SIMULATION AND MODELLING TURBULENT SPRAY DYNAMICS

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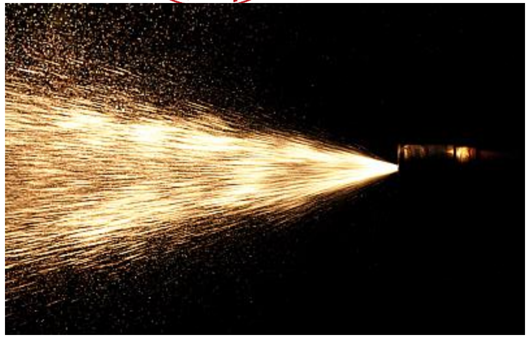
DATE: 11/09/2020

Motivation

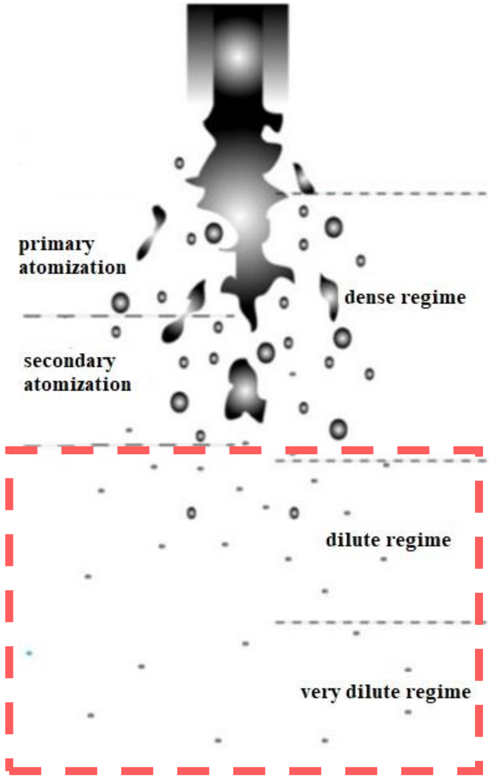
❑ Turbulent spray

- Complex multiphase flows where two distinguished phases mutually interact exchanging mass, momentum and energy in a turbulent environment.
- Evaporation, preferential concentration, mixing process, combustion, pollutant formation……
- Unsteady, multiphase, multiscale…
- A satisfied understanding? The capability to modeling?



❑ Diluted regime

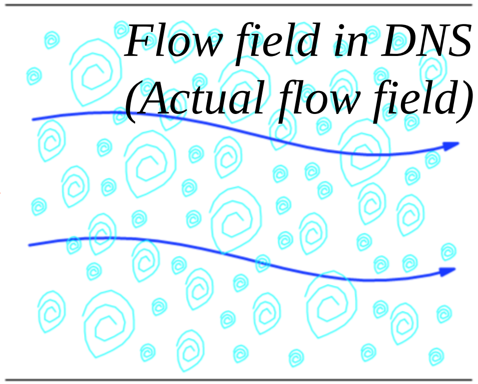
- Dispersed droplets: **Point-droplet approximation**
- **No break-up** : surface tension >> aerodynamic forces
- No collision / coalescence : **low volume fraction** ($\Phi < 10^{-3}$)
- 1-way or **2-way** coupling method
- Main region occurring evaporation and combustion



Sketch of various regimes in turbulent sprays [Jenny.2012]

Description of numerical approaches for turbulent flows

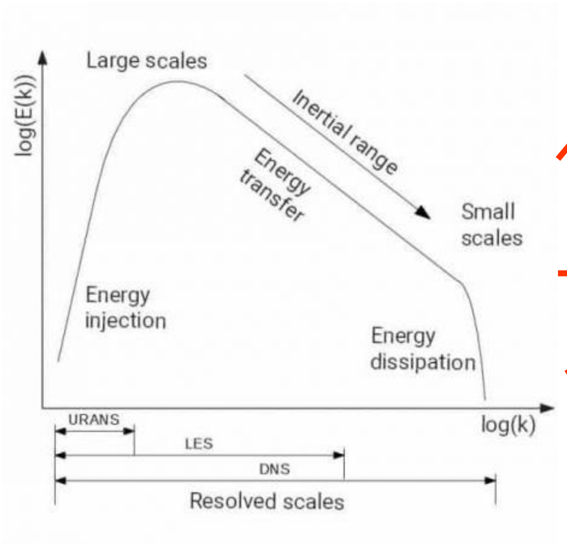
- **Basic tool for research**

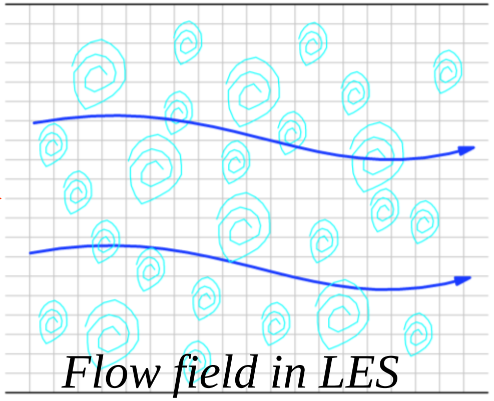


Flow field in DNS (Actual flow field)

- More flow details available

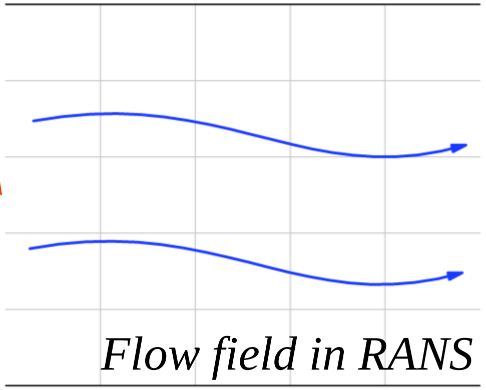
Increase in resolution & computational cost





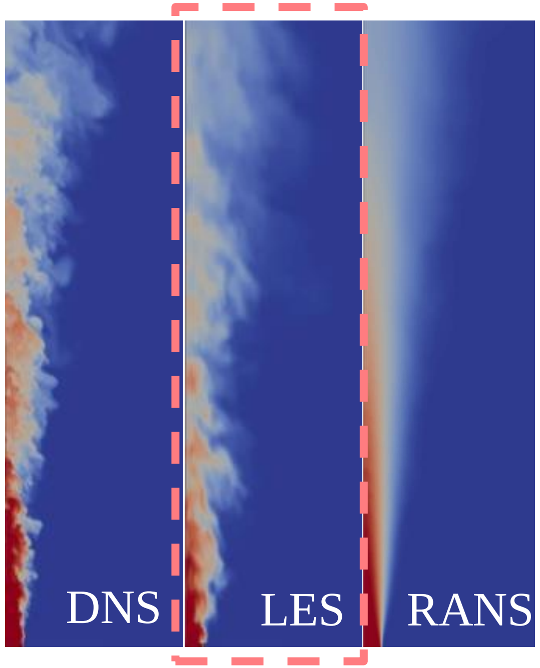
Flow field in LES

- **Popular tools for industrial application**



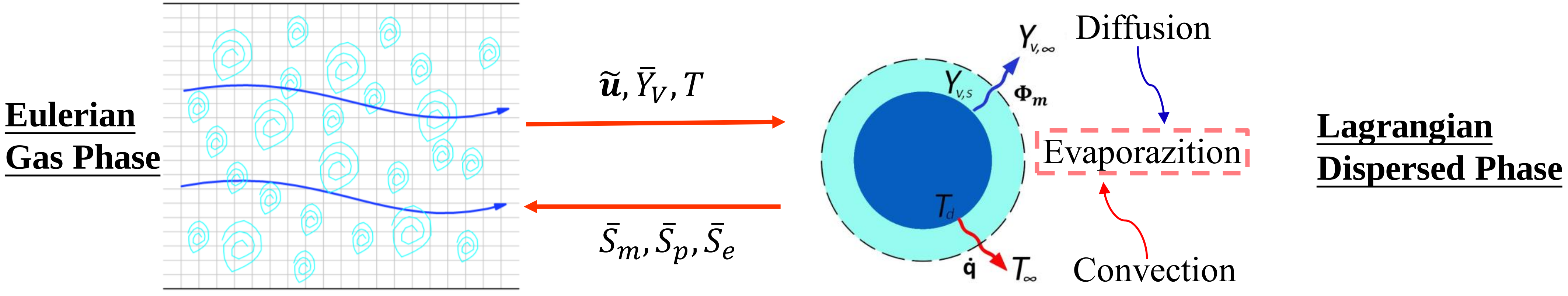
Flow field in RANS

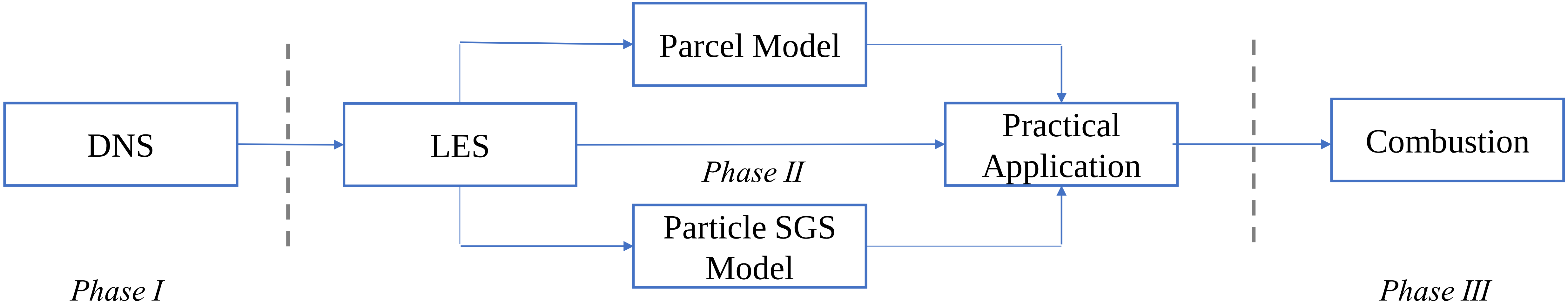
- Decent computational cost



Comparison between numerical methods for flow

- Is it possible to further **enhance the computational efficiency** in LES approach?
- Is it possible to further **improve the prediction accuracy** in LES approach?





Numerical tool and Formulations for DNS

❑ Numerical Tool: CYCLONE

- Fully turbulent flow
- Staggered mesh
- Low Mach number NS & Point-droplet equations
- Cylindrical coordinate
- MPI parallelization

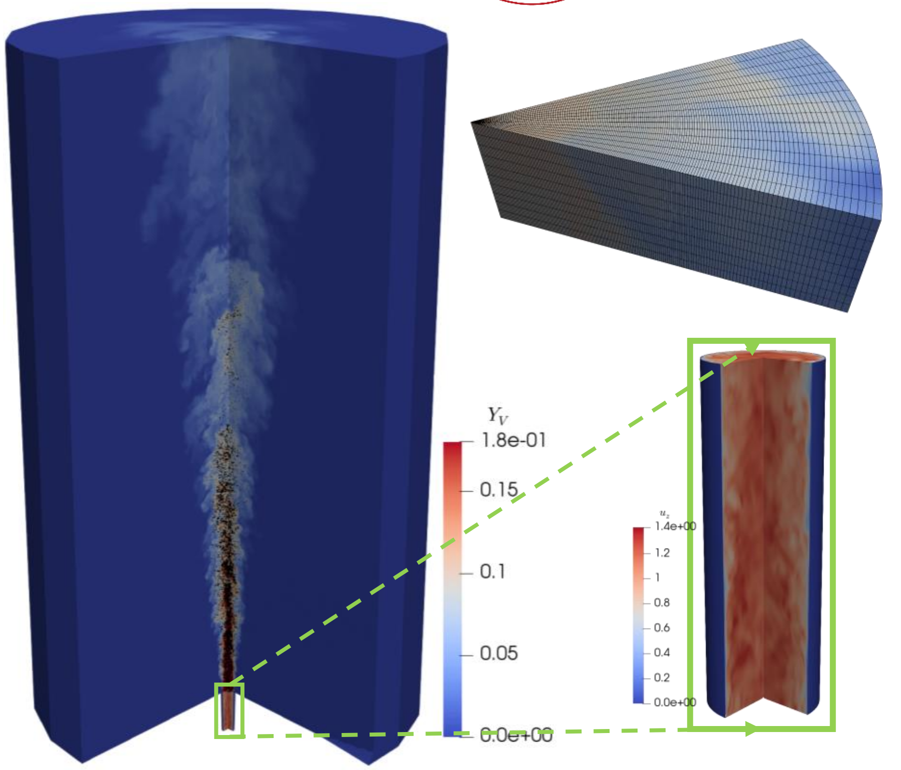
❑ Formulations for DNS

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

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

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



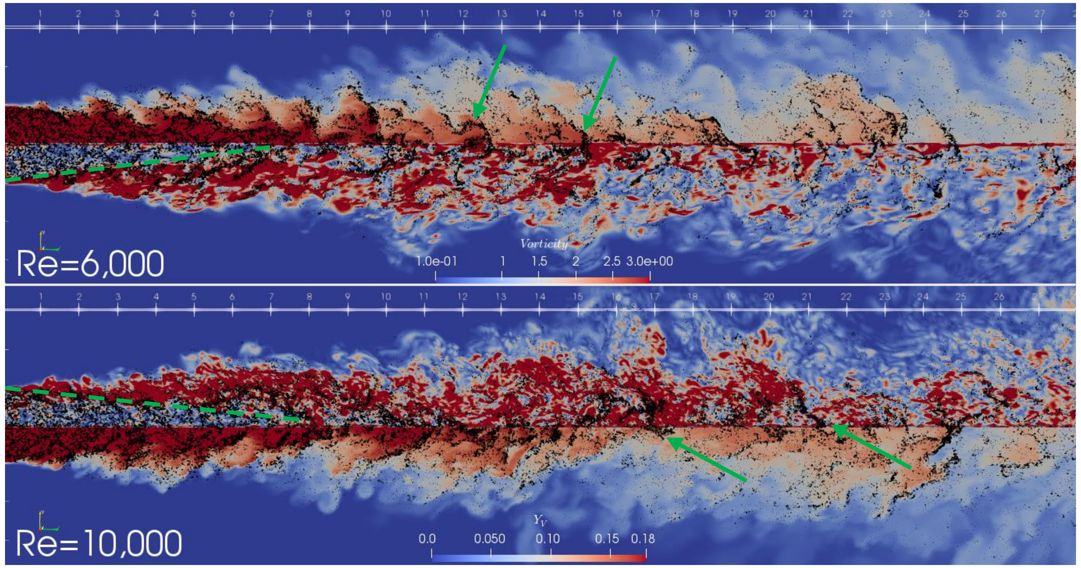
A sketch of the 3D cylindrical domain

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

Benchmark simulation parameters

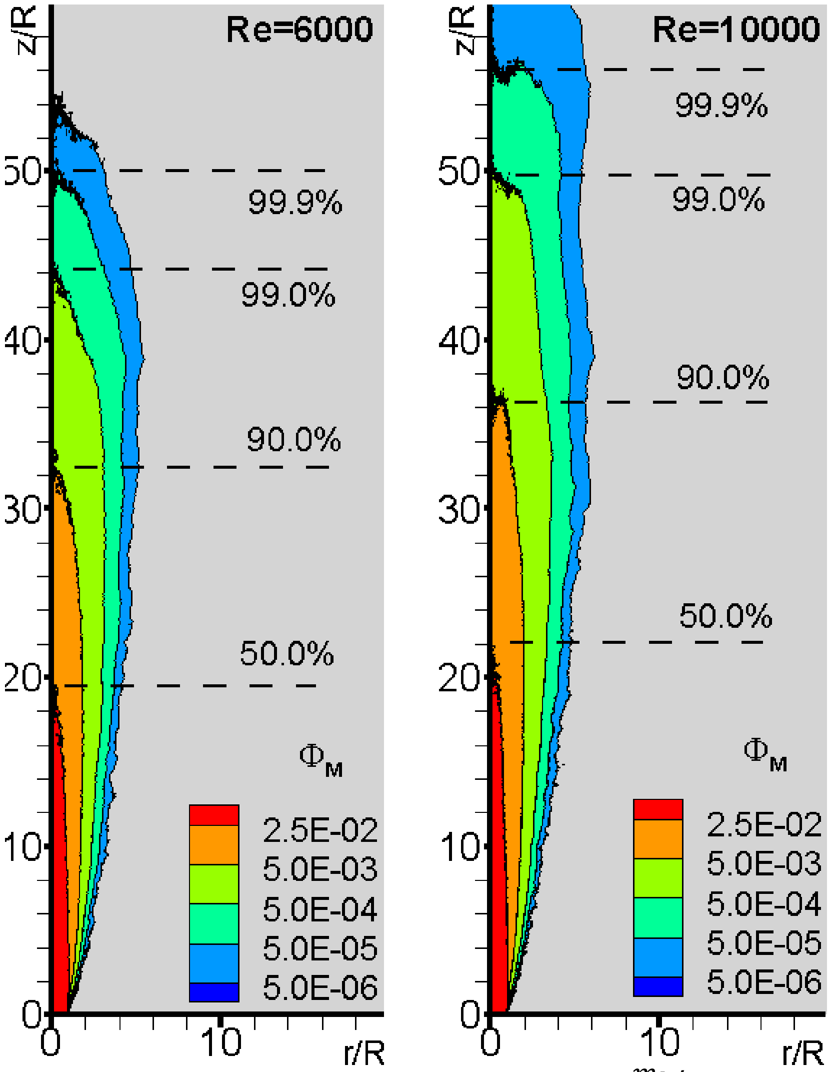
- **Benchmark simulation parameters** *(DNS)*
  - Monodisperse acetone droplets at the inflow ($r_{d,0}$=6μm)
  - Turbulent inflow with saturated gas (S=0.99, T=275 K)
  - Reynolds number : Re=$2U_0R/\nu$=6,000 &10,000 (**U_0=8.1 m/s & U_0=13.9 m/s**)
  - Quiescent environment of dry air
  - Non-uniform mesh 46 M points
  - ~3M evaporating droplets with mass fraction Φ≈0.05

Radial slices of instantaneous distribution for vapor mass fraction, $Y_v = {}^{\rho_v}/_{\rho_g}$, and vorticity.

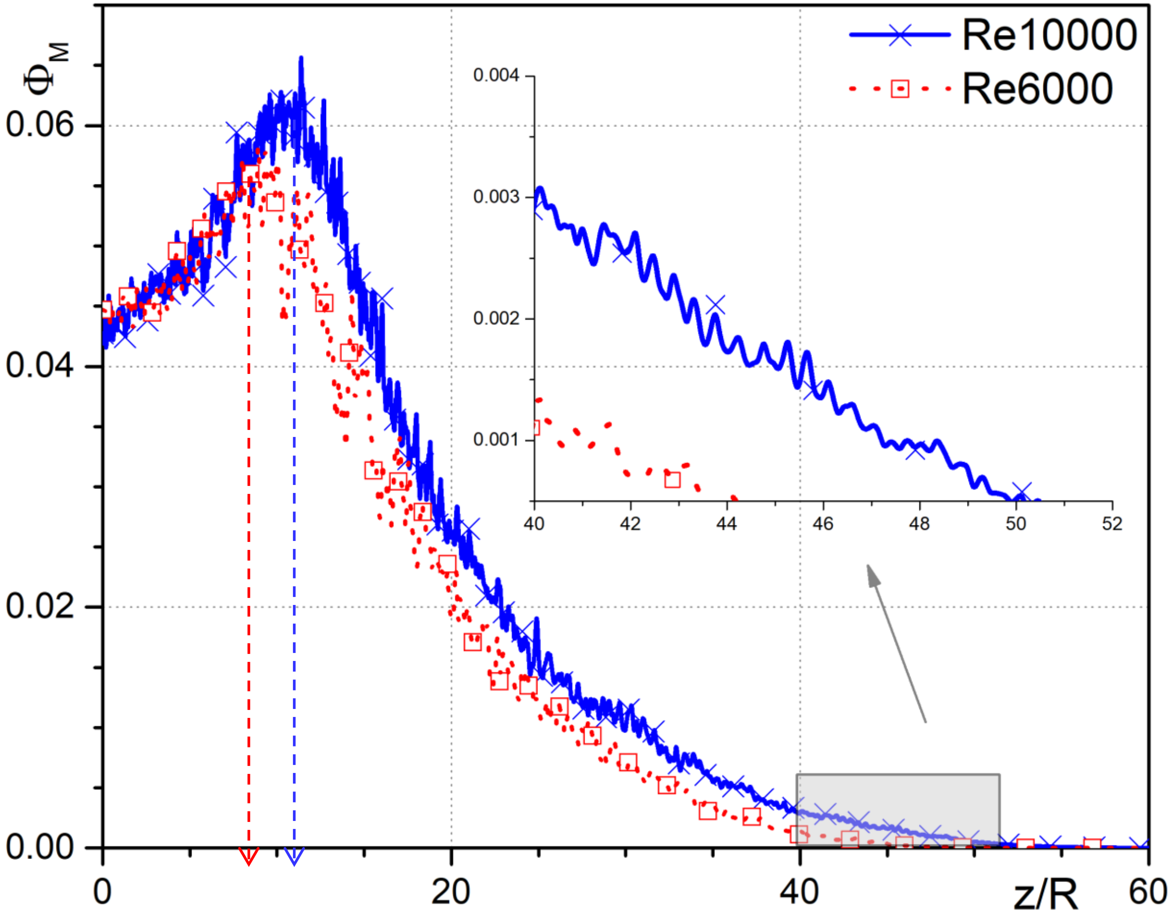


- **A qualitive view**
  - The preferential concentration is evident for both cases.
  - A longer self-potential core is observable in Re=10,000 case.

Mean field results



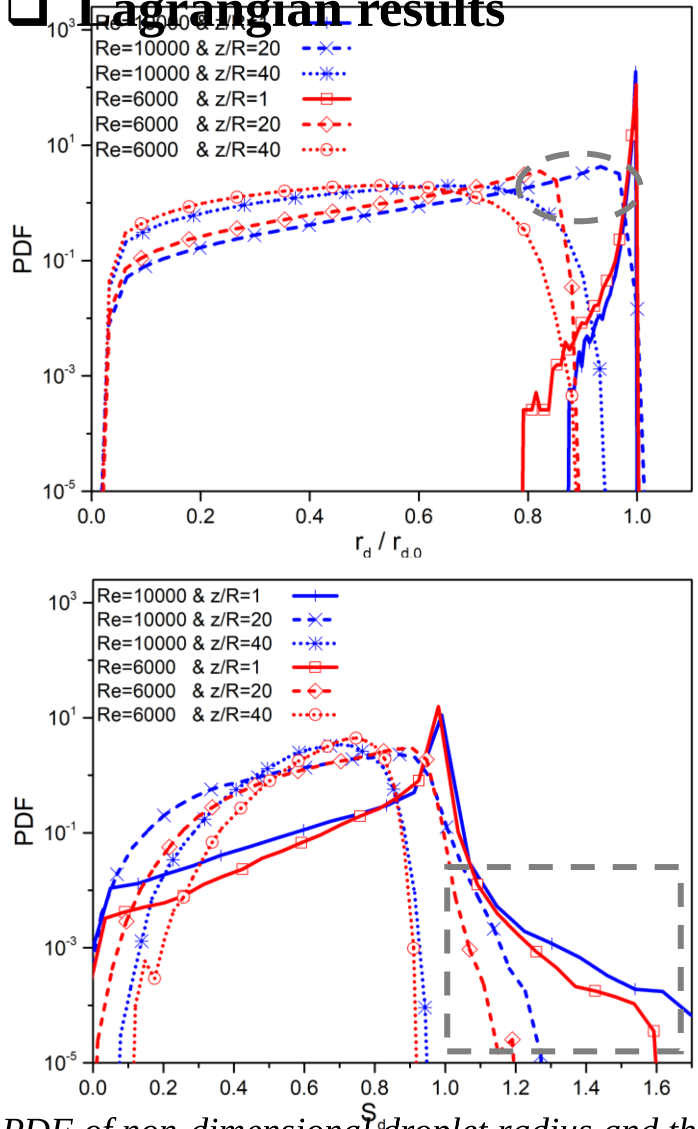
Mean liquid mass fraction, $\Phi_M = {m_l}/{m_g}$



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

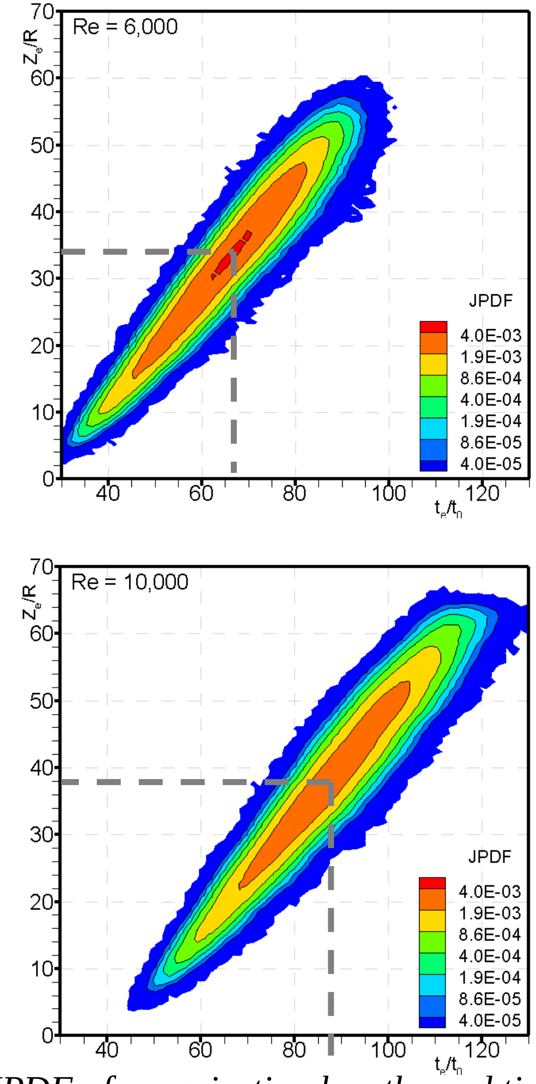
- A longer vaporization length (99%) is shown in Re = 10,000 case.
- The Φ_M exhibits a near-field hump shape along the center axis.

❑ Lagrangian results



PDF of non-dimensional droplet radius and the saturation field at droplets surface

- Towards the intermediate-fields and far-fields region, **more robust spread of the droplet size spectrum is shown in Re = 10,000 case.**
- Certain amount of droplets stay in range $S_d > 1$, *i.e.* supersaturation, which is more intensive in higher Re sprays.



JPDF of vaporization lengths and times of the droplets computed over the whole droplet population

- A strong linear correlation between the droplet vaporization length and time while different slope rates are observable.
- In Re = 10,000 case, the median vaporization times is $t_e/t_0 = 90$, which is larger than its correspondent value, $t_e/t_0 = 70$ in Re = 6,000 case.

LES – Basic Equations

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

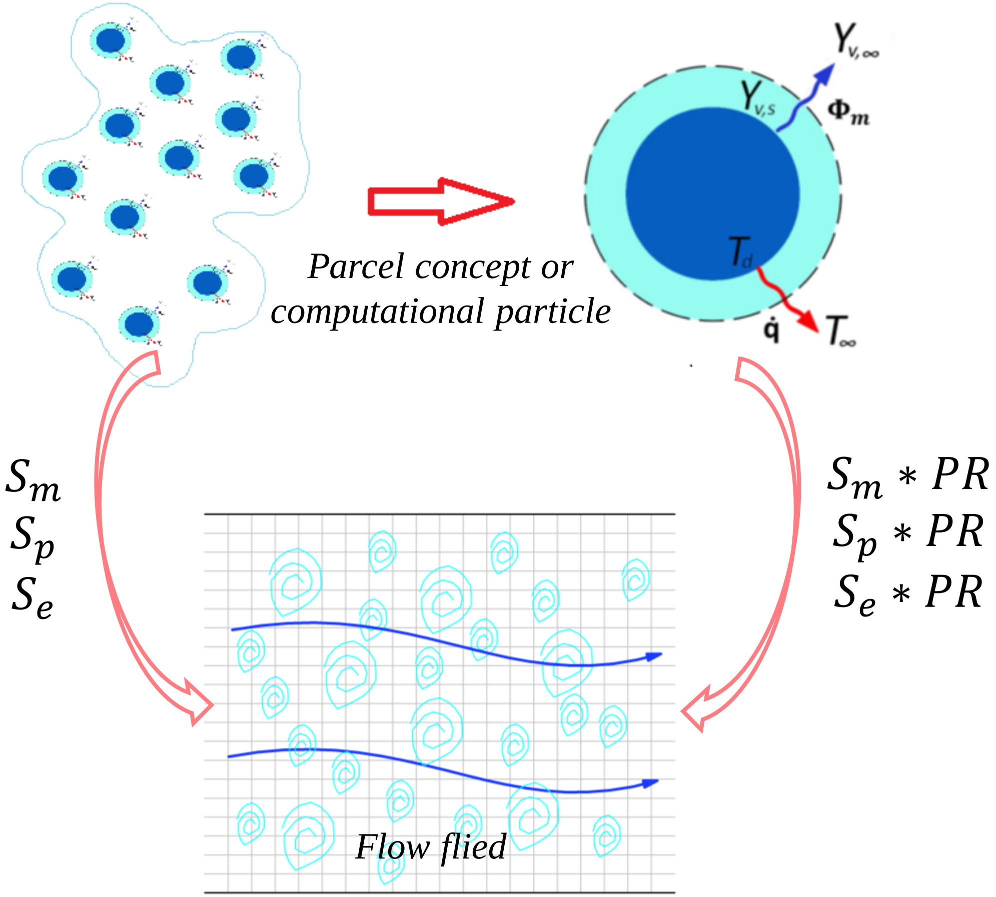
$$\bar{S}_m = \int S_m G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r} \qquad \bar{S}_e = \int S_e G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r} \qquad \bar{S}_p = \int S_p G_\Delta(\mathbf{x}, \boldsymbol{r})d\boldsymbol{r}$$

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

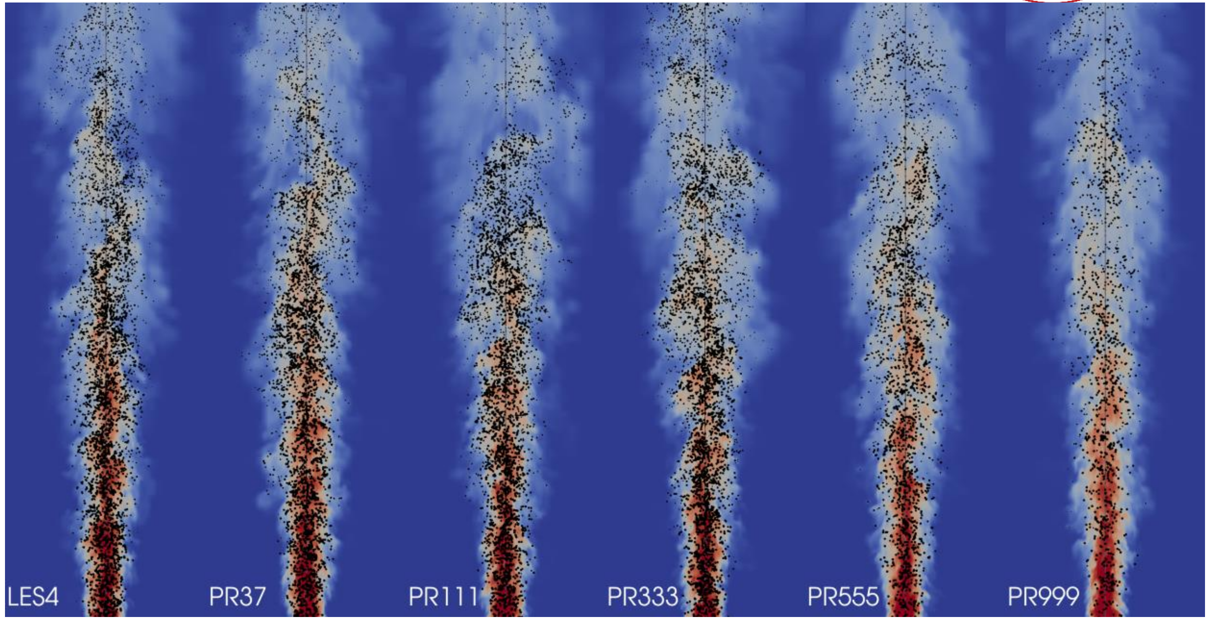
Smagorinsky Model: $\mu_{SGS} = \bar{\rho}(C_S\Delta)^2|\tilde{S}|$ $\quad |\tilde{S}| = (2\tilde{S}\tilde{S})^{1/2}$ $\quad \Delta = (r\Delta\theta\Delta r\Delta z)^{1/3}$

- The classical Smagorinsky SGS model is employed in the LES approach.
- All LES simulations are based on formulations listed above.

- The mesh for LES is coarsen from DNS mesh by increasing mesh size 4 times in each direction. The total number is ~ 0.7 M points.



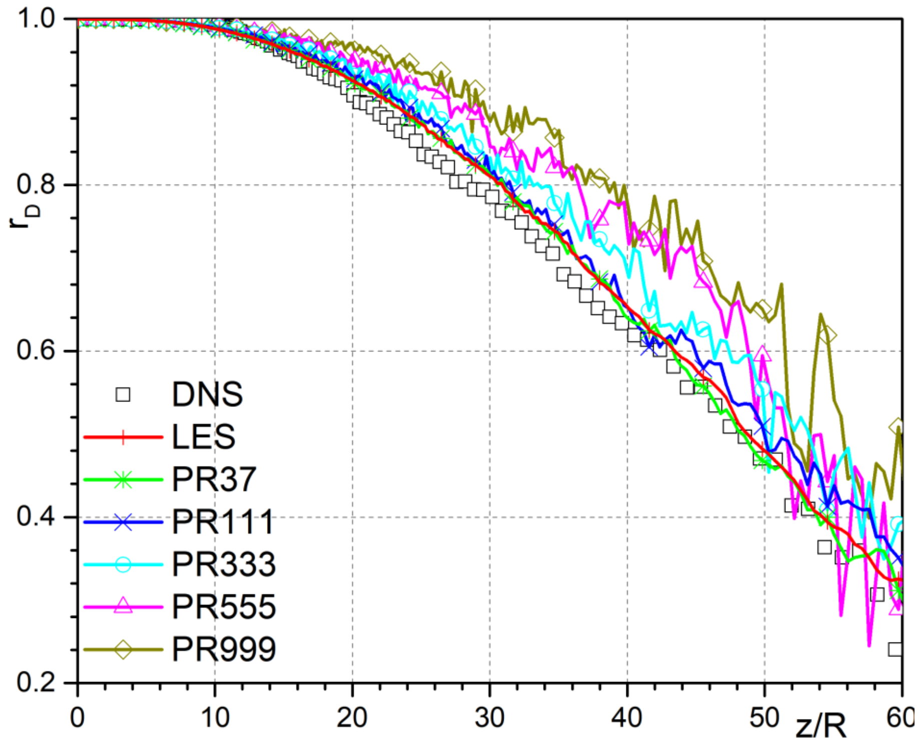
❑ Results



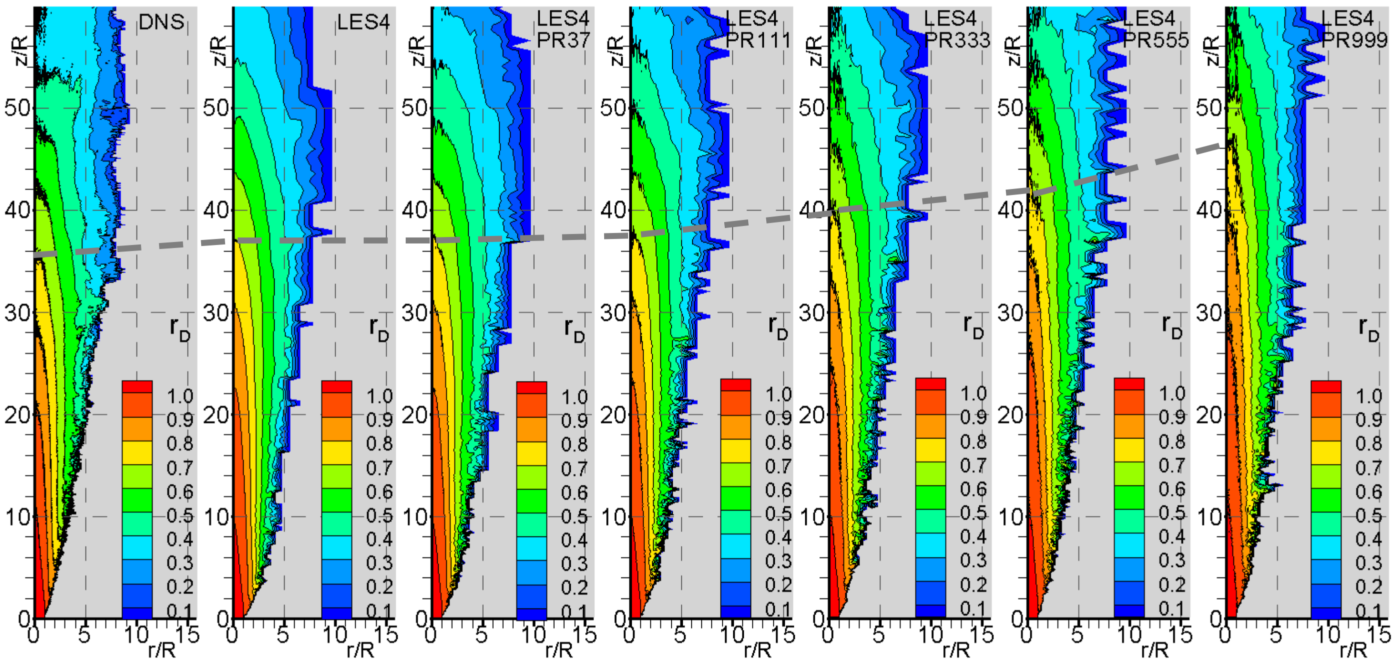
Radial slices of instantaneous distribution for vapor mass fraction, Y_V, with different Parcel Ratios (PR)

- A cluster of droplets with similar properties are represented by one “parcel”, e.g. temperature, radius and velocity.
- **Parcel model is added in our code package successfully.**
- From the qualitive point-of-view, no remarkable difference is observable among LES simulations with different PRs.

❑ *Results*



Mean droplet radius near the jet center axis, r/R<0.2



Mean droplet radius rescaled by the droplet initial radius, r_d, with different Parcel Ratios (PR)

- Droplet vaporization: The lifetime of droplets could be prolonged if large PR values are used in modeling spray dynamics.
- **<u>PR =111</u> is recommended considering the computational efficiency and prediction accuracy.**

LES – Particle SGS Model

❑ *Model description*

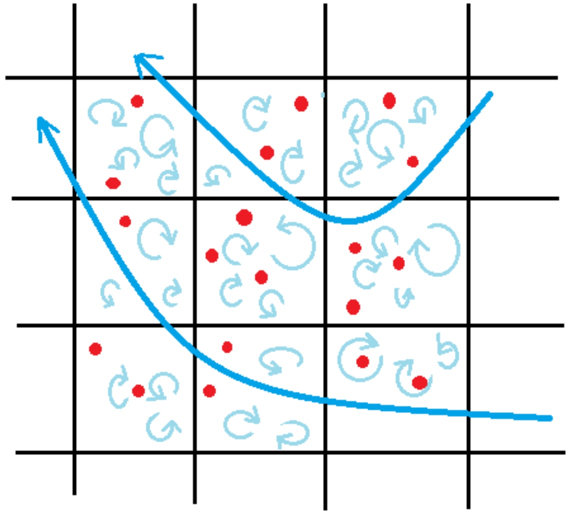
$$\frac{d\mathbf{u}_d}{dt} = \frac{(\tilde{\mathbf{u}} + \boldsymbol{u}_{sgs} - \mathbf{u}_d)}{\tau_d}\left(1 + 0.15\mathrm{Re}_d^{0.687}\right)$$

$$\boldsymbol{u}_{sgs} = \chi\sqrt{\frac{2}{3}\frac{\mu_t}{\bar{\rho}C_k\bar{\Delta}Re}}$$, (SGS velocity)

$\chi \sim \mathbb{N}(0,1)$, (Gaussian distribution)

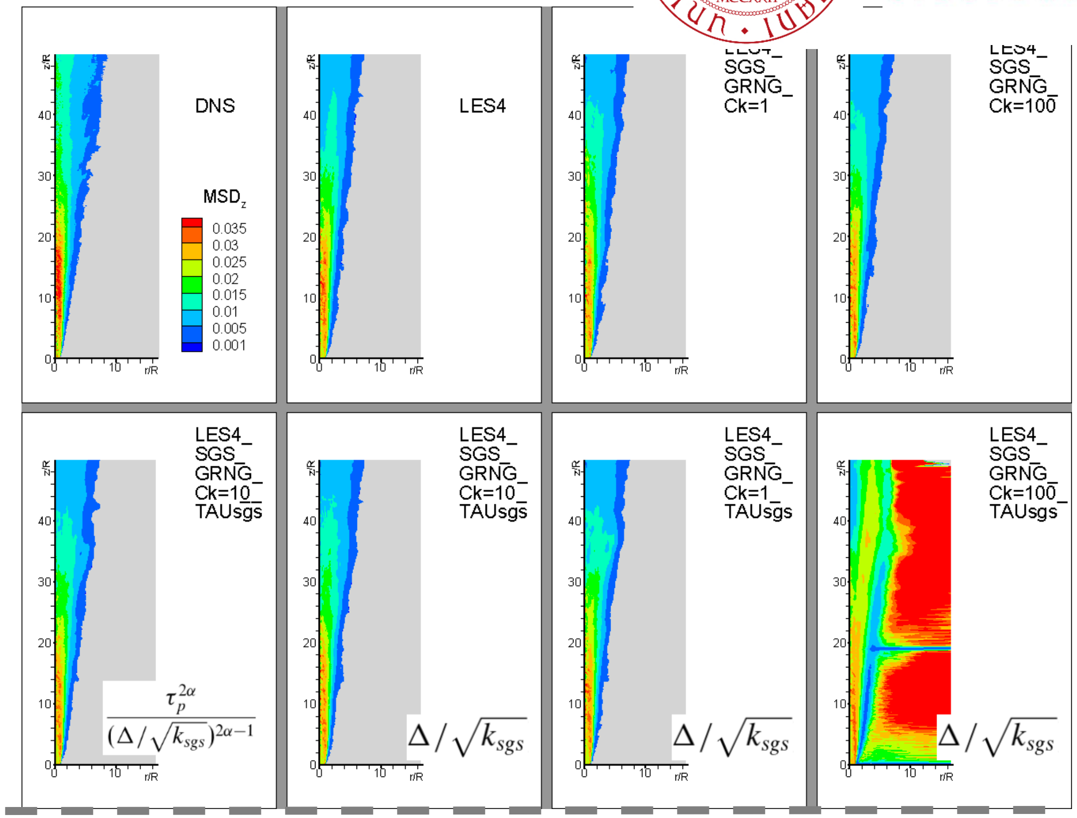
$$\tau_{sgs} = \frac{\bar{\Delta}Re}{\mu_t} \ \& \ \tau_{sgs} = {\tau_d}^{1.6} / \left(\frac{\bar{\Delta}Re}{\mu_t}\right)^{0.6}$$

, (SGS time scale)



Top: Schematics of particles in LES framework

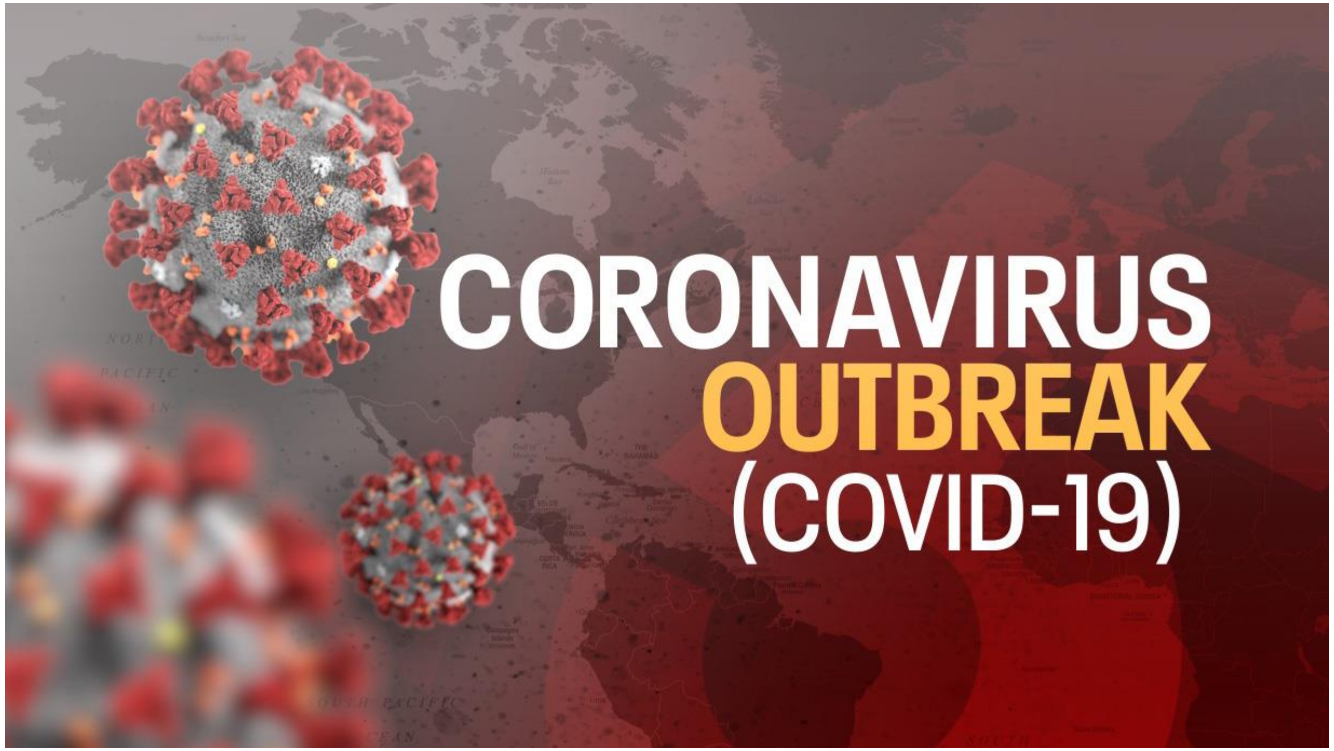
❑ *Results*

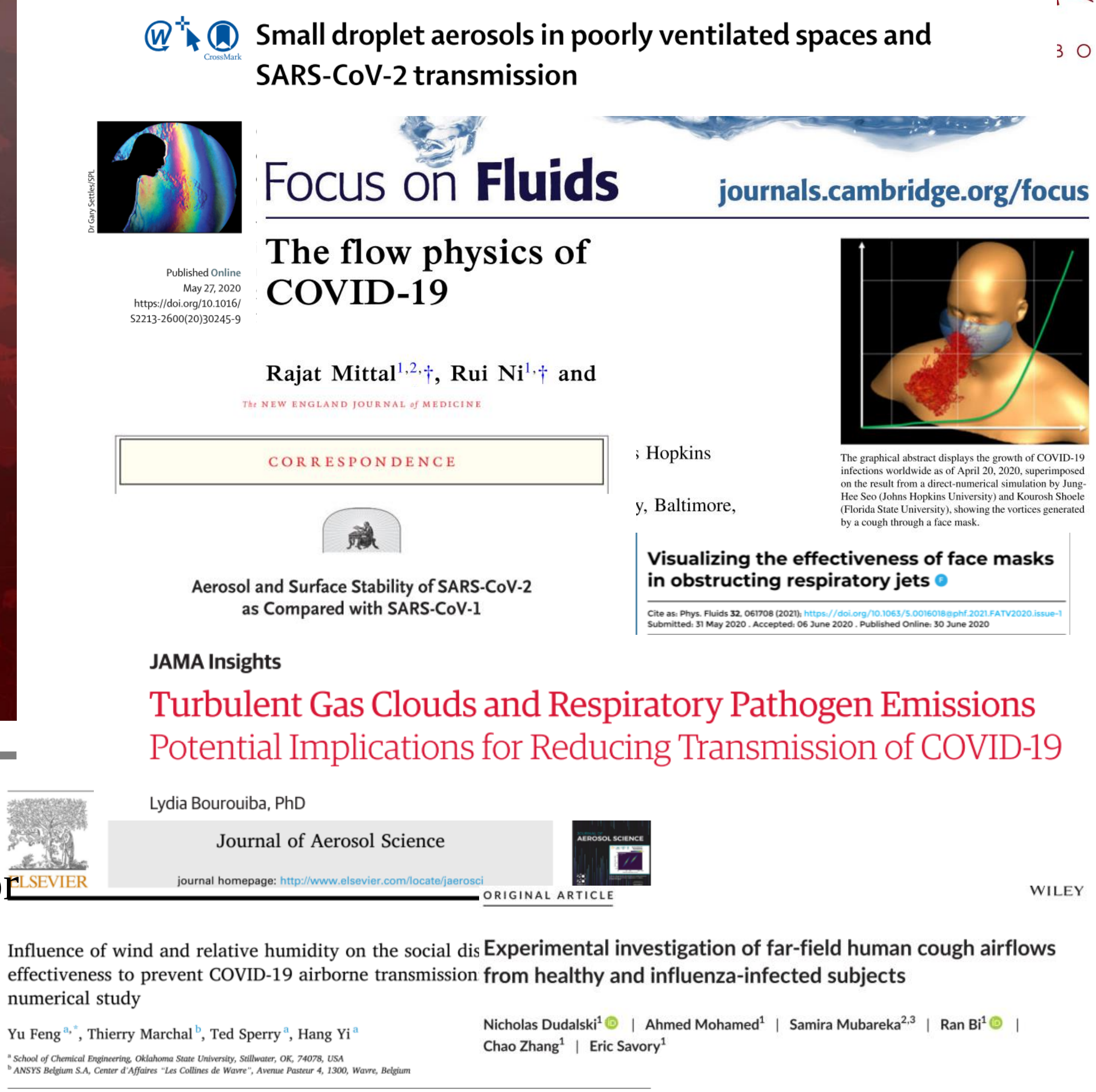


Right: Mean square displacement (MSD) in z direction for DNS, original LES and LES cases with different particle SGS models or model coefficients

- A stochastic model to account for the SGS part in particle momentum equation is proposed and implemented in our code.
- The Ziggurat method [Marsaglia.2000] is adopted to generate a Ganssian random number for the SGS model.
- **<u>No significant improvement compared to the original LES has been observed.</u>** Further investigations is undergoing.

- ***COVID-19***





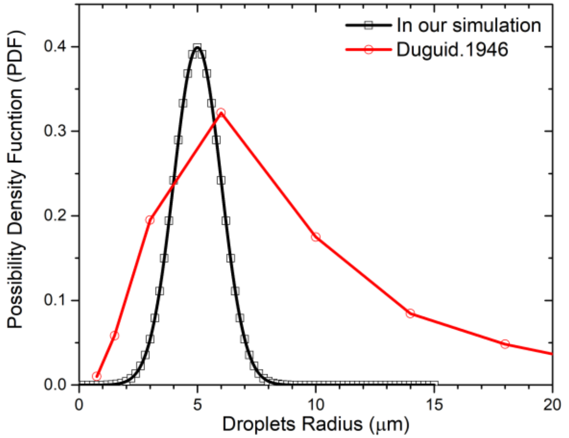
- To fill scientific gaps in our understanding of critical issues.
- To better prepare ourselves to tackle the next break of COVID-19 or a similar disease.
- **The behaviors of droplets laden with virus under different ambient conditions.**

❑ *Coughing jets: Initial Conditions, Boundary Conditions and Parameters Setup*

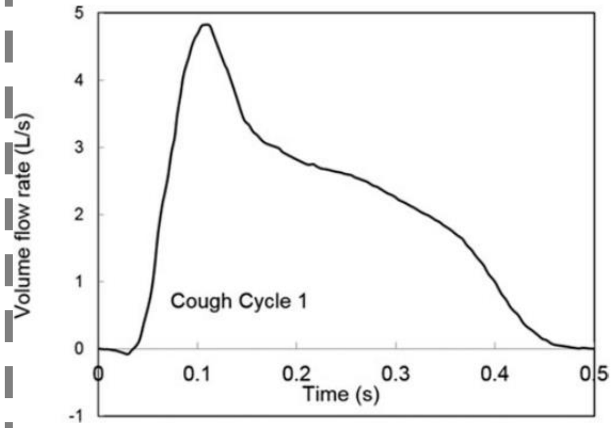
Parameters	Value
Inlet radius[m]	1×10^{-2}
Inlet temp.[K]	310.15
Inlet RH[%]	100
Max. inlet vel.[m/s]	10.93
Initial pressure[Pa]	101300
Ambient Temp.[K]	296.15
Ambient RH[%]	19 & 50 & 90
Droplets radius[m]	$\mathbb{N}(5 \times 10^{-6}, 1)$
Liquid volume fraction[%]	1.9×10^{-7}
Bulk Re	12000
Computational domain $(\theta \times r \times z)$[m]	$2\pi \times 1 \times 2$
Mesh	$64 \times 280 \times 600$
Time step [s]	1×10^{-5}

An enhanced image of a sneeze process

- Other thermodynamic parameters for humid air is calculated based on *[Picard.2008 &Tsilingiris.2008]*.
- Buoyancy force is added in both gas phase and particle phase.
- The quantity of injected droplets per time steps is proportional to the prescribed velocity condition.



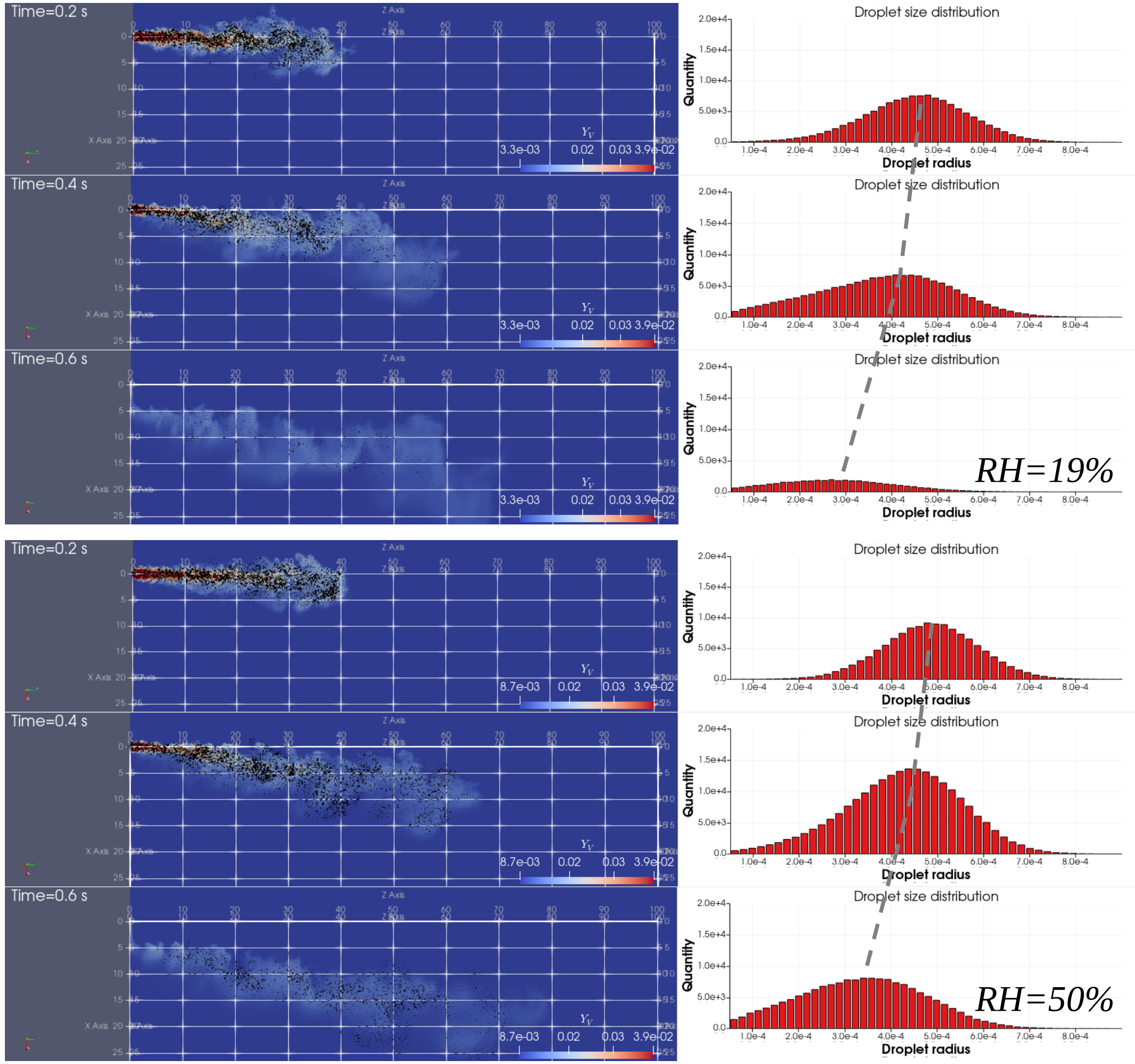
Droplets radius distribution



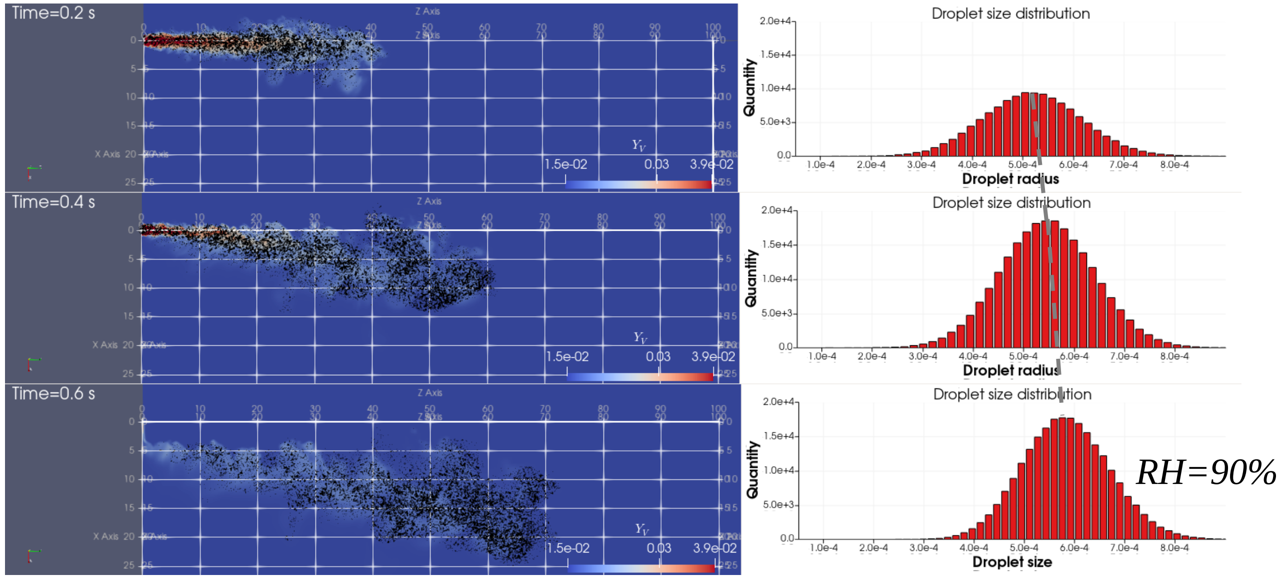
Inlet flow rate [Thatiparti.2016]

LES – A Practical Application (3/3)

❑ *Coughing jets: Preliminary Results*



The instantaneous vapor mass fraction distribution sampling with droplets under different Relative Humidity (RH) conditions: 19%, 50%, 90%.



- Slower vaporization is obvious as RH is increased from 19% to 90%.
- **Droplets can "grow up" in high RH conditions.**

Summary

- ✓ The spray dynamics of an evaporating turbulent acetone jet in Re = 10, 000 has been investigated with DNS framework.
  - A longer vaporization length compared to our previous work (Re=6,000) was found together with delayed preferential concentration phenomena*.

- ✓ 3D LES cases has been performed to obtain the influence of parcel model on Lagrangian phase behaviors.
  - An optimal PR was found to maintain the prediction accuracy*.

- ✓ The impact other submodels on particle dynamics has been checked.

Work in progress

- ➢ Particle SGS model
- ➢ Coughing jet simulation with different ambient conditions
- ➢ A manuscript is preparing for publication*; another one is under writing*.

THE END

Thank you for your attention!