CURRICULUM: SCIENCES AND TECHNOLOGIES FOR AERONAUTICS AND SATELLITE APPLICATIONS (STASA)

SIMULATION AND MODELLING TURBULENT SPRAY DYNAMICS

Year I: Turbulent Spray Evaporation Modelling

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DATE: 12/09/2019

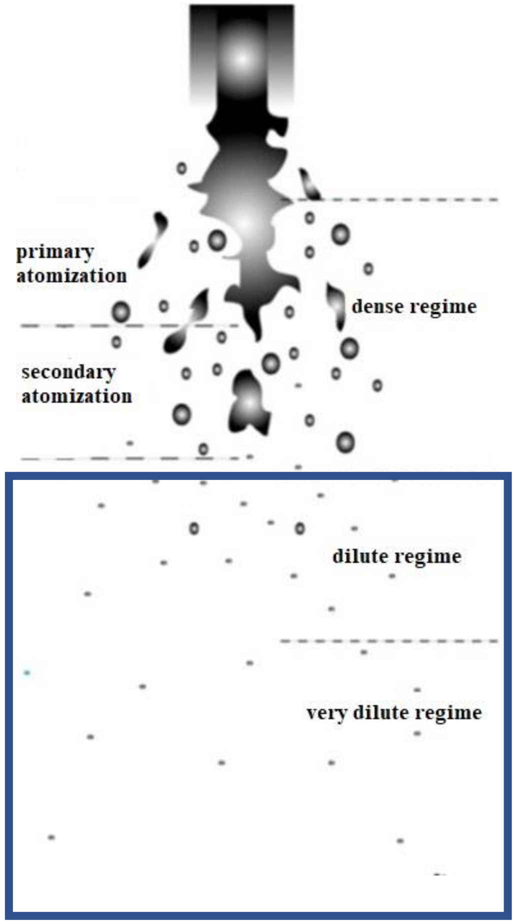
Spray Evaporation & Combustion

- A **chaotic multiphase** and **multiscale** flow where chemical reactions occur together with phase exchange during combustion:
  - Physical phenomena: evaporation, mixing and combustion
  - Turbulence : unsteady, irregular, random and chaotic
  - Multiphase: gas, liquid (and solid)
  - Multiscale: From submicron (e.g. reaction) to meter size turbulent motion

- It plays an important role both in nature and technology:
  - **Industrial application**: Clean and efficient internal combustion engine
  - **Natural phenomena**: Dust storms, sediment transport in rivers, flash clouds and volcanic ash dispersion in the atmosphere

- A satisfactory comprehension of turbulent spray dynamics, considering evaporation and combustion, has not yet been achieved
- The capabilities of existing models of reproducing these phenomena are still limited

Modelling Regime description



- ❑ Liquid jet break-up : K-H & R-T instabilities
- ❑ Collision and coalescence
- ❑ Low evaporation rates
- ❑ 4-way coupling method

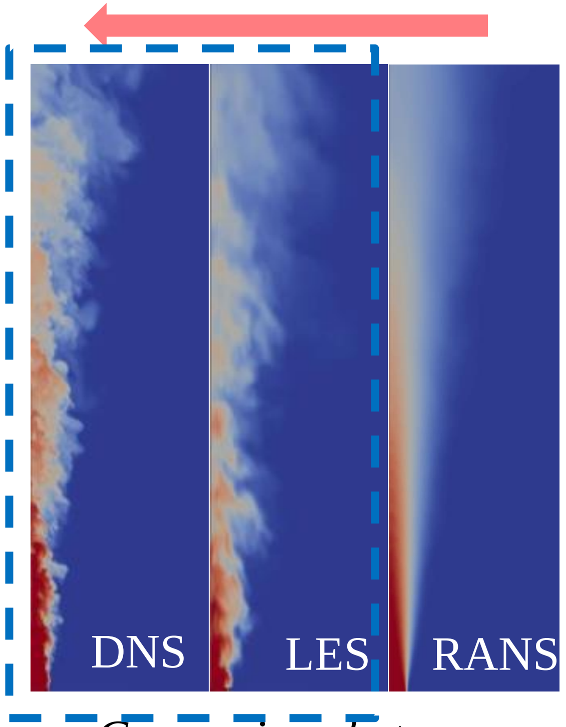
- ❑ Dispersed droplets: **Point-droplet approximation**
- ❑ **No break-up** : surface tension >> aerodynamic forces
- ❑ **No collision / coalescence** : low volume fraction ($\Phi < 10^{-3}$)
- ❑ 2-way coupling method
- ❑ **Main region occurring evaporation and combustion**

Jenny et al. PECS 2012

Numerical methods for turbulent flow and combustion

Flow		Combustion	
DNS (Direct Numerical Simulation) : **No model**	→	Detailed Chemical Mechanism (Hundred of species with thousands of reaction steps)	Research tool
LES (Large Eddy Simulation): **Model in small scales**	→	Reduced Chemical Mechanism (Species below 100)	
RANS (Reynolds-average Navier-Strokes): **Model in all scales**	→	Various Combustion Model (e.g. CMC, PDF, FGM……)	Industry application

Increase in resolution & computational cost

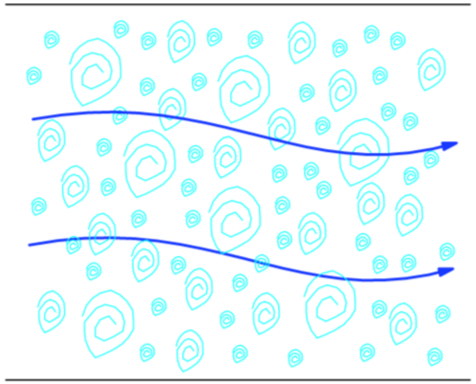


Comparison between numerical methods for flow

- Higher the jet speed, i.e. the Reynolds number Re=Ud/n, more expensive are the simulations
- Our idea is to advance the current understanding of spray dynamics with DNS approach, then develop and optimize proper model for this complex phenomena in the framework of LES
- We applied for computational resources on CINECA via ISCRA C application, and a budget of 360000 core hours on Marconi cluster has been granted.

Description of DNS & LES

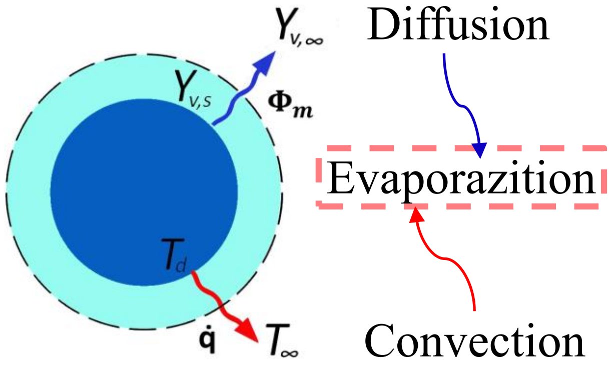
Flow field in DNS



Eulerian gas Phase

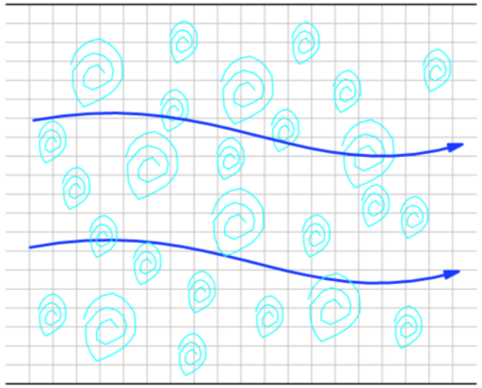
$\mathbf{u}$, Y_v, T →

← Source term



Lagrangian dispersed phase

Filter: $G_\Delta(\mathbf{x}, \boldsymbol{r})$



Flow field in LES

$\mathbf{u}$

Resoloved component:

$$\tilde{\mathbf{u}} = \int \mathbf{u} G_\Delta(\mathbf{x}, \boldsymbol{r}) d\boldsymbol{r}$$

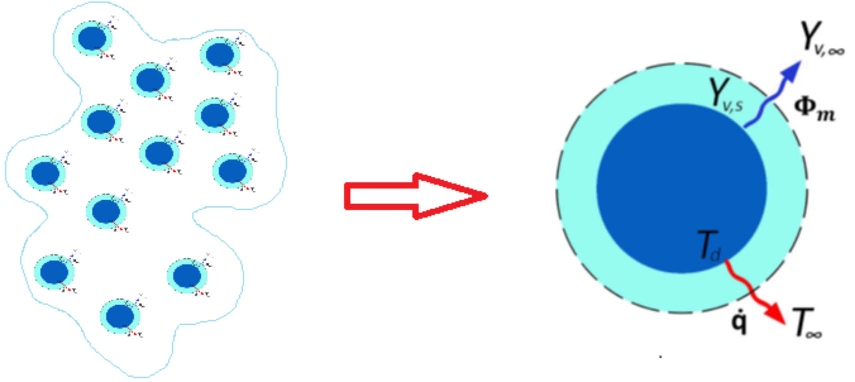
Favre filtering:

$$\tilde{\mathbf{u}} = \frac{\overline{\rho \mathbf{u}}}{\bar{\rho}}$$

Subgrid component:

$$\mathbf{u}' = \mathbf{u} - \tilde{\mathbf{u}}$$ (Need modeling)

Representative model for droplets



A cluster of droplets are represented by one "parcel"

Numerical Method - DNS

Eulerian Gas Phase (Low Mach Navier- Stokes)	**Lagrangian dispersed phase (Point-droplet equations)**
$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = S_m$	$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d$
$\frac{\partial}{\partial t}(\rho Y_V) + \nabla \cdot (\rho Y_V \mathbf{u}) = \nabla \cdot (\rho \mathcal{D} \nabla Y_V) + S_m$	$\frac{d\mathbf{u}_d}{dt} = \frac{(\mathbf{u} - \mathbf{u}_d)}{\tau_d}\left(1 + 0.15\mathrm{Re}_d^{0.687}\right)$
$\frac{\partial}{\partial t}(\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = \nabla \cdot \boldsymbol{\sigma} - \nabla P + S_P$	$\frac{dr_d^2}{dt} = -\frac{\mu_g}{\rho_l}\frac{\mathrm{Sh}}{\mathrm{Sc}}\ln(1 + B_m)$
$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho E \mathbf{u}) = -\nabla P \mathbf{u} + \nabla \cdot (\boldsymbol{\sigma} \otimes \mathbf{u}) - \nabla q + S_e$	$\frac{dT_d}{dt} = \frac{\mathrm{Nu}}{3\mathrm{Pr}}\frac{c_{p,g}}{c_{p,l}}\frac{T - T_d}{\tau_d} + \frac{L_v}{c_{p,l}}\frac{\dot{m}_d}{m_d}$

2-way coupling terms

$$S_m = -\sum_{i=1} \frac{dm_{d,i}}{dt}\delta(\mathbf{x} - \mathbf{x}_{d,i})$$

$$S_e = -\sum_{i=1} \frac{d}{dt}(m_{d,i} c_{p,l} T_{d,i})\,\delta(\mathbf{x} - \mathbf{x}_{d,i}) \qquad S_p = -\sum_{i=1} \frac{d}{dt}(m_{d,i}\mathbf{u}_{d,i})\,\delta(\mathbf{x} - \mathbf{x}_{d,i})$$

More details: Miller R.S., et al. J. Fluid Mech. (1999) & Mashayek F., Int. J. Heat Mass Transf.(1998) & Bukhvostova A. et al., J. Comp. Phys. (2015)

Numerical Method - LES

Eulerian Gas Phase (Low Mach Navier- Stokes)	**Lagrangian dispersed phase (Point-droplet equations)**
$\frac{\partial \bar{\rho}}{\partial t} + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}}) = \bar{S}_m$	$\frac{d\mathbf{x}_d}{dt} = \mathbf{u}_d$
$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_V) + \nabla \cdot (\bar{\rho}\tilde{Y}_V\tilde{\mathbf{u}}) = \nabla \cdot (\bar{\rho}\tilde{\mathrm{D}}\nabla\tilde{Y}_V) - \nabla q_{Y_V} + \bar{S}_m$	$\frac{d\mathbf{u}_d}{dt} = \frac{(\tilde{\mathbf{u}} - \mathbf{u}_d)}{\tau_d}(1 + 0.15\mathrm{Re}_d^{0.687}) + \chi$
$\frac{\partial}{\partial t}(\bar{\rho}\tilde{\mathbf{u}}) + \nabla \cdot (\bar{\rho}\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}) = \nabla \cdot \bar{\boldsymbol{\sigma}} - \nabla \cdot \boldsymbol{\tau}^R - \nabla\bar{P} + \bar{S}_P$	$\frac{dr_d^2}{dt} = -\frac{\bar{\mu}_g}{\rho_l}\frac{\mathrm{Sh}}{\mathrm{Sc}}\ln(1 + B_m)$
$\frac{\partial}{\partial t}(\bar{\rho}\tilde{e}) + \nabla \cdot (\bar{\rho}\tilde{e}\tilde{\mathbf{u}}) = -\nabla\overline{P\mathbf{u}} + \nabla \cdot \overline{(\boldsymbol{\sigma} \otimes \mathbf{u})} - \nabla\bar{q} - \nabla q_e + \bar{S}_e$	$\frac{dT_d}{dt} = \frac{\mathrm{Nu}}{3\mathrm{Pr}}\frac{\bar{c}_{p,g}}{c_{p,l}}\frac{T - T_d}{\tau_d} + \frac{L_v}{c_{p,l}}\frac{\dot{m}_d}{m_d}$

$$\bar{S}_m = \int S_m G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r} \qquad \bar{S}_e = \int S_e G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r} \qquad \bar{S}_p = \int S_p G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r}$$

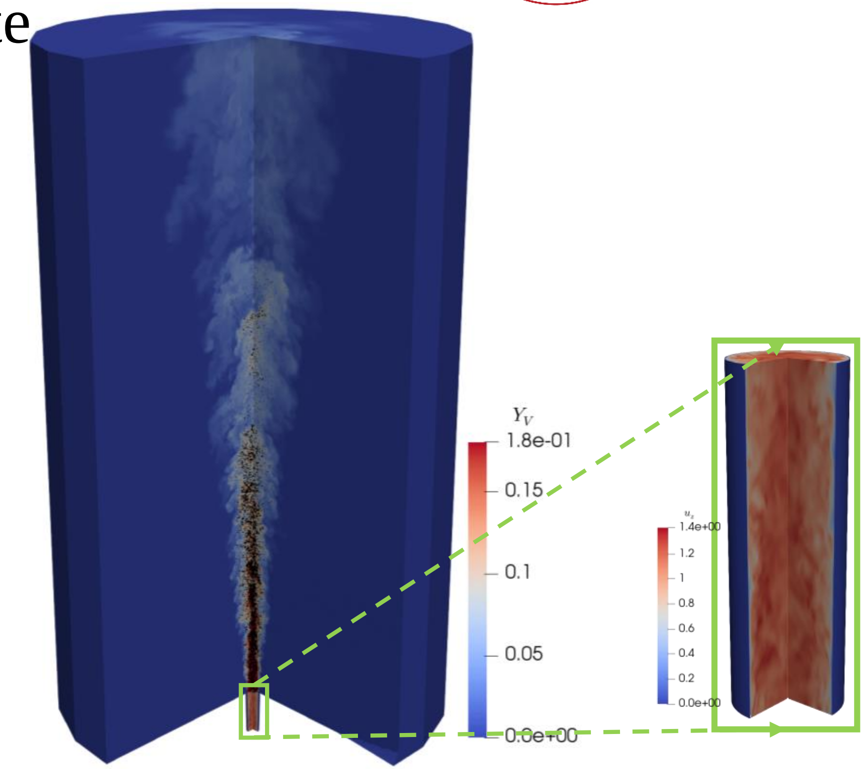
Boussinesq Hypothesis: $\boldsymbol{\tau}^R = -2\mu_{SGS}(\tilde{S} - 1/3\tilde{S}\mathbf{I})$ $\quad \tilde{S} = 0.5(\nabla\tilde{\mathbf{u}} + \nabla\tilde{\boldsymbol{u}}^T)$

Smagorinsky Model: $\mu_{SGS} = \bar{\rho}(C_S\Delta)^2|\tilde{S}|$ $\quad |\tilde{S}| = (2\tilde{S}\tilde{S})^{1/2}$ $\quad \Delta = (r\Delta\theta\Delta r\Delta z)^{1/3}$

- During the 1st year of Ph.D. course, the Smagorinsky model has been modified to conduct the research.

❑ Numerical Tool: CYCLONE

- II order centered FD space
- III order RK time
- Fully turbulent flow
- Low Mach number NS & Point-droplet equations
- Staggered mesh
- Cylindrical coordinate
- MPI parallelization



❑ Parameter Setup & Boundary Conditions

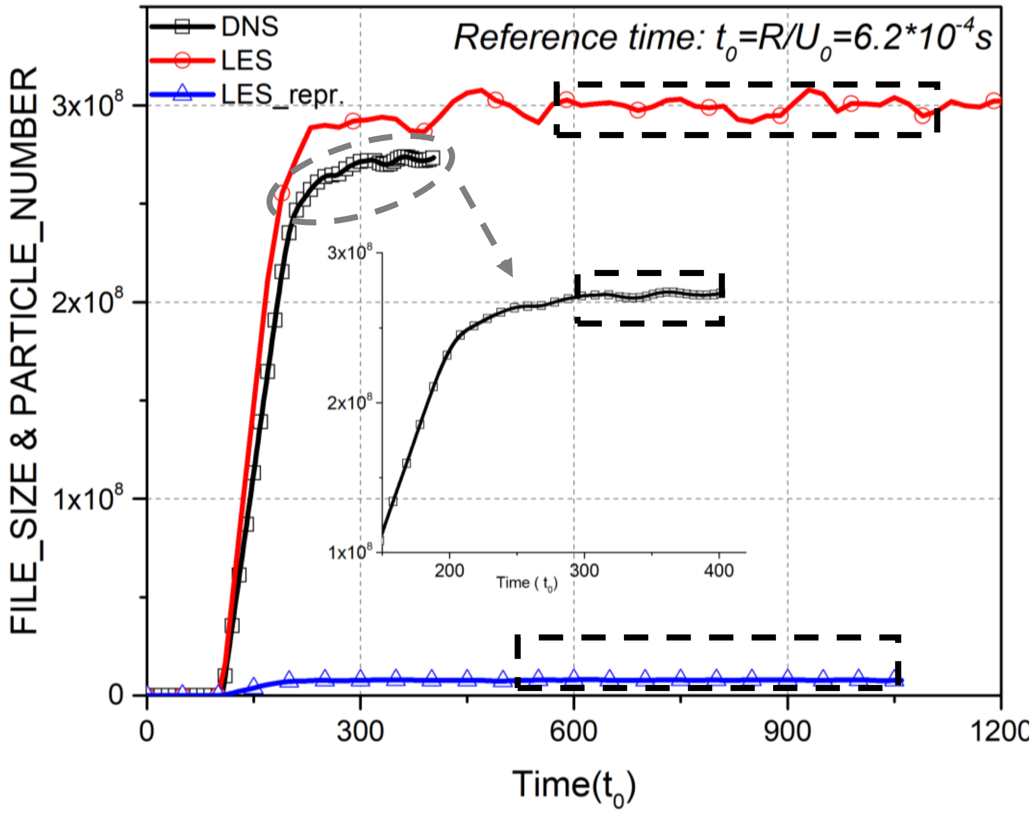
- Monodisperse acetone droplets at the inflow ($r_{d,0}$=6μm)
- Turbulent inflow with saturated gas (S=0.99, T=275 K)
- <u>Reynolds number : Re=$2U_0R/\nu$=10000</u>
- Quiescent environment of dry air
- <u>Non-uniform mesh 46 M (DNS) / 0.7 M (LES) points</u>
- ~3M evaporating droplets with mass fraction $\Phi\approx0.05$, volume fraction $\Psi\approx10^{-5}$

More details:Battista et al. PoF 2011 and Dalla Barba & Picano PRF 2018

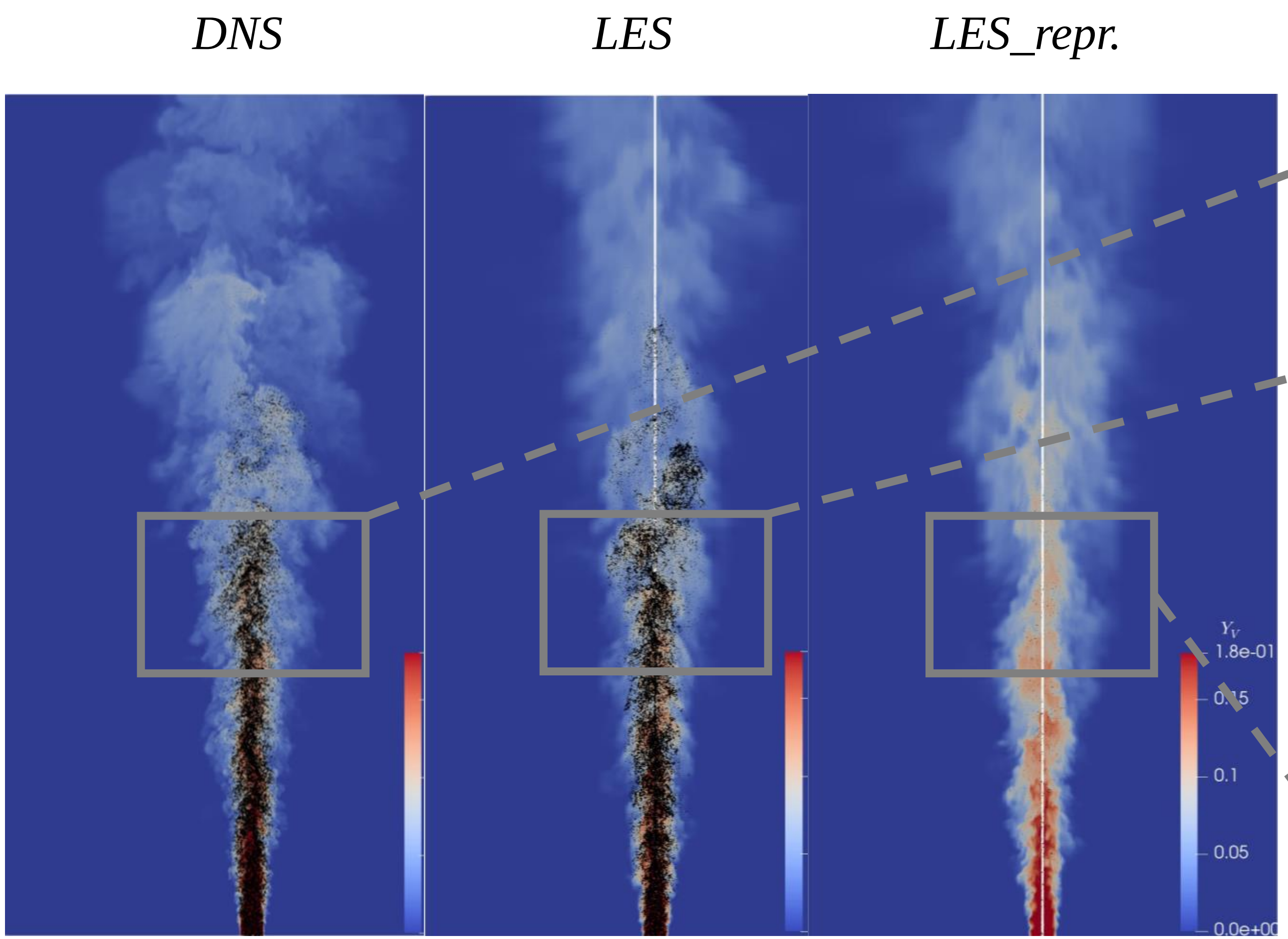
❑ Three simulations have been performed:

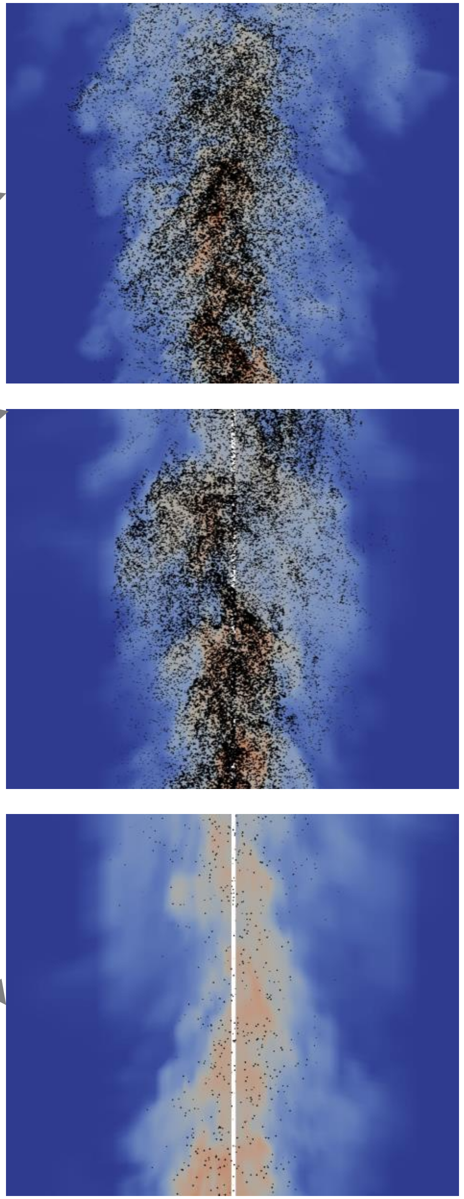
	DNS	LES	LES_repr.
SGS Model	\	Smagorinsky model	
Mesh	192*211*1152	48*52*288	
Particle number	~3M	~3M	~0.08M
Core number	96 in Marconi	2	
Time step	0.001	0.01	
duration	~3 months	~20 days	3 days

- Computation details for these simulations



- Data collected after simulations reach the statistic stable situation

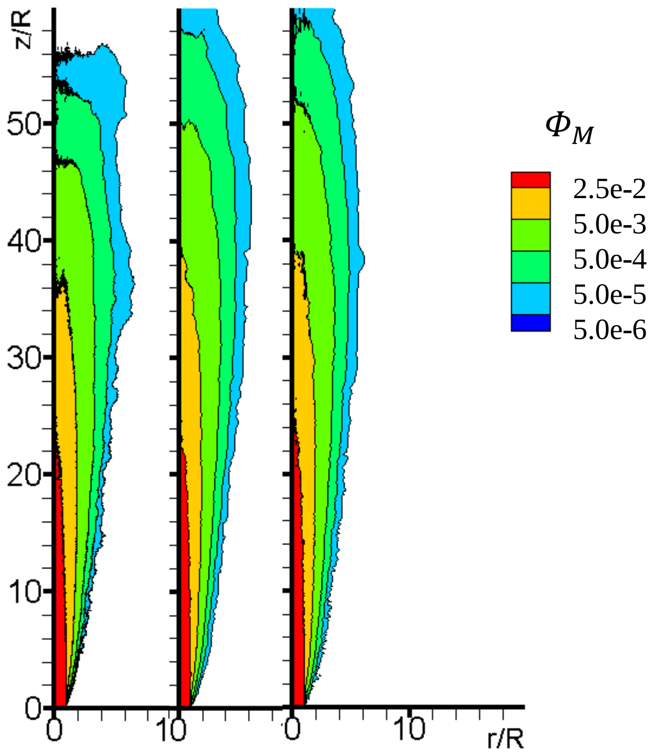




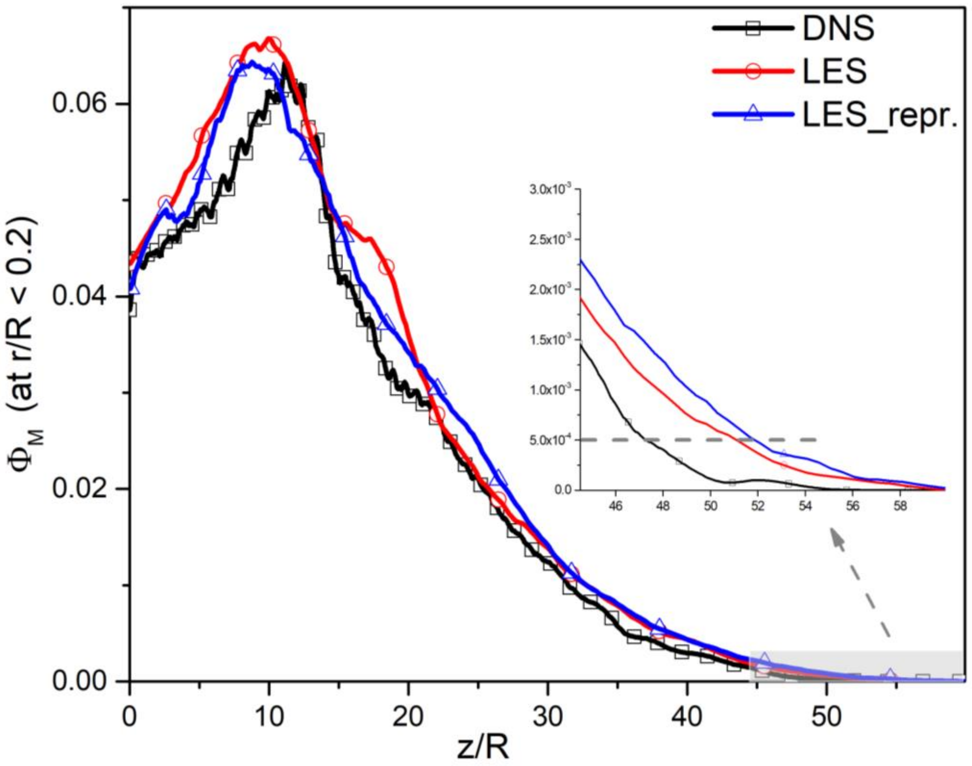
Instantaneous distribution of droplets and vapor mass fraction (up) and corresponding enlargements of jet regions centered at z/R = 30 (right)

- Less details about the gas phase are shown in LES case
- Droplets distributions are different. More droplets populate the turbulent spray core in LES
- LES only provides an approximation of the filtered velocity
- Interpolation errors due to the coarse-grained domains
- However, the peculiar phenomenon characterizing dispersed multiphase turbulent flow – the preferential segregation – is still evident in LES.

- ***DNS*** *V.S.* ***LES*** *V.S.* ***LES_repr.***



Mean liquid mass fraction,
$\Phi_M = {}^{m_l}/_{m_g}$



Mean liquid mass fraction near the jet center axis, r/R<0.2

Additional analyses are in progress…

- The overall vaporization length : 99 % of droplet mass have evaporated
- In LES, the overall vaporization length for droplets is larger which means slower evaporation compared to DNS
- We are working to improve the model to capture this prediction

Summary of The Research Activity & Perspective Plan

- ✓ A detailed literature review concerning spray evaporation in different engineering and scientific fields has been produced
- ✓ The numerical tool CYCLONE has been learnt and tuned to conduct research
- ✓ **An application for computation resources** (ISCRA C)has been approved by CINECA and a budget of 360000 core-hours on Marconi cluster has been granted
- ✓ High Reynolds number simulations **DNS case (largest in the word) and two corresponding LES cases** have been properly setup and **completed**
- ✓ From preliminary results, Droplets in LES case evaporates more slowly compared to DNS case
- ➢ Try different LES SGS model, improve the prediction accuracy of Lagrangian dispersed phase
- ➢ Reactive flow simulation

Thank you for your attention!