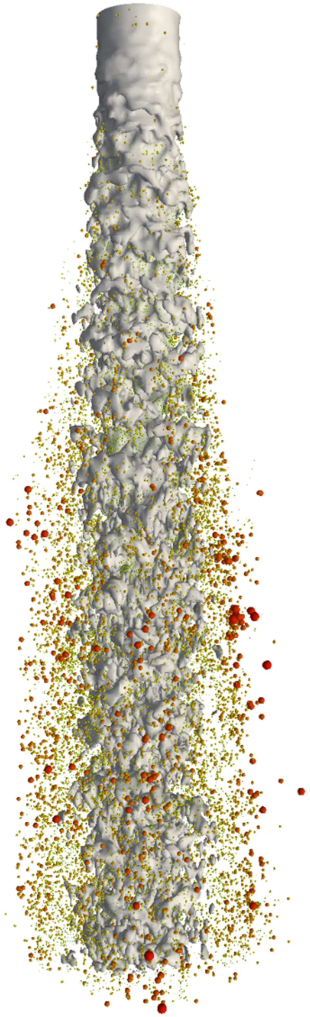
Early prediction of spray characteristics from curvature distribution analysis and other problems …



F.X. Demoulin, B. Duret, J. Reveillon

PhDs:

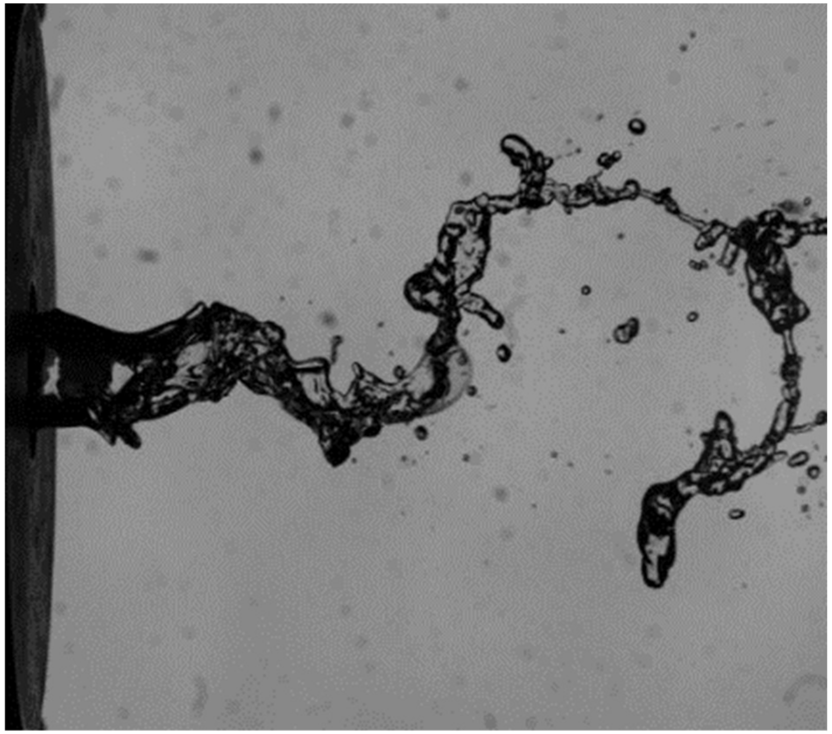
P.A. Beau
R. Lebas
G. Luret
Y. Meslem
B. Duret
N. Hecht
S. Puggelli
F. Dabonneville
J. Anez
R. Canu
A. Ahmed
A. Remigi
L. Palenti
D. Ferrado

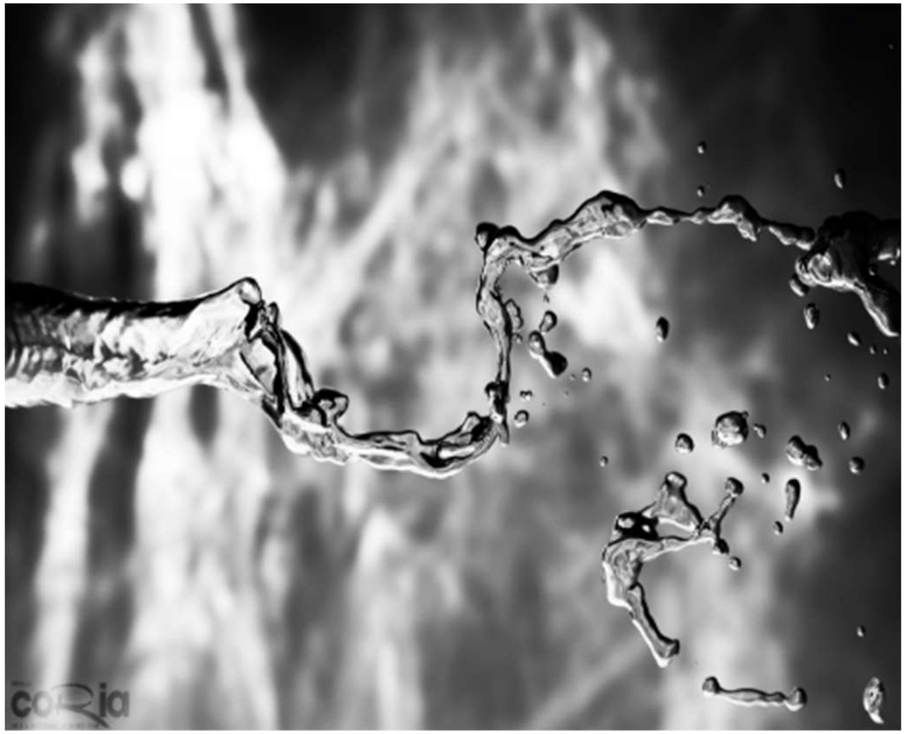
DNS and ICM ➔ Amazing results

To perform simulation of atomization the best known approach rely on:

- Navier-Stokes equations
- Directly resolved by numerical simulation (DNS)
- Appropriate numerical method : interface capturing method (ICM)

CORIA Berlemont A., Ménard T. et al.





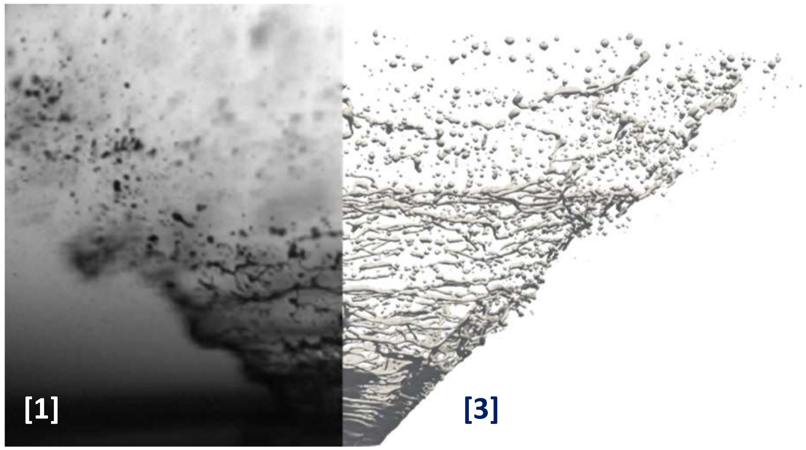
But … DNS-ICM : Accurate and Computationally expensive

Can we go beyond ?

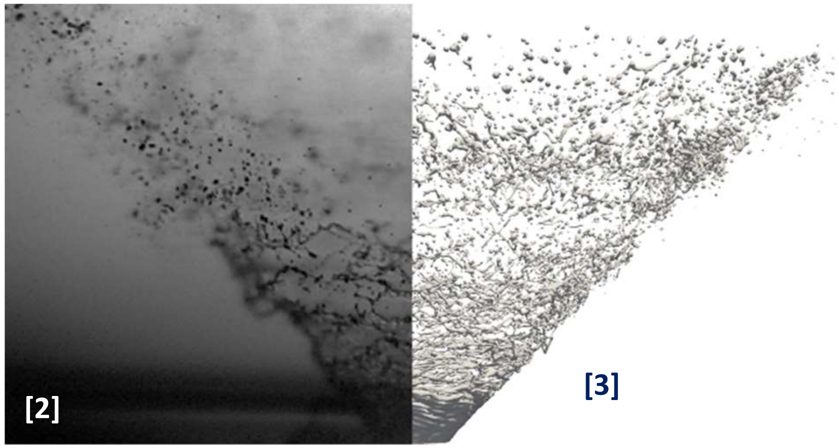
DNS Simplex Swirl Atomizer

(limited to primary break up)

Ambient Temperature

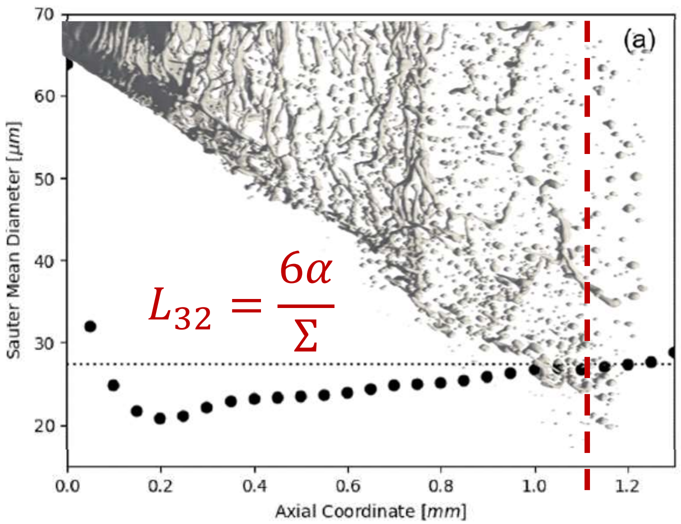


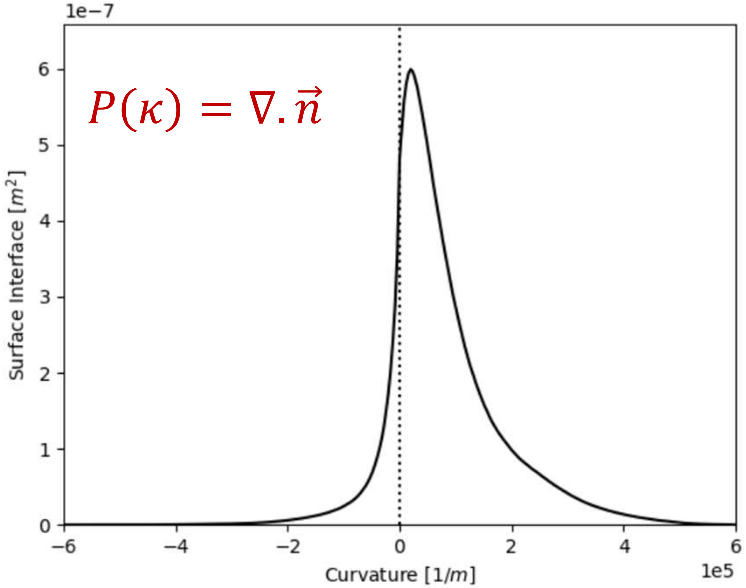
High Temperature

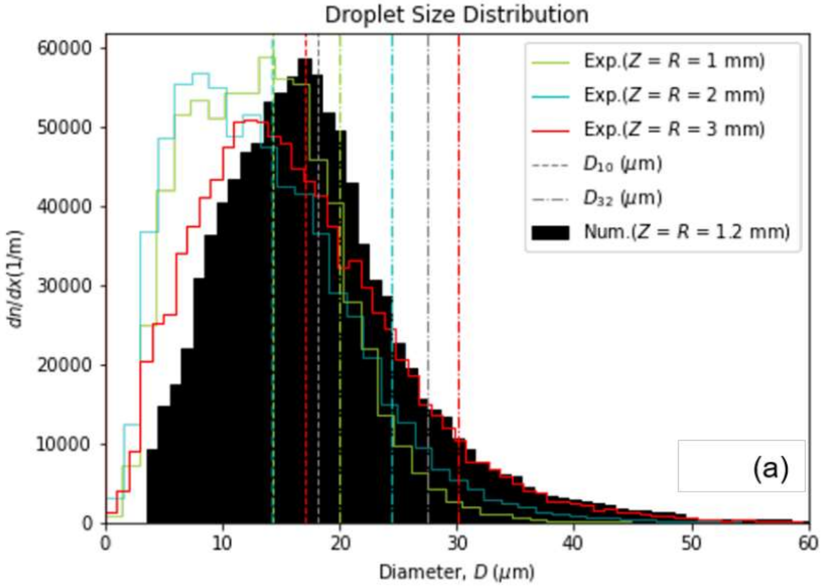


[1] Verdier. PhD Thesis, 2017
[2] Marrero. PhD Thesis, 2018
[3] Ferrando,D. PhDThesis, 2022

Curvature analysis ➔ drop size distribution







Beyond : Computation ⇔ Model

ELSA

Generalized liquid-gas flows:

1) Single flow with two phase
2) Turbulent liquid flux
3) Surface density
4) Switch to Blobs / Droplets

WBE

Blobs / Droplets : Multiphase flow

1) Carrier Phase and Discrete phase
2) Liquid and Gas velocity
3) Droplet radius

Most Used : "Lagrangian method"
J. K. Dukowicz, 1980.
Eulerian method available also :
Multiphase, sectional, Qmom,…

WBE: Williams-Boltzmann equation kinetic approach

ELSA : Eulerian Lagrangian Spray Atomization

Principles of the approach

A. Vallet and R. Borghi, *Modélisation Eulerienne de L'atomisation d'un Jet Liquide. C. R. Acad. Sci., Paris, Sér. II b,* ***327: p. 1015–1020, 1999***

First application to Co-axial injector

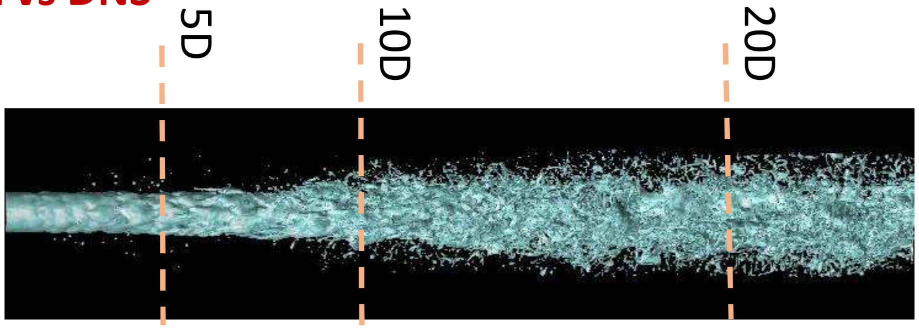
A. Vallet, A.A. Burluka, and R. Borghi, *Development of a Eulerian model for the "Atomization" of a liquid jet. Atomization and Sprays,* ***11(6): p. 619-642, 2001***

First transition to Lagrangian ➔ name ELSA

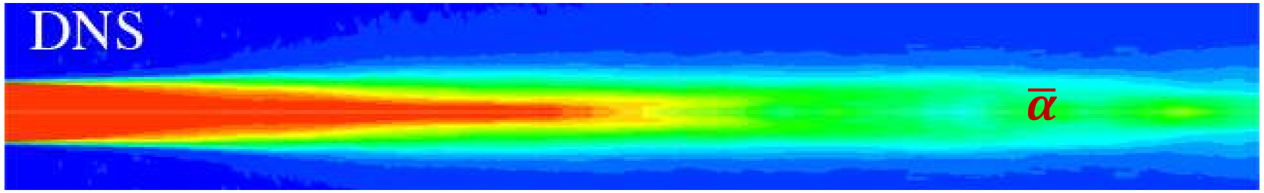
G. Blokkeel, R. Borghi, and B. Barbeau, *A 3d Eulerian model to improve the primary breakup of atomizing jet. SAE Technical Papers,* ***2003-01-0005, 2003***

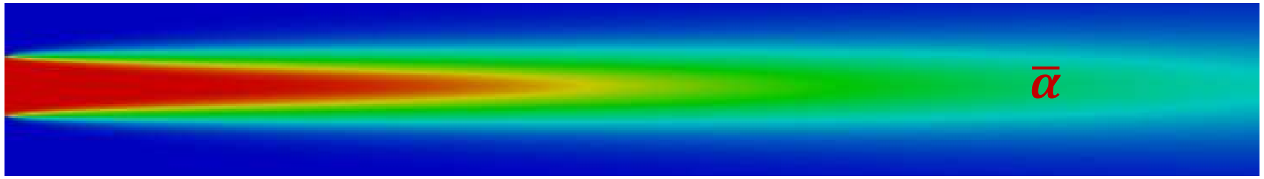
Turbulent liquid flux: Drift/Diffusion

Validation vs DNS

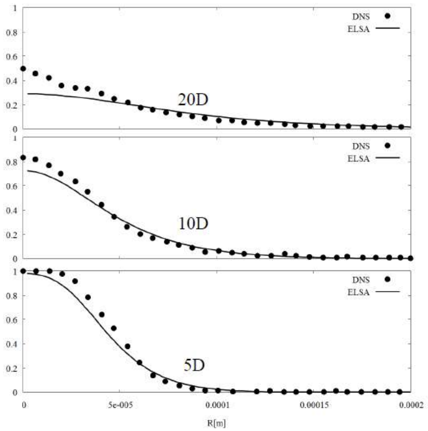


⇨ Mean liquid volume fraction $\bar{\alpha}$





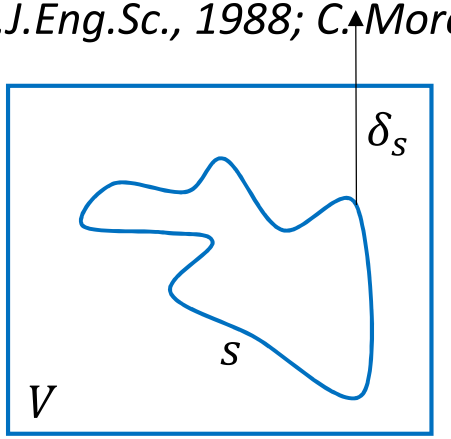
$\bar{\alpha}$



FX Demoulin, Foam extend workshop, 2014

Liquid-Gas Surface Density : $\Sigma = \frac{area}{volume}\ [m^{-1}]$

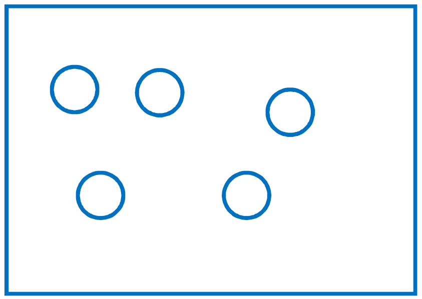
Material surface carried by turbulence *[D. Drew, SIAM J. Appl. Math., 1990; S.B. Pope, Int.J.Eng.Sc., 1988; C. Morel, IJMF, 2007]:*



δ_S : Dirac generalized function at the interface

$$\Sigma = \frac{\iiint_V \delta_S dv}{V}$$

$$\Sigma\, \bar{\varphi}\Big|_{\Sigma} = \iiint_V \delta_S \varphi\, dv$$



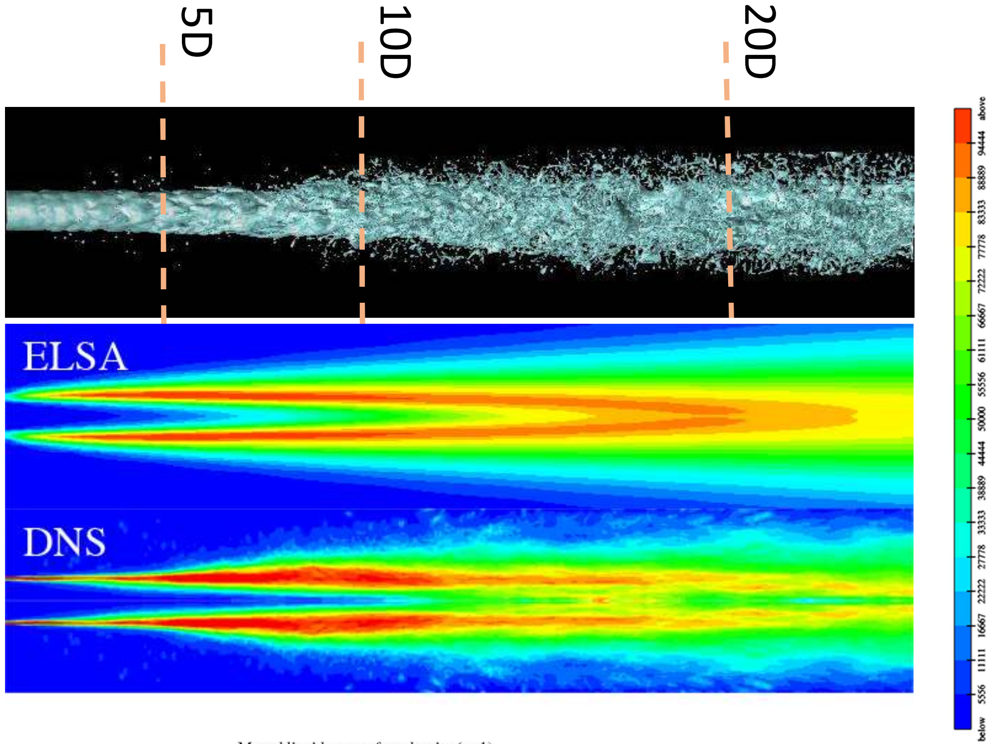
$$\mathrm{D} = \frac{6\alpha}{\Sigma} \rightarrow L_{32} = \boxed{D_{32} = \frac{6\alpha(1-\alpha)}{\Sigma}}$$

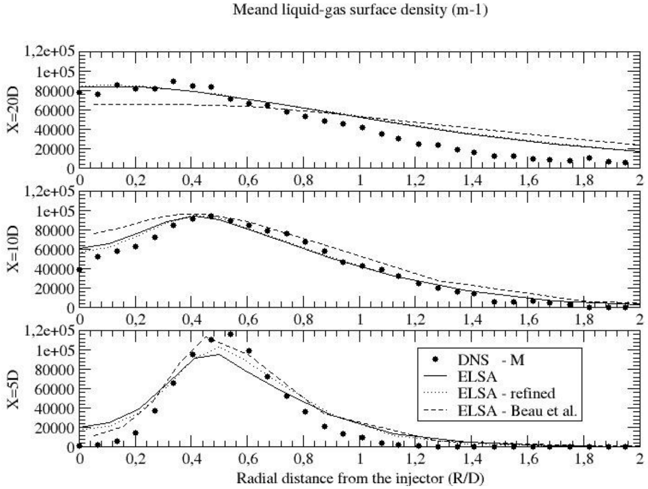
The Sauter mean diameter

Surface density equation ?

$$\frac{\partial \Sigma}{\partial t} + \nabla . \bar{u}\Sigma = \nabla . \underbrace{\left(\bar{u}\Sigma - \overline{u\delta_S}\right)}_{\overline{R_\Sigma}} + source\ terms = \nabla . \Sigma(\bar{u} - \bar{u}|_{\Sigma}) + source\ terms$$

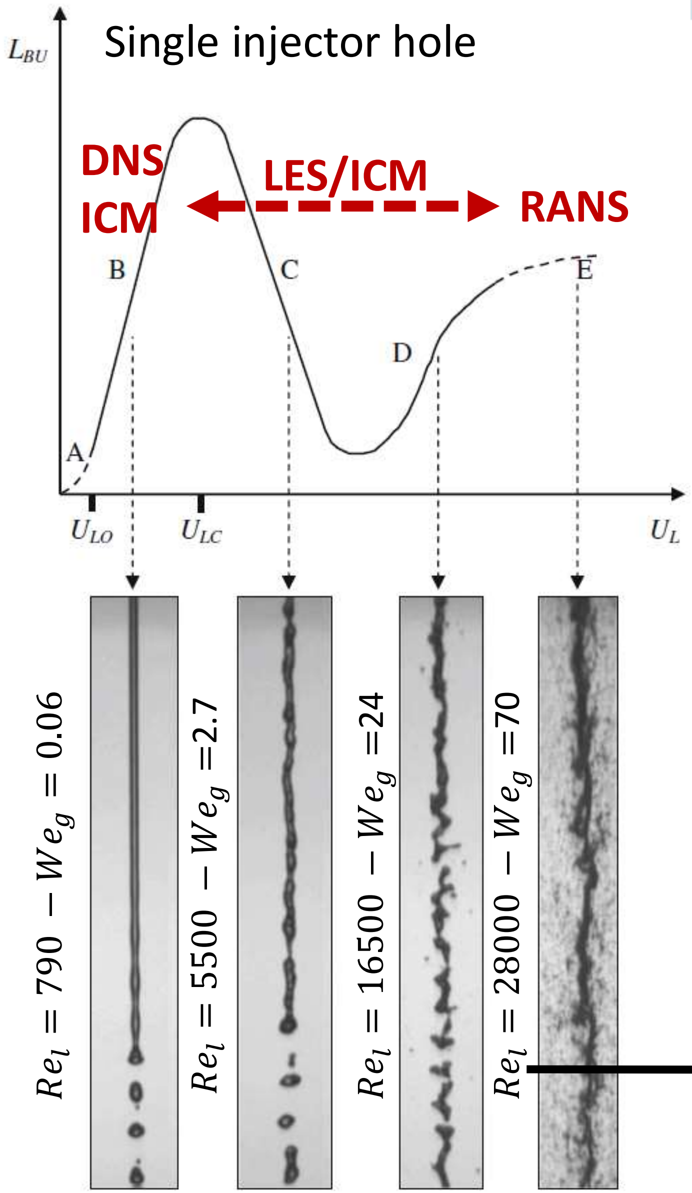
Overall DNS Validation: postulated equation for Σ





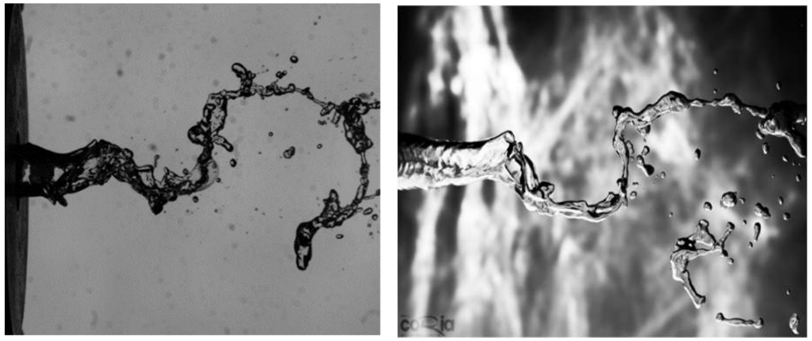
LES and ICM

Single injector hole



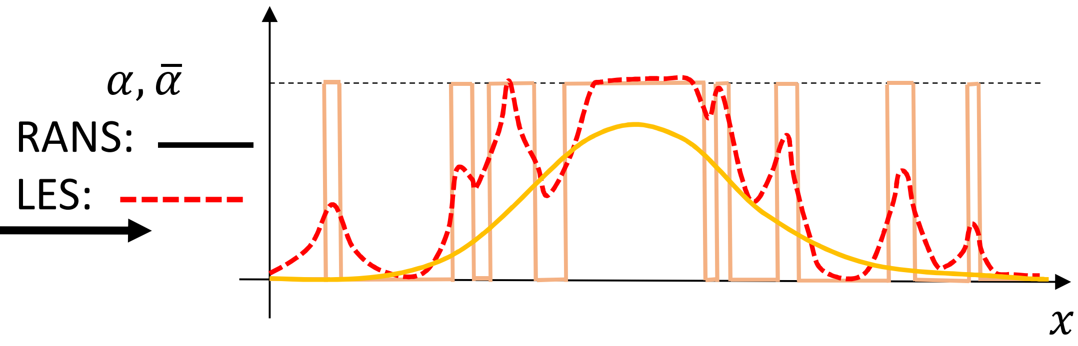
C. Dumouchel,2008

- DNS and ICM ➔ Amazing results



CORIA Berlemont A., Ménard T. et al.

- RANS: $\bar{\alpha}$ is mean, average
- LES: $\bar{\alpha} = \iiint \alpha(x,t) K_\Delta(x - x_0, t)\, dv$

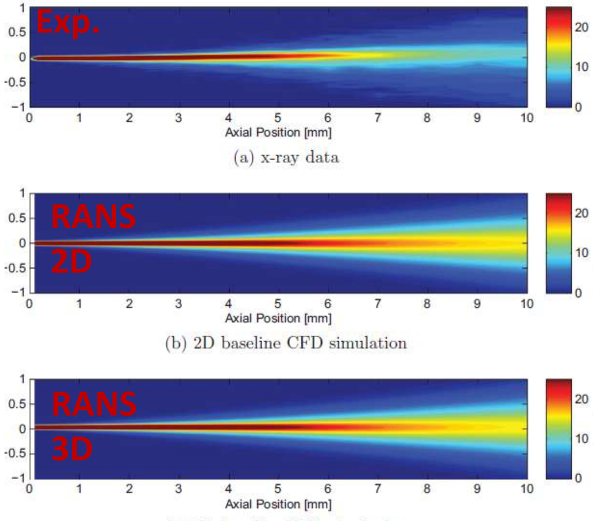


Experimental validations:

X-Ray: PMD, ECN spray A

CMT, U-Mass

- Mass formulation : $\widetilde{\boldsymbol{Y}}, \widetilde{\boldsymbol{R_Y}}$
- $C_{\varepsilon 1} = 1.44 \rightarrow 1.60$
- $Sc_t = 0.9$



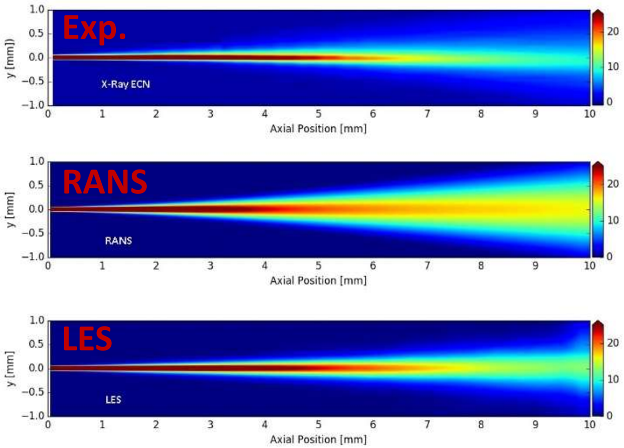
(a) x-ray data

(b) 2D baseline CFD simulation

(c) 3D baseline CFD simulation

CORIA

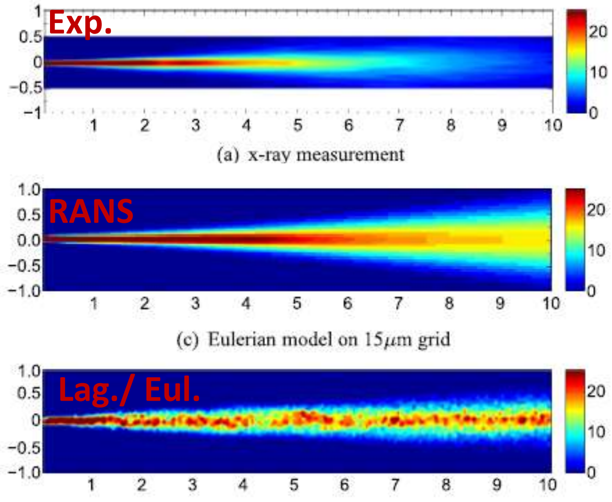
- Vol. formulation : $\overline{\boldsymbol{\alpha}}, \overline{\boldsymbol{R_\alpha}}$
- $C_{\varepsilon 1} = 1.44 \rightarrow 1.60$
- $Sc_t = 1.0$



Argonne, Convergent Science, U-Mass

- Mass formulation : $\widetilde{\boldsymbol{Y}}, \widetilde{\boldsymbol{R_Y}}$
- $C_{\varepsilon 1} = 1.44 \rightarrow 1.60$
- $Sc_t = 0.9$

Q. Xue et al., IJMF, 2015



(a) x-ray measurement

(c) Eulerian model on 15μm grid

(d) Lagrangian model

LES

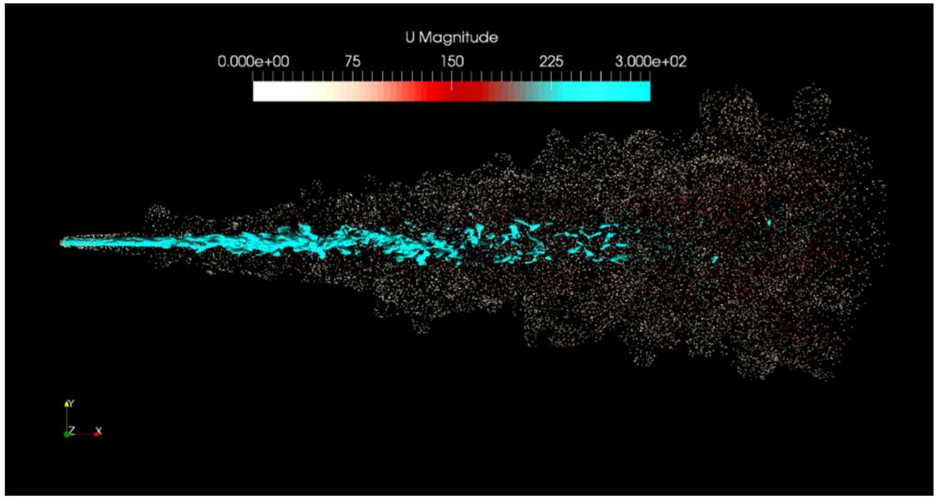
- CMT- Mass formulation *(J.M. Desantes et al., ILASS 2017)*
- CORIA –Volume formulation *(J. Anez et al., ILASS 2017)*

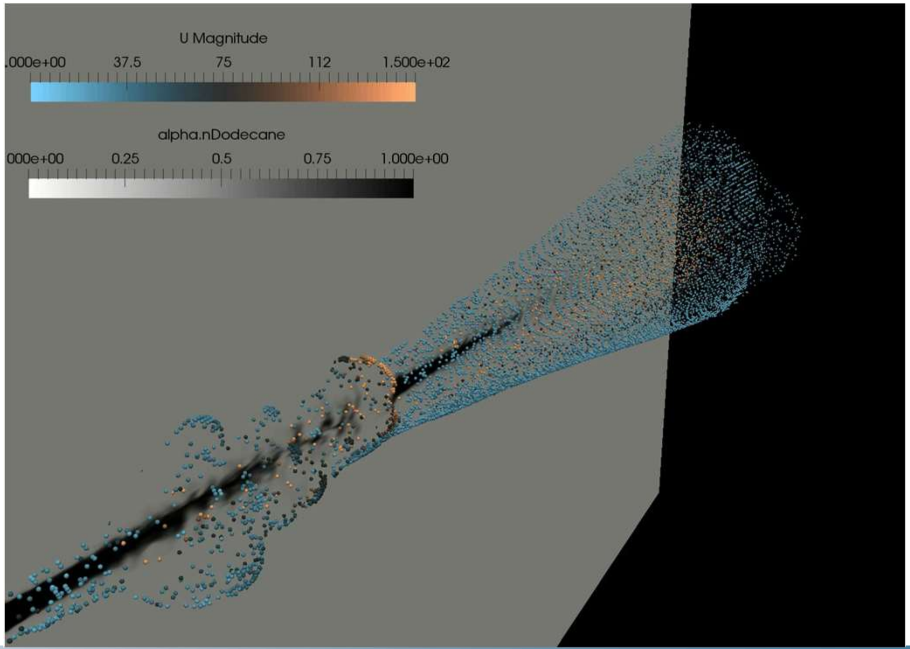
Transfering Eulerian α, Σ to Lagrangian approach (WBE + Monte Carlo)

Acknowledgments:
CPU's resource center: GENCI, TGCC, CINES, IDRIS, CRIHAN

Industrial support: Renault, PSA Peugeot Citroën, CONTINENTAL, Safran, AVL, Vinci Technologies, INERIS, …

Region Normandie
European MARIE CURIE ITN "HAoS"



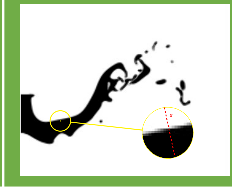
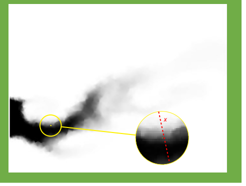


Some dust under the carpet …

or

Opportunities/needs to establish more firmly the different approaches

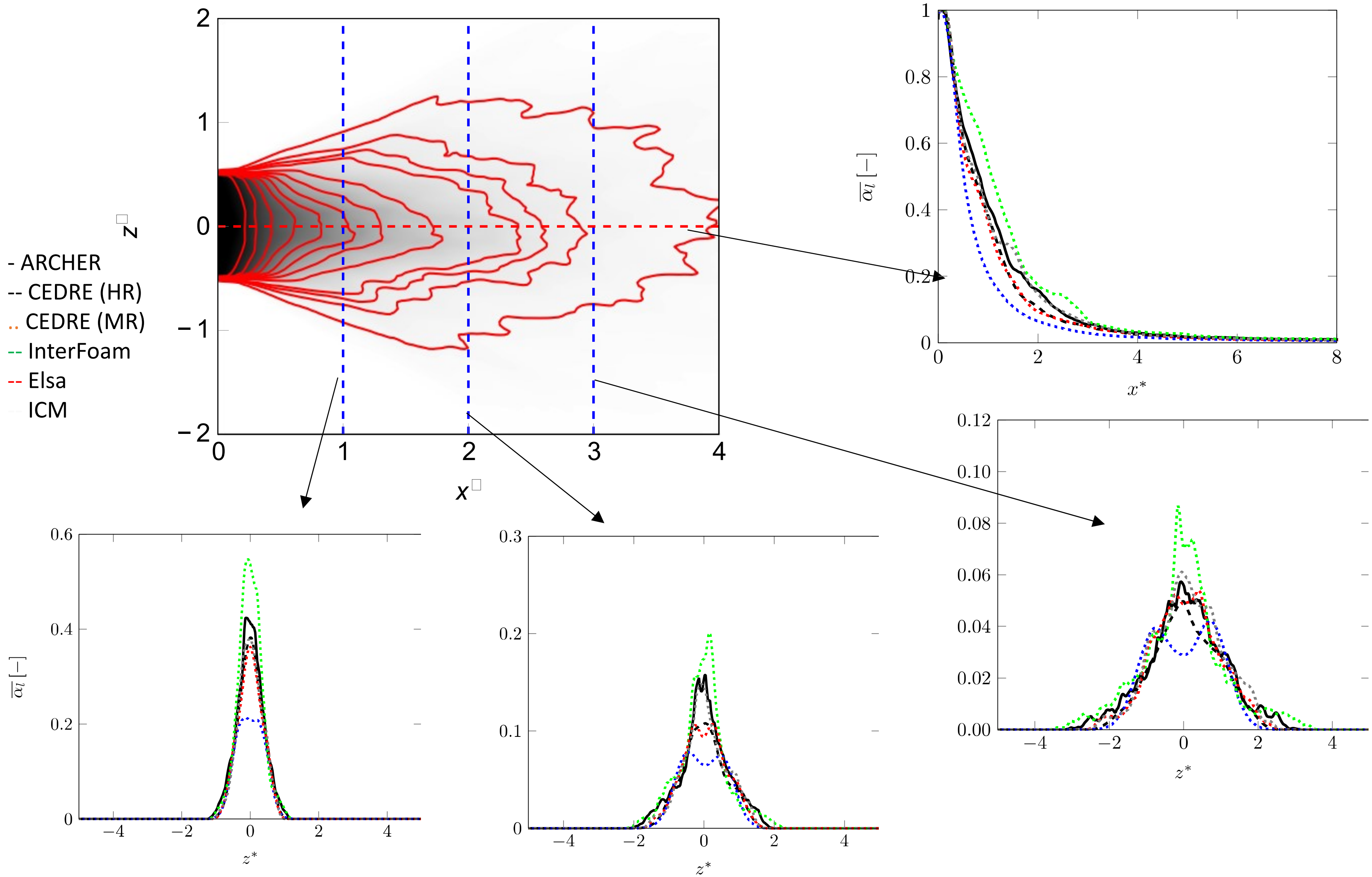
1) ICM: So many approaches : properties, rules ?

Method	Separated  Diffused 
ARCHER	Separated
interFoam	Diffused at Δ_x
CEDRE	Diffused
Elsa	Diffused phy-model
IcmElsa	Separated/diffused

Dynamic well reproduced by all the models.
Differences mainly in the small features.

PhD A. Remiggi, 2021, P. Cordesse *et al.*, *Flow Turbulence Combust*, 2020

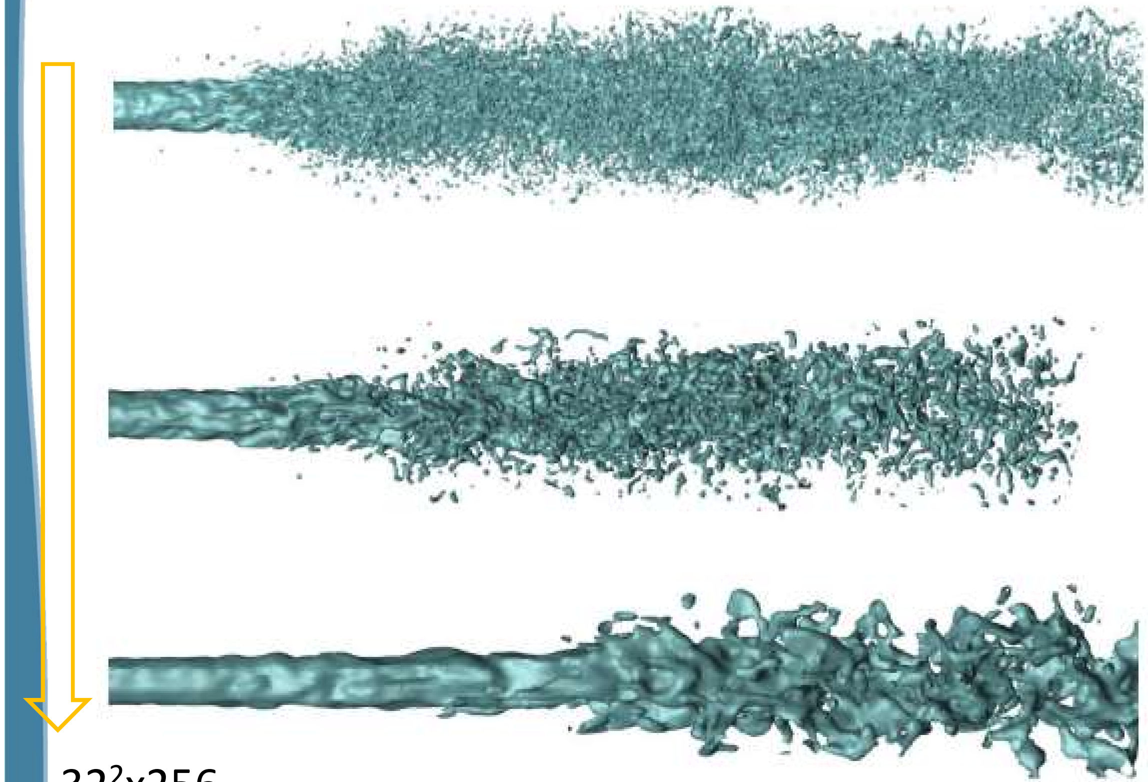
Global agreement, but noticeable differences : mean $\overline{\alpha}$



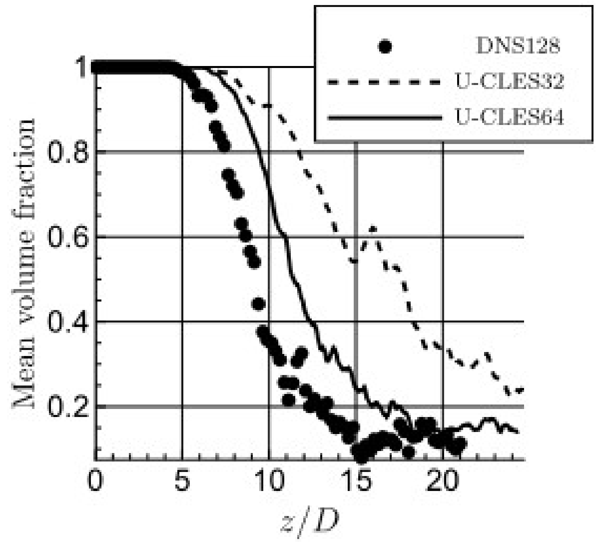
More pronounced : small scales features, variance, Σ, …

2) Under resolution effect – subgrid models ?

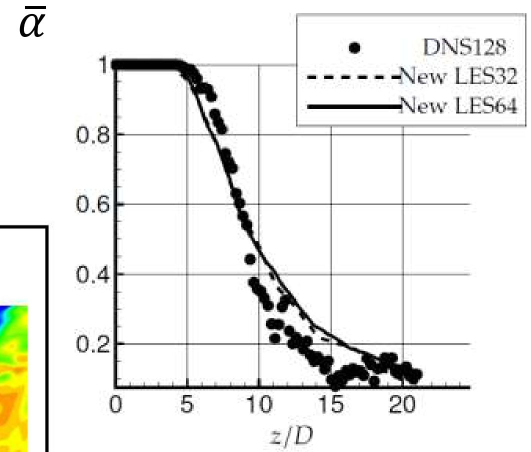
128^2x1024



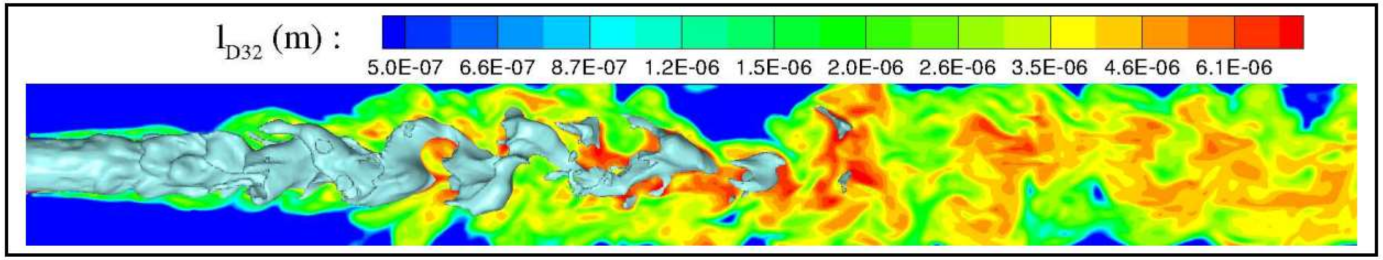
32^2x256



Low resolution → Low dispersion



J. Chesnel, et *al.*, *Large eddy simulation of liquid jet atomization.* Atomization and Sprays, **21**(9): p. 711-736, 2011



3) Subgrid turbulent liquid flux $\overline{R_\alpha}$

Mass formulation :

$$\frac{\partial \bar{\rho}\tilde{Y}}{\partial t} + \nabla.\bar{\rho}\tilde{u}\tilde{Y} = \nabla.\bar{\rho}\underbrace{\left(\tilde{u}\tilde{Y} - \widetilde{uY}\right)}_{\widetilde{R_Y}} = \nabla.\bar{\rho}\tilde{Y}(\tilde{u} - \bar{u}|_l) = \nabla.\bar{\rho}\tilde{Y}(1-\tilde{Y})\left(\bar{u}|_l - \bar{u}|_g\right)$$

Volume formulation :

$$\frac{\partial \bar{\alpha}}{\partial t} + \nabla.\overline{u\alpha} = \nabla.\underbrace{\left(\bar{u}\,\bar{\alpha} - \overline{u\alpha}\right)}_{\overline{R_\alpha}} = \nabla.\bar{\alpha}(\bar{u} - \bar{u}|_l) = \nabla.\bar{\alpha}(1-\bar{\alpha})\left(\bar{u}|_l - \bar{u}|_g\right)$$

$\widetilde{R_Y}$ and $\overline{R_\alpha}$ are the turbulent liquid flux

1. **Correlation: Turbulent velocity/concentration**
2. **Slip motion between phase**

Single phase flows:

➔ Turbulent diffusion (1)

\+ Slip motion (2)

Multi phase flows:

➔ Slip motion (2)

\+ Drift motion (1)

P. Février and O. Simonin, VKI, 2000

Mass formulation : $\widetilde{R_Y} \approx \frac{\widetilde{\nu_t}}{Sc_t}\nabla\tilde{Y}$

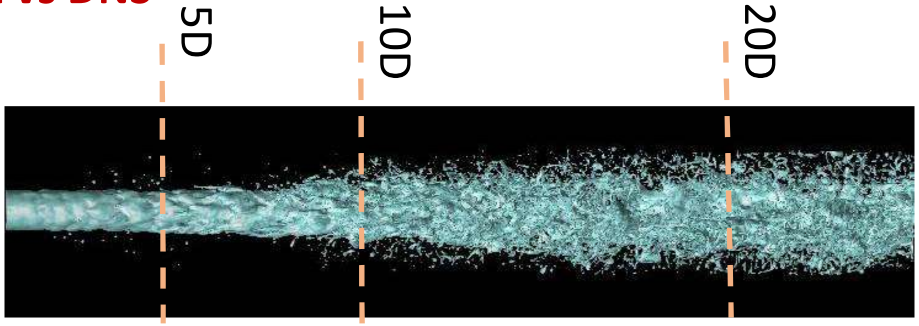
Volume formulation $\overline{R_\alpha} \approx \frac{\overline{\nu_t}}{Sc_t}\nabla\bar{\alpha}$

4) Mean or filter value : Density/Volume weighted

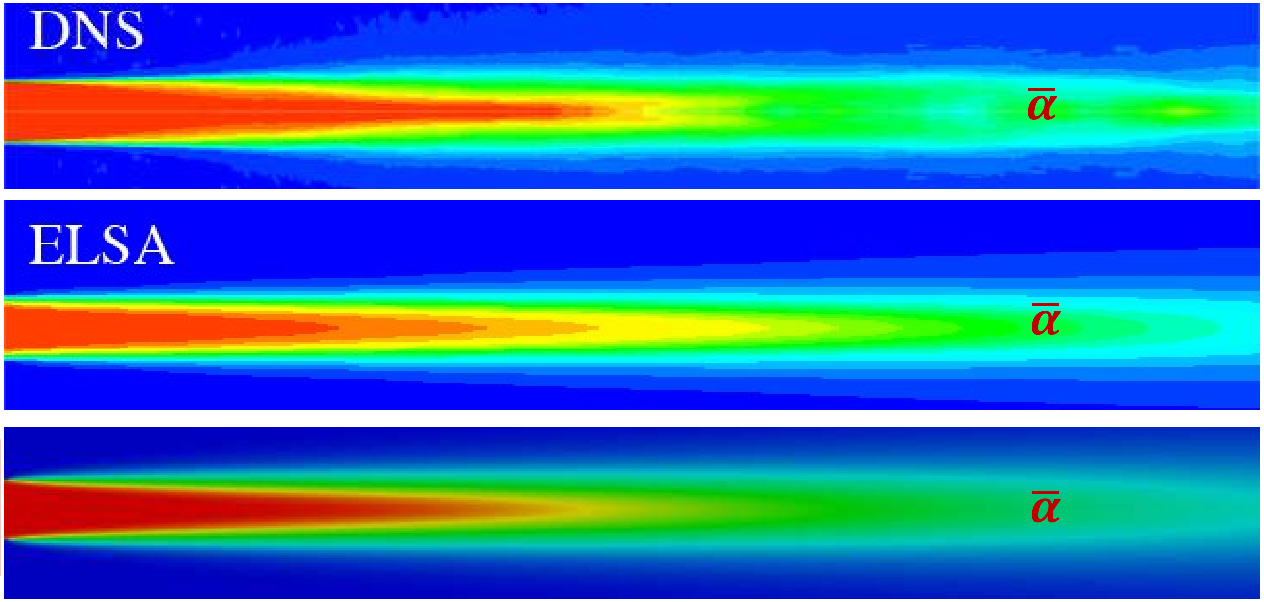
Example: Turbulent liquid flux

Mass formulation : $\widetilde{\boldsymbol{R}_{\boldsymbol{Y}}} \approx \frac{\widetilde{\nu_t}}{Sc_t} \nabla \widetilde{\boldsymbol{Y}}$ ⟷ Volume formulation $\overline{\boldsymbol{R}_{\boldsymbol{\alpha}}} \approx \frac{\overline{\nu_t}}{Sc_t} \nabla \overline{\boldsymbol{\alpha}}$

Validation vs DNS



⇨ Mean liquid volume fraction $\overline{\boldsymbol{\alpha}}$



$\widetilde{\boldsymbol{R}_{\boldsymbol{Y}}}$… Sc_t=1.0

R. Lebas et al. IJMF, 2009

$\overline{\boldsymbol{R}_{\boldsymbol{\alpha}}}$… Sc_t=0.7

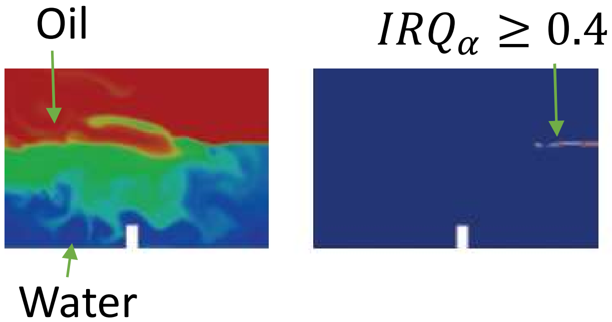
FX Demoulin, Foam extend workshop, 2014

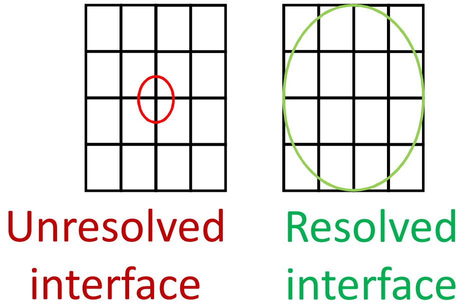
5) Interface Resolution Quality : Multi-Scale ELSA

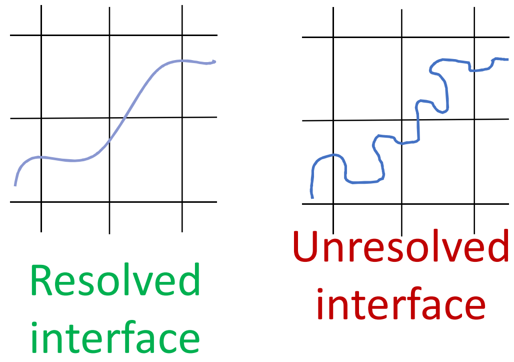
$$IRQ_\alpha = \frac{|\nabla\alpha|}{\max(|\nabla\alpha|)} \text{ [1]}$$

$$IRQ_\kappa = \frac{1}{\Delta x|\kappa|} \text{ [2]}$$

$$IRQ_\Sigma = \frac{\Sigma}{\Sigma_{min}} \text{ [3]}$$







[1]K. E. Wardle et H. G. Weller, *International Journal of Chemical,* 2013.
[2]R. Canu et al., *Atomization and Sprays*, 2020.
[3]Anez, J. *et al.*. *International Journal of Multiphase Flow* (2018)

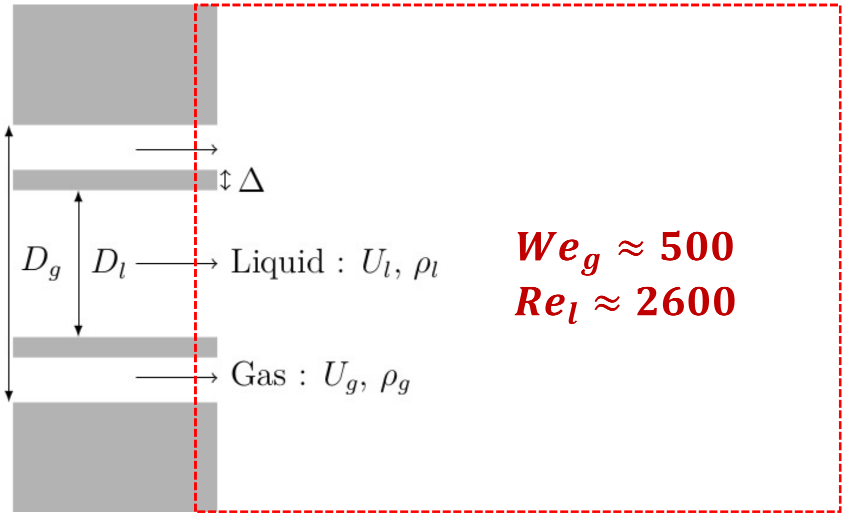
➔ **To switch between ICM and DI (diffused interface) based on IRQs**

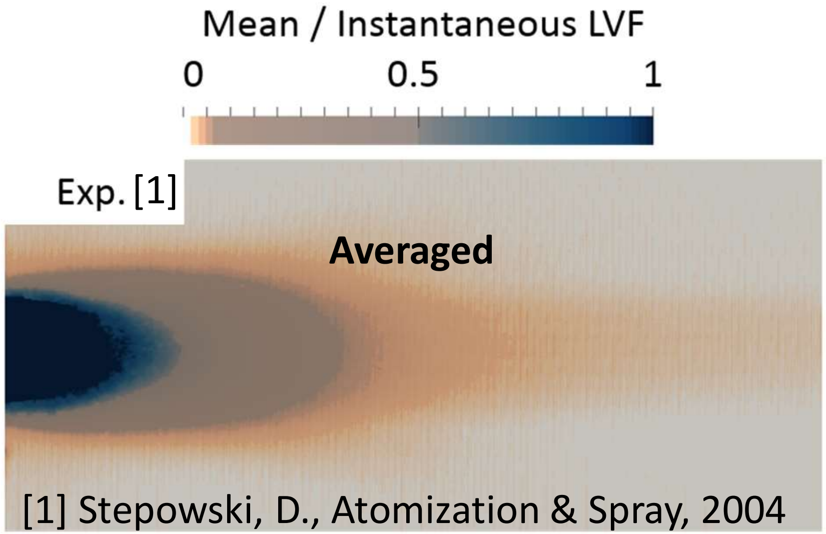
LES – Multi-Scale :

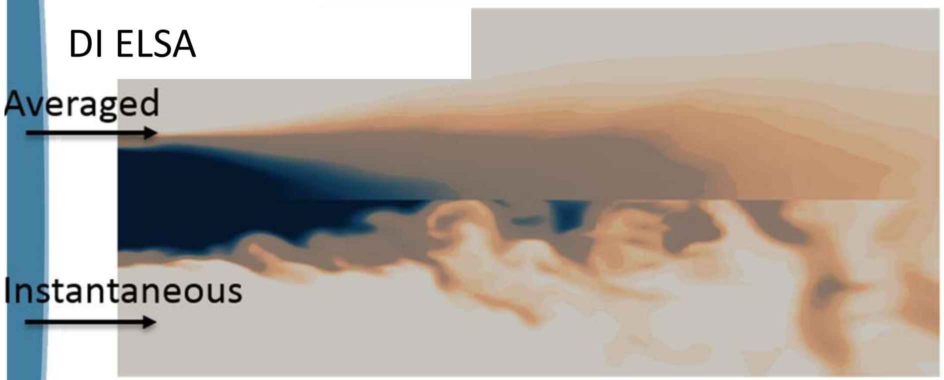
- LES-DI ⇔ LES-ICM
- IRQ: Interface Resolution Quality

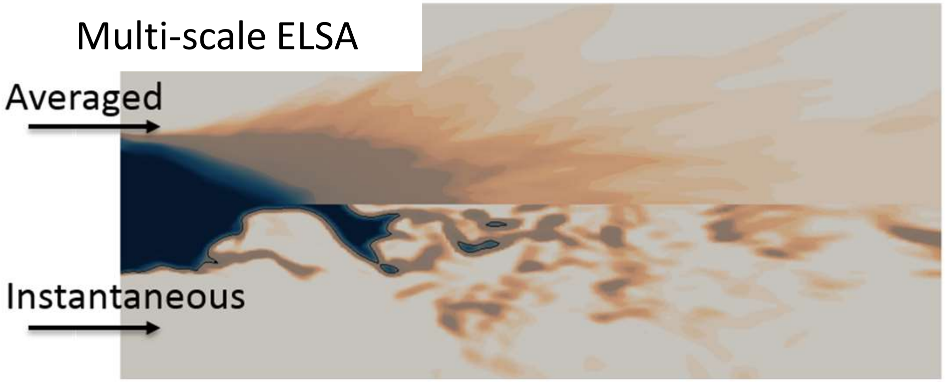
$$\frac{\partial\bar{\alpha}}{\partial t} + \frac{\partial\bar{u}_j\,\bar{\alpha}}{\partial x_j} + \underbrace{\frac{\partial C_\alpha u_{Cj}\bar{\alpha}(1-\bar{\alpha})}{\partial x_j}}_{\text{ICM}} = \underbrace{(1-C_\alpha)\frac{\partial \overline{R_{\alpha j}}}{\partial x_j}}_{\text{DI}}$$

Air-blast: Mean/Instantaneous LVF





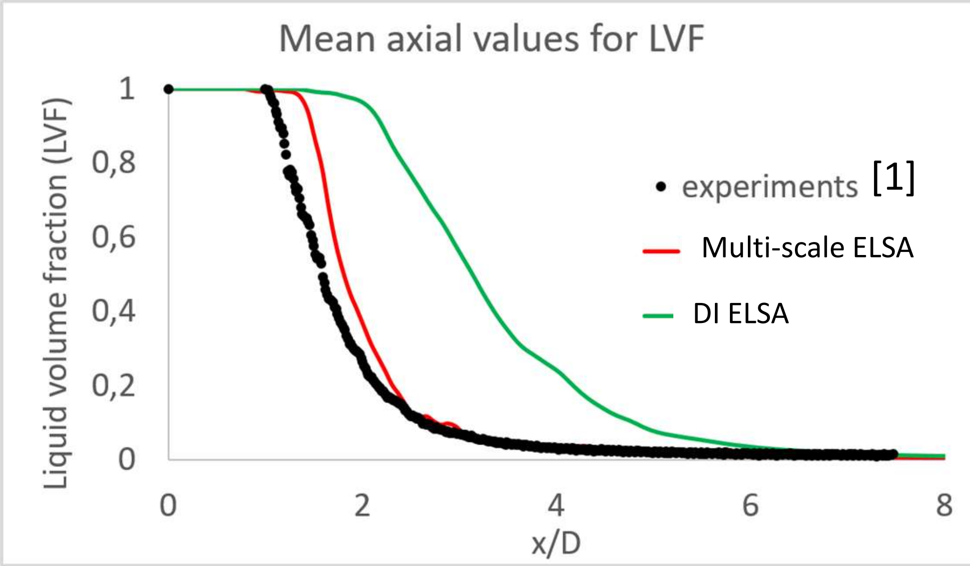


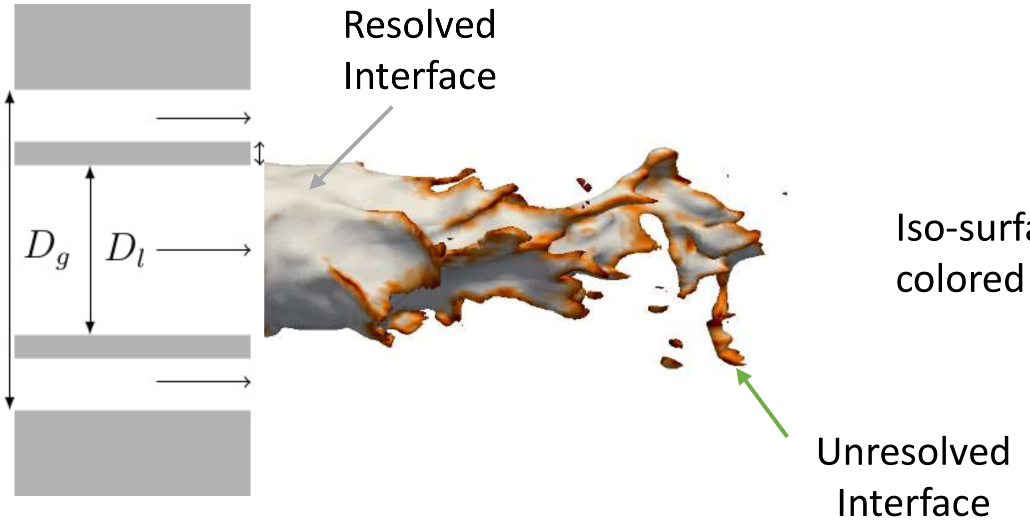


- **Unresolved approach,** is overpredicting the liquid penetration. Sub-grid modeling not addequate to represent the turbulence development delay.
- In this case of low Re and We number, the mesh resolution is suitable enough to capture some details near nozzle exit, compared with experiments.

Air-blast: Axial LVF profiles

- **Unresolved approach** is unadapted in this case,.
- Multi-scale model is able to adapt dynamically to the fluctuating field.



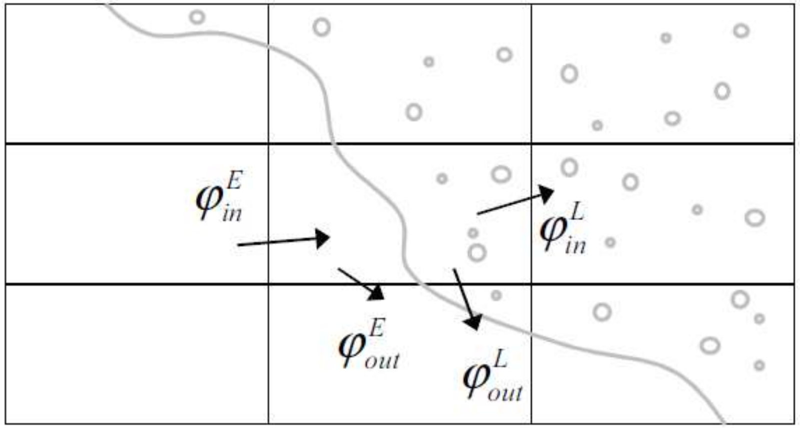


Iso-surface at 0.5 LVF, colored by C_α

6) From Euler to Lagrange (MC)

Direct switch at a dynamic boundary

Lagrange Only



Euler Only

Drawbacks:
Eulerian net flux
Lagrangian total flux
The boundary location is moving
Eulerian equation on the whole domain
Discard Lagrangian droplet in Euler Zone
Lagrangian statistic convergence

Using Both on the whole domain ?

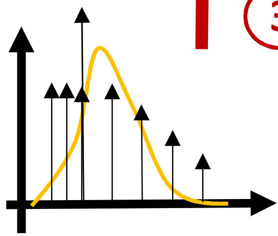
Euler: Known Moment Equations
$(\bar{\alpha}, \Sigma, \bar{u}, \bar{u}|_l, \bar{k})$

Lagrange:
Known stochastic sample

1

2

Improved spray distribution



3

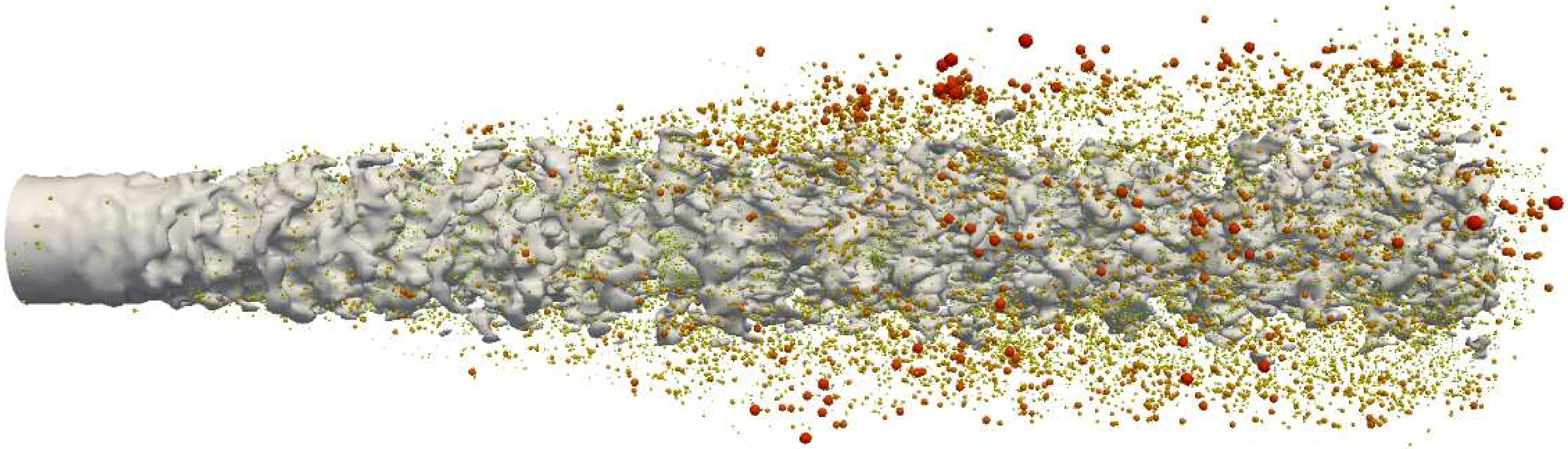
Improved source terms:
$(\dot{\bar{\alpha}}, \dot{\Sigma}, \dot{\bar{u}}, \dot{\bar{u}}|_l, \dot{\bar{k}})$

Correction Eq.

4

R. Lebas, et al., ASME,2006

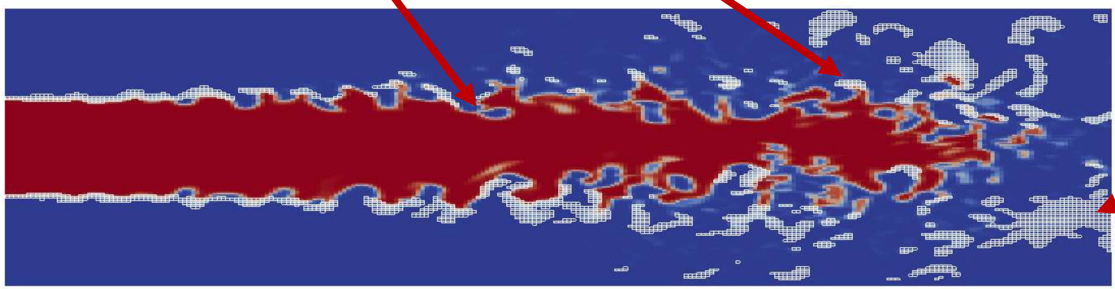
Multi-scale ELSA + Lagrange
Dynamic adaptive numerical methods



Resolved Interface

Under Resolved Interface

Subgrid Spray



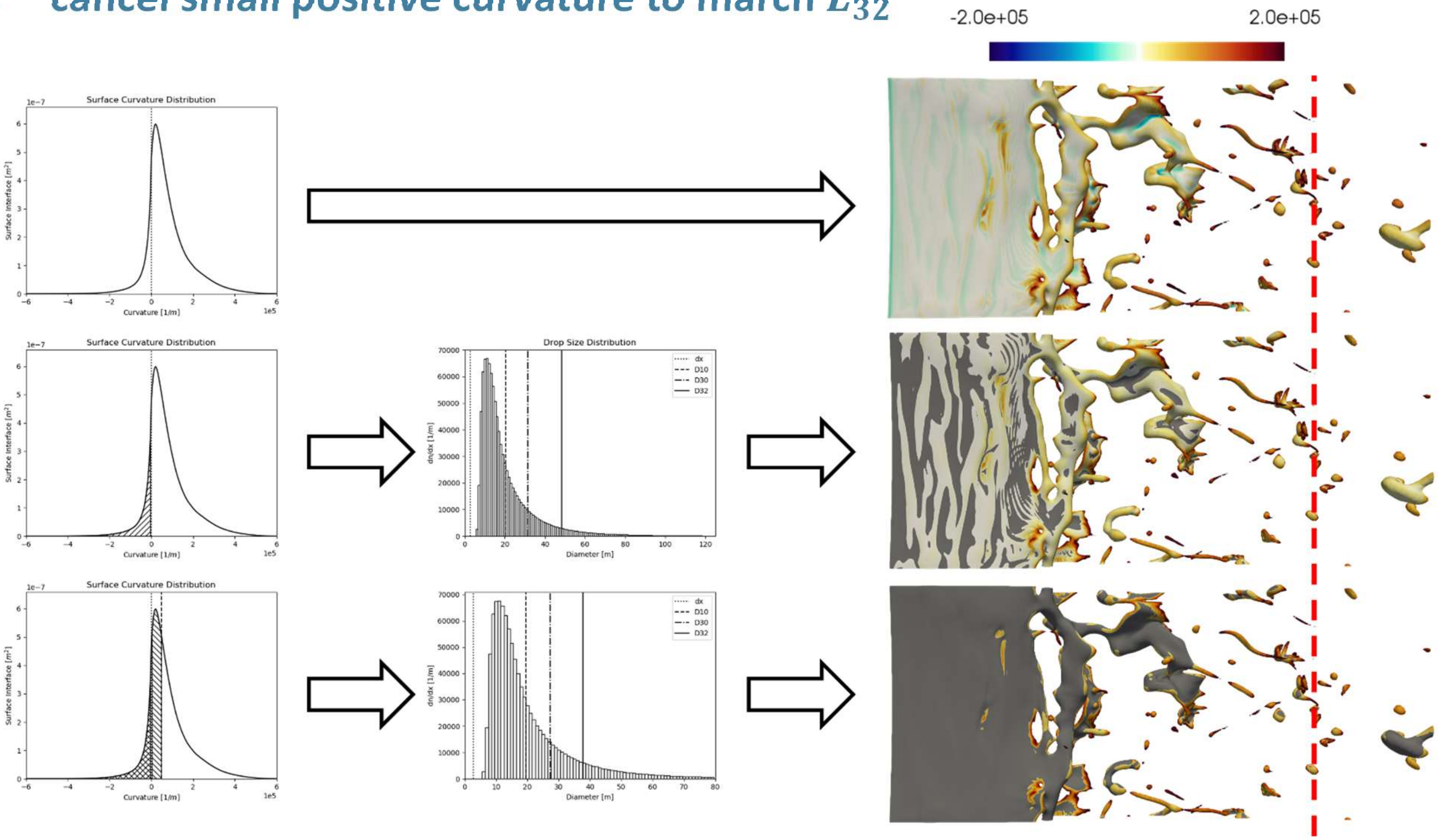
To be continued ….

7) Curvature Analysis to drop size distribution

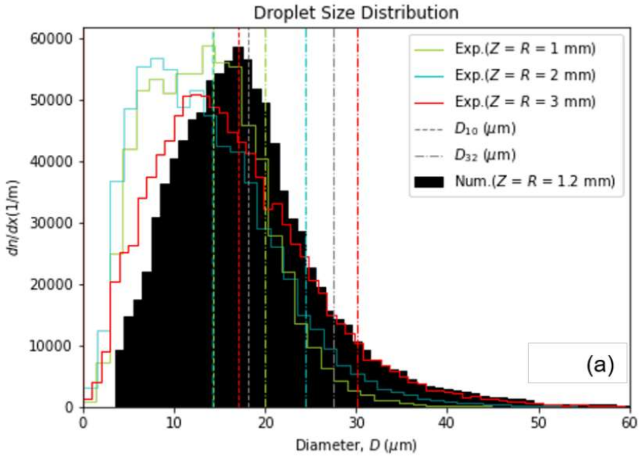
a) Compute surface and curvature

b) Discard negative curvatures

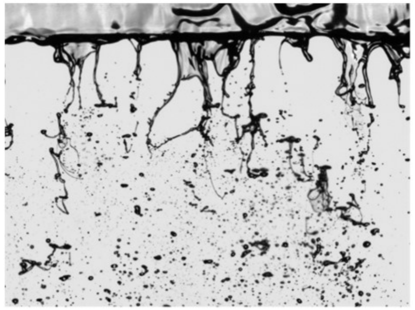
c) *cancel small positive curvature to march* L_{32}

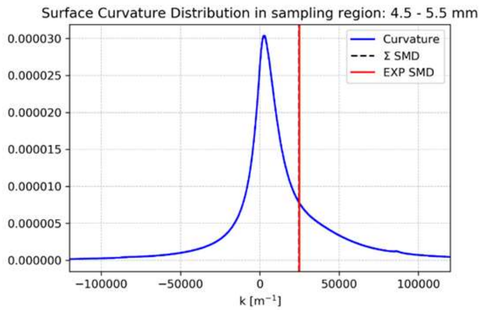


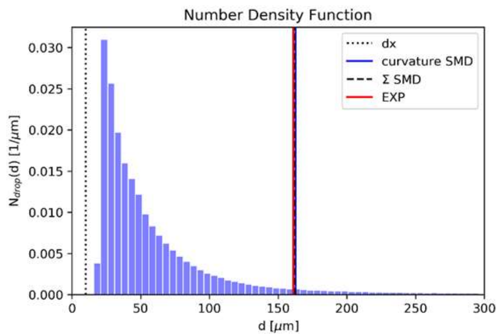
Curvature analysis ➔ drop size distribution



Gepperth, S et al , ICLASS 2012
Chaussonnet, G. et al., IJMF, 2016







	Num.	Exp.
D_{32}	161	161.9
D_{10}	56.80	58.35
D_{30}	97.55	97.49

Many open issues 1,2,3,4,5,6,7 …

Open for discussion, suggestion, help …

demoulin@coria.fr