

# CFD Simulation of Injection Processes in OpenFOAM: Under-expanded Jets and Lagrangian Sprays

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Francesco Duronio<sup>a</sup>, Michele Battistoni<sup>b</sup>, Anqi Zhang<sup>c</sup>, Emma Zhao<sup>c</sup>,  
Angelo De Vita<sup>a</sup>, Andrea Di Mascio<sup>a</sup>

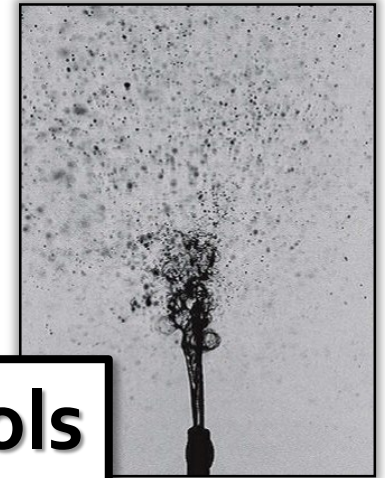
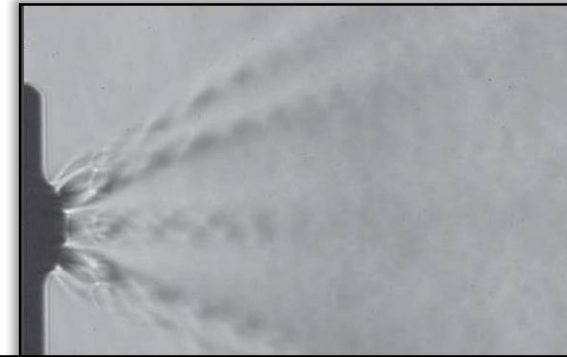
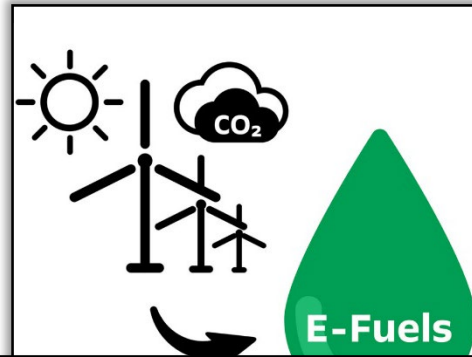
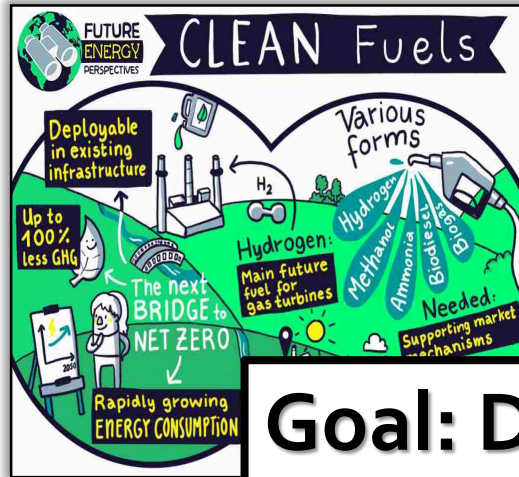
*a - Università degli Studi dell'Aquila*

*b - Università degli Studi di Perugia*

*c - Aramco Americas: Aramco Research Center – Detroit*



# Motivations: Sprays & Innovative Fuels



**Goal: Development of ad-hoc simulation tools**

Poursadegh, F., Lacey, J.S., Brear, M.J., Gordon, R.L., Petersen, P., Lakey, C., Butcher, B., Ryan, S. and Kramer, U. On the phase and structural variability of directly injected propane at spark ignition engine conditions.

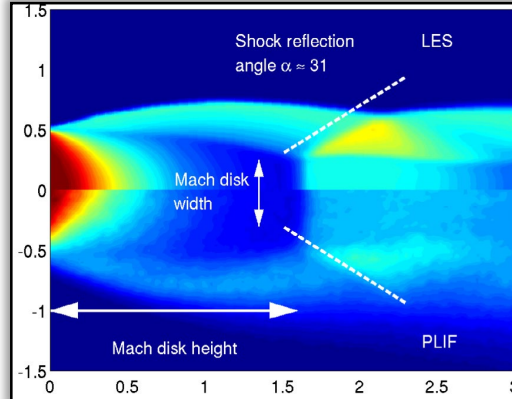
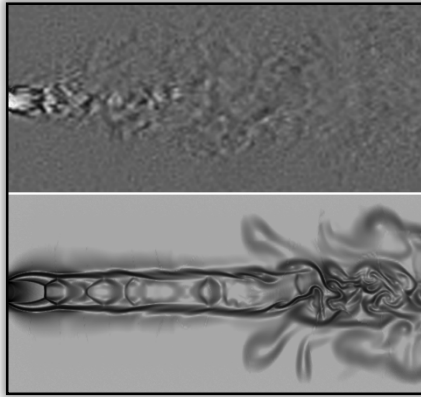
- ✓  $H_2$ ,  $MeOH$ ,  $C_3H_8$ ,  $NH_3$ , e-fuels, ..
- ✓ Sprays: different physical behavior
- ✓ Under-expanded jets

- ✓ Often injected in critical conditions or as gases
- ✓ Phase transition ruled by flash boiling



# Challenges on Injection Processes CFD Simulation

## Near Nozzle: Eulerian Approach

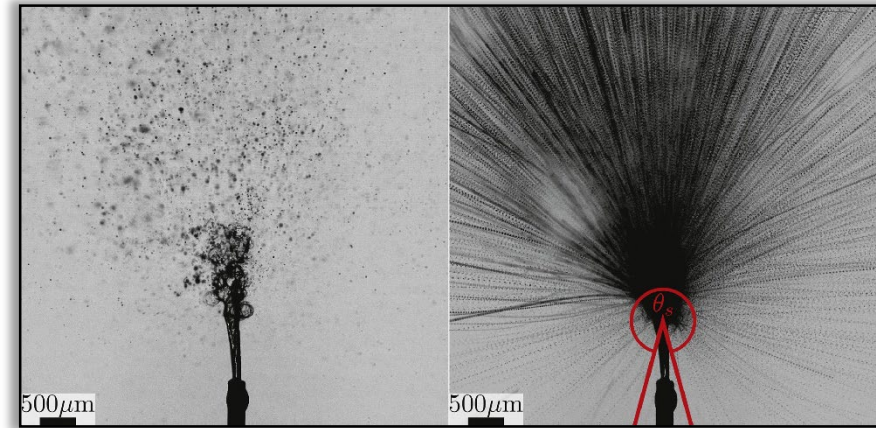


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Yu J, Vuorinen V, Kaario O, Sarjovaara T, Larmi M. Characteristics of High Pressure Jets for Direct Injection Gas Engine

- ✓ Strong compressibility effects and handle trans-critical fluids
- ✓ Under-expanded jets
- ✓ Limit numerical dissipation
- ✓ Development of low order methods

## Whole Spray: Eulerian-Lagrangian Approach



- ✓ Flash boiling onset
- ✓ Extreme tuning of:
  - Breakup model constants
  - Spray angles
- ✓ Droplets sizing inaccurate
- ✓ Difficulties in catching spray collapse



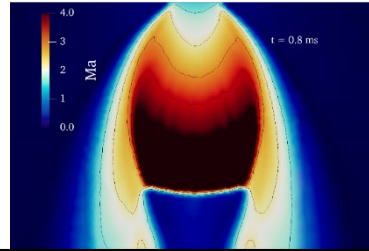
# Simulation of Near-Nozzle Multi-phase Flow



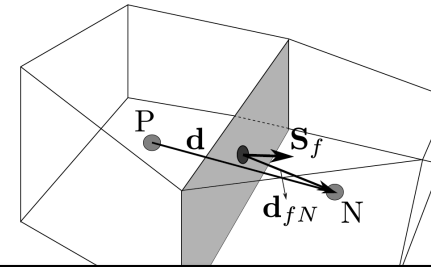
## Fluid Properties

- ✓ **UniPG Real Fluid Pkg**
- ✓ Peng Robison EOS
- ✓ Cp, Cv: Modified Janaf
- ✓ Dyn Visc: Chung

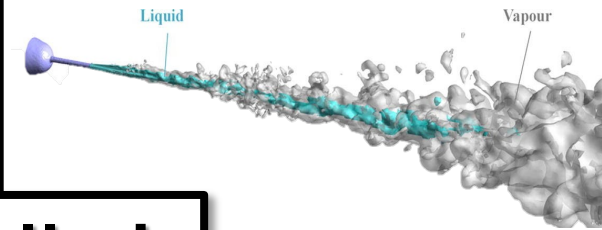
## Adequate Numerics



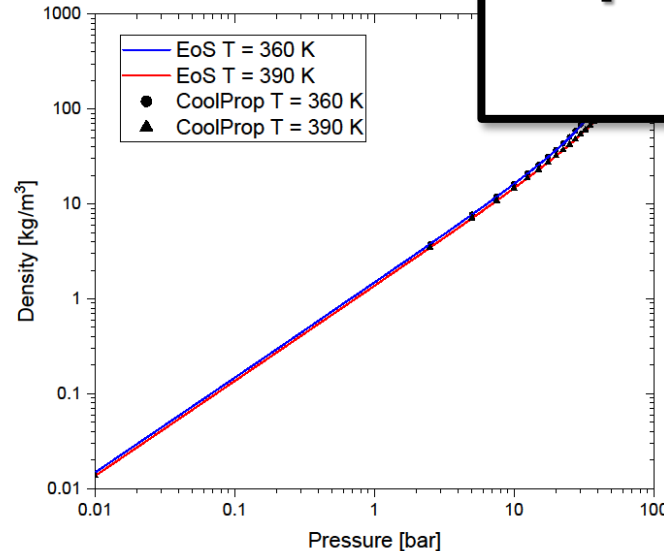
Montanaro, A., Ranieri, S. and De Angelis, L., 2015. Effects of dynamic conditions and geometry in gaseous direct injection process for internal combustion engines.



## Phase Transition Model



**OpenFOAM developed solver was called**  
**realCentralHRMFoam**



- ✓ Under-expanded jets
- ✓ **Low numerical dissipation!**
- ✓ Flux splitting: Kurganov Noelle Petrova
- ✓ Crank Nicholson 2°temporal int.
- ✓ MUSCL scheme for reconstruction

Internal non-equilibrium



**Homogeneous Relaxation Model**

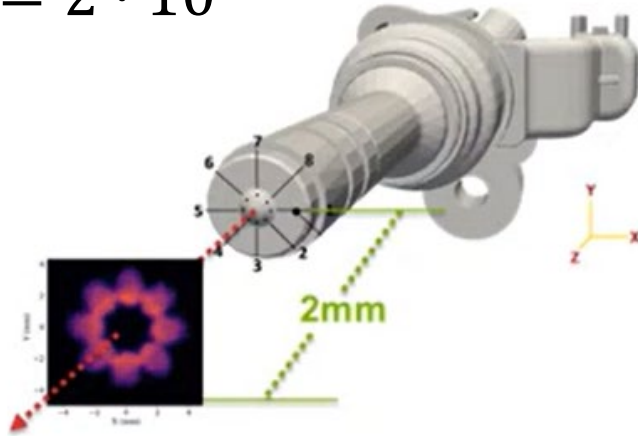




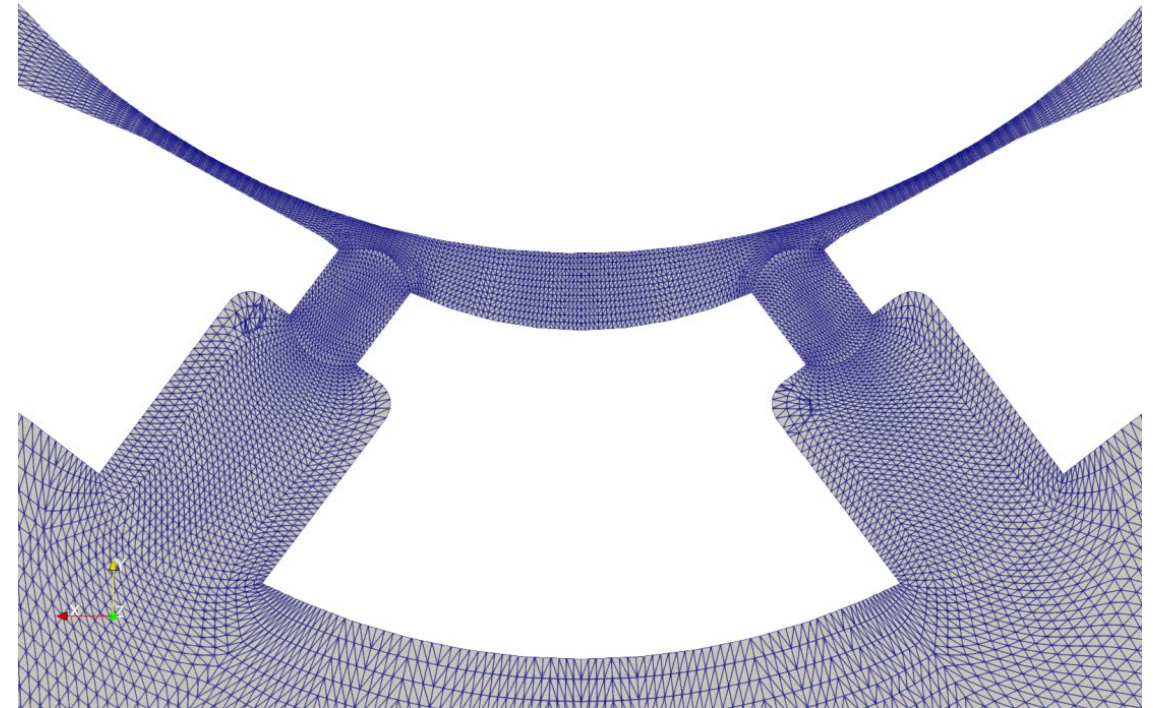
# Validation on G2 Injection (flashing case)



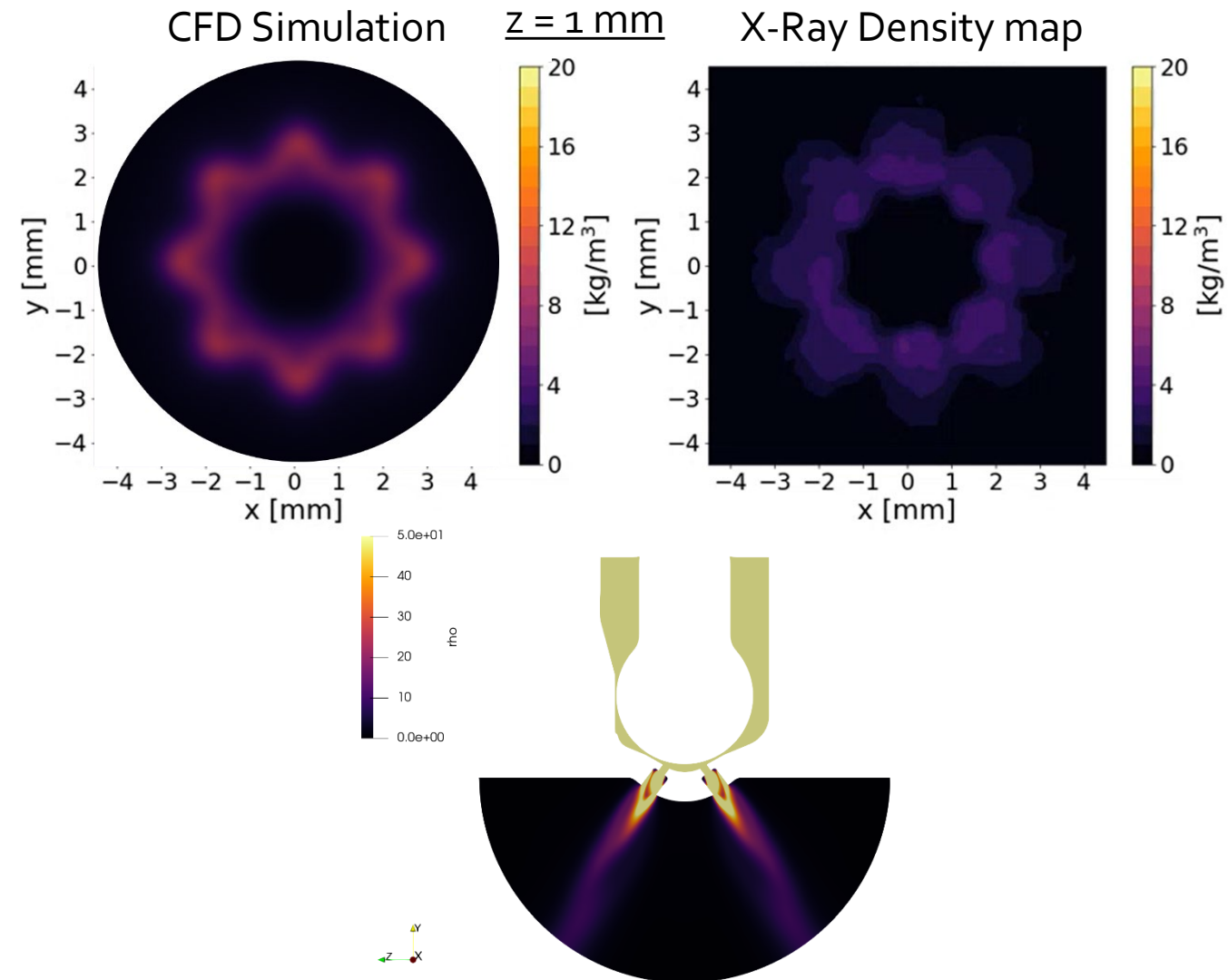
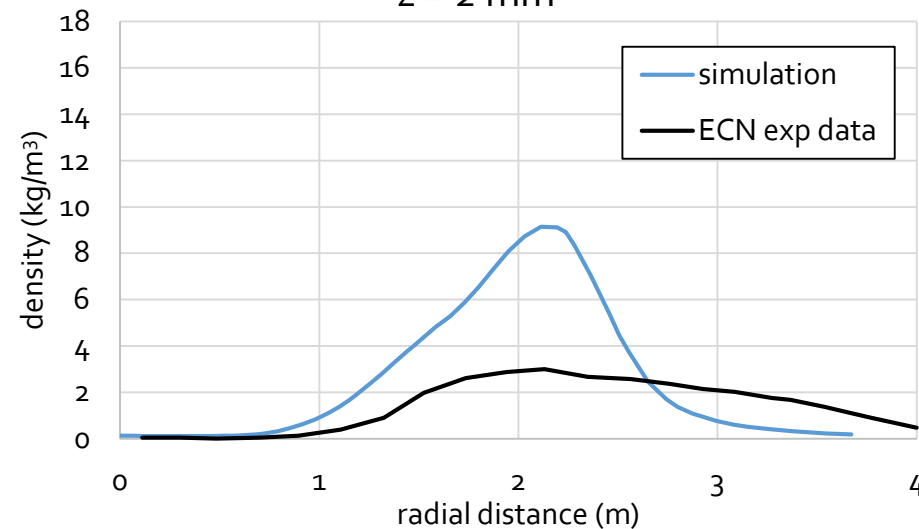
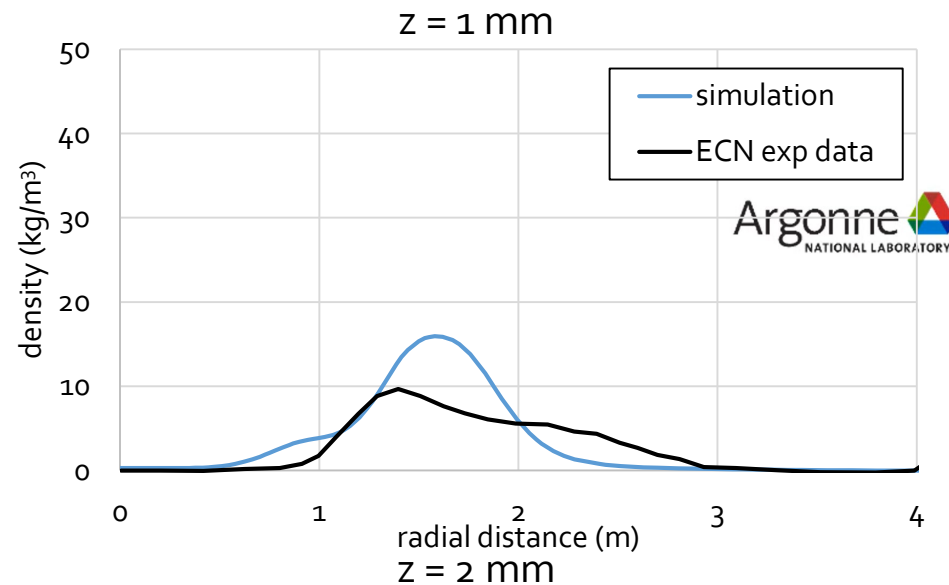
- ✓ ECN Spray G condition G2:
  - ✓ Fuel temp: 363 K
  - ✓ Ambient temp: 333 K
  - ✓ Ambient Pressure 0.5 bar
- ✓ Argonne X-Ray data: density maps
- ✓ Fuel:  $\text{IC}_8\text{H}_{18}$
- ✓ Turbulence: LES Dynamic kEqn
- ✓ HRM:  $\vartheta_0 = 2 \cdot 10^{-10}$



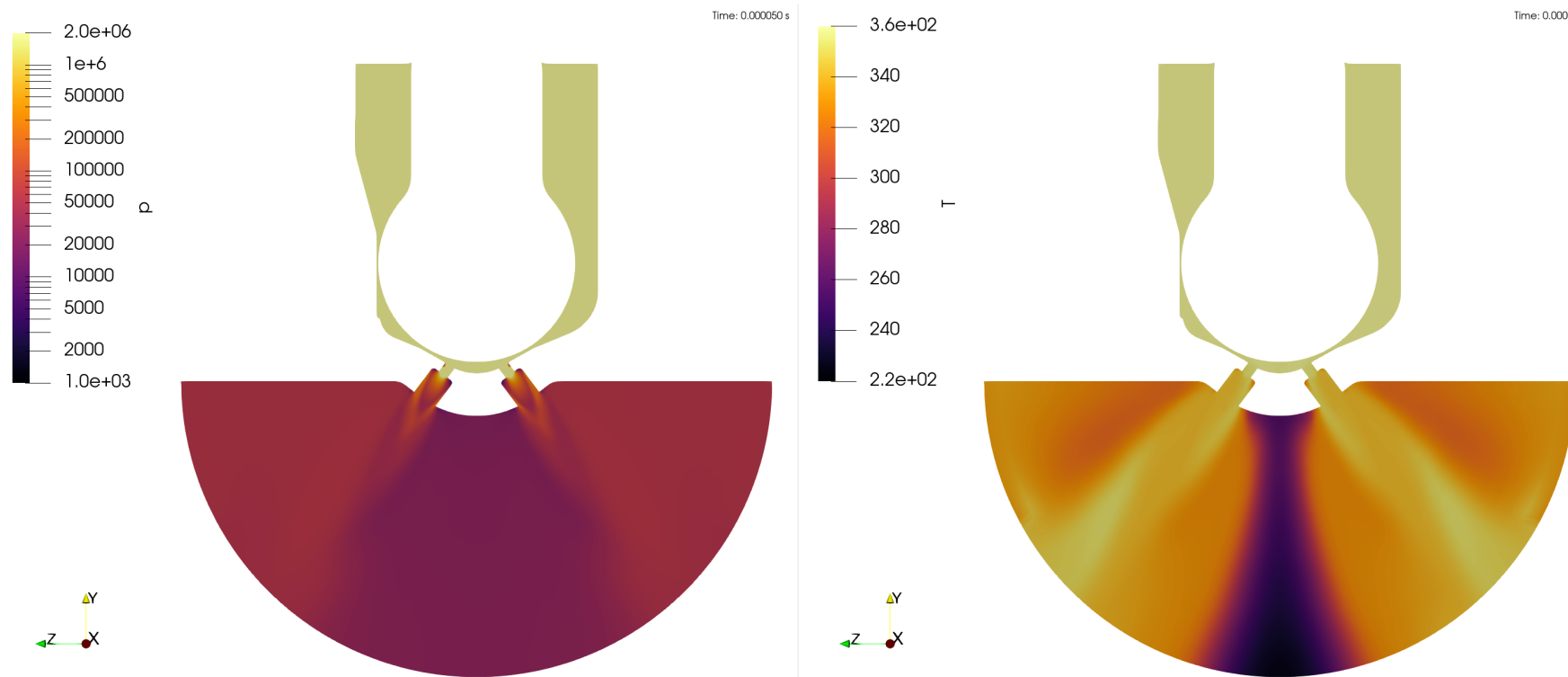
- ✓ Mesh: GridPro provided @ ECN website, Structured up to  $5 \mu\text{m}$  (refineMesh - **9 M**)
- ✓ Injector + 9 mm cap
- ✓ Fixed Needle: 50 mm



# Validation on G2 Injection (flashing case)



# Validation on G2 Injection (flashing case)



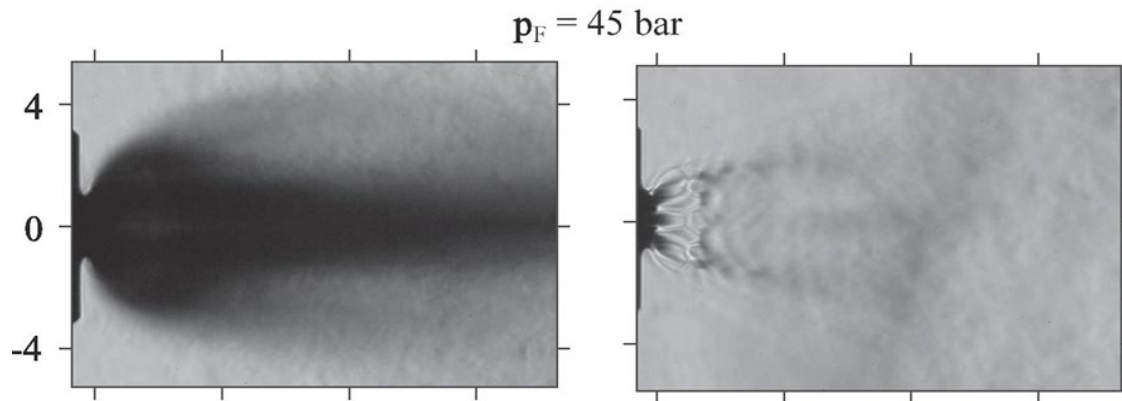
- ✓ Pressure field shows a slight internal depressurization
- ✓ Temperature field also shows a strong decrease in the internal region among jets



# Case Study: Spray G - C<sub>3</sub>H<sub>8</sub> Injection



- ✓ Validation: Schlieren images of Poursadegh et al.
- ✓ Fuel: C<sub>3</sub>H<sub>8</sub>
- ✓ Turbulence: LES Dynamic kEqn
- ✓ HRM:  $\vartheta_0 = 3.84 \cdot 10^{-8}$



Poursadegh, F., Lacey, J.S., Brear, M.J., Gordon, R.L., Petersen, P., Lakey, C., Butcher, B., Ryan, S. and Kramer, U. On the phase and structural variability of directly injected propane at spark ignition engine conditions.

- ✓ Mesh: GridPro provided @ ECN website, Structured
  - Base grid: up to 10  $\mu\text{m}$  (1.5 M)
  - Fine grid: up to 5  $\mu\text{m}$  (refineMesh - 9 M)
- ✓ Injector + 9 mm cap
- ✓ Fixed Needle: 50 mm

	Sub Critical	Super Critical
Inj Press. [bar]	45	
Ambient Press. [bar]	0.5	
Amb. Temp. [K]	390	
Fuel Temp. [K]	360	390

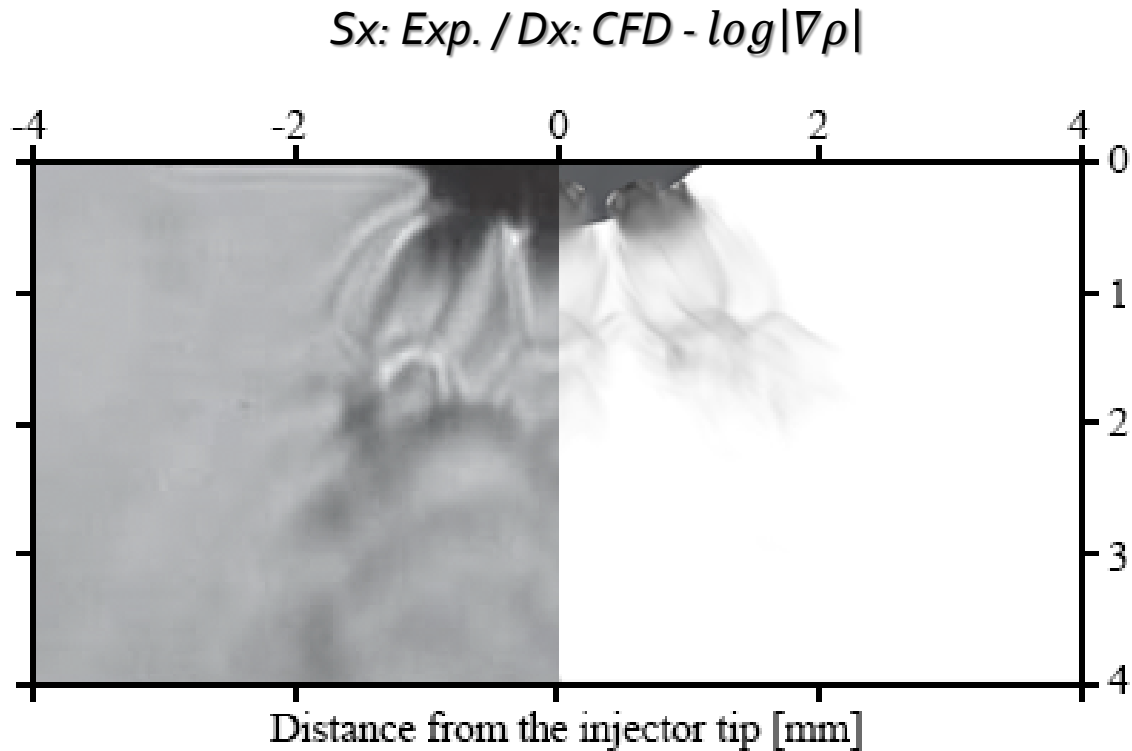




# Comparison with Schlieren Images

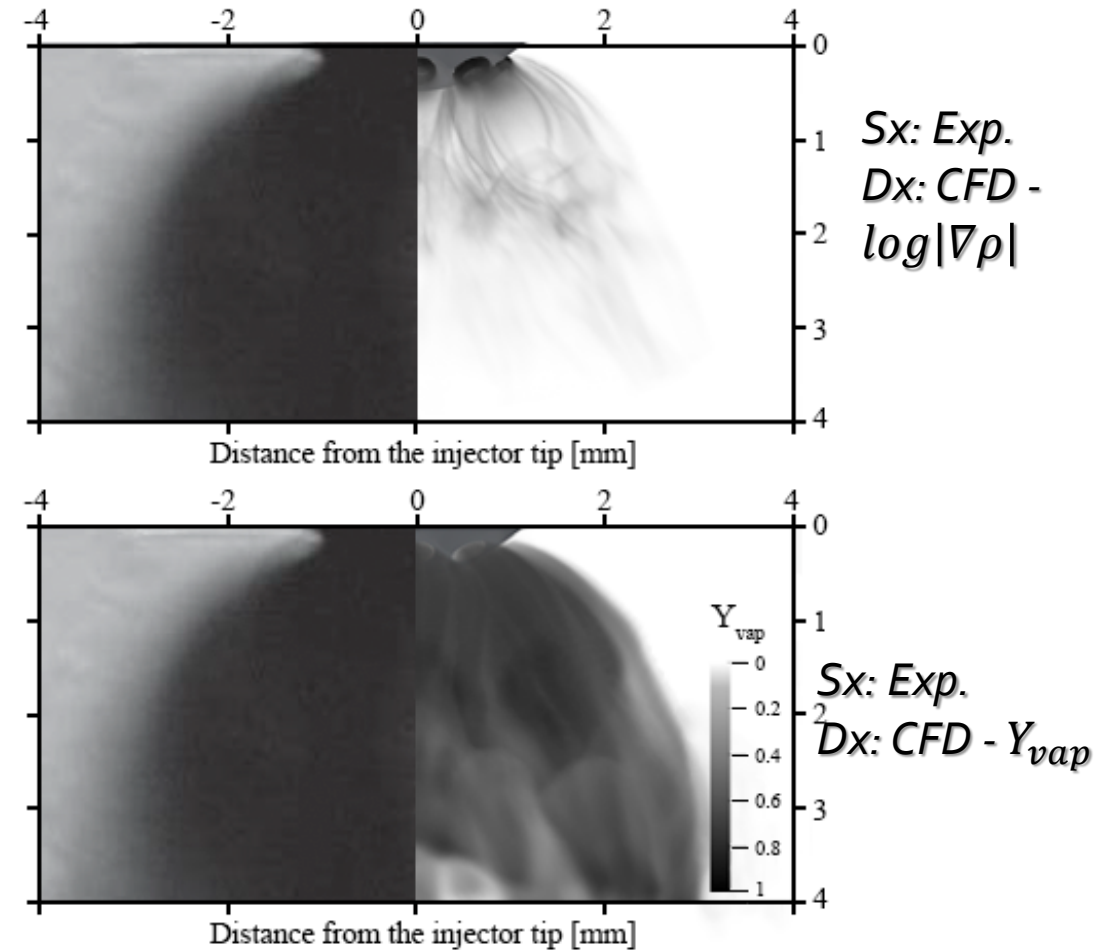


## Super-Critical Injection



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## Sub-Critical Injection

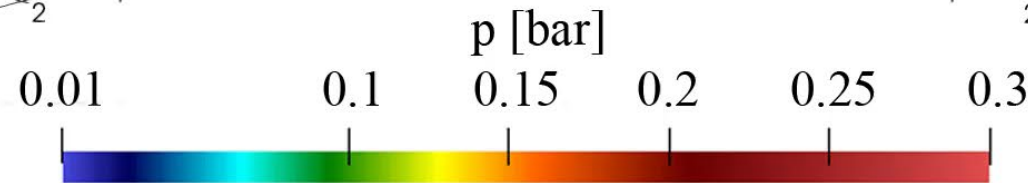
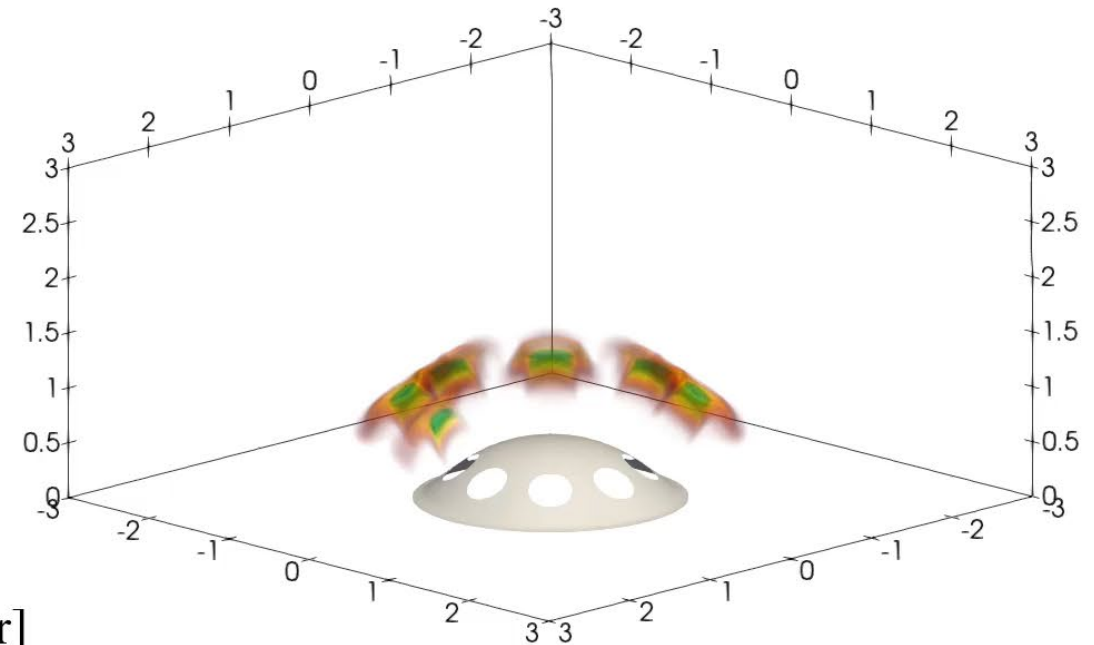
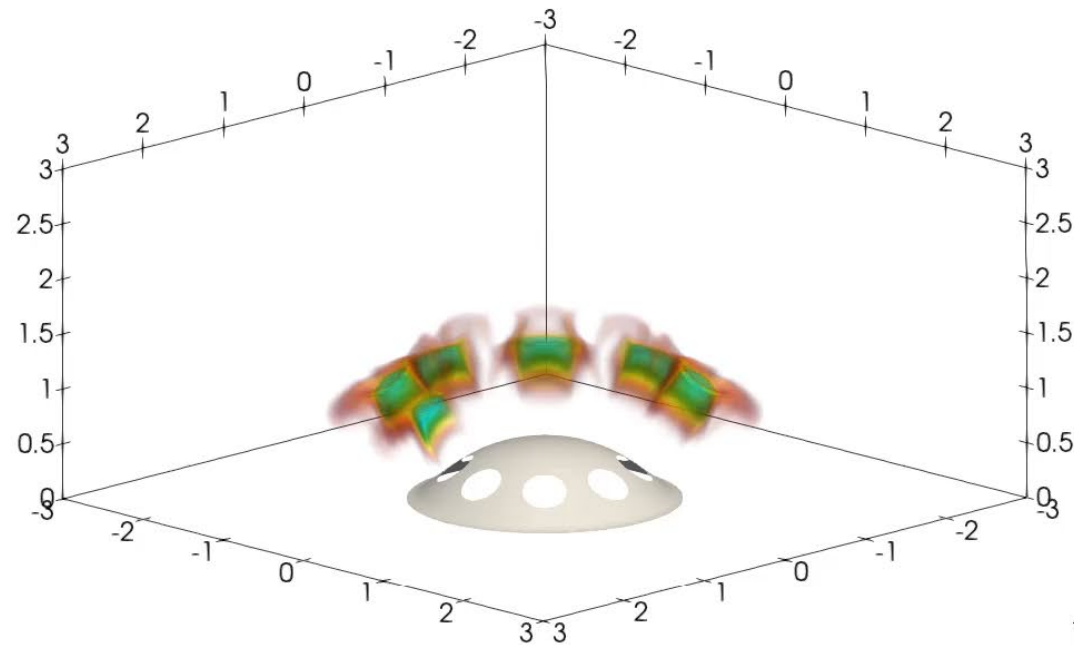


# Temporal Evolution



## Super-Critical Injection

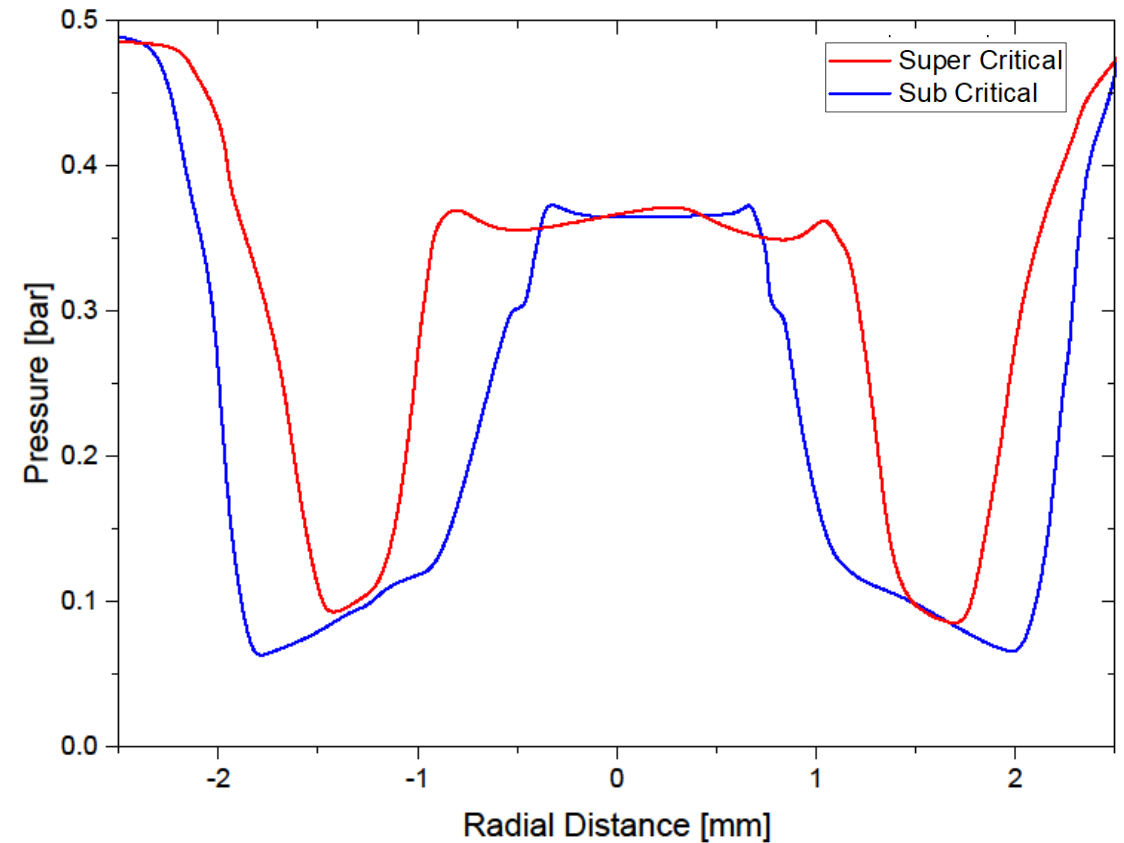
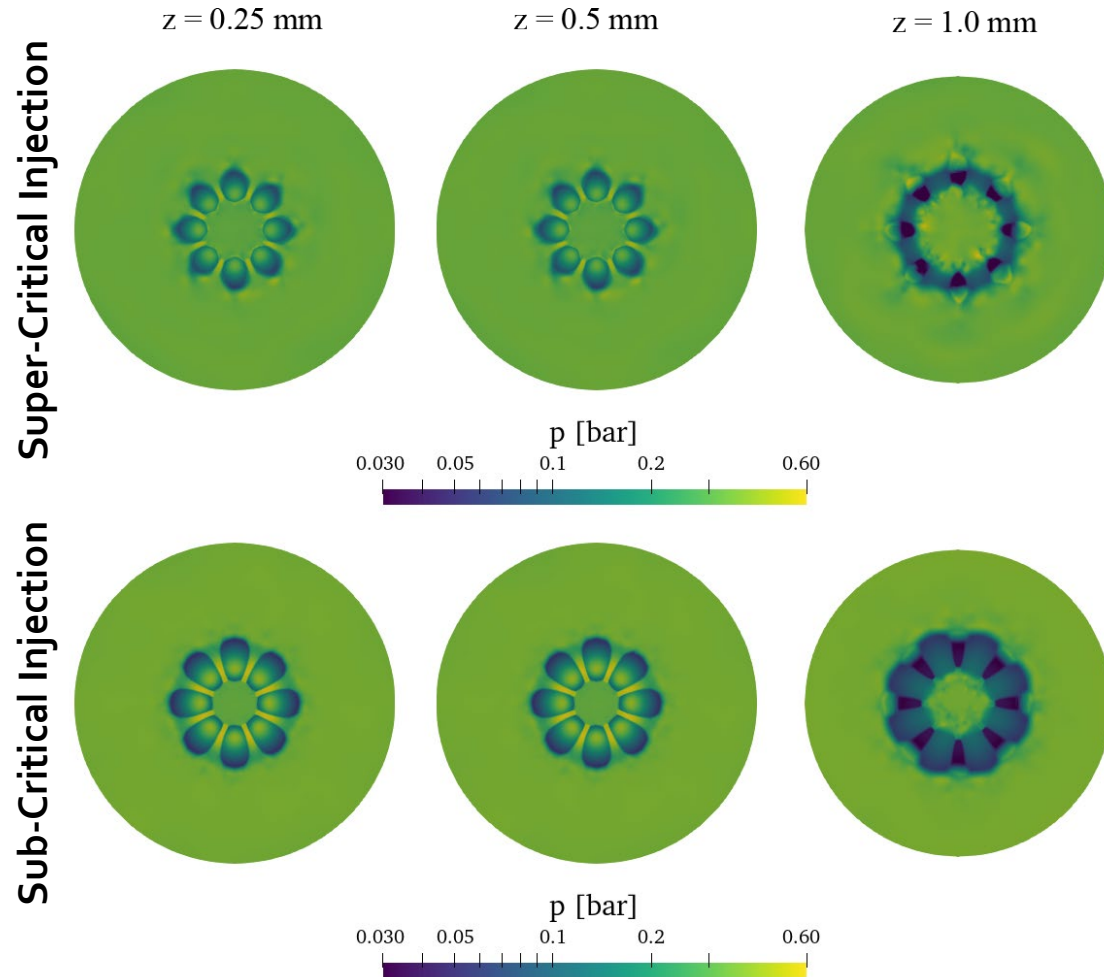
## Sub-Critical Injection



Duronio F, Battistoni M, Di Mascio A., De Vita A., Rahantamialisoa F. N. Z., Zembi J., A real-fluid low-dissipative solver for flash boiling simulations of non-equilibrium mixtures, International Journal of Heat and Mass Transfer, Volume 225, 2024,



# Pressure Field: Axial Cross Sections

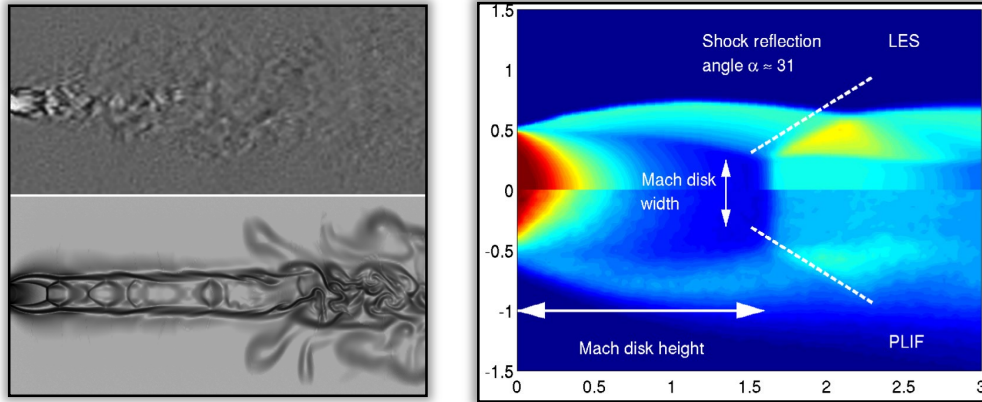


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# Challenges on Injection Processes CFD Simulation

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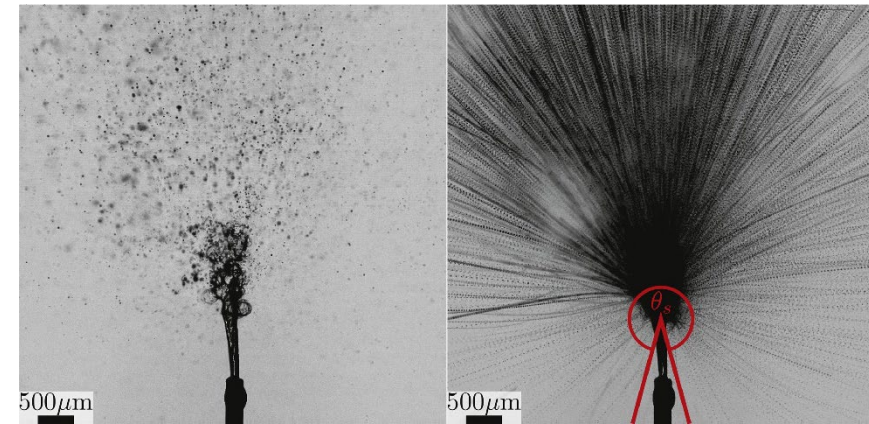


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## Whole Spray: Eulerian-Lagrangian Approach

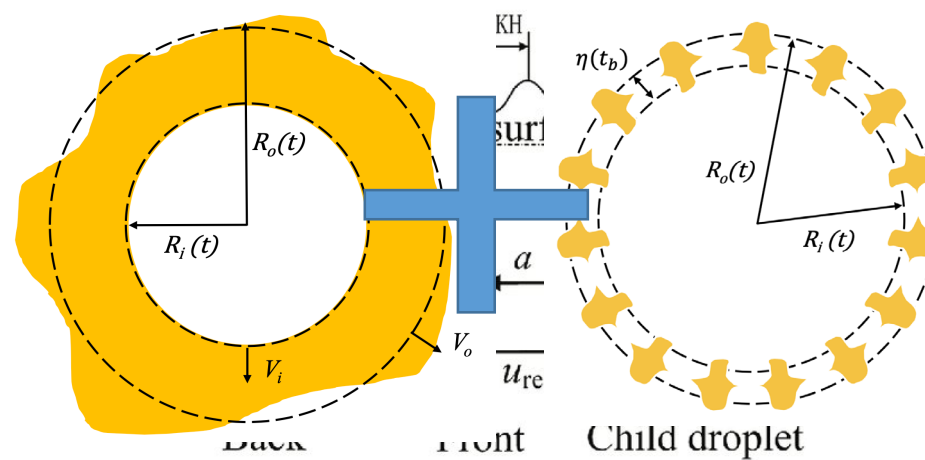


### Key Models:

- ✓ Phase change: Adachi/Price
- ✓ Breakup: ...  
Rayleigh-Plesset Equation !?



# fbBreakup model: Flash Boiling Breakup



## Aerodynamic breakup mechanisms are:

- driven by aero-dynamic instabilities on droplet surface
- mainly function of liquid-gas relative velocity

## Flash boiling induced breakup is:

- driven by bubbles  $R_i(t)$  growing within the droplets  $R_o(t)$
- influenced by the liquid thermodynamic properties (especially saturation pressure!)
- Breakup occurs when the instability amplitude  $\eta(t)$  grows larger than a «characteristic length» of the spray



# fbBreakup model: Parameters

Breakup criterion:

$$\eta_0 e^{\int_0^t \omega dt} > k_b (R_o(t) - R_i(t))$$

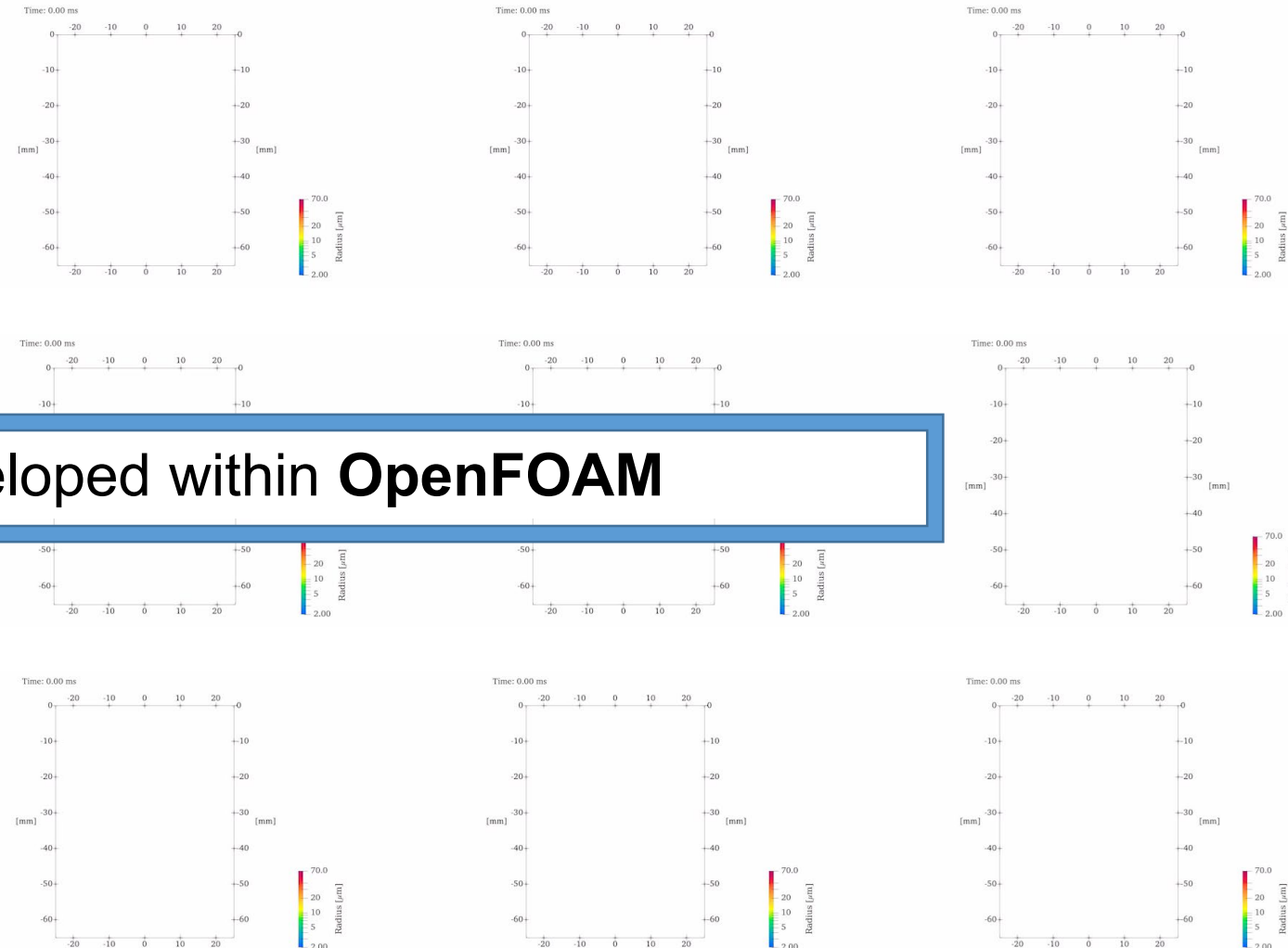
$R_o(t), R_i(t)$  growth rate is  $p_{sat}$  dependent:

fbBreakup was developed within OpenFOAM

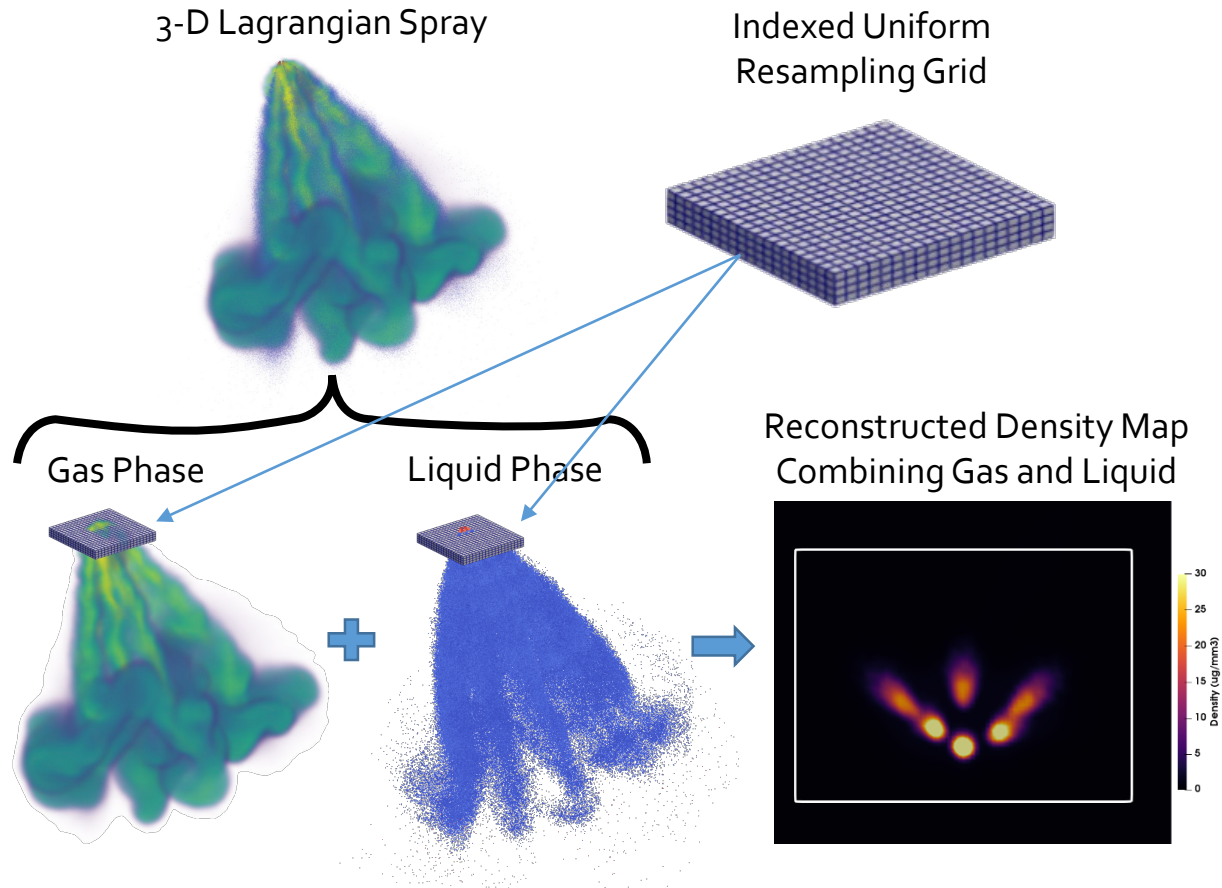
After breakup added a radial component:

$$U_r = k_v \frac{3R_i^2 V_i (R_o - R_i)}{R_o^3 - R_i^3}$$

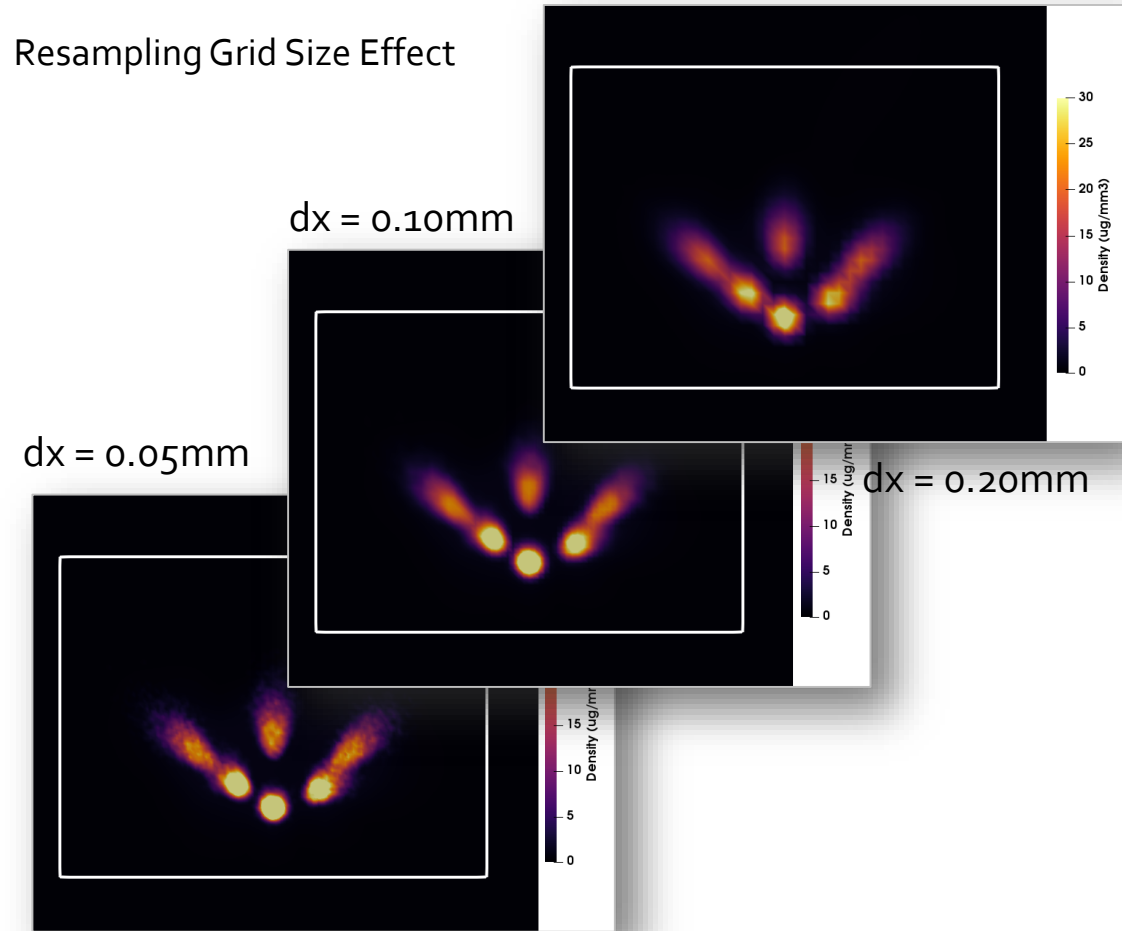
Assessment of Lagrangian Spray Simulation Procedure using Realistic GDI Injector and Fuel under Flash-Boiling Condition - *Francesco Duronio, Anqi Zhang, Le Zhao and Angelo De Vita*



# Post-processing approach



Resampling Grid Size Effect



Robust post-processing developed to enable subsequent model performance evaluation

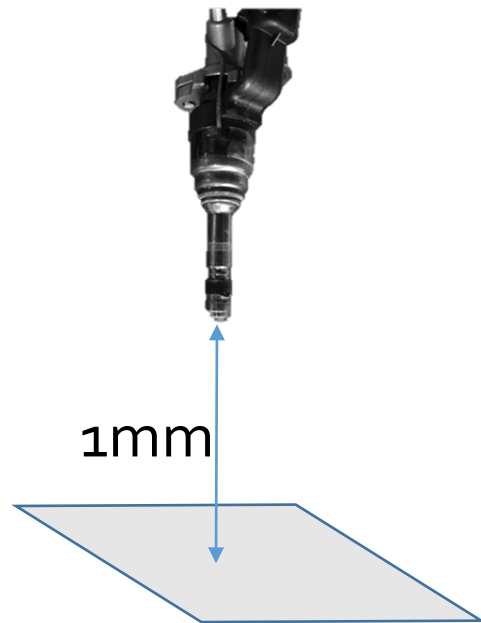
# Near Nozzle Validation: Exp. Campaign

- Bosch GDI injector
- 6-hole side-mounted

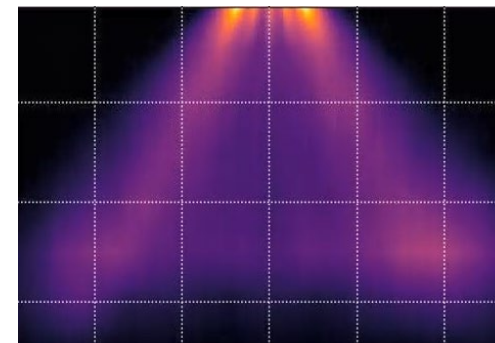
- EU5 : real gasoline surrogate properties developed @



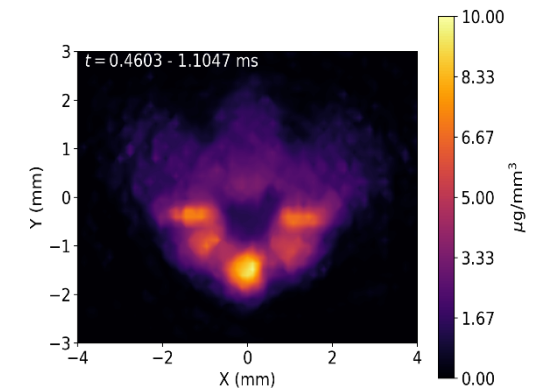
Fuel Temp. [K]	Amb. Temp. [K]	Amb. Press. [bar]	Injection Press. [bar]
363.15	298.15	0.4	50



Near-Nozzle Fuel Density



Spray Tomography

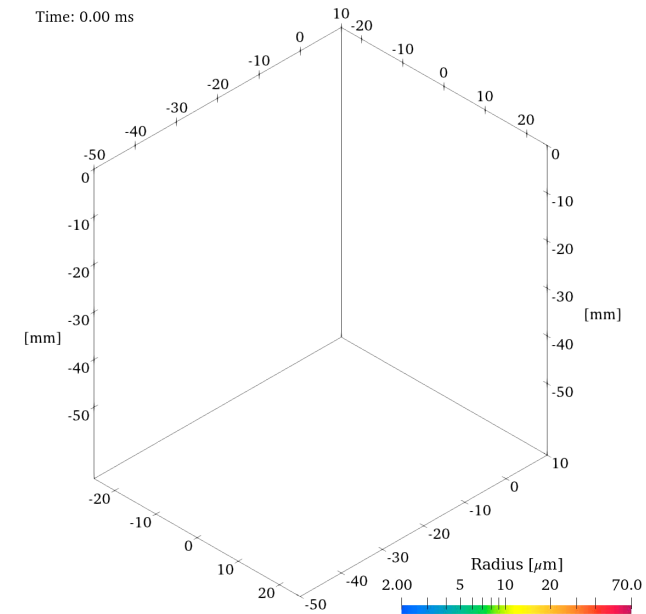
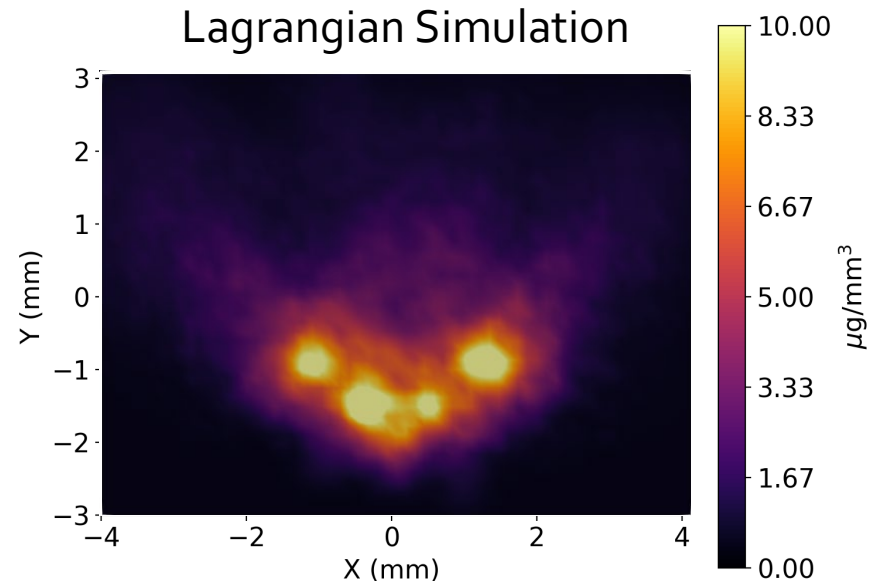
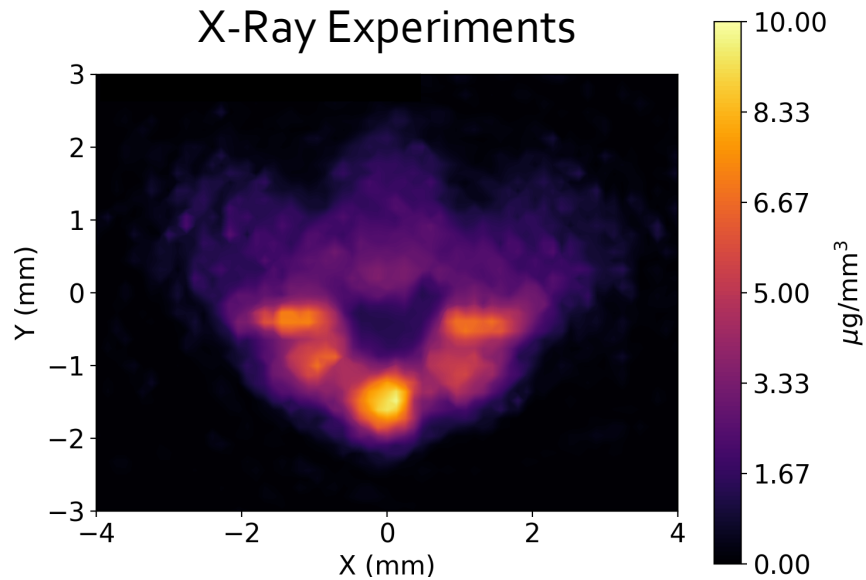


# Near Nozzle Validation: CFD Model

EULERIAN FRAMEWORK	
Integration domain	Cylindrical, 100 x 85 mm
Base Grid	1 x 1 x 1 mm
Near Nozzle Grid	0.125 mm
Turbulence	RANS RNG $k$ - $\varepsilon$

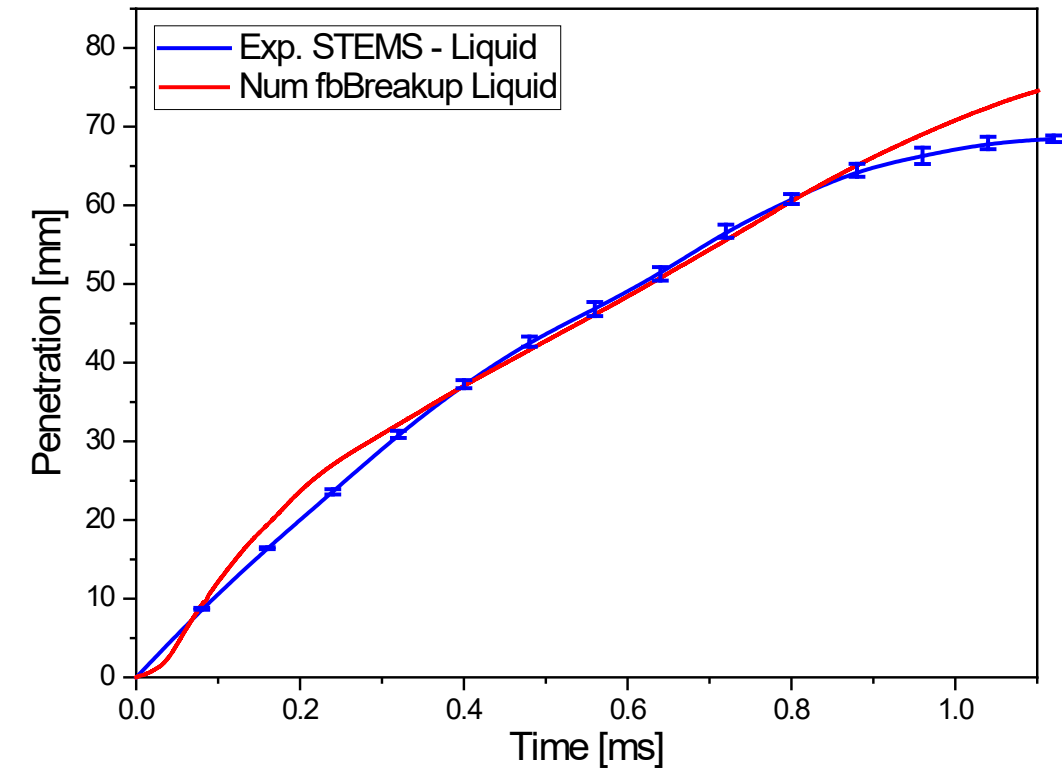
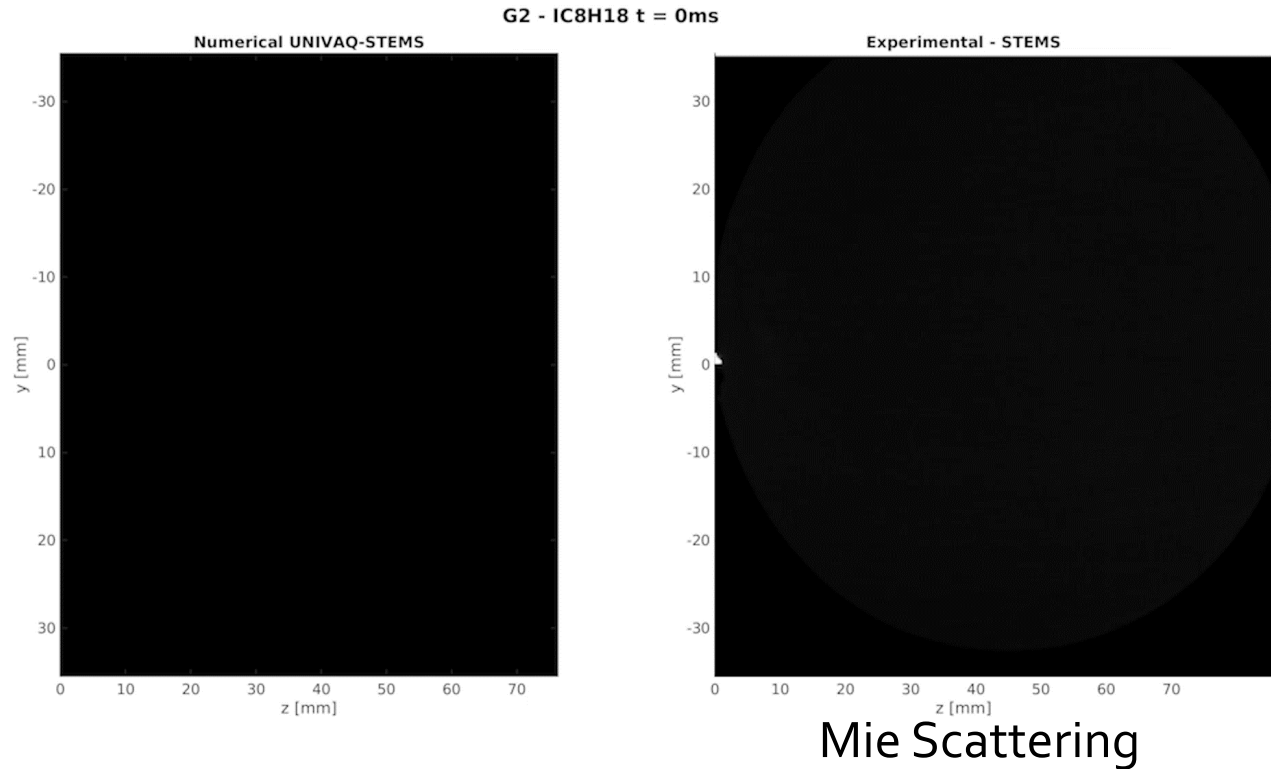
Plume cone angle and plume direction set equal to the nominal value obtained from the manufacturer

LAGRANGIAN FRAMEWORK	
Injection method	Uniform
Effervescent Breakup	<b>fbBreakup</b> $k_v = 2.5$ $k_b = 2$ and $k_{vb} = 3$
Aereodynamic Breakup	Reitz Diwakar
Vaporization	Adachi + Price (flash-boiling vaporization)



# Spray G Validation: G2<sub>SFB</sub>

G2<sub>SFB</sub>: G2 with lower ambient pressure 0.2 bar



✓ Aereodynamic Breaup: Reitz Diwakar

✓  $k_b = 2.5 k_{vb} = 2.5 k_v = 3.5$

✓ Plume Cone Angle:  $27^\circ$

✓ Plume direction:  $35^\circ$

Duronio, F., Ranieri, S., Montanaro, A., Allocca, L. and De Vita, A., 2021. ECN Spray G injector: Numerical modelling of flash-boiling breakup and spray collapse. *International Journal of Multiphase Flow*, 145, p.103817.

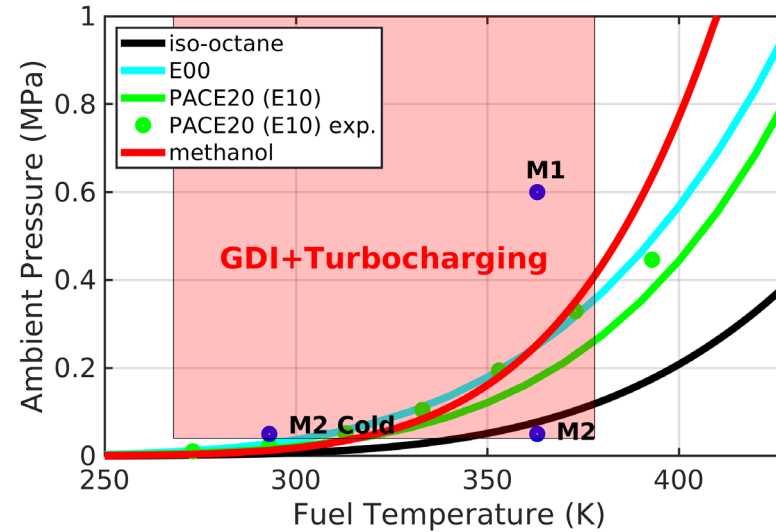
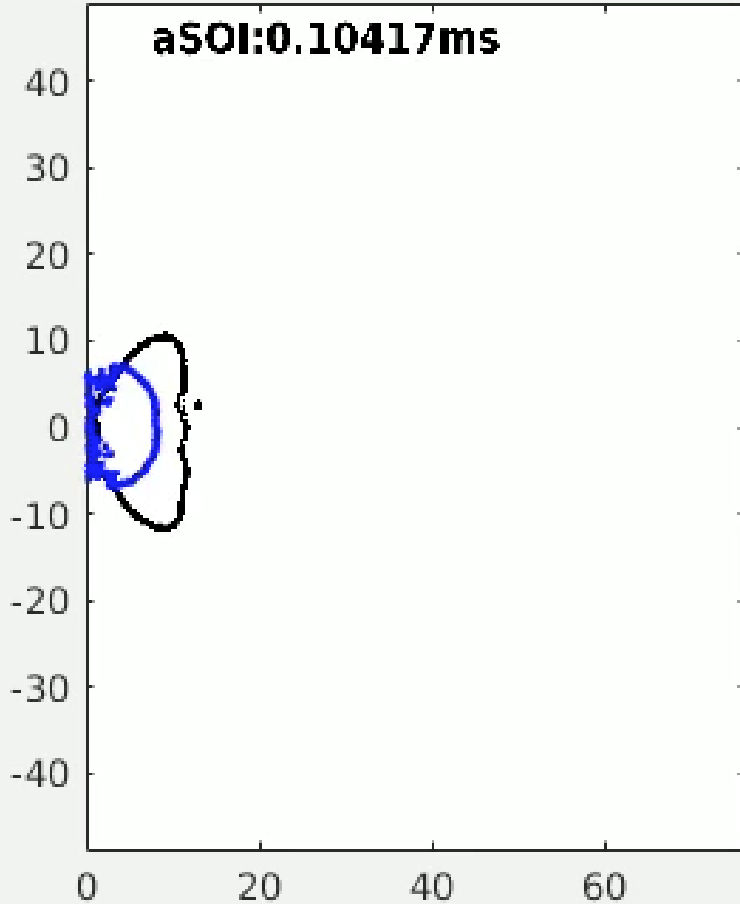


# ECN 9 – Spray M - MeOH & PACE20

## M2 - Methanol

Simulation time = 0.100000ms

aSOI:0.10417ms



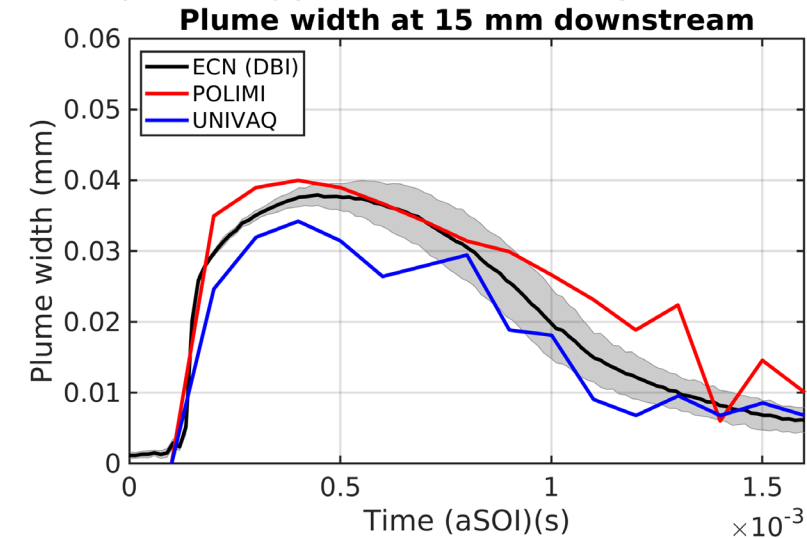
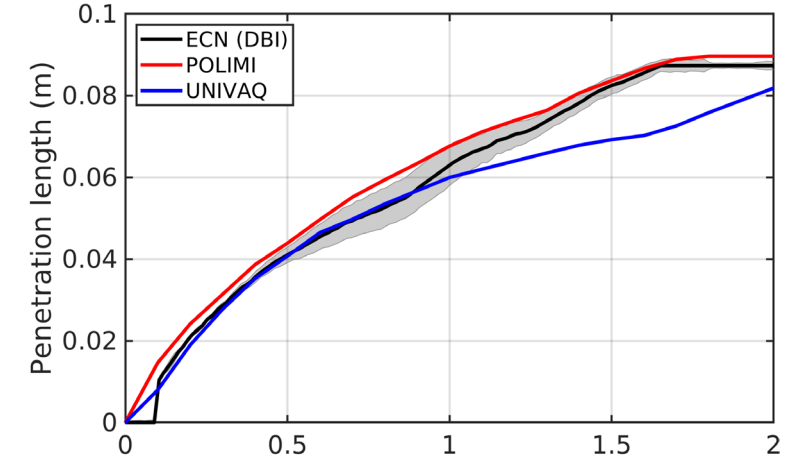
$$R_p = \frac{p_{amb}}{p_{sat}(T_0)} \begin{cases} R_p < 0.3 & \text{Flash boiling} \\ 0.3 < R_p < 1 & \text{Transition regime} \\ R_p > 1 & \text{Non-flash boiling} \end{cases}$$

$$\text{C}_8\text{H}_{18}: R_p = 0.69$$

$$\text{PACE 20}: R_p = 0.21$$

$$\text{MeOH}: R_p = 0.197$$

## M2 – PACE 20



# Conclusions

## Near Nozzle: Eulerian Approach

- ✓ Development of a low dissipative code for simulating multiphase flows with:
  - Flux-splitting schemes for compressible flows
  - Real fluid properties
  - HRM phase change model
- ✓ Validation with Spray G2 data and  $C_3H_8$  injections: promising performances reproducing multiphase under-expanded jets

} **realCentralHRMFoam**

## Whole Spray: Eulerian-Lagrangian Approach

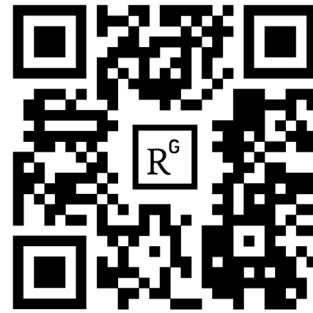
- ✓ Effervescent breakup model allow to predict quite well fb spray morphology both in the near nozzle zone and in the far field
- ✓ fbBreakup model is **capable to reproduce spray collapse without changing spray angles**
- ✓ fbBreakup model is sensible to the fuel properties



# Contact Info



# Thank you !



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Job: **Research Fellow**

Email: **francesco.duronio@univaq.it**



# STEMS

