Eulerian high order moment models for polydisperse evaporating sprays

D. Kah*, M. Massot, F. Laurent, S. Jay*

Q. H. Tran*, S. de Chaisemartin*, L. Fréret[1]

Laboratoire EM2C - UPR CNRS 288 - Ecole Centrale Paris

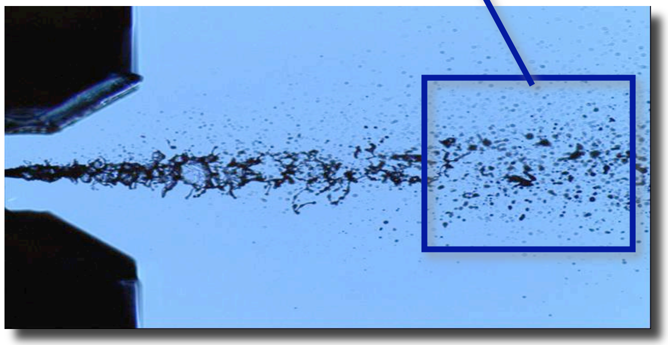
*IFP Energies nouvelles

[1] Université Pierre et Marie Currie

Context

- Sprays in internal combustion engines
- Numerical simulation of reactive multiphase flow

Dispersed liquid phase
Large size spectrum



(Source C. Dumouchel, CORIA Rouen)

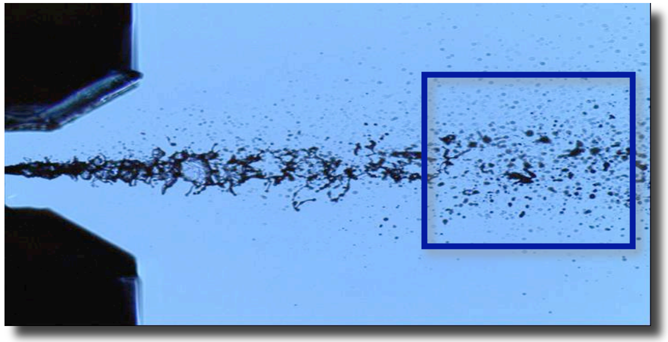
(Source Prof. Edwards, Stanford)

Accurately predict fuel fraction in gas before combustion

CENTRALE PARIS
CNRS
IFP Energies nouvelles

Context: Modeling

- **Droplet - gas interactions**
  → evaporation, drag and heat transfer
- **Droplet - droplet interactions**
  → coalescence, break-up, …



(Source C. Dumouchel, CORIA Rouen)

(Source Prof. Edwards, Stanford)

Key parameter : size
Description of polydispersity

Context: Modeling

Kinetic model

- $f(t, \boldsymbol{x}, S, \boldsymbol{u}, T)$: number density function
- Williams-Boltzmann equation

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

Resolution framework of the PhD

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

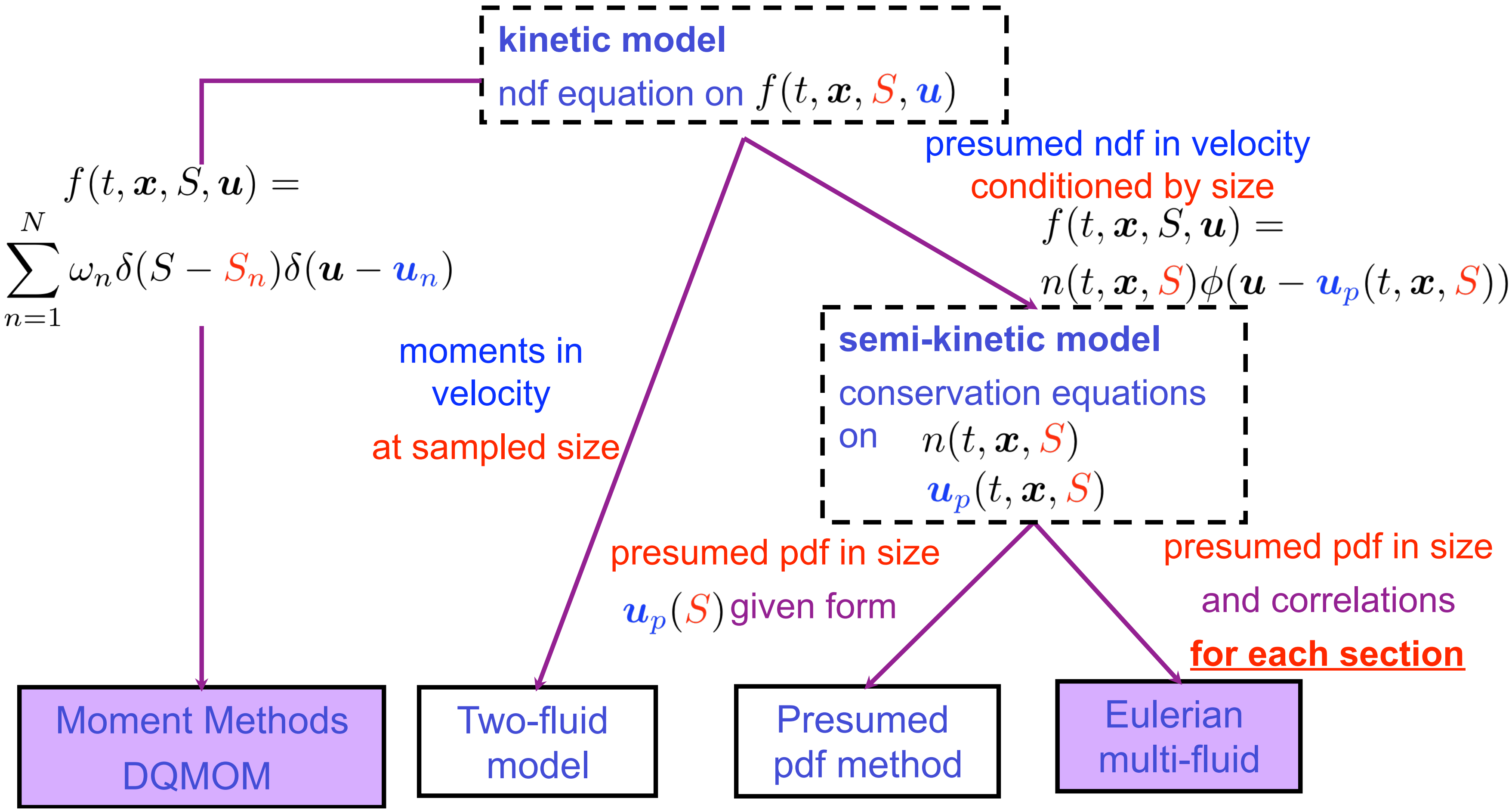
$$\partial_t f + \underbrace{\nabla_{\boldsymbol{x}} (\boldsymbol{u} f)}_{\text{advection}} + \underbrace{\partial_S (K f)}_{\text{evaporation}} + \underbrace{\nabla_{\boldsymbol{u}} (\boldsymbol{D}_{\mathrm{r}} f)}_{\text{drag}} = 0$$

- Dimensionless quantities, $S \in [0, 1]$; d^2 law, $K = constant$; One way coupling

Eulerian resolution: Resolution of moments of f

- Definition of moments: $$\mathcal{M}_{k,\boldsymbol{l}} = \int_0^1 \int_{\mathbb{R}} S^k \boldsymbol{u}^{\boldsymbol{l}} f \, \mathrm{d}\boldsymbol{u} \mathrm{d}S$$
- Size moments: $m_k = \mathcal{M}_{k,\boldsymbol{0}}$
- Velocity moments: $M_{\boldsymbol{l}} = \mathcal{M}_{0,\boldsymbol{l}}$, Mean droplet velocity: $\boldsymbol{u}_p = \dfrac{\mathcal{M}_{0,\boldsymbol{1}}}{\mathcal{M}_{0,\boldsymbol{0}}}$

Modeling: Resolution strategies in Eulerian framework

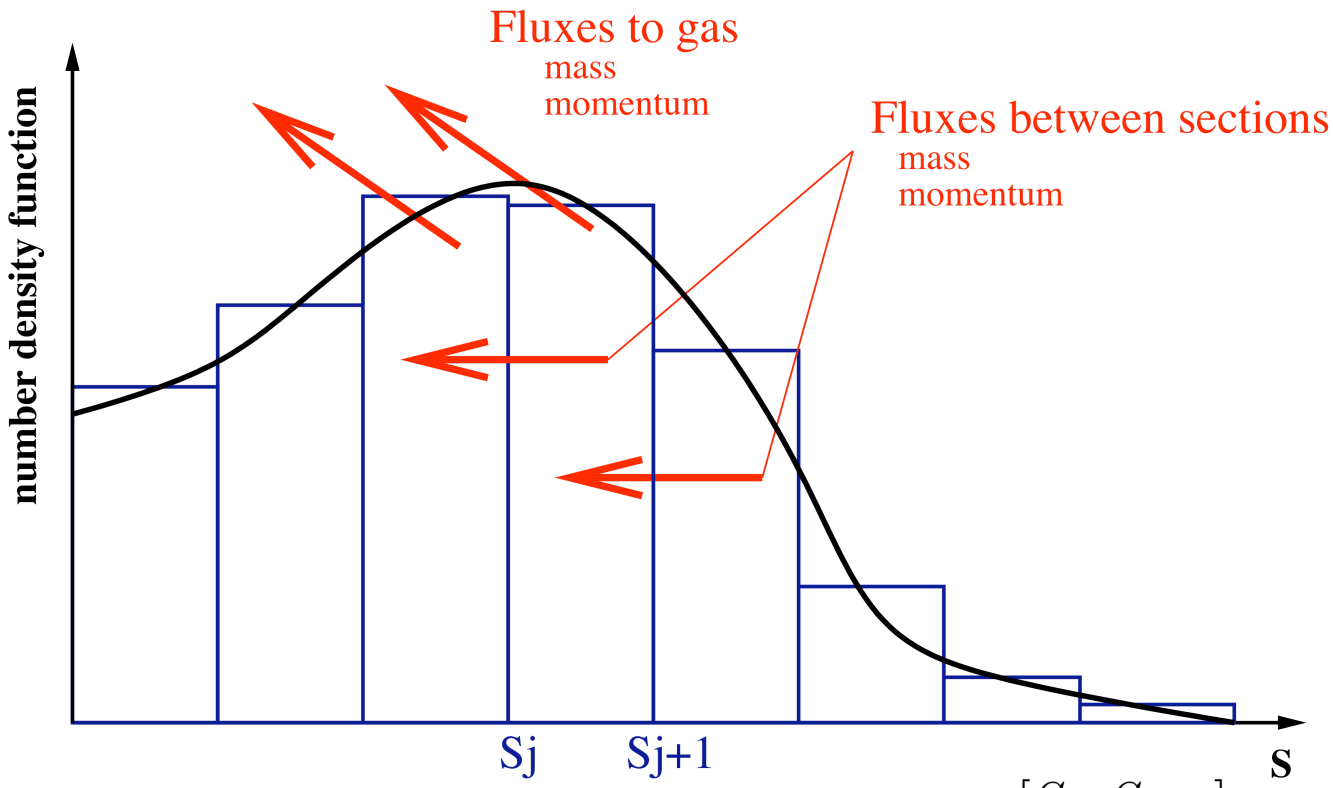


(Marchisio et al., 05; Fox et al., JCP 08)

(Mossa, 05)

(Massot and Laurent, 01; de Chaisemartin 09)

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 and momentum $m_{3/2,j}$, $m_{3/2,j}\boldsymbol{u}_{p,j}$ (monokinetic assumption in a section)
- For the evaporation process, the section quantities are impacted by fluxes from adjacent sections

Multi-Fluid model: Limitations

- Discretization in the size phase is first order accurate *(Laurent 2006)*

  Important computational cost, prohibitive for an industrial application

  Aim: Increase the number of size moments: Eulerian Multi-Size Moment (EMSM) model

  ➡ Decrease the number of section (**Up to ONE**)

  Difficulties:

  - Mathematics: closure problems
  - Scheme: stable and accurate numerical scheme

- Unable to describe Particle Trajectory Crossing (PTC) for high Knudsen number flow

  Equivalent to Pressureless Gas Dynamics (PGD) *(Bouchut 1994)*

Outline of the presentation

- EMSM model: General resolution strategy
- Evaporation term resolution
- Advection term resolution

EMSM model: General resolution strategy

Basis kinetic equation

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

Expression of the NDF

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

Monokinetic assumption

Quantities resolved

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

$$\boldsymbol{u}_p = \frac{\mathcal{M}_{0,\boldsymbol{1}}}{\mathcal{M}_{0,\boldsymbol{0}}}$$

EMSM model: General resolution strategy

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

↓ Velocity moments of order 0 and 1: $\int_{\mathbb{R}} \boldsymbol{u}^{\boldsymbol{l}} f \, \mathrm{d}\boldsymbol{u}$

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

Velocity moments **conditioned by size**

↓ 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: General resolution strategy

Moment equation system

We aim to solve the following system:

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

$$\vdots$$

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

$$\partial_t m_1 \boldsymbol{u}_p + \underbrace{\nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p)}_{\text{advection}} = \underbrace{-Km_0 \boldsymbol{u}_p}_{\text{evaporation}} - \nabla_{\boldsymbol{x}} P + \underbrace{\boldsymbol{D}}_{\text{drag}}$$

EMSM model: General resolution strategy

Moment equation system

We aim to solve the following system:

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

$$\vdots$$

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

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

Unclosed terms

$f(t, \boldsymbol{x}, S, \boldsymbol{u}) = n(t, \boldsymbol{x}, S)\delta(\boldsymbol{u} - \boldsymbol{u}_p)$ ➡ $P = 0$ (velocity dispersion)

$n(t, \boldsymbol{x}, S = 0) = \Phi(m_0, ..., m_N)(t, \boldsymbol{x})$ pointwise value of the size NDF

EMSM model: General resolution strategy

- Operator splitting strategy *(Descombes and Massot 04)*

  to treat each operator with a dedicated scheme: limit diffusion
- Successive resolution of
  - **Evaporation**
  - Advection
  - Drag

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

$$\vdots$$

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

$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = -Km_0 \boldsymbol{u}_p + \boldsymbol{D}$$

EMSM model: General resolution strategy

- Operator splitting strategy *(Descombes and Massot 04)*
  to treat each operator with a dedicated scheme: limit diffusion
- Successive resolution of
  - Evaporation
  - **Advection**
  - Drag

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

$$\vdots$$

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

$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = -K m_0 \boldsymbol{u}_p + \boldsymbol{D}$$

EMSM model: General resolution strategy

- Operator splitting strategy *(Descombes and Massot 04)* to treat each operator with a dedicated scheme: limit diffusion
- Successive resolution of
  - Evaporation
  - Advection
  - **Drag**

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

$$\vdots$$

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

$$\partial_t m_1 \boldsymbol{u}_p + \nabla_{\boldsymbol{x}}(m_1 \boldsymbol{u}_p \otimes \boldsymbol{u}_p) = -K m_0 \boldsymbol{u}_p + \boldsymbol{D}$$

Outline of the presentation

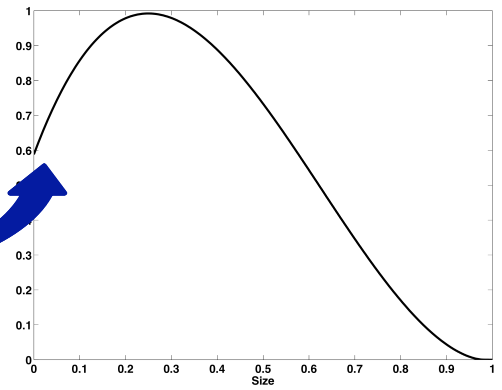
- EMSM model: General resolution strategy
- Evaporation term resolution
- Advection term resolution

EMSM model: Evaporation Model

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:

Realizability condition

EMSM model: Evaporation Model

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

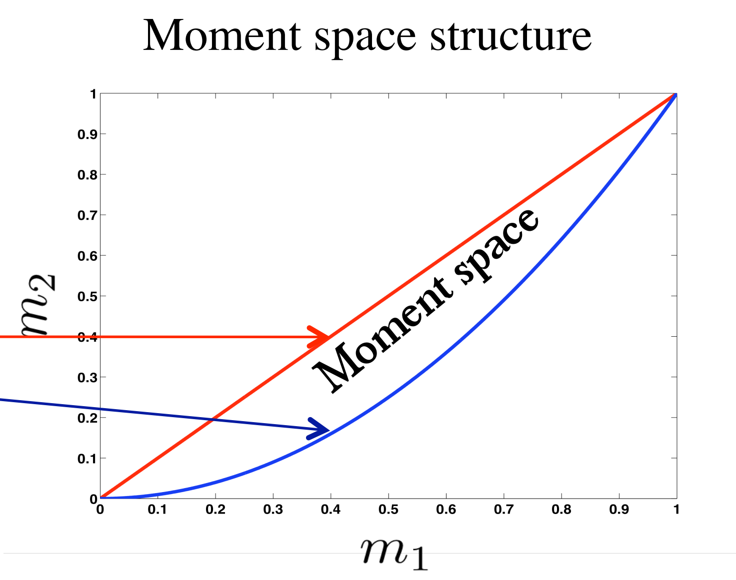
Example of moment space geometry

- Set of PDF such as $m_0 = \int_0^1 n \, \mathrm{d}S = 1$, on [0,1]
- Condition on m_1 and m_2

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

$$m_2 = \int_0^1 S^2 \, n \, \mathrm{d}S, \quad m_1^2 < m_2 < m_1$$

low border (m_1^2), high border (m_1)

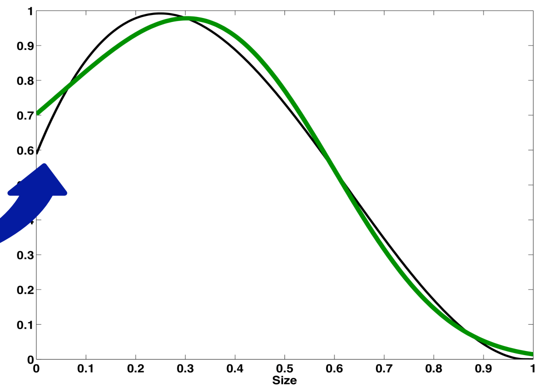


EMSM model: Evaporation Model

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

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



- 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: Evaporation Model

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
- Moment update using DQMOM

} *(Massot et al. SIAM 2010)*

Principle of a kinetic scheme

Flux computation lies on the equivalence between the two descriptions:

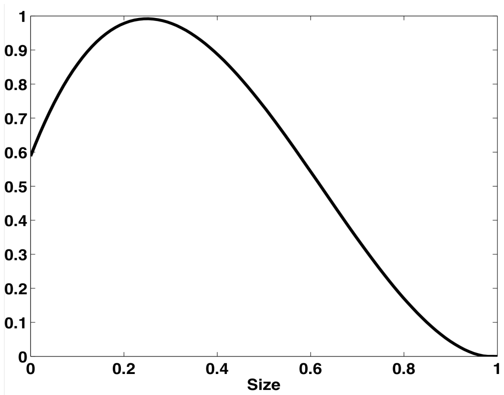
- Kinetic: $\partial_t n - \partial_S (K\, n) = 0$
- Macroscopic: $\mathrm{d}_t \boldsymbol{m}_N = -\mathbf{A}\, \boldsymbol{m}_N - \boldsymbol{\phi}_-$

CENTRALE PARIS · CNRS · IFP Energies nouvelles

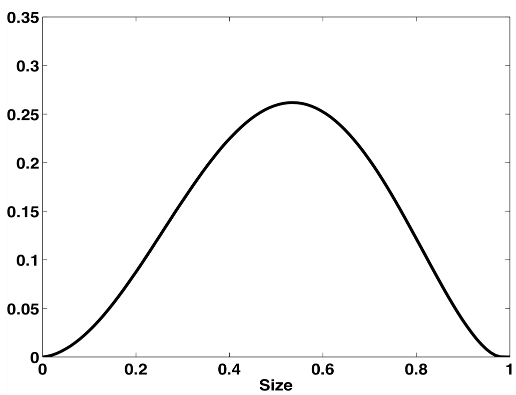
EMSM model: Evaporation Validation

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

Number density



Mass density

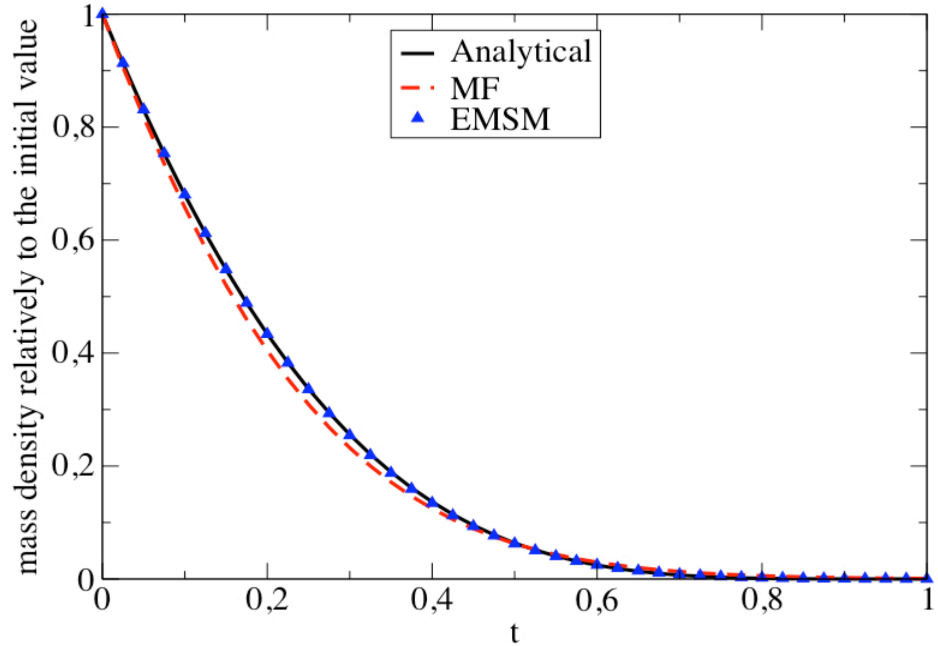


Comparison between EMSM and MF models

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

EMSM model: Evaporation Validation

Results



- Very good level of comparison
- **EMSM with 1 section more precise than MF with 10 sections**

Outline of the presentation

- EMSM model: General resolution strategy
- Evaporation term resolution
- Advection term resolution

EMSM model: 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:

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

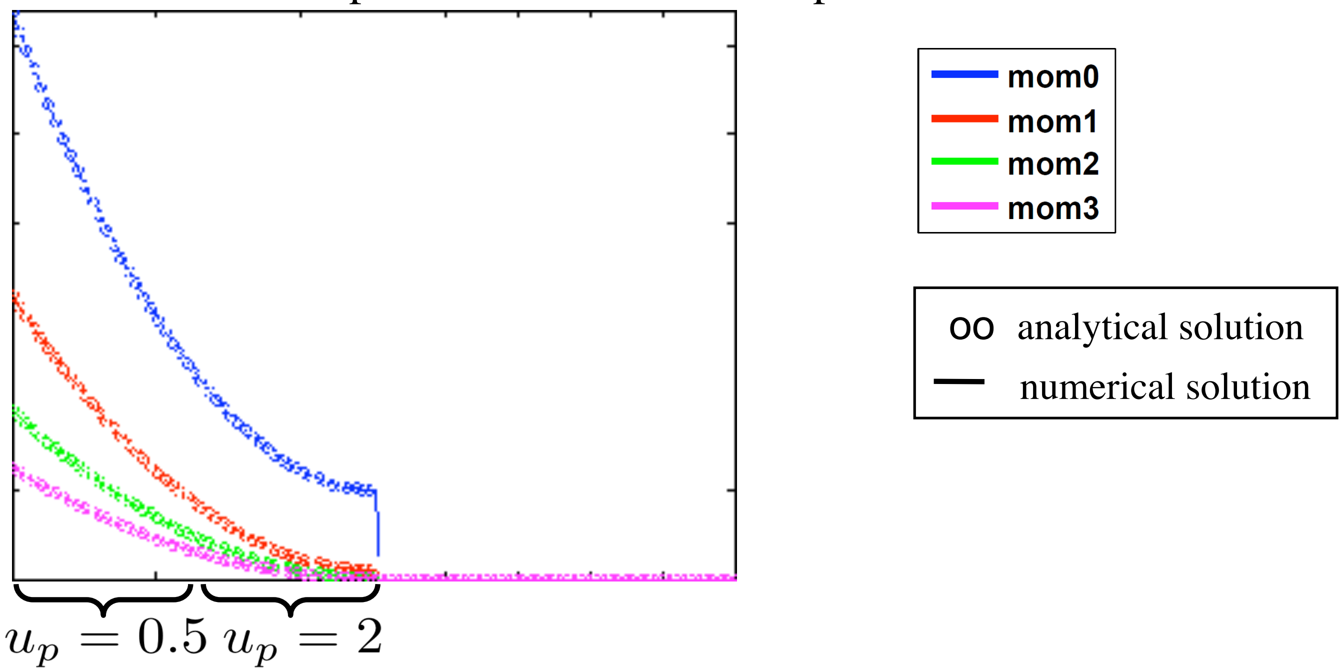
Challenges

- Pressureless gas dynamics (PGD)– delta choc, vacuum zones
  - Dedicated scheme designed in *(de Chaisemartin, PhD 09)* from the kinetic scheme *(Perthame 02, Bouchut 03)* and using dimensional splitting
- **Realizability condition**
  - Reconstruction of quantities given by the Canonical Moment Therory *(Dette and Studden, 1997)*

(Kah et al. 2011)

EMSM model : Quantitative validation

Validation of the evaporation and advection operator

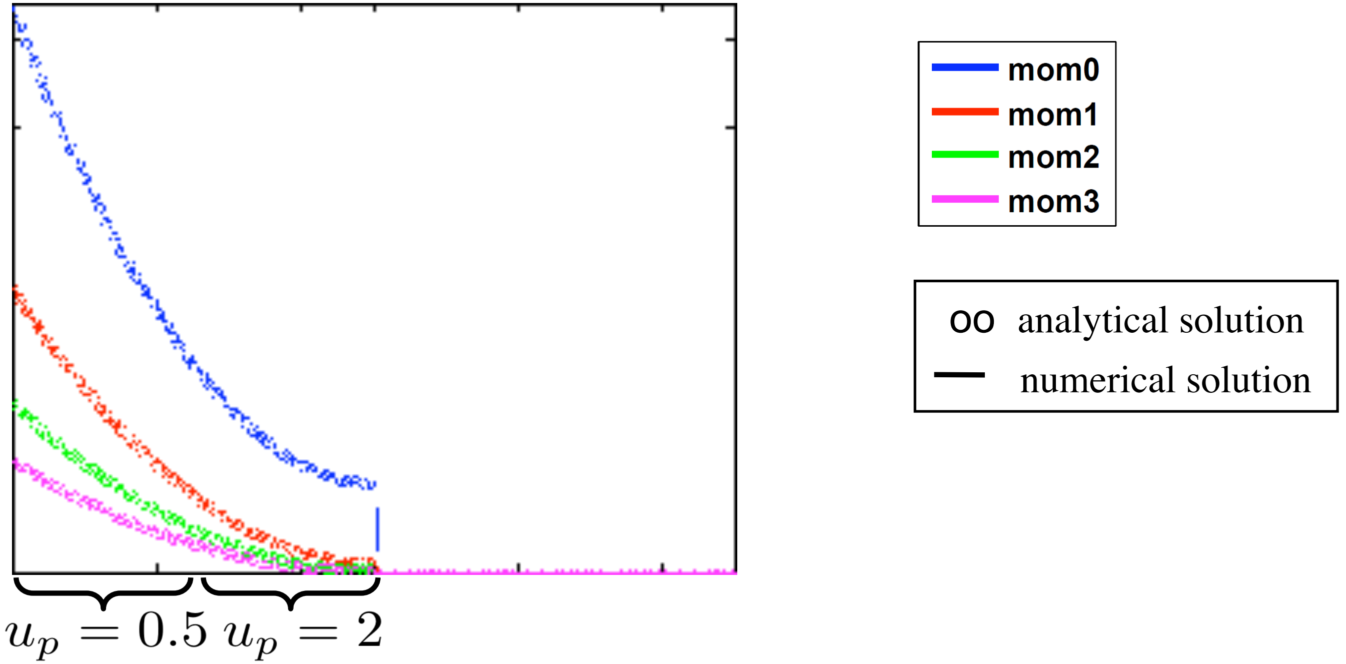


Interest of the test case

- Velocity discontinuity → Creation of Vacuum zone
- Periodic boundary conditions → Singularity formation
- Inhomogeneous size NDF profile → Reconstruction with non null slope

EMSM model : Quantitative validation

Validation of the evaporation and advection operator



Conclusion

- **Very good level of comparison with the analytical solution**
- **Vacuum zone well described- Singularity (delta-shock) well captured**
- **Illustration of the monokinetic assumption limitation**

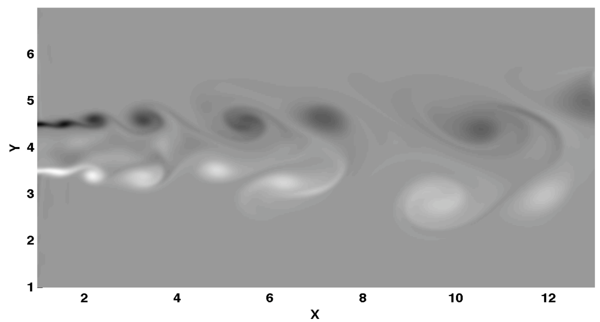
Comparison with the MF model : Free jet test case

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

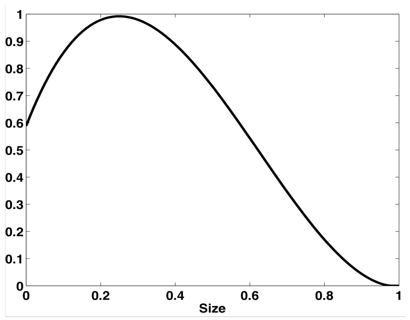
- Complex case: injected turbulence in the gas phase
- Time resolved dynamics, compared to the MF model

Presentation of the configuration

- Gas vortices field at time t=20



- Size NDF for the droplet



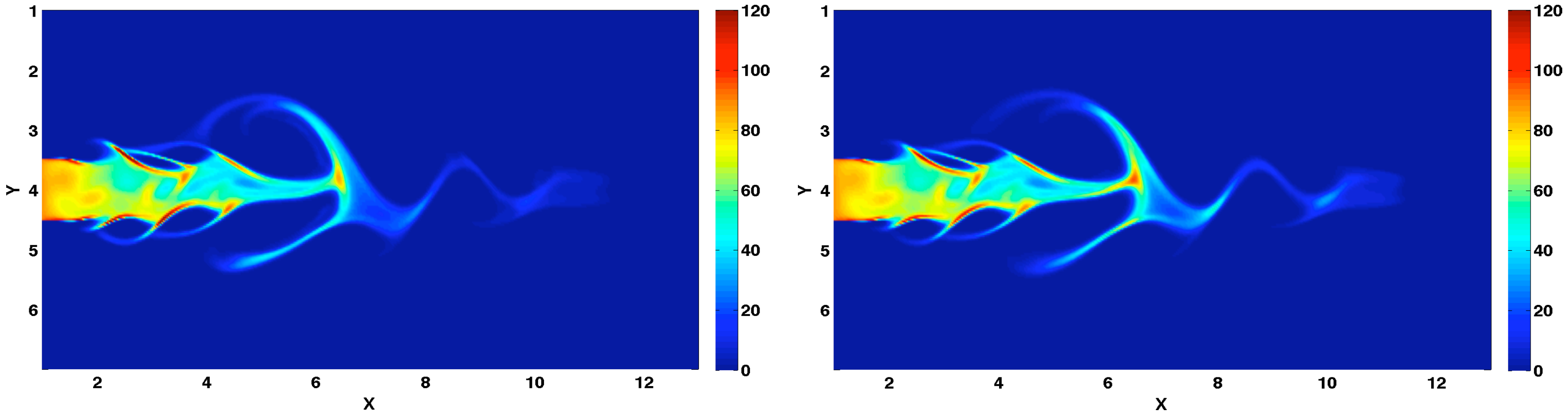
- $\mathrm{St}_{max} = 0.75$
- Comparison of $m_{3/2}, Y_F$ (evaporated fuel mass fraction)
- Multi-Fluid: 10 sections / 1 moment
- EMSM: 1 section / 4 moments

Comparison with the MF model : Free jet test case

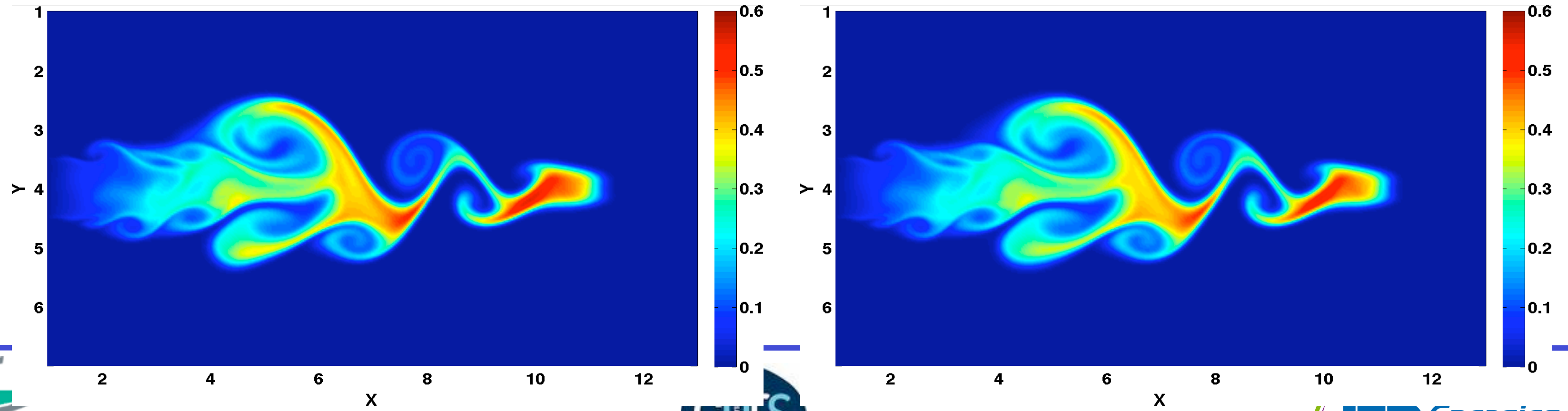
Results at t =10

EMSM model | MF model

$m_{3/2}$



Y_F



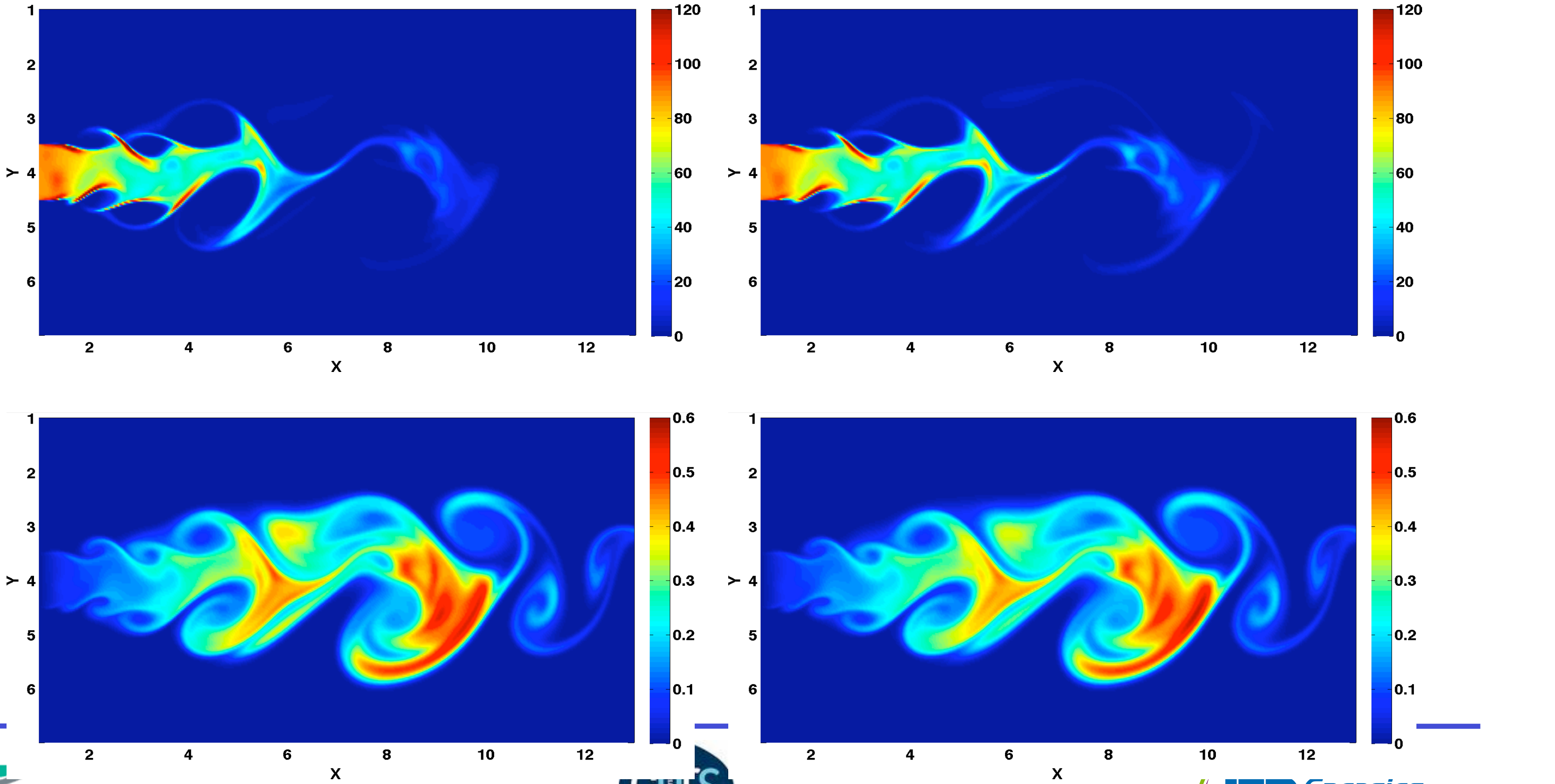
Comparison with the MF model : Free jet test case

Results at t =15

- EMSM model
- MF model

$m_{3/2}$

Y_F



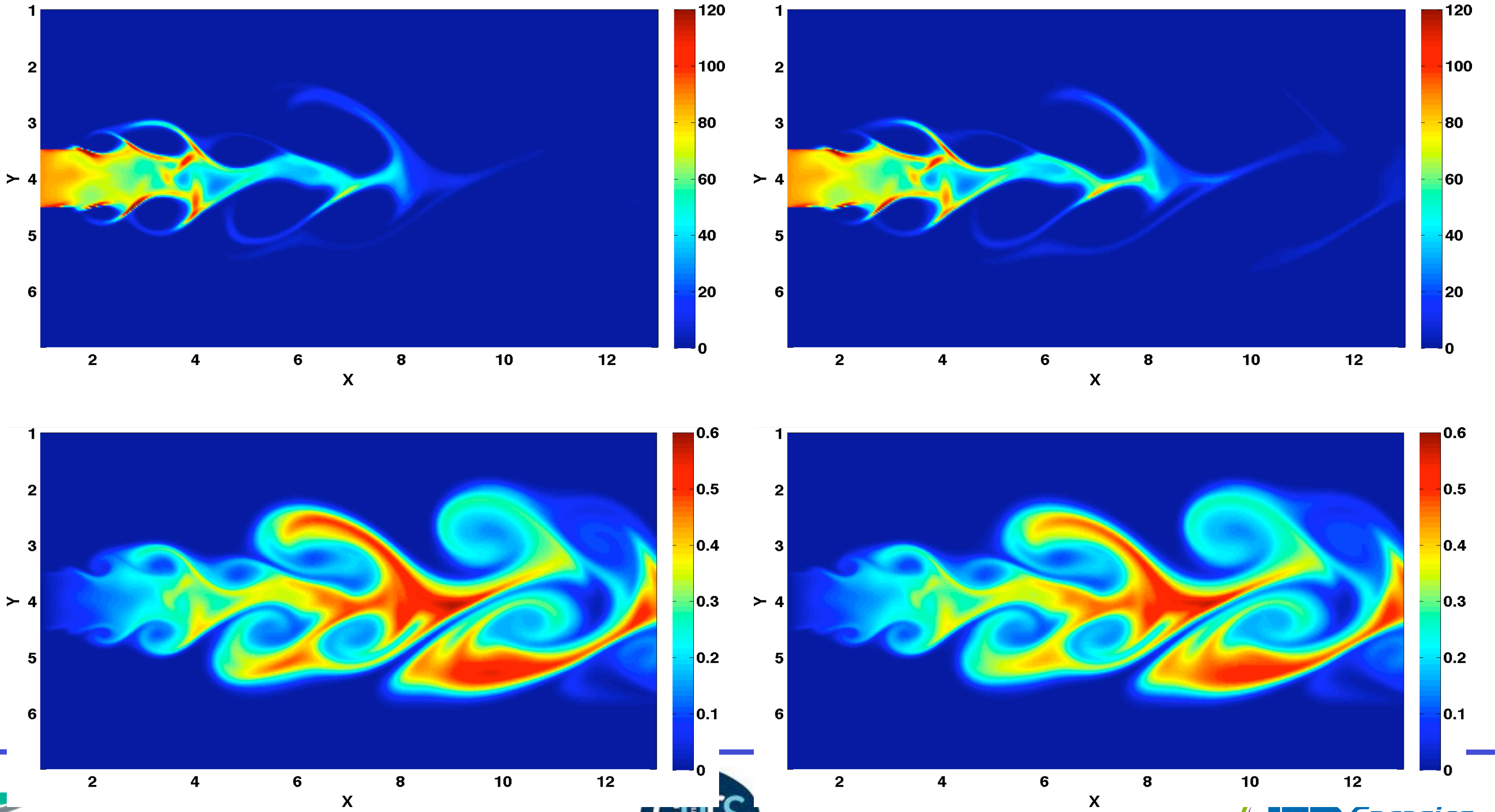
Comparison with the MF model : Free jet test case

Results at t =20

- EMSM model
- MF model

$m_{3/2}$

Y_F



Free jet case : Conclusions

- Jet dynamics resolved
  - High order moment method, with
  - high order advection scheme

➡ **Transport of a moment set enforcing the realizability condition.** This difficulty has been stated in *(wright07, mcgraw07)*

- Excellent level of comparison with the MF model

➡ **Validates the EMSM model and numerical tools**

- In terms of CPU time

➡ 2D case of evaporating spray dynamics in Taylor-Green vortices

EMSM 4 times faster than Multi-Fluid in 2D. Expected even better ratio in 3D

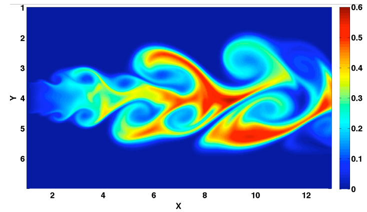
Conclusions

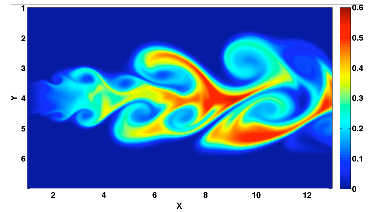
MF model: Eulerian sectional model for polydisperse evaporating sprays

first order in size (CPU cost)

EMSM model: polydispersity resolution with **one section and reasonnable CPU cost** for industrial computation (4 times faster than MF with 10 sections in 2D)

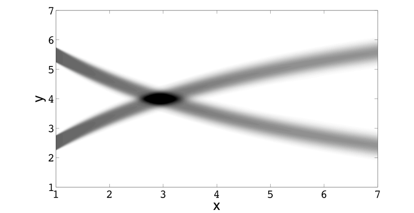
- Mathematics: Entropy Maximization; Moment Theory
- Numerical scheme: Kinetic scheme



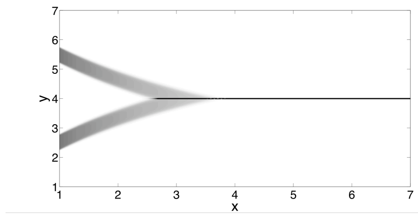


Unable to describe particle trajectory crossings (PTC)

Kinetic solution



Multi-Fluid solution

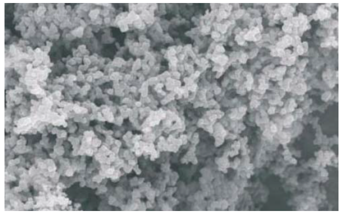


EMVM model: Eulerian Multi-Velocity Moment model – based on QMOM *(Mc Graw 97)*

- Mathematic study of 1D model *(Chalons et al., 11)*
- Multi-Dimensional model *(2 Proceedings CTR 08, Stanford), (de Chaisemartin et al., 09), (Kah et al., 10)*

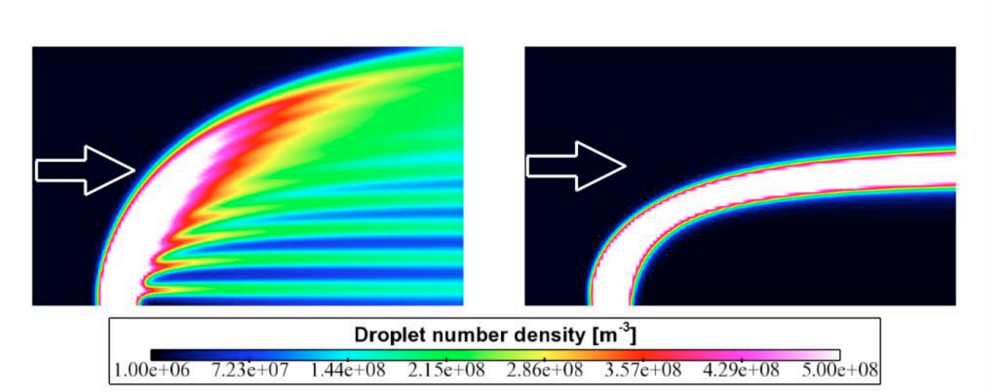
Perspectives

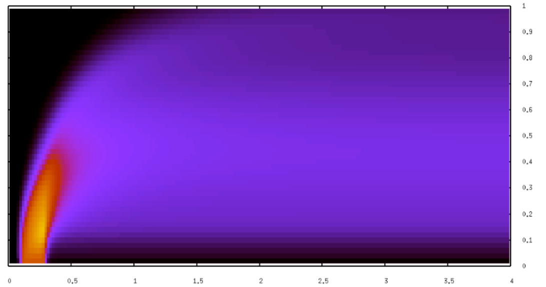
- Extension to aerosol or soot oxydation and transport

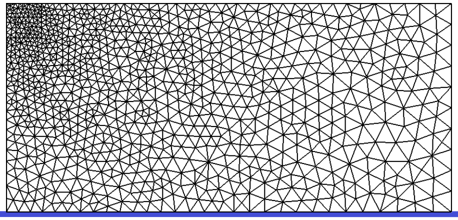


- Description of size/velocity correlations using only one section (Aymeric Vié)

Multi-Fluid 10 sections — EMSM 1 section — EMSM 1 section with correlation







- High order scheme for transport in unstructured grids