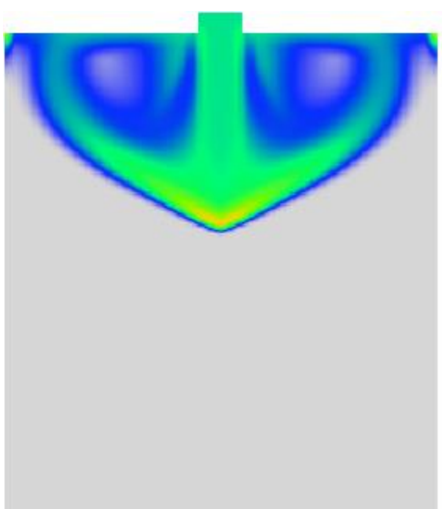
Implementation of the EMSM model in IFP-C3D
Injection cases

Eulerian evaporating spray

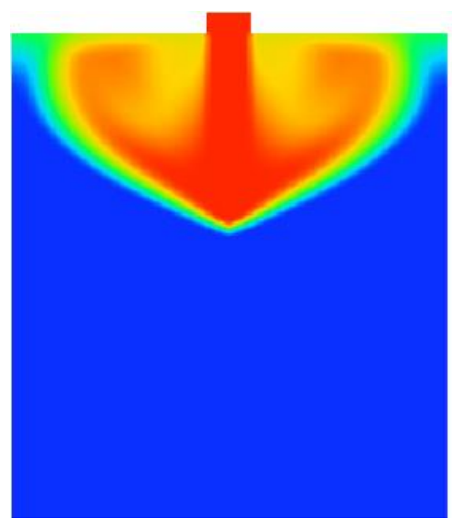
Parameters

- One-way coupling
- $t=10^{-2}$ s
- $smd = 5\mu m$

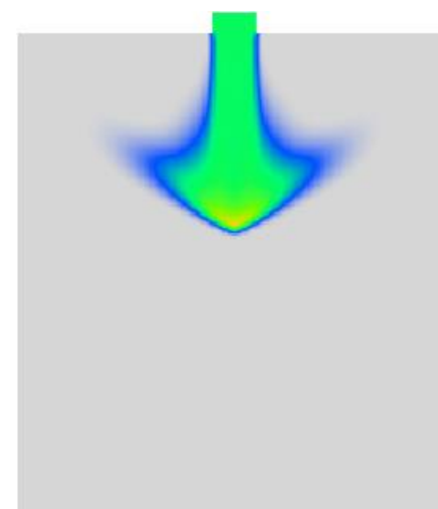
Non Evaporating case



Non Evaporating case



Evaporating case



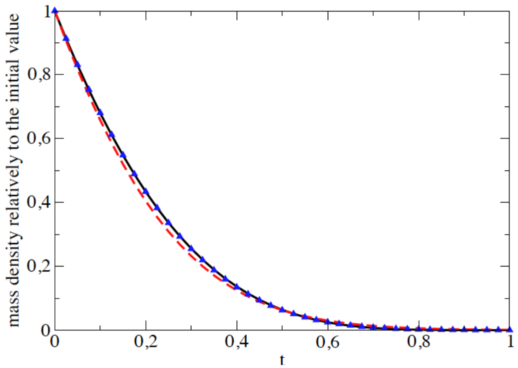
Conclusions and Perspectives

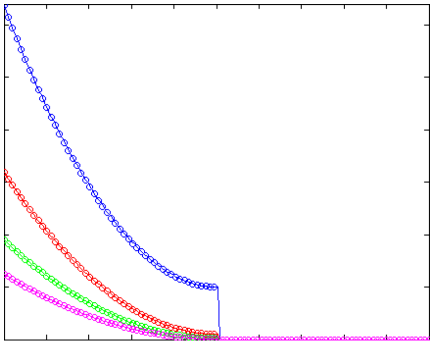
Achievements of the PhD

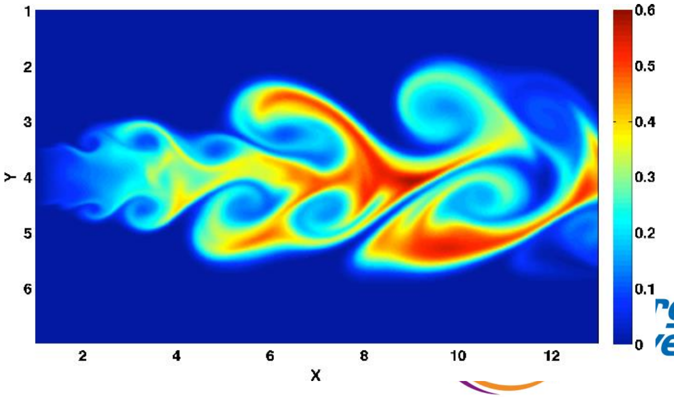
- Description of polydispersity:

  Eulerian Multi-Size Moment (EMSM) model

Development of the EMSM model and numerical tools
• Evaporation ➡ EMSM model with 1 section as accurate as MF model with 10 sections • Advection of a moment set ➡ High order scheme enforcing the Realizability condition and Pressureless Gas Dynamics • Validation of the EMSM model ➡ Implementation in the Muses3D code Comparison with the MF model





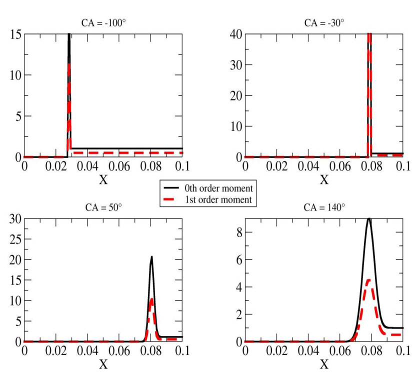


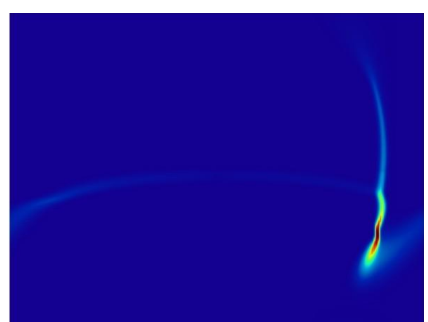
Achievements of the PhD

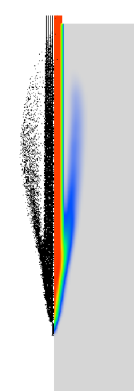
- Description of polydispersity:

  Eulerian Multi-Size Moment (EMSM) model

Extension to an industrial context
• Adaptation of the designed schemes to the ALE formalism ➡ High order advection scheme in ALE formalism • Implementation of the EMSM model in IFP-C3D and validation ➡ Validation with moving grid Taylor-Green computation compared with Muses3D Jet computation compared with Lagrangian: spray injection demonstrated







Achievements of the PhD

- Description of particle trajectory crossing

  Eulerian Multi-Velocity Moment (EMVM) model

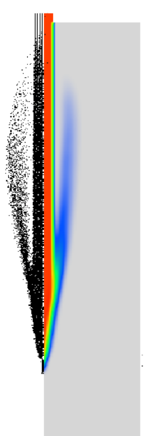
Development of the EMVM model and numerical tools
• 1D problem: Mathematical study of the closed system in order to prepare the design of high order advection schemes: • Multi-D problem: study on closure of the ill-posed problem and evaluation of the EMVM model ➡ Implementation of the EMVM and EMFVM model in Muses3D Validation by comparison with Lagrangian results

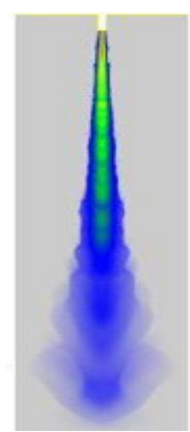
Perspectives
Short term

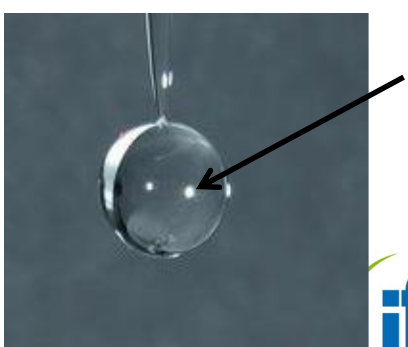
- Conclude the validation process on injection with a real injection case, and with the exact same framework for both the Eulerian and Lagrangian model

- Extend the implementation of the EMSM model in IFP-C3D to turbulence modeling with RANS formalism

- Study the relevance to consider compressible droplets, in the perspective to couple the EMSM model to the compressible two-fluid model for separate phase flow



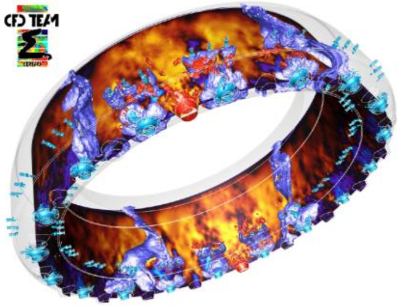




Pressure ?

Perspectives
Spray models

- Extend the Eulerian spray models discussed in this PhD to a two-way coupling formalism *(Doisneau, PhD)*
- For the EMSM model, to be able to describe size/velocity correlation using only one section *(Vié)*
- Consider turbulence modeling in LES framework, and going beyond the monokinetic assumption *(Boileau)*



- EMVM model
  - Design, on the basis of the study done in *(CMS 10)*, high order advection schemes
  - Continue the initiated research work on an optimized closure in multi-dimensional configurations: CQMOM *(Yuan, 10)*
  - Consider turbulence modeling in LES framework *(Chalons, 10)*

Perspectives
Long term perspective

- Research on high order kinetic schemes for advection problems on unstructured grids

- Couple the EMSM model with the Eulerian two-fluid model for the separate phase