Méthodes multi-fluides eulériennes pour la description de brouillards de gouttes polydispersés qui s'évaporent

F. Laurent, M. Massot, S. de Chaisemartin

CENTRE NATIONAL DE LA RECHERCHE SCIENTIFIQUE

Laboratoire EM2C
CNRS - Ecole Centrale Paris

CENTRALE PARIS

en collaboration avec J. Réveillon

CORIA UMR 6614

Laboratoire CORIA
CNRS - Université de Rouen

UNIVERSITÉ DE ROUEN

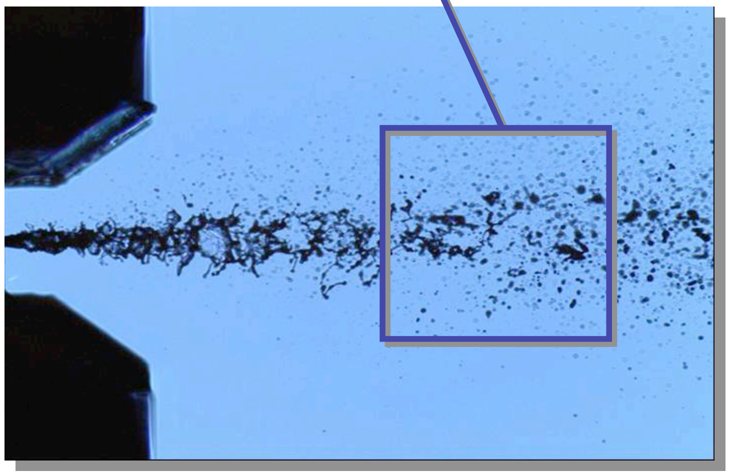
Unstationary polydispersed spray flames

Injection of polydispersed spray

Dispersed liquid phase

+

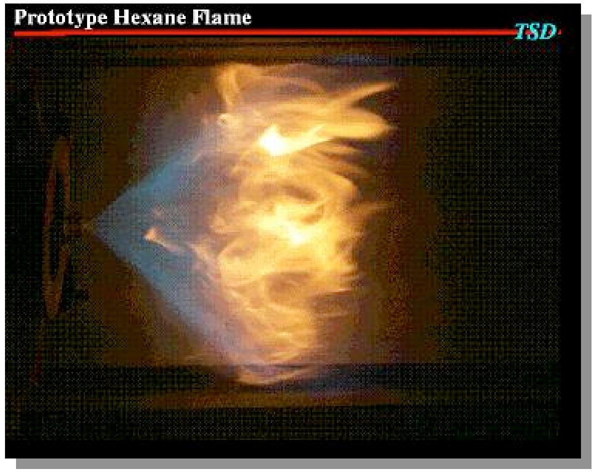
Large spectrum of sizes



(Source C. Dumouchel, CORIA Rouen)

Spray flame

- Mass fraction of fuel in the gaseous phase
- Flame structure and dynamics
- Combustion efficiency
- Pollutants produced

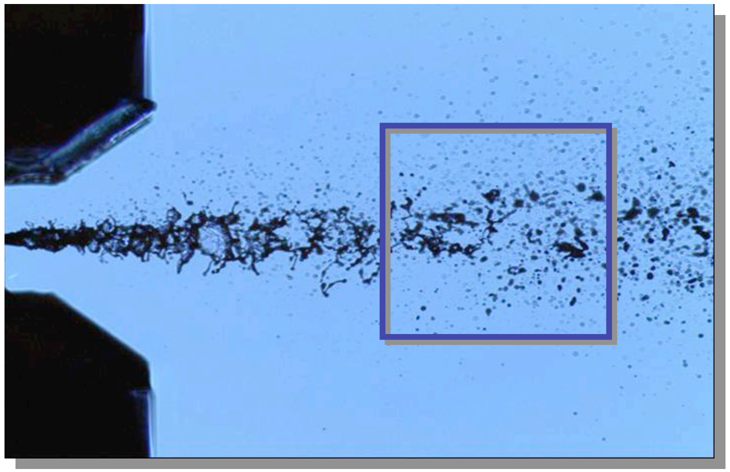


(Source Prof. Edwards, Stanford)

Unstationary polydispersed spray flames

Modeling of the dispersed phase

- **Interactions droplets – gas**
  → evaporation, drag, heat transfer
- **Interactions between droplets**
  → coalescence, breakup, …



Key parameter : **size**

Unstationary polydispersed spray flames

Modeling of the dispersed phase

- **Interactions droplets – gas**
  $\rightarrow$ evaporation, drag, heat transfer
- **Interactions between droplets**
  $\rightarrow$ coalescence, breakup, …

Statistical model $f^{\phi}(t, x, \phi, \mathbf{u_l}, \mathbf{T_l})$: probability density of droplets

Transport equation of Boltzmann type (Williams 1958):

$$\underbrace{\partial_t f^{\phi} + \partial_x \cdot (u_l f^{\phi})}_{\text{free transport}} + \partial_{\phi}(R_{\phi} f^{\phi}) + \partial_{\mathbf{u_l}} \cdot (F f^{\phi}) + \partial_{\mathbf{T_l}}(E f^{\phi}) = \Gamma$$

evaporation, drag, heat transfer

operators of coalescence and breakup

Unstationary polydispersed spray flames

Modeling of the dispersed phase

- **Interactions droplets – gas**
  $\rightarrow$ evaporation, drag, heat transfer
- **Interactions between droplets**
  $\rightarrow$ coalescence, breakup, …

Statistical model $f^{\phi}(t, x, \phi, \mathbf{u_l}, \cancel{\mathbf{T_l}})$: probability density of droplets

Transport equation of Boltzmann type (Williams 1958):

$$\underbrace{\partial_t f^{\phi} + \partial_x \cdot (u_l f^{\phi})}_{\text{free transport}} + \underbrace{\partial_{\phi}(R_{\phi} f^{\phi})}_{\text{evaporation}} + \underbrace{\partial_{\mathbf{u_l}} \cdot (F f^{\phi})}_{\text{drag}} + \underbrace{\partial_{\mathbf{T_l}}(E f^{\phi})}_{\text{heat transfer}} = \underbrace{\cancel{\Gamma}}_{\text{operators of coalescence and breakup}}$$

Unstationary polydispersed spray flames

Modeling of the dispersed phase

- **Interactions droplets – gas**
  $\rightarrow$ evaporation, drag, heat transfer
- **Interactions between droplets**
  $\rightarrow$ coalescence, breakup, …

Statistical model $f^{\phi}(t, x, \phi, \mathbf{u_l}, \cancel{\mathbf{T_l}})$: probability density of droplets

Transport equation of Boltzmann type (Williams 1958):

$$\underbrace{\partial_t f^{\phi} + \partial_x \cdot (u_l f^{\phi})}_{\text{free transport}} + \partial_{\phi}(R_{\phi} f^{\phi}) + \partial_{\mathbf{u_l}} \cdot (F f^{\phi}) + \cancel{\partial_{\mathbf{T_l}}(E f^{\phi})} = \cancel{\Gamma}$$

evaporation drag heat transfer

operators of coalescence and breakup

Plan

- **Types of models developed for the spray simulation**

  ↪ choice to satisfy key points for evaporating spray :

  polydispersion and correlations size/velocity

- **Multi-fluid model**

  ↪ derivation of the method

- **Ejection of spray by vortices**

  ↪ comparisons between multi-fluid model and Lagrangian

Plan

- **Types of models developed for the spray simulation**

  ↪ choice to satisfy key points for evaporating spray :

  polydispersion and correlations size/velocity

- **Multi-fluid model**

  ↪ derivation of the method

- **Ejection of spray by vortices**

  ↪ comparisons between multi-fluid model and Lagrangian

Simulation methods

Lagrangian methods

” Stochastic Parcel Method “ sampling of the probability density function

O’Rourke 81, Duckowicz 80

Simulation methods

Lagrangian methods

” Stochastic Parcel Method “ sampling of the probability density function

O’Rourke 81, Duckowicz 80

Advantages:

- usable in most cases
- no numerical diffusion

Simulation methods

Lagrangian methods

” Stochastic Parcel Method “ sampling of the probability density function

O’Rourke 81, Duckowicz 80

Advantages:

- usable in most cases
- no numerical diffusion

Disadvantages:

- coupling: Eulerian description of the gas / Lagrangian description for the droplets
- cost for unstationnary problems

Simulation methods

Lagrangian methods

” Stochastic Parcel Method “ sampling of the probability density function

O’Rourke 81, Duckowicz 80

Eulerian methods

Goal: give alternative discretization methods to largely used lagrangien ones

3 levels of modeling

- distribution in size
- distribution in velocity
- correlations size/velocity

$$f^{\phi}(t, x, \phi, u_l)$$

Objective : develop eulerian methods, with a **cost as weak as possible,** accurate for

- the description of the **polydispersed** aspect
- the description of the **dynamic** of the droplets
- the **correlations size/velocity**

Link between Eulerian "models"

kinetic model
pdf equation on $f^{\phi}(t, x, \phi, u_l)$

Link between Eulerian "models"

kinetic model

pdf equation on $f^\phi(t, x, \phi, u_l)$

presumed pdf in velocity

conditioned by size

$$f^\phi(t,x,\phi,u_l) = n^\phi(t,x,\phi)\,\varphi_\sigma(u_l - u_d(t,x,\phi))$$

semi-kinetic model

conservation equations on

$n^\phi(t,x,\phi) \quad u_d(t,x,\phi)$

...

Link between Eulerian "models"

kinetic model
pdf equation on $f^\phi(t, x, \phi, u_l)$

presumed pdf in velocity
conditioned by size
$$f^\phi(t, x, \phi, u_l) = n^\phi(t, x, \phi)\, \varphi_\sigma(u_l - u_d(t, x, \phi))$$

semi-kinetic model
conservation equations on

$n^\phi(t, x, \phi)$ $u_d(t, x, \phi)$
...

presumed pdf in size
and correlations
for each section

Eulerian
multi-fluid

Link between Eulerian "models"

kinetic model
pdf equation on $f^{\phi}(t, x, \phi, u_l)$

presumed pdf in velocity
conditioned by size

$$f^{\phi}(t, x, \phi, u_l) = n^{\phi}(t, x, \phi)\, \varphi_{\sigma}(u_l - u_d(t, x, \phi))$$

semi-kinetic model
conservation equations on

$n^{\phi}(t, x, \phi) \quad u_d(t, x, \phi)$

...

presumed pdf in size
$u_d(\phi)$ given form

presumed pdf in size
and correlations
for each section

Presumed pdf method

Eulerian multi-fluid

Link between Eulerian "models"

kinetic model
pdf equation on $f^{\phi}(t, x, \phi, u_l)$

presumed pdf in velocity
conditioned by size

$$f^{\phi}(t, x, \phi, u_l) =$$
$$n^{\phi}(t, x, \phi)\, \varphi_{\sigma}(u_l - u_d(t, x, \phi))$$

moment in velocity
at sampled size

semi-kinetic model
conservation equations on

$n^{\phi}(t, x, \phi)$ $\quad u_d(t, x, \phi)$
...

presumed pdf in size
$u_d(\phi)$ given form

presumed pdf in size
and correlations
<u>for each section</u>

Bi-fluid model

O. Simonin et al.

Presumed pdf method

Mossa, INPT 2005

Eulerian multi-fluid

Link between Eulerian “models”

kinetic model
pdf equation on $f^{\phi}(t, x, \phi, u_l)$

$$f^{\phi}(t, x, \phi, u_l) = \sum_{n=1}^{N} w_n \delta(\phi - \phi_n)\delta(u_l - u_n)$$

moment in velocity
at sampled size

presumed pdf in velocity
conditioned by size

$$f^{\phi}(t, x, \phi, u_l) = n^{\phi}(t, x, \phi)\, \varphi_{\sigma}(u_l - u_d(t, x, \phi))$$

semi-kinetic model
conservation equations on

$n^{\phi}(t, x, \phi)$ $\quad u_d(t, x, \phi)$

...

presumed pdf in size
$u_d(\phi)$ given form

presumed pdf in size
and correlations
<u>for each section</u>

Moment Methods
DQMOM

McGraw, Rosner, Fox

Bi-fluid
model

O. Simonin et al.

Presumed
pdf method

Mossa, INPT 2005

Eulerian
multi-fluid

Plan

- **Types of models developed for the spray simulation**

  ⤷ choice to satisfy key points for evaporating spray :

  polydispersion and correlations size/velocity

- **Multi-fluid model**

  ⤷ derivation of the method

- **Ejection of spray by vortices**

  ⤷ comparisons between multi-fluid model and Lagrangian

Previous work

Eulerian multi-fluid model

- **Modeling**

  diluted laminar case

  F. Laurent, M. Massot

  laminar case with coalescence or/and breakup

  F. Laurent, M. Massot, P. Villedieu + G. Dufour

  turbulent case

  J. Réveillon, M. Massot, C. Péra + R. Knikker

- **Numerical analysis** of the evaporation and higher order methods

  F. Laurent / G. Dufour

- **Mathematic analysis** : plane flames, multi-fluid models

  F. Laurent, M. Massot / G. Dufour, M. Massot

William's Transport Equation

$f(t, x, S, u_l)$: probability density of droplets

Transport equation :

$$\partial_t f + \partial_x \cdot (u_l f) + \partial_S (R_s f) + \partial_{u_l} \cdot (F f) = 0$$

Stokes law for drag

$$F(S, u_{gaz}, u_l) = \frac{u_{gaz} - u_l}{\tau_p}$$

d^2 law for evaporation

$$R_s = \text{cste}$$

Derivation of the multi-fluid model

Semi-kinetic model: equations on

$$n(t,x,S) = \int f(t,x,S,u_l)du_l$$

$$u_d(t,x,S) = \frac{1}{n(t,x,S)} \int u_l f(t,x,S,u_l)\,du_l$$

Derivation of the multi-fluid model

Semi-kinetic model: equations on

$$n(t,x,S) = \int f(t,x,S,u_l)du_l$$

$$u_d(t,x,S) = \frac{1}{n(t,x,S)} \int u_l f(t,x,S,u_l)\, du_l$$

presumed pdf $f(t,x,S,u_l) = n(t,x,S)\delta(u_l - u_d(t,x,S))$

➢ Assumptions :

H1 Only one characteristic velocity at a given droplet size

H2 No dispersion of *f* at a given size for the velocity. → laminar case

Derivation of the multi-fluid model

Semi-kinetic model: equations on

$$n(t,x,S) = \int f(t,x,S,u_l)du_l$$

$$u_d(t,x,S) = \frac{1}{n(t,x,S)} \int u_l f(t,x,S,u_l)\, du_l$$

presumed pdf $f(t,x,S,u_l) = n(t,x,S)\delta(u_l - u_d(t,x,S))$

$$\boxed{\begin{cases} \partial_t n + \partial_x \cdot (n\, u_d) + \partial_\phi (n\, R_s) = 0 \\ \partial_t (n\, u_d) + \partial_x \cdot (n\, u_d \otimes u_d) + \partial_\phi (n\, R_s\, u_d) = nF \end{cases}}$$

➢ Assumptions :

H1 Only one characteristic velocity at a given droplet size

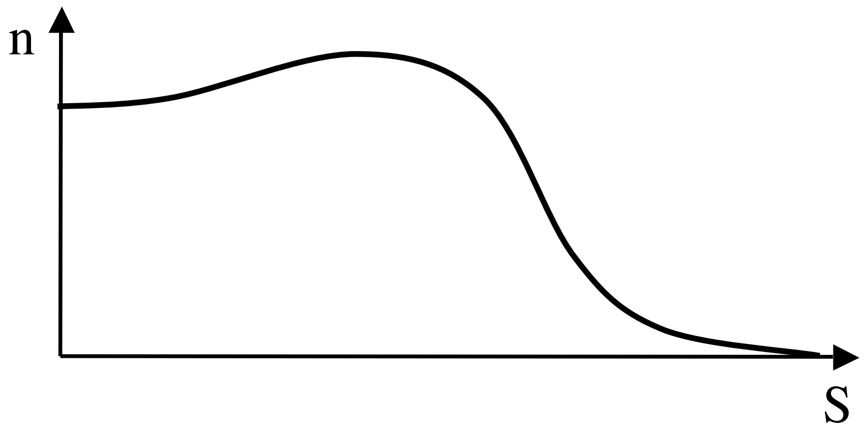
H2 No dispersion of *f* at a given size for the velocity. → laminar case

Derivation of the multi-fluid model

Semi-kinetic model: equations on
$$n(t,x,S) = \int f(t,x,S,u_l)du_l$$
$$u_d(t,x,S) = \frac{1}{n(t,x,S)} \int u_l f(t,x,S,u_l)\, du_l$$

presumed pdf $f(t,x,S,u_l) = n(t,x,S)\delta(u_l - u_d(t,x,S))$

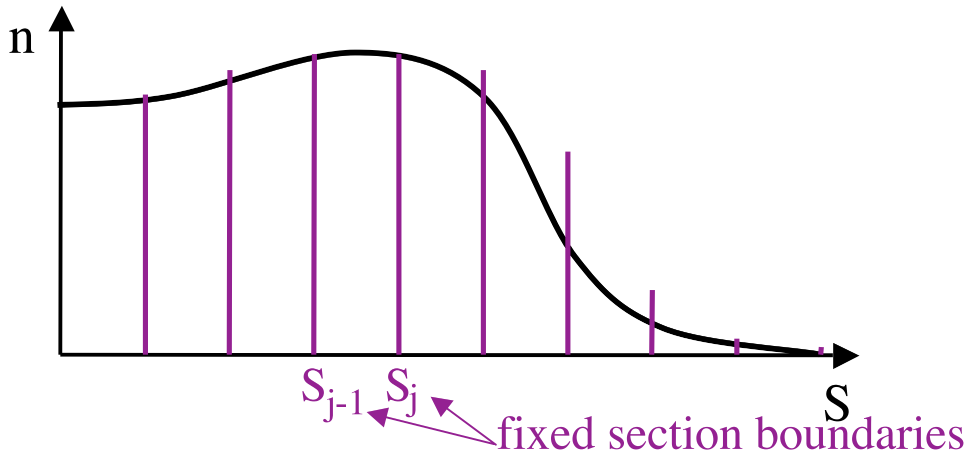
$$\boxed{\begin{cases} \partial_t n + \partial_x \cdot (n\, u_d) + \partial_\phi (n\, R_s) = 0 \\ \partial_t (n\, u_d) + \partial_x \cdot (n\, u_d \otimes u_d) + \partial_\phi (n\, R_s\, u_d) = nF \end{cases}}$$



Derivation of the multi-fluid model

Multi-fluid model: finite volume discretization of $n(t, x, S)$

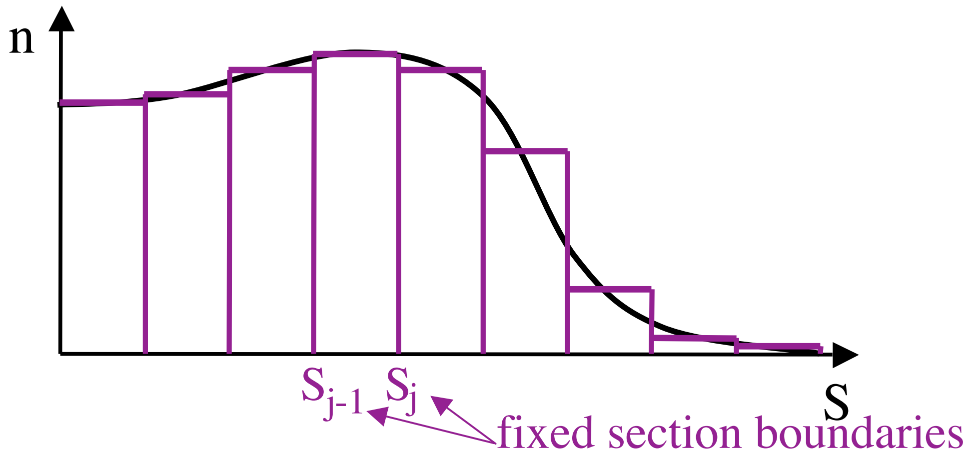
presumed profile of the distribution in each section



Derivation of the multi-fluid model

Multi-fluid model: finite volume discretization of $n(t, x, S)$

presumed profile of the distribution in each section



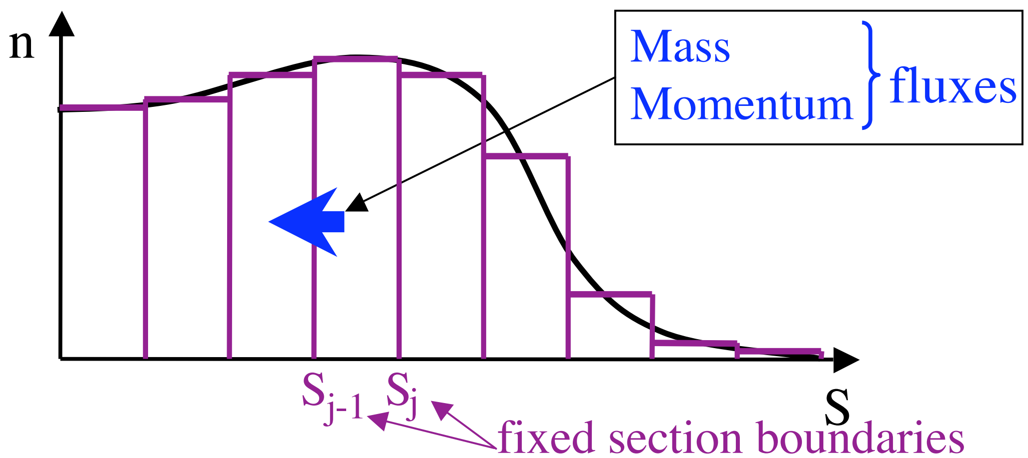
Derivation of the multi-fluid model

Multi-fluid model: finite volume discretization of $n(t, x, S)$

presumed profile of the distribution in each section

unknowns : $m_j(t,x) = \int_{S_{i-1}}^{S_i} \rho_l \frac{S^{3/2}}{6\sqrt{\pi}} n(t,x,S)dS \qquad u_d^{(j)}(t,x)$

$$\boxed{\begin{cases} \partial_t m^{(j)} + \partial_x \cdot (u_d^{(j)} m^{(j)}) = -(E_1^{(j)} + E_2^{(j)}) m^{(j)} + E_1^{(j+1)} m^{(j+1)} \\ \partial_t (m^{(j)} u_d^{(j)}) + \partial_x \cdot (m^{(j)} u_d^{(j)} \otimes u_d^{(j)}) = \\ \qquad -(E_1^{(j)} + E_2^{(j)}) m^{(j)} u_d^{(j)} + E_1^{(j+1)} m^{(j+1)} u_d^{(j+1)} + m^{(j)} F^{(j)} \end{cases}}$$



Extensions the multi-fluid model

Scheme for the evaporation phenomenon

- Classical multi-fluid method : 1^{st} order method (F. Laurent M2AN 2006)

Extensions the multi-fluid model

Scheme for the evaporation phenomenon

- Classical multi-fluid method : 1st order method (F. Laurent M2AN 2006)
- Second order multi-fluid methods :
  - G. Dufour, P. Villedieu, M2AN 2006
    the profile of the distribution is exponential in each section

    unknowns $n_j(t,x) = \int_{S_{j-1}}^{S_j} n(t,x,S)\,dS$, $m_j(t,x) = \int_{S_{i-1}}^{S_i} \rho_l \frac{S^{3/2}}{6\sqrt{\pi}} n(t,x,S)dS$
  - F. Laurent, M2AN 2006
    the profile of the distribution is bi-affine in each section

    unknowns $n_j(t,x) = \int_{S_{j-1}}^{S_j} n(t,x,S)\,dS$, $\widetilde{nS}_j(t,x) = \int_{S_{j-1}}^{S_j} S\,n(t,x,S)\,dS$

Numerical scheme

Transport part: pressureless gas

$$\begin{cases} \partial_t(\rho) + \partial_x \cdot (\rho u) & = & 0 \\ \partial_t(\rho u) + \partial_x \cdot (\rho u \otimes u) & = & 0 \end{cases}$$

- Weakly hyperbolic system

  $\Rightarrow$ Development of delta-shocks

  $\Rightarrow$ Emergence of the vacuum state

Numerical scheme

Transport part: pressureless gas

$$\begin{cases} \partial_t(\rho) + \partial_x \cdot (\rho u) & = & 0 \\ \partial_t(\rho u) + \partial_x \cdot (\rho u \otimes u) & = & 0 \end{cases}$$

Transport scheme:

- Numerical approximations of pressureless gas

  ↪ Finite volume kinetic scheme

  Bouchut, Jin and Li, SIAM Numerical Analysis (2003)

- Scheme properties
  - Ability to treat delta shock and vacuum
  - Maximum principle on the velocity
  - Positivity of the density

Numerical scheme

Transport part: pressureless gas

$$\begin{cases} \partial_t(\rho) + \partial_x \cdot (\rho u) & = & 0 \\ \partial_t(\rho u) + \partial_x \cdot (\rho u \otimes u) & = & 0 \end{cases}$$

Transport scheme:

- Numerical approximations of pressureless gas

  ↪ Finite volume kinetic scheme

  Bouchut, Jin and Li, SIAM Numerical Analysis (2003)

Splitting

- Separated treatment of transport, drag and evaporation

  ↪ Strang splitting: Time 2^{nd} order

Plan

- **Types of models developed for the spray simulation**

  ↪ choice to satisfy key points for evaporating spray :

  polydispersion and correlations size/velocity

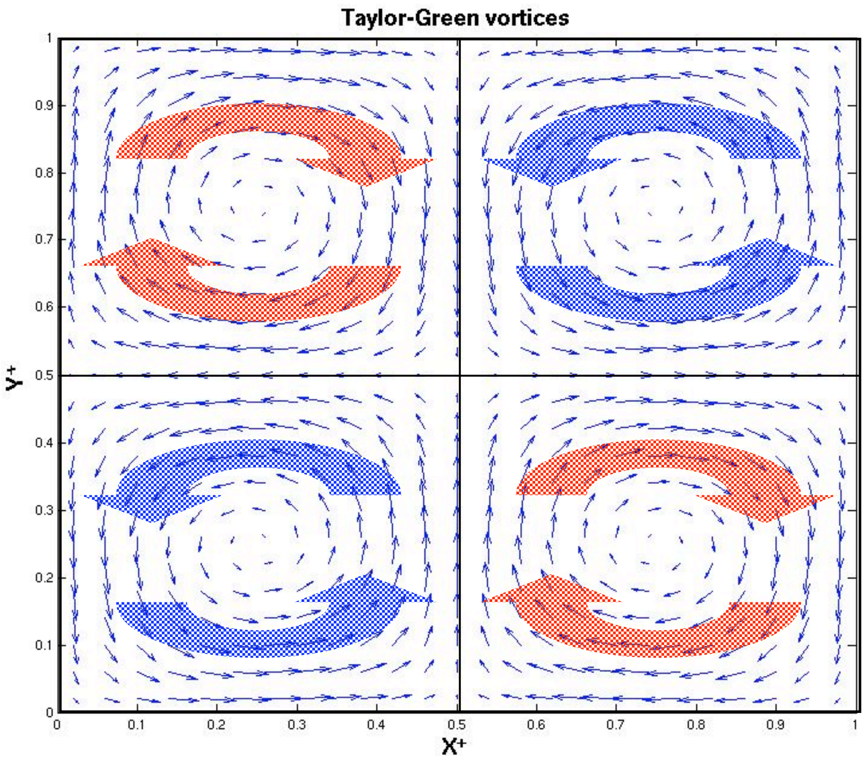
- **Multi-fluid model**

  ↪ derivation of the method

- **Ejection of spray by vortices**

  ↪ comparisons between multi-fluid model and Lagrangian

Gas configuration



- 2D Taylor-Green vortices

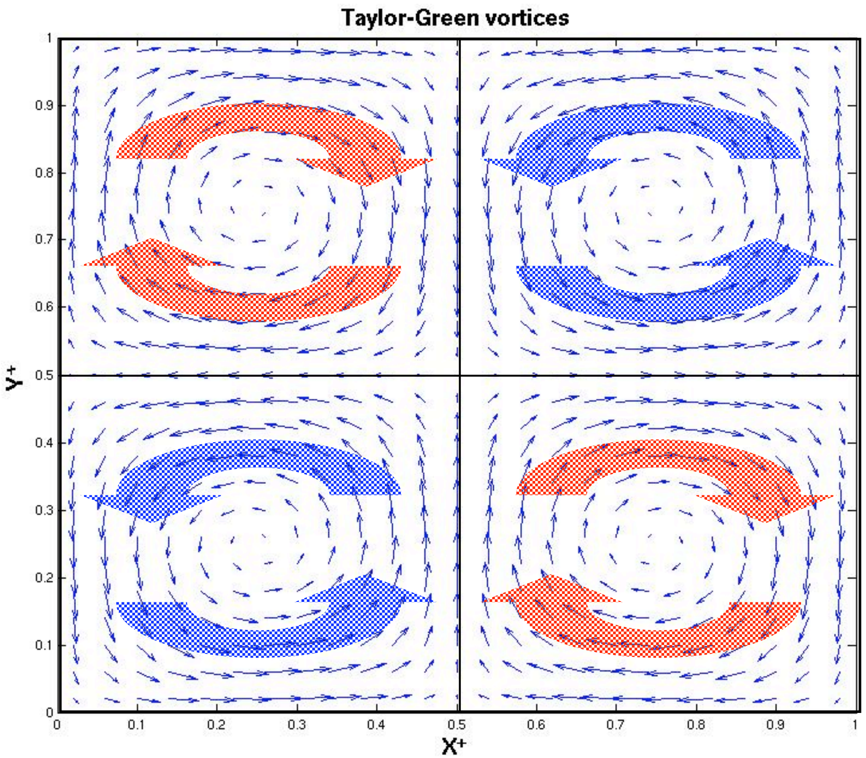
  ↪ Euler stationary solution

$$\begin{cases} U_x(x,y) & = & A\, sin(\frac{2\pi x}{\lambda}) cos(\frac{2\pi y}{\lambda}) \\ U_y(x,y) & = & -A\, cos(\frac{2\pi x}{\lambda}) sin(\frac{2\pi y}{\lambda}) \end{cases}$$

- One way steady simulation

$\Rightarrow$ Study of the dynamic of droplets ejection by vortices

Gas configuration



- 2D Taylor-Green vortices

  ↪ Euler stationary solution

$$\left\{ \begin{array}{lcl} U_x(x,y) & = & A\,sin(\frac{2\pi x}{\lambda})cos(\frac{2\pi y}{\lambda}) \\ U_y(x,y) & = & -A\,cos(\frac{2\pi x}{\lambda})sin(\frac{2\pi y}{\lambda}) \end{array} \right.$$

- One way steady simulation

⇒ Study of the dynamic of droplets ejection by vortices

- Critical Stokes $St = \frac{\tau_p A}{\lambda} \longrightarrow St_c = \frac{1}{8\pi}$

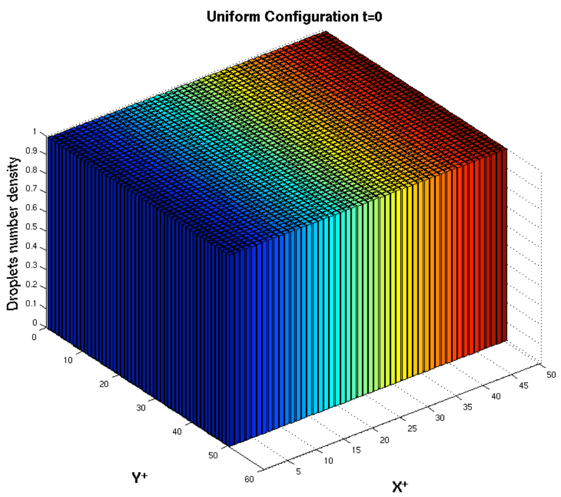
Droplet configuration

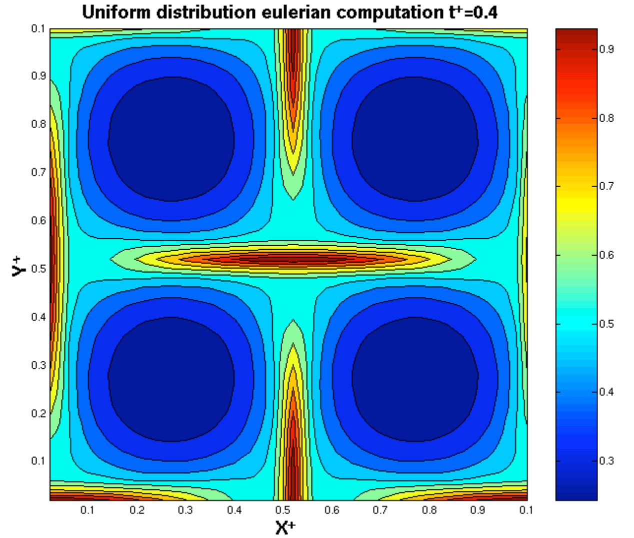
- Non-dimensional equation

$$\underbrace{\partial_{t^+} f + \partial_{x^+} \cdot (u^+ f)}_{\text{free transport}} + \underbrace{K \cdot \partial_{S^+}(f)}_{\text{vaporisation}} + \underbrace{\partial_{u^+}\left(\frac{u^+_{gas} - u^+}{St} f\right)}_{\text{drag}} = 0$$

$$St = \frac{\tau_p}{\tau_{gas}} \qquad K = \frac{\tau_{gas}}{\tau_{vap}}$$

- Uniform space distribution





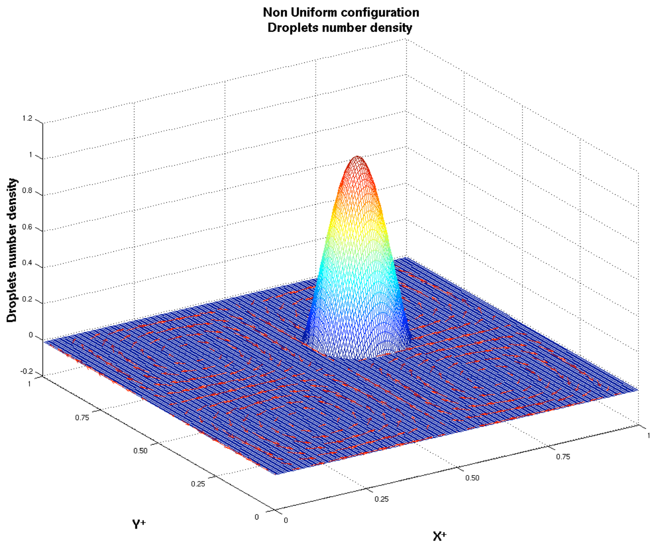
Droplet configuration

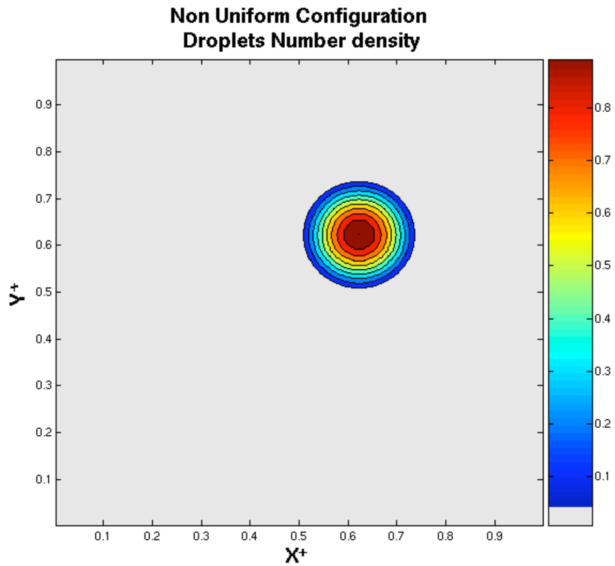
- Non-dimensional equation

$$\underbrace{\partial_{t^+} f + \partial_{x^+} \cdot (u^+ f)}_{\text{free transport}} + \underbrace{K \cdot \partial_{S^+}(f)}_{\text{vaporisation}} + \underbrace{\partial_{u^+}\left(\frac{u^+_{gas} - u^+}{St} f\right)}_{\text{drag}} = 0$$

$$St = \frac{\tau_p}{\tau_{gas}} \qquad K = \frac{\tau_{gas}}{\tau_{vap}}$$

- Non-uniform space distribution





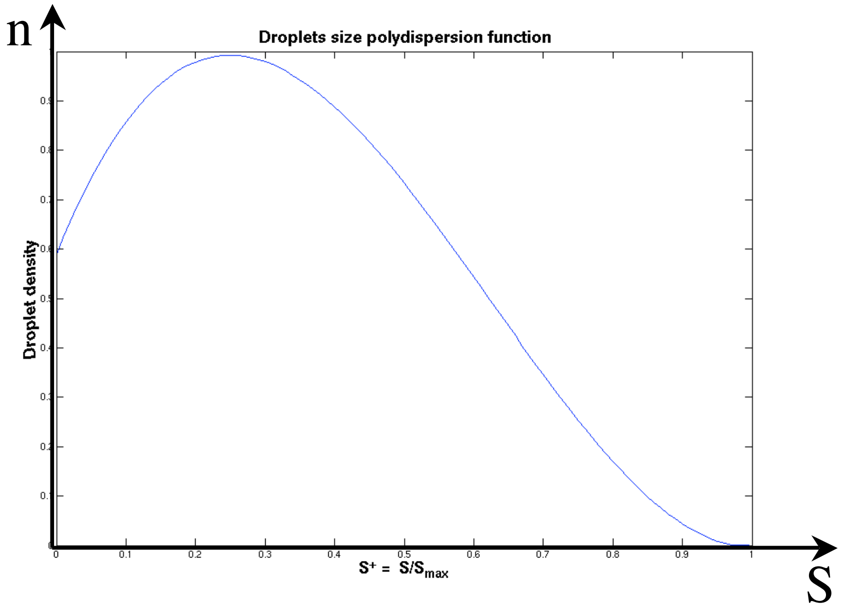
Droplet configuration

- Non-dimensional equation

$$\underbrace{\partial_{t^+} f + \partial_{x^+} \cdot (u^+ f)}_{\text{free transport}} + \underbrace{K \cdot \partial_{S^+}(f)}_{\text{vaporisation}} + \underbrace{\partial_{u^+}\left(\frac{u^+_{gas} - u^+}{St} f\right)}_{\text{drag}} = 0$$

$$St = \frac{\tau_p}{\tau_{gas}} \qquad K = \frac{\tau_{gas}}{\tau_{vap}}$$

- Polydisperse case

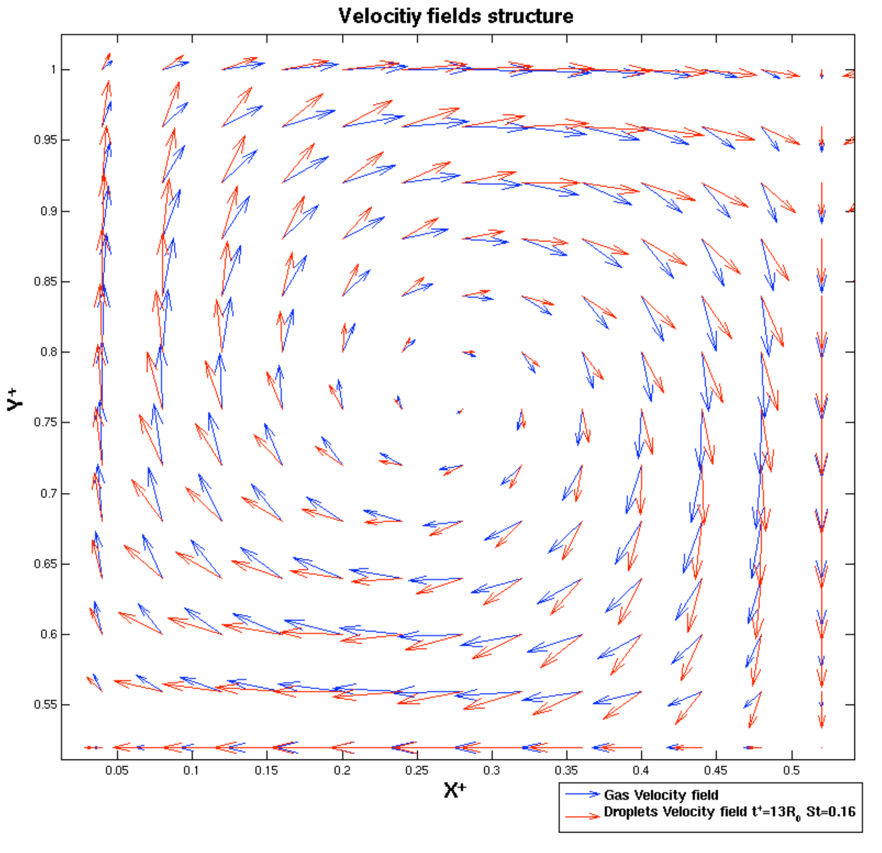


Eulerian result analysis

- Toward a steady velocity structure for the droplets

  → Observed and proved in 1D sinus case

  → Observed in our Taylor-Green configuration



Eulerian result analysis

- Toward a steady velocity structure for the droplets

  → Observed and proved in 1D sinus case

  → Observed in our Taylor-Green configuration

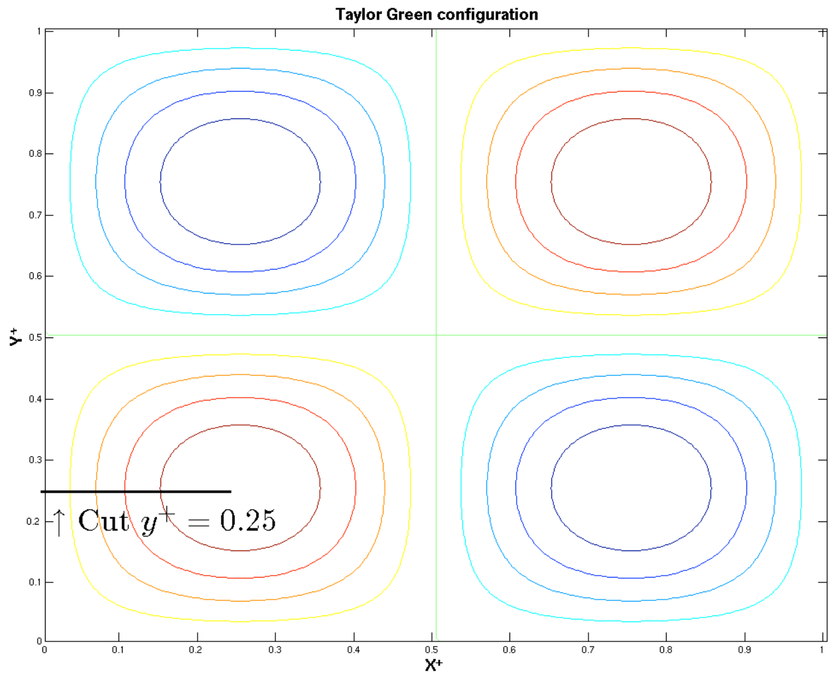
- Ejection from the vortices: characteristic time

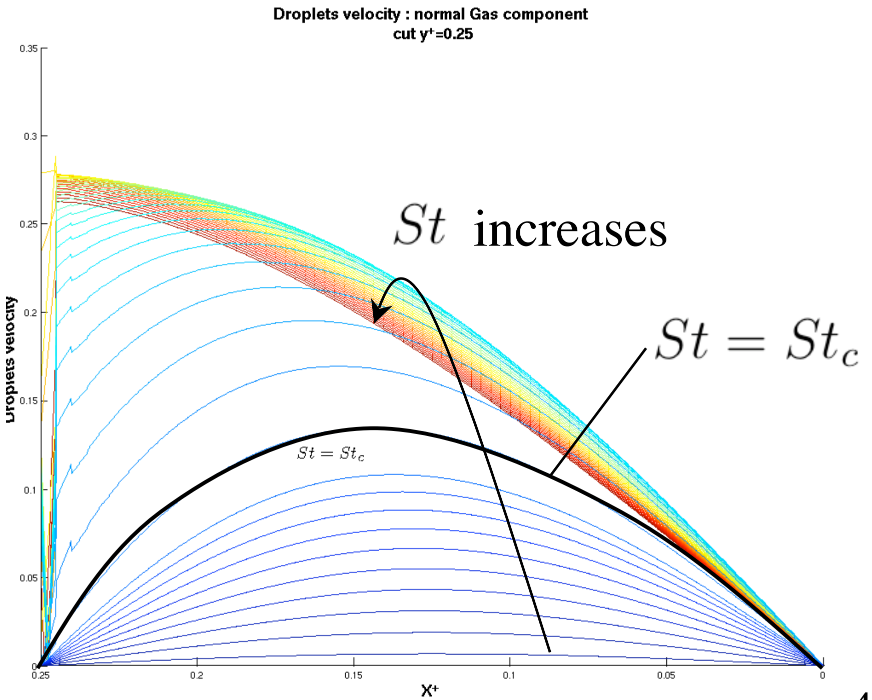
  - Defined from the characteristic velocity of each droplet size

  - Allows characterization of the droplets dynamics

Eulerian result analysis

- Toward a steady velocity structure for the droplets
  - $\rightarrow$ Observed and proved in 1D sinus case
  - $\rightarrow$ Observed in our Taylor-Green configuration
- Ejection from the vortices: characteristic time

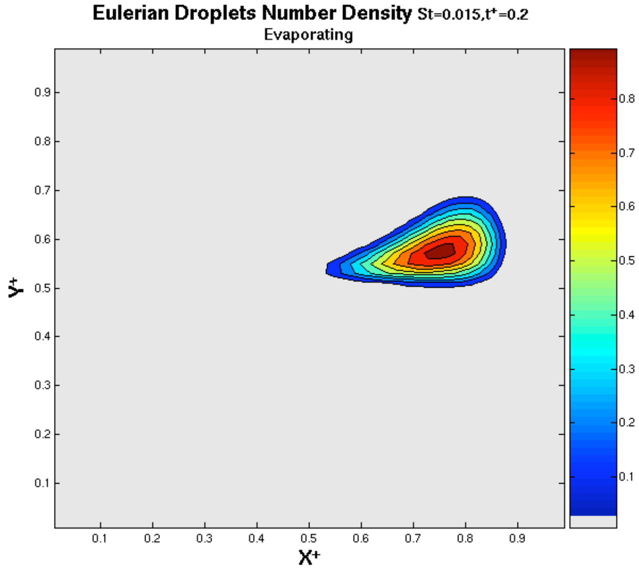


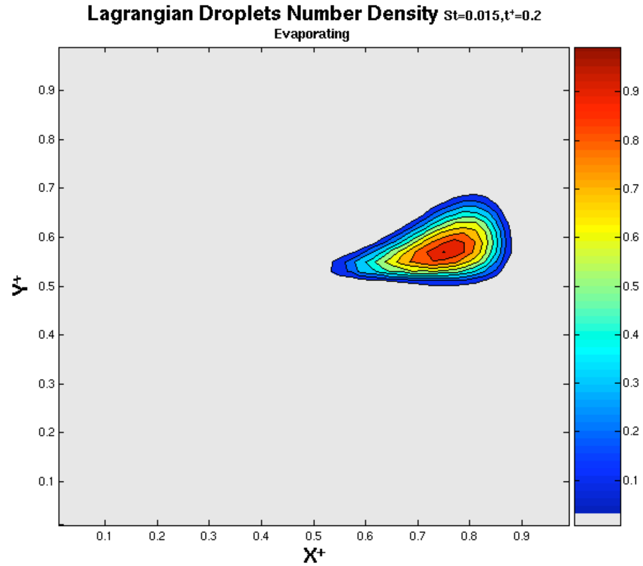


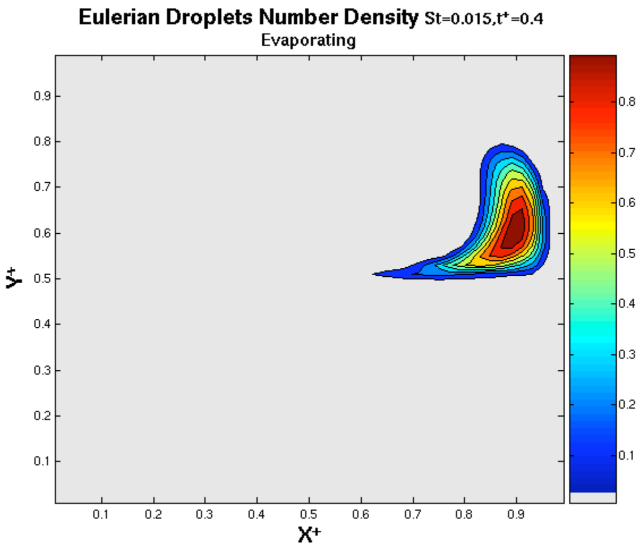
Eulerian Lagrangian comparison

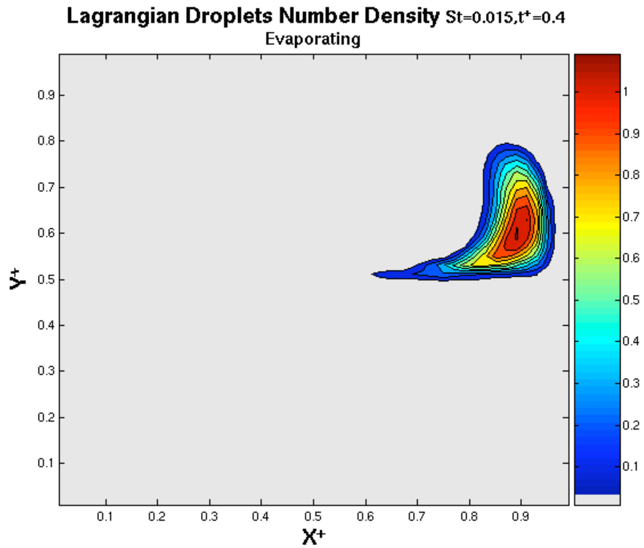
Eulerien

Lagrangien





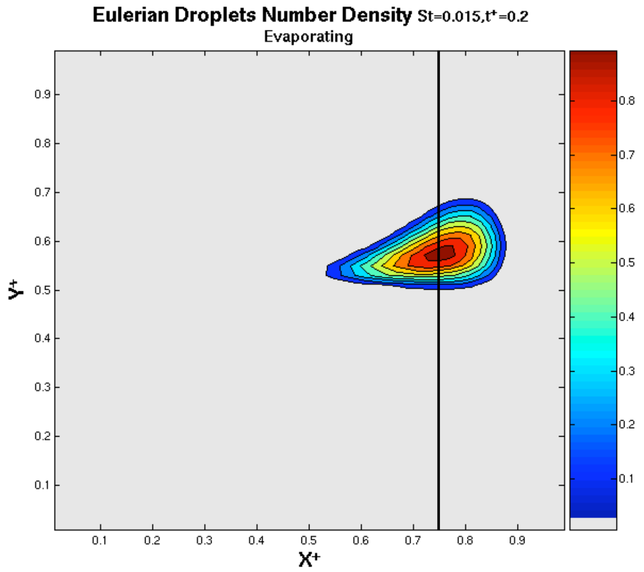


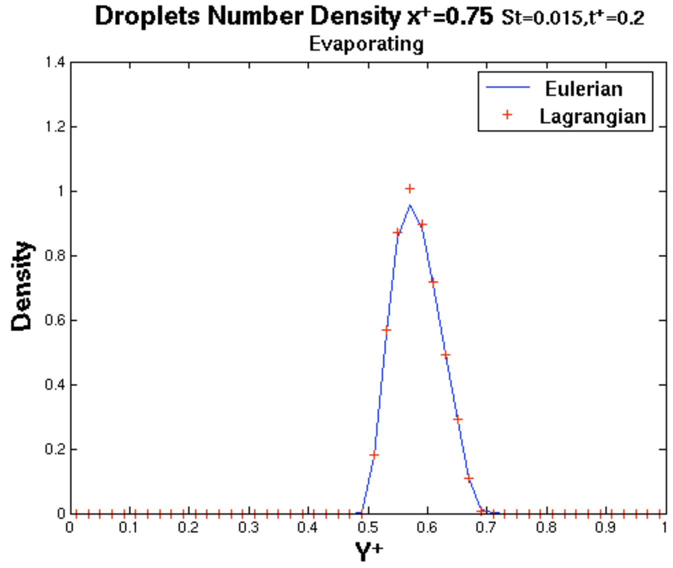


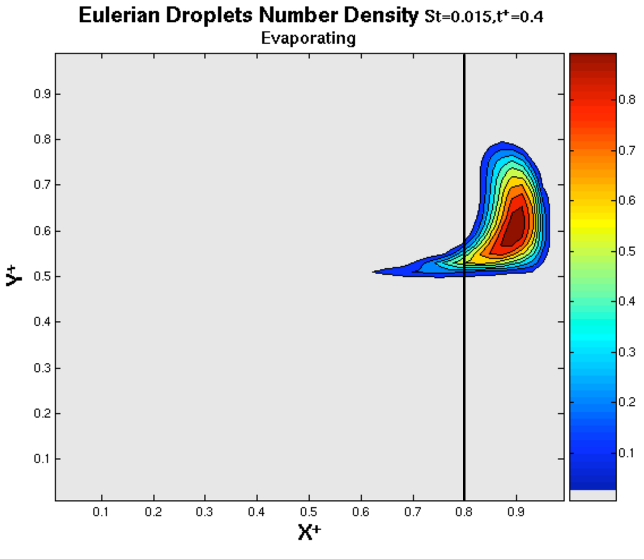
Eulerian Lagrangian comparison

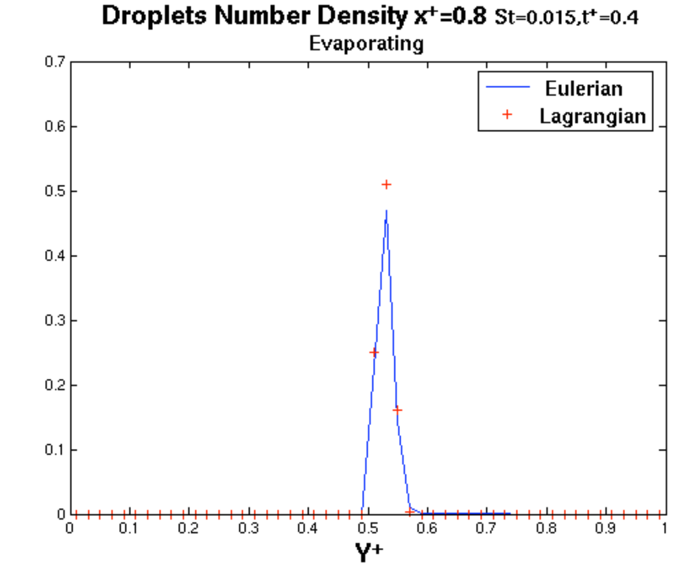
Eulerien

coupes



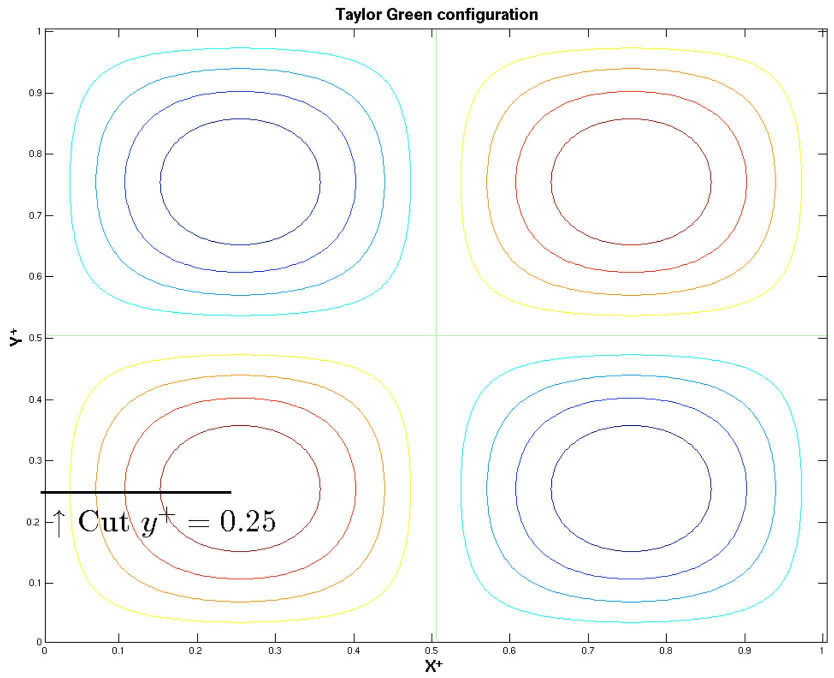


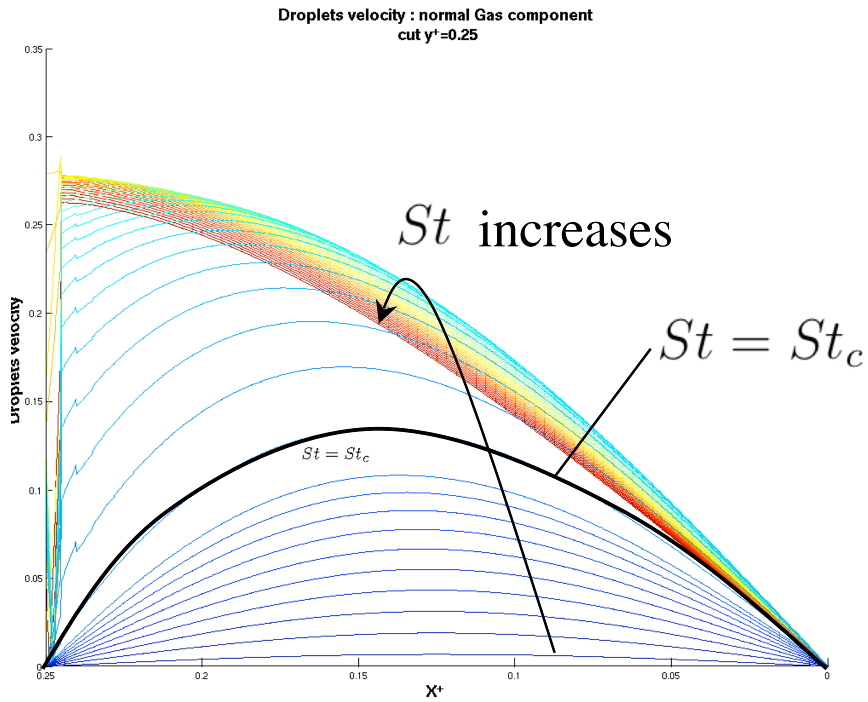




Further results

- Case St = 0.8 >> St_c Eulerian non-uniform simulation





- Case St > St_c Lagrangian uniform simulation
- Limit of the validity of the kinetic equation considered

  ⇒ consideration of particles interactions

Conclusion and Future work

Eulerian Multi-fluid method

- Derivation of a Eulerian method: validity domain
- Extension to higher order method for the evaporation phenomenon

Results on the studied configurations

- Interesting information extracted from the Eulerian simulation
- Encouraging Eulerian-Lagrangian comparisons results

Future work

- Going farther with the Taylor-Green configuration : analysis of the Eulerian results
- Addition of the collision phenomenon
- Working on new configurations: 2D-axis or 3D jet with turbulence
- Comparison of the classical multi-fluid method with the higher order methods and the DQMOM method

Références principales

- F. Laurent, M. Massot *Multi-fluid Modeling of Laminar Poly-dispersed Spray Flames : Origin, Assumptions and Comparison of the Sectional and Sampling Method* CTM 2001
- F. Laurent, M. Massot, P. Villedieu, *Eulerian multi-fluid modeling for the numerical simulation of coalescence in polydisperse dense liquid sprays* JCP 2004
- G. Dufour *Modélisation eulérienne des écoulements diphasiques à inclusions dispersées* PhD Thesis, Université Paul Sabatier Toulouse 2005
- G. Dufour, P. Villedieu *The sectional method revisited for evaporating sprays* M2AN 2006
- F. Laurent *Numerical analysis of eulerian multi-fluid models in the context of kinetic formulations for dilute evaporating sprays* M2AN 2006
- S. Jin, F. Bouchut, X. Li *Numerical approximations of pressureless and isothermal gas dynamics* Siam J. Numer. Anal. 2003

Financement

Projet européen TIMECOP (2006-2007)

coordinateur de la tâche : F. Laurent, M. Massot

ACI Nouvelles Interfaces des Mathématiques, Ministère de la Recherche (2003-2006)

coordinateurs : M. Massot, S. Descombes

ANR jeune équipe dynamique des sprays en évaporation et en combustion (2005-2008)

coordinateur : M. Massot