UNIVERSITÀ DEGLI STUDI DI PADOVA

High-fidelity simulation and modeling of turbulent sprays

Xiang'en Kong - 38th Cycle

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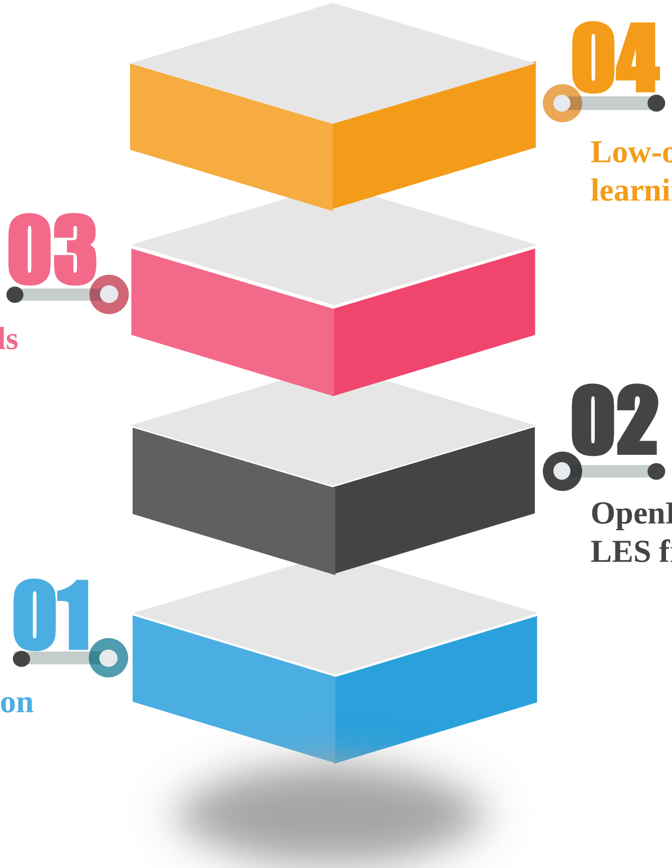
Co-supervisor: Dr. Federico Dalla Barba

Meeting - 13/09/2023

Research plan



Low-order simulations using Machine-learning models

Training Machine-learning models using datasets from step 2

OpenFOAM simulation of sprays in LES framework

Theoretical Knowledge Preparation

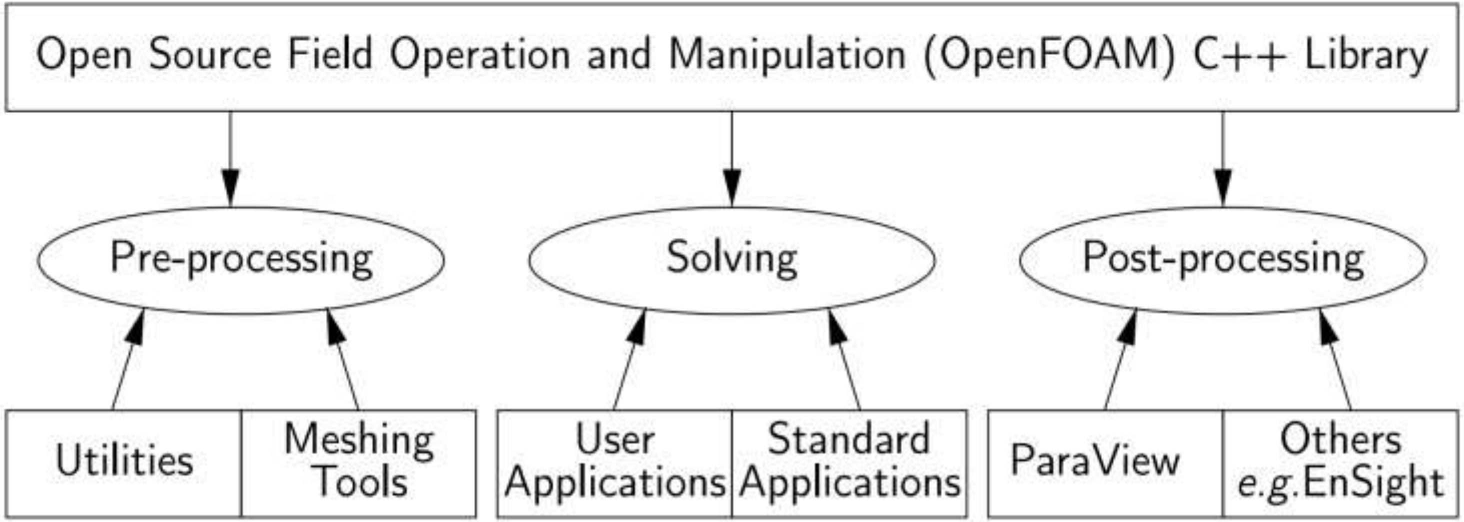
Work done

Bibliographical Research
- Fluid Mechanics
- Turbulent Flows Theory
- Multiphase Flow Theory

OpenFOAM Simulation
- Training for OpenFOAM
- 19th Multiphase Flow Conference & Short Course
- Simulation of “Spray A” (non-reacting)

Introduction to OpenFOAM

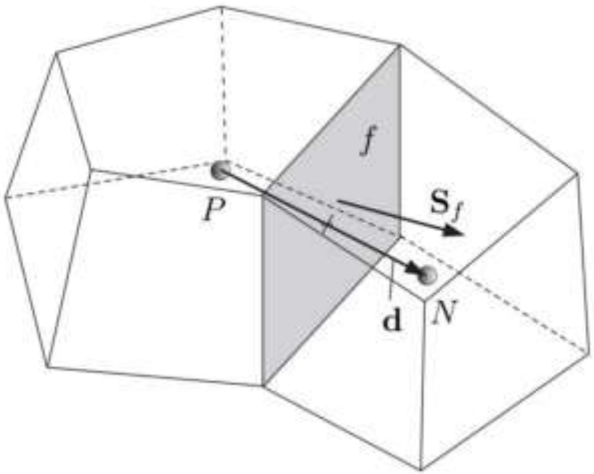
OpenFOAM (for "Open-source Field Operation And Manipulation") is a C++ toolbox for the development of customized numerical solvers, and pre-/post-processing utilities for the solution of continuum mechanics problems, most prominently including computational fluid dynamics (CFD).



OpenFOAM user's guide

Finite Volume Method (FVM)

A control volume is defined around every single grid point and the conservation laws must be respected if fluxes from any quantity are calculated through the interface between two different volumes. Due to this conservation property, FVM is more stable and hence chosen for solving CFD problems.



Details of discretised control volume (OpenFOAM user's guide)

Introduction to sprayFoam solver

sprayFoam is a transient PIMPLE solver for compressible, laminar or turbulent flows with a spray particle cloud.

sprayFoam uses Eulerian-Lagrangian approach and the interaction between the continuous phase and discrete phase is given by two-way coupling.

Governing Equations

Eulerian Phase (LES)

Mass equation

Momentum equation

Energy equation

Mass fraction equation

$$\begin{cases} \dfrac{\partial \overline{\rho}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\mathbf{v}}) = \overline{\dot{\rho}_l} \\ \dfrac{\partial \overline{\rho}\tilde{\mathbf{v}}}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{\mathbf{v}} \otimes \tilde{\mathbf{v}}) = -\nabla \overline{p} + \nabla \cdot \overline{\boldsymbol{\tau}} + \overline{\rho}\mathbf{g} + \overline{\mathbf{f}_l} - \nabla \cdot \mathbf{B} \\ \dfrac{\partial \overline{\rho}\tilde{H}_K}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{H}_K\tilde{\mathbf{v}}) = \dfrac{\partial \overline{p}}{\partial t} + W + \nabla \cdot (\overline{\alpha}\nabla\tilde{h}) + \overline{\dot{q}_c} + \overline{\dot{q}_l} - \nabla \cdot \mathbf{b_E} \\ \dfrac{\partial \overline{\rho}\tilde{Y}_i}{\partial t} + \nabla \cdot (\overline{\rho}\tilde{Y}_i\tilde{\mathbf{v}}) = \nabla \cdot (D_i\nabla\tilde{Y}_i) + \overline{\dot{\omega}_{ic}} + \overline{\dot{m}_{il}} - \nabla \cdot \mathbf{b_i} \end{cases}$$

Lagrangian Phase

Mass equation

$$\frac{\mathrm{d}m_d}{\mathrm{d}t} = \frac{m_d}{\tau_i}$$

Momentum equation

$$m_d \frac{\mathrm{d}u_d}{\mathrm{d}t} = -\frac{\pi D^2}{8}\rho C_d |u_d - u|(u_d - u) + F_G + F_P$$

Energy equation

$$m_d \frac{\mathrm{d}h_d}{\mathrm{d}t} = \dot{m}_d h_v(T_d) + \pi D \cdot k_v \cdot Nu \cdot (T - T_d) f$$

Governing Equations

Lagrangian Phase

Particle Forces

Drag force $$F_D = C_D \frac{\pi D_p^2}{8} \rho_f (u_f - u_p)|u_f - u_p|$$

where

- Schiller-Naumann (1935)

$$C_D = \begin{cases} \frac{24}{Re_p}(1 + 0.15 Re_p^0.687) & if \quad Re_p \leq 1000 \\ 0.44 & if \quad Re_p > 1000 \end{cases}$$

- Putnam (1961)

$$C_D = \begin{cases} \frac{24}{Re_p}(1 + \frac{1}{6} Re_p^{2/3}) & if \quad Re_p \leq 1000 \\ 0.424 & if \quad Re_p > 1000 \end{cases}$$

Governing Equations

Lagrangian Phase

Gravity/Buoyancy force

$$F_G = m_p g\left(1 - \frac{\rho_f}{\rho_p}\right)$$

Pressure gradient force

$$F_P = -\frac{\pi D_p^3}{6}\nabla p$$

Other forces:

- **Added mass force**
- **Thermophoretic force**
- **Slip-rotation lift force**
- **Slip-shear lift force**

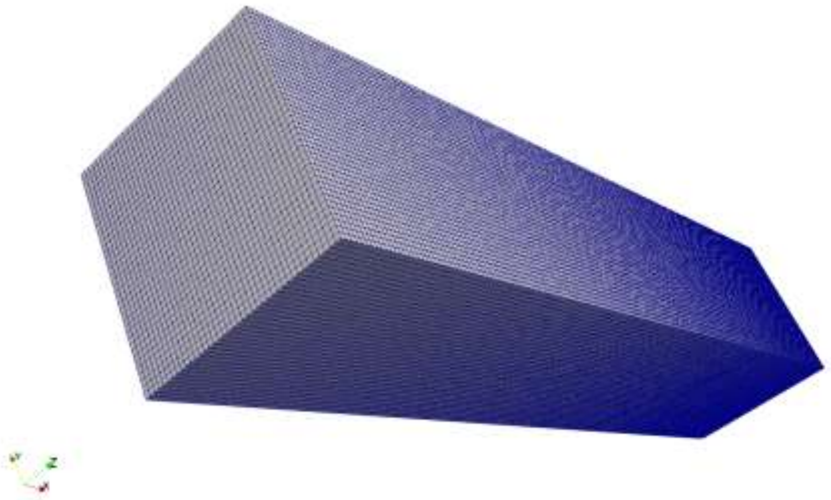
Introduction to Spray A

ECN (Engine Combustion Network) refers to the spray of n-dodecane as Spray A

Specifications for Spray A operating condition of the Engine Combustion Network		Combustion chamber gas composition (volume fraction)		
Ambient gas temperature/K	900		Non-reacting	Reacting
Ambient gas pressure/MPa	Near 6.0	$\psi(O_2)$ / %	0	15
Ambient gas density/ kg/m^3	22.8	$\psi(N_2)$ / %	89.71	75
Ambient gas oxygen (by volume)/ %	15 (reacting); 0 (non-reacting).	$\psi(H_2O)$ / %	6.52	6.38
Fuel injector nominal nozzle outlet diameter/mm	0.090	$\psi(CO_2)$ / %	3.77	3.62
Nozzle K factor	1.5			
Number of holes	1			
Orifice orientation	Axial			
Fuel injection pressure/ Mpa	50			
n-dodecane density/ kg/m^3	698			
Fuel temperature at nozzle /K	363			
Injection duration / ms	1.5			
Injection mass / mg	1.92			

https://ecn.sandia.gov/diesel-spray-combustion/target-condition/spray-ab/

Mesh details

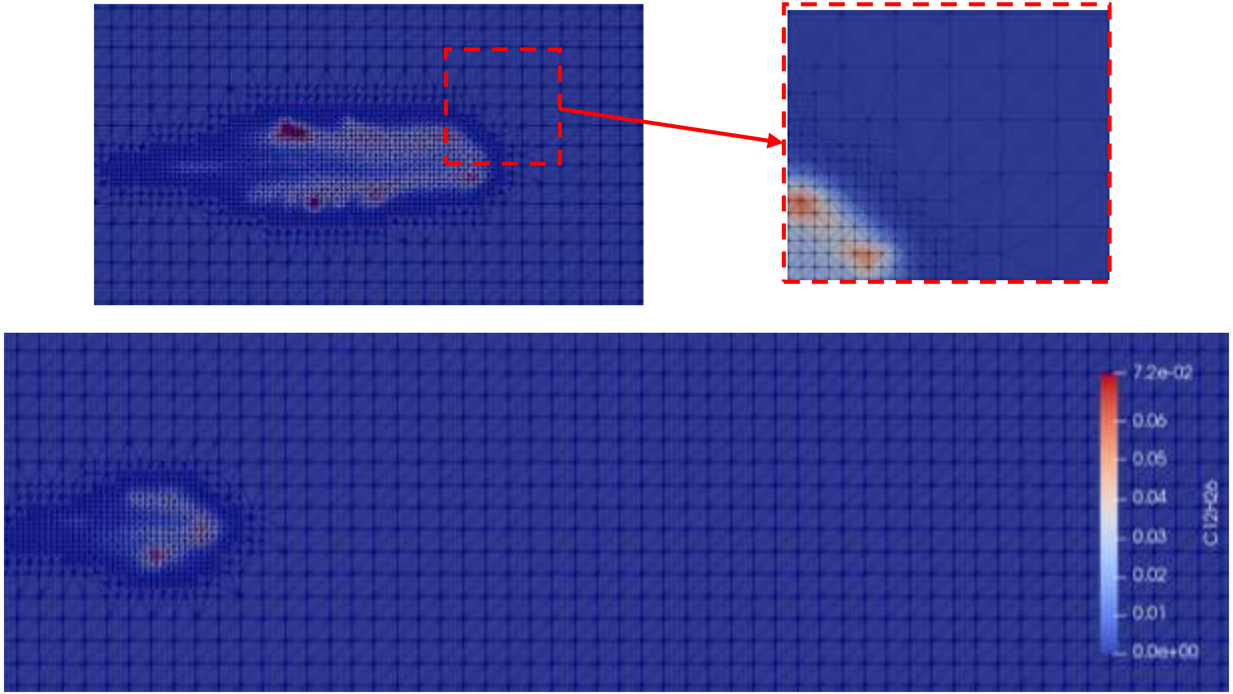


Length	Width	Height
20mm	20mm	100mm

	Case1	Case2
grids	320000	871808
Min size	0.125mm	0.09mm

Mesh details

Adaptive mesh refinement (AMR) is relevant for CFD since it can greatly reduce the computational effort needed to solve a lot of cases.



Cut plane of the 3-D computational domain and the illustration of AMR

Numerical method

Perssure-velocity coupling: PIMPLE algorithm

LES Model: one-equation eddy viscosity model (kEqn)

Injection Model:

Initial droplet distribution： RosinRammler

breakup Model: ReitzKHRT

Simulation results

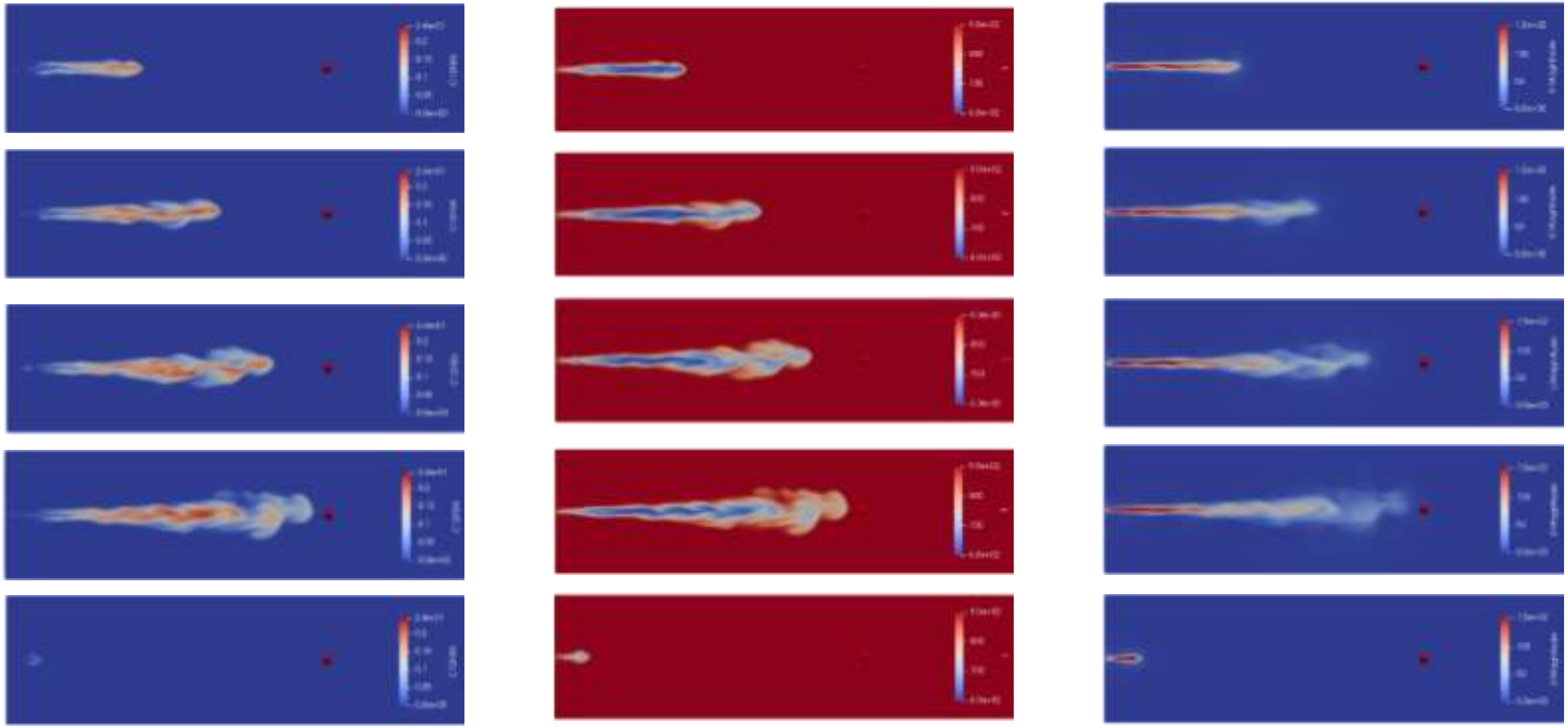
Case1 — C12H26 | T | U

0.25ms

0.50ms

0.75ms

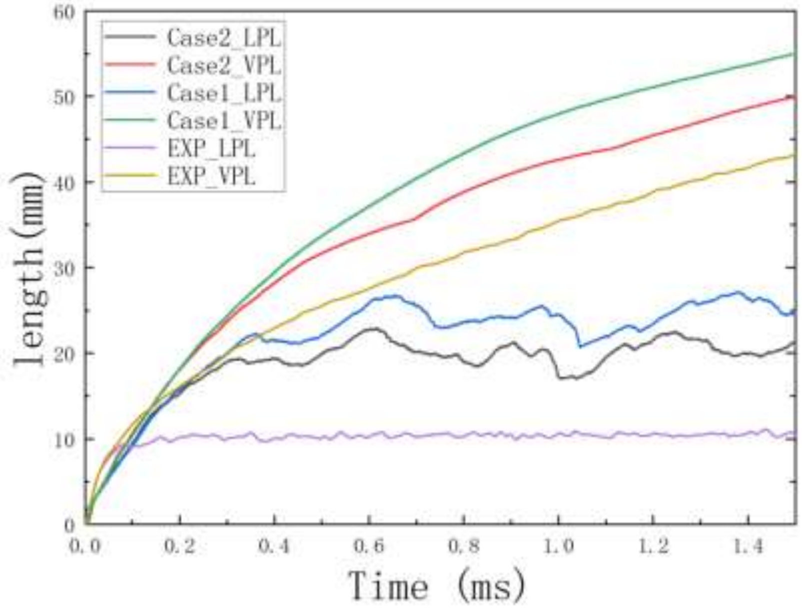
1.00ms



Simulation results

Liquid penetration length (LPL): the axial distance covering 95% of the injected liquid fuel mass

Vapour penetration length (VPL): distance from the nozzle tip to the location where the fuel mass fraction is 0.1% of its maximum value

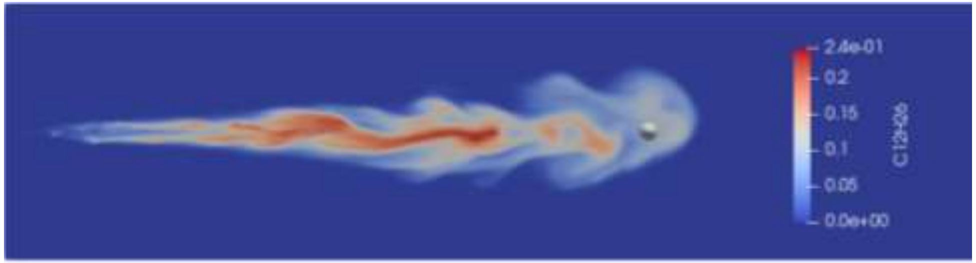


- Simulations have longer LPL and VPL than experiment
- Refining the mesh can shorten LPL and VPL
- It is necessary to adjust the parameters of the injection model to optimize the simulation results and make them more consistent with the experimental results

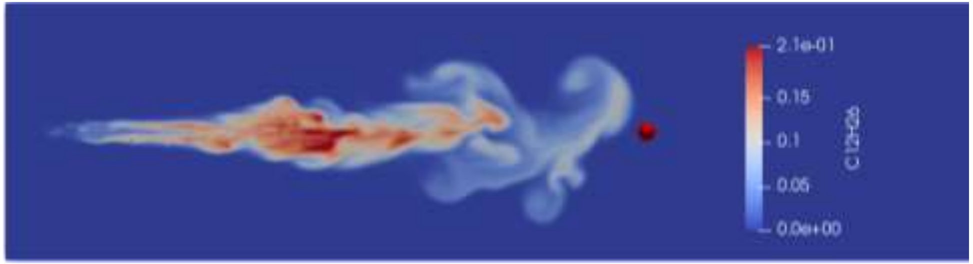
Simulation results

1.45 ms

Case1



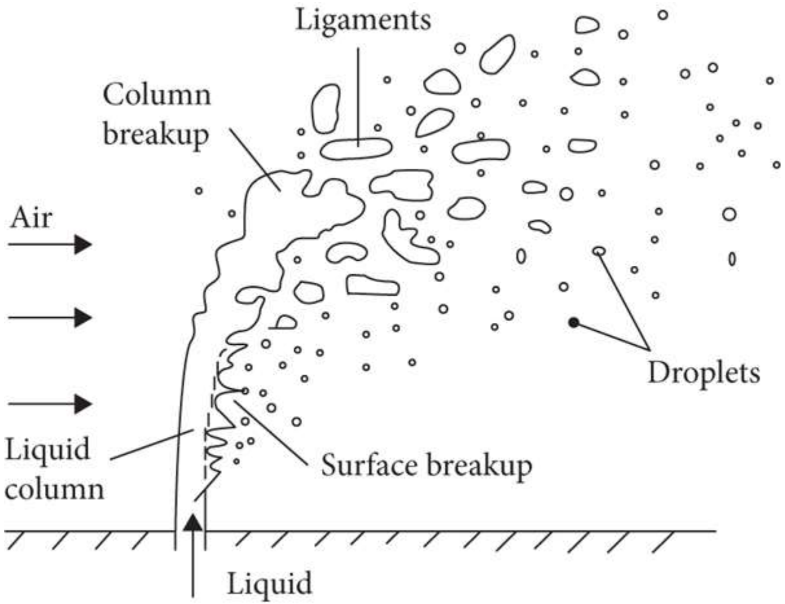
Case2



With decreasing the mesh size, the carrier gas radial dispersion increases

Following work

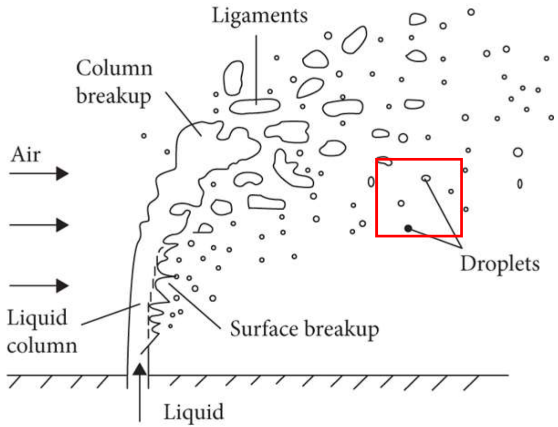
The following work will develop physics-based and AI-based model for spray dynamics considering dispersed droplet in a shear-layer



Droplet Size Spatial Distribution Model of Liquid Jets Injected into Crossflow

Following work

- **Different kinds of LES models will be applied in OpenFOAM to simulate the spray in crossflow**
- **Specific regions (Inside the red box) of the spray will be investigated for the dynamical behavior of the dispersed droplets**
- **The obtained data will then be used to train the AI model**



Thanks for the attention

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