Topic 2 – Near Nozzle Flow

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Contributors

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  - Qingluan Xue, Sibendu Som
  - Michele Battistoni from University of Perugia during sabbatical
- Bosch Research and Technology Center (Bosch)
  - Edward Knudsen, Eric Doran
- CMT
  - Pedro Marti, Raul Payri
- IFPEN
  - Chawki Habchi
- Sandia National Laboratory (Sandia)
  - Francois Doisneau, Marco Arienti, Joe Oefelein
- Experimental Data: Argonne National Laboratory
  - Chris Powell, Alan Kastengren

Modeling Objectives

- Focus on the near nozzle region (within first 10-15 mm)
- Encourage high-fidelity simulations of fuel sprays to understand the primary atomization physics
- Capture the SOI and EOI physics for single and multi-hole injectors
- Capture the spray physics during the main injection process for both single and multi-hole injectors
- Study the capability of the different modeling approaches (Lagrangian-Eulerian, Eulerian-Eulerian) and CFD frameworks (RANS, LES, DNS) for capturing the near nozzle physics
- Assess the importance of different models and modeling artifacts: Turbulence, Compressibility, primary and secondary atomization, …?

Conditions of Interest for Simulations

- Spray A and Spray B operating conditions from Argonne: (http://www.sandia.gov/ecn/refs.php?nam=Kastengren-2012-a#Kastengren-2012-a)
  - Spray A: 675; Spray B: 201
  - Priority 1: P_{inj} = 1500 bar; Priority 2: P_{inj} = 500 bar
  - Fuel temperature: Spray A - 343 K; Spray B – 338 K

Ambient gas temperature	**303 (K)**
Ambient gas pressure	2.0 (MPa)
Ambient gas density	**22.8 (kg/m3)**
Ambient gas N_2 (by volume)	100%

Data Needed from Spray A Simulations

- Mass flow rate at the nozzle exit
- Fuel spray penetration vs. time
- Contour plots of projected density at 0.1 and 0.5 ms
- Transverse mass distribution (projected density across the spray) in ug/mm^2 @ x = 0.1, 0.6, 2, 6, and 10 mm downstream to nozzle exit:
  - between 0.5 – 1.0 ms after SOI
- 2D contours of LVF at x = 0.1, 0.6, 2, 6, 10 mm at 0.5 and 1.0 ms
- Mean droplet size (SMD) at x = 1, 4, 8 mm at 0.5 ms after SOI
  - Mean SMD at the above axial positions vs. axial position
  - Distributions of SMD vs. radial position at the above axial positions

Set-up conditions from Argonne

Outline

- Spray A Comparison between all groups
  - Aachen, ANL, Bosch, CMT, IFPEN, Sandia
  - Description of Simulation set-up from all groups
  - Side-by-side comparisons
    - Liquid penetration, mass flow rate at nozzle exit
    - Liquid volume fractions, projected mass density, SMD
- Parametric variations
  - RANS vs. LES (ANL)
  - Effect of Injection pressure (Bosch)
  - Effect of wall temperature (CMT)
  - Effect of fixed vs. moving needle (CMT)
  - Effect of primary atomization modeling (IFPEN)
- Spray A vs. Spray B dynamics (ANL)
- Concluding Remarks/Suggestions

Comparison between different groups

Model description

Institution	Model approach	CFD Code	Compressibility	Turbulence model
Aachen	Two-Fluid Eulerian/Lagrangian	CIAO	Low Mach	LES/DNS Smagorinsky
Argonne	Single-mixture Eulerian	CONVERGE	Compressible liquid Compressible gas (EOS)	RANS (k-e) and LES (DS)
Bosch	Two-Fluid multi-species Eulerian	Cascade Technologies	Compressible liquid & gas Peng-Robinson EOS	LES Vreman
CMT	Single-mixture Eulerian	OpenFOAM (ESA)	Compressible liquid (function of P, T) and gas EOS	RANS SST k-omega
IFPEN	Two-fluid model with Lagrangian-Eulerian coupling and Primary atomization	IFP-C3D	Compressible liquid and gas	LES Smagorinsky
Sandia (two-phase)	Eulerian Multi-Fluid with multi-component gas and dense spray	Raptor	Liquid: Singularly compressible Gas: Perfect gas EOS	LES Dynamic Smagorinsky

Simulation set up (Spray A)

Institution	Mesh resolution	Needle motion	Initial conditions inside injector	2-D or 3-D
Aachen	Nozzle: 2.7 µm; Prim. Breakup: 1.5 µm; Lag. Spray: 0.25 mm	Fixed needle lift	Fuel filled sac and orifice; 150 MPa and 343 K in Sac and orifice	3-D
Argonne	10 µm inside nozzle and first 6 mm	Transient needle motion – with wobble	Fuel filled sac and orifice; 150 MPa and 343 K otherwise	3-D Height = 200 mm D = 50 mm
Bosch	Voronoi polyhedra; 10 µm inside nozzle; coarsens downstream	Fixed needle lift	Liquid fuel halfway through nozzle; 156 MPa rail pressures; 900K & 300K gas	3-D 45 mm long chamber
CMT	About 30 µm uniform	Fixed and moving needle lift	Fuel filled sac and orifice: 150 MPa and 343 K in sac and orifice	2-D axisymmetric Height = 12 mm Width = 6 mm
IFPEN	Non-uniform hexahedra : Min. size=(5µm in the hole,2µm in the seat, 15µm near-nozzle region)	With needle motion - Without wobble	Chamber-needle-seat : (0.999, 150 Mpa, 343K) Sac and hole : (0.0001,2MPa,, 343K) Chamber : (0.0001,2MPa,303K)	3D configuration including: - control volume - Chamber (bore=6 cm, height =6cm)
Sandia	Cartesian 12.5µm	Fixed needle lift	6MPa, 900K/363K	3D

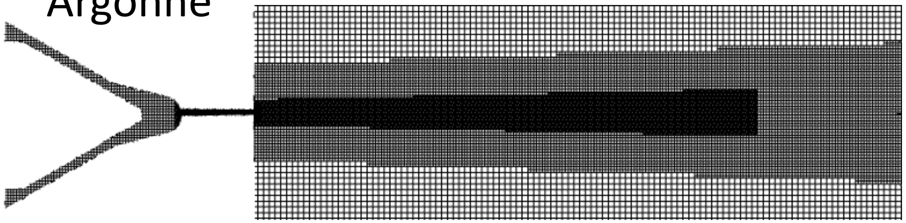
Spray A: Computational time (first 100μs)

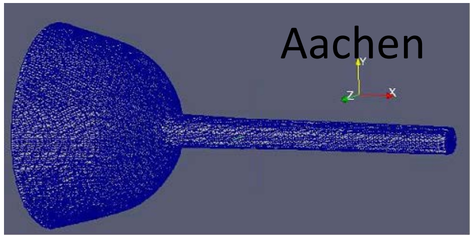
Institution	Geometry (210675)	Total number of computational cells	Computational time for first 100 microseconds (CPU hours)
Aachen	Low resolution	Nozzle: 300 million Primary Breakup: 900 million Lagrange Spray: 7 million	
Argonne	Low resolution	4.50 millions	12,288
Bosch	Low resolution	3.20 million	7,000
CMT	Low resolution	0.09 millions	160: fixed needle 1350: moving needle
IFPEN	High-resolution (CNRS scanned)	3 millions	11,776
Sandia (two-phase)	Box 9.6x3.2x3.2mm^3	50 millions	86,000

- The computational domain size, initial conditions, and needle motions are different for the institutions

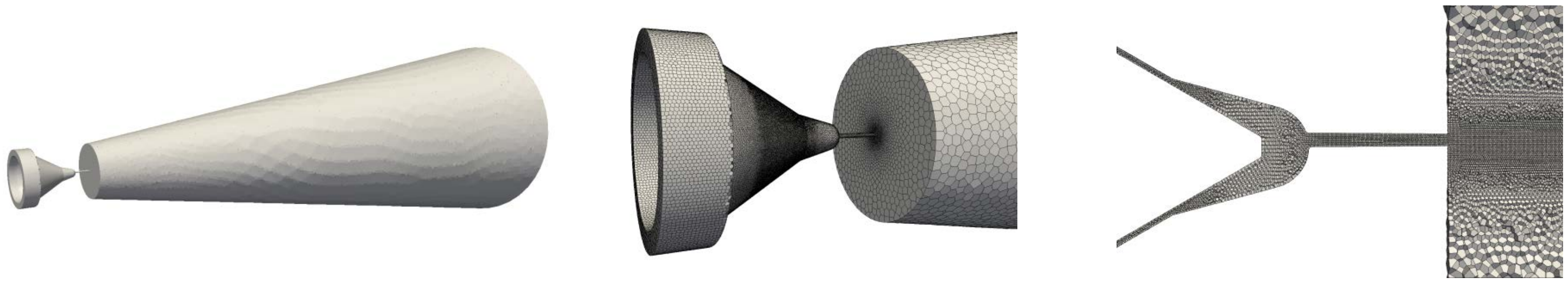
Computational domain and mesh image

Argonne

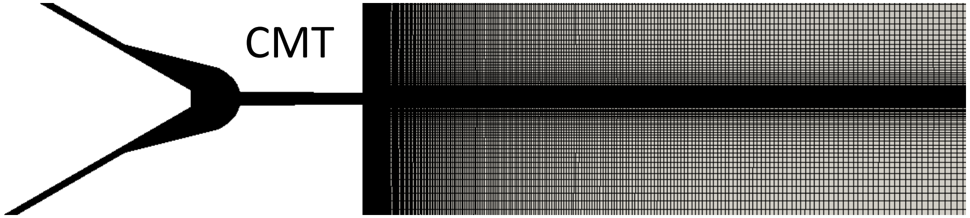


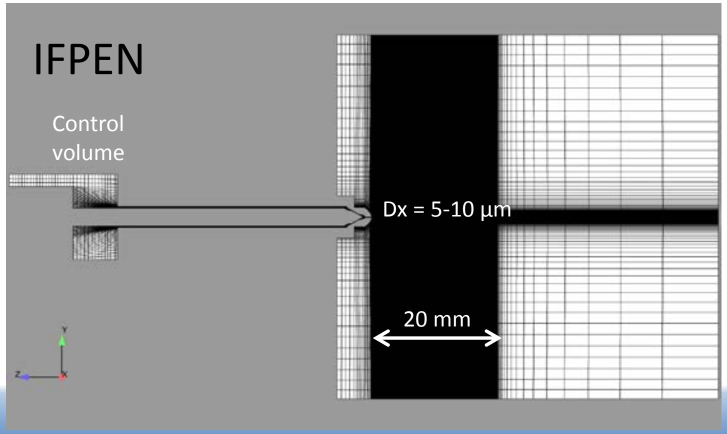


Bosch

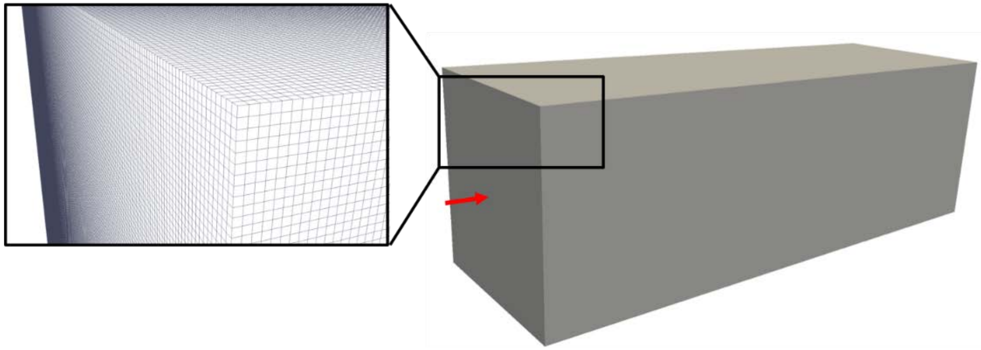


CMT

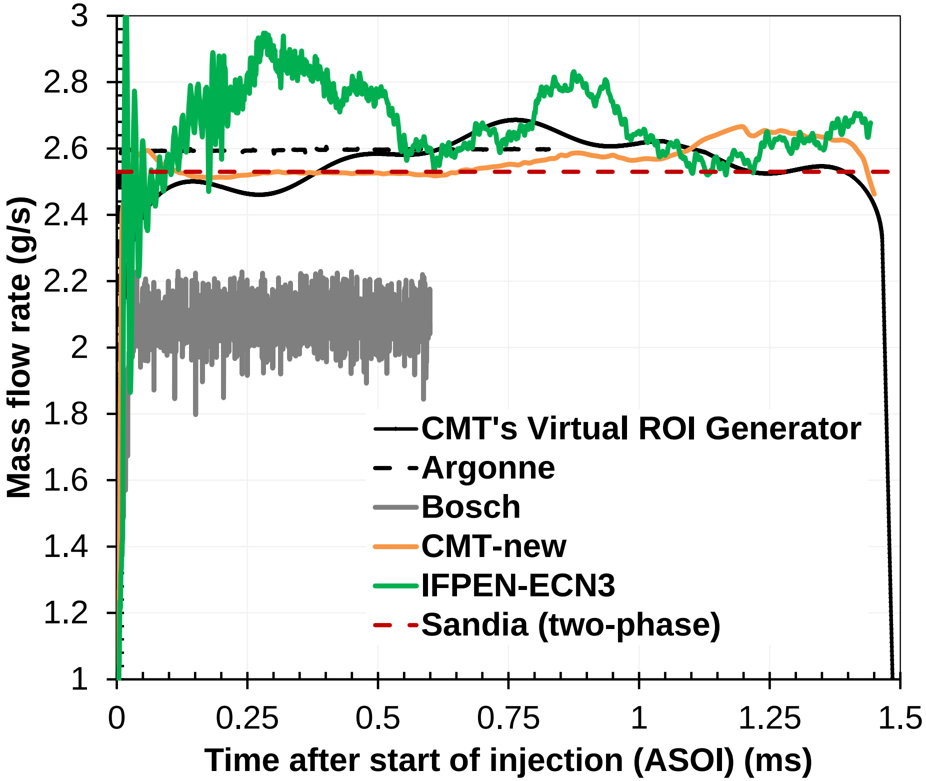


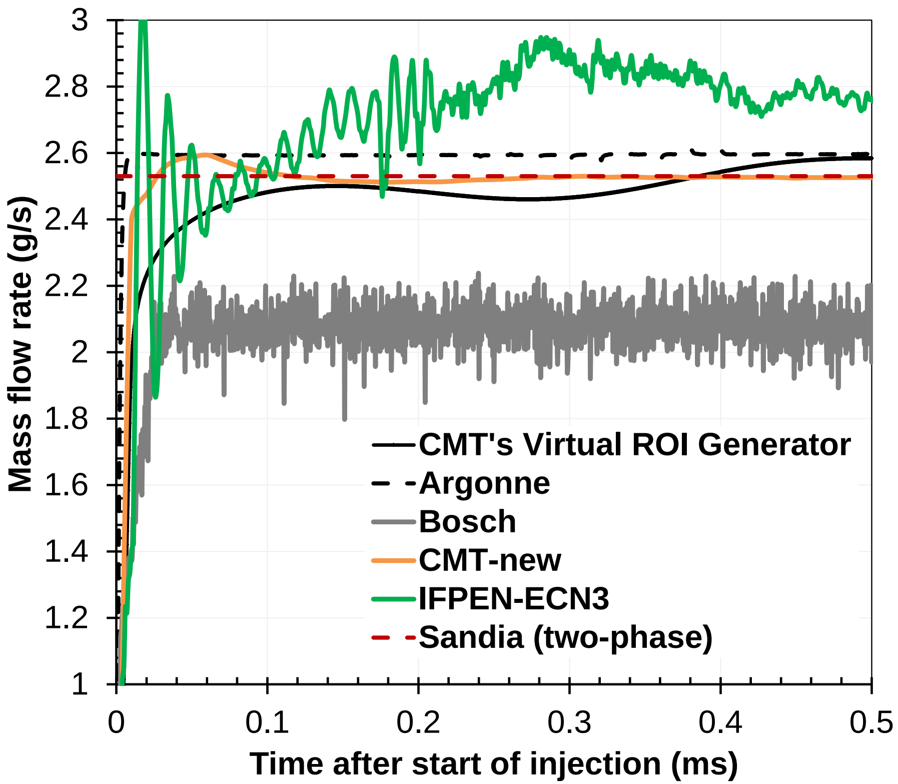


Sandia



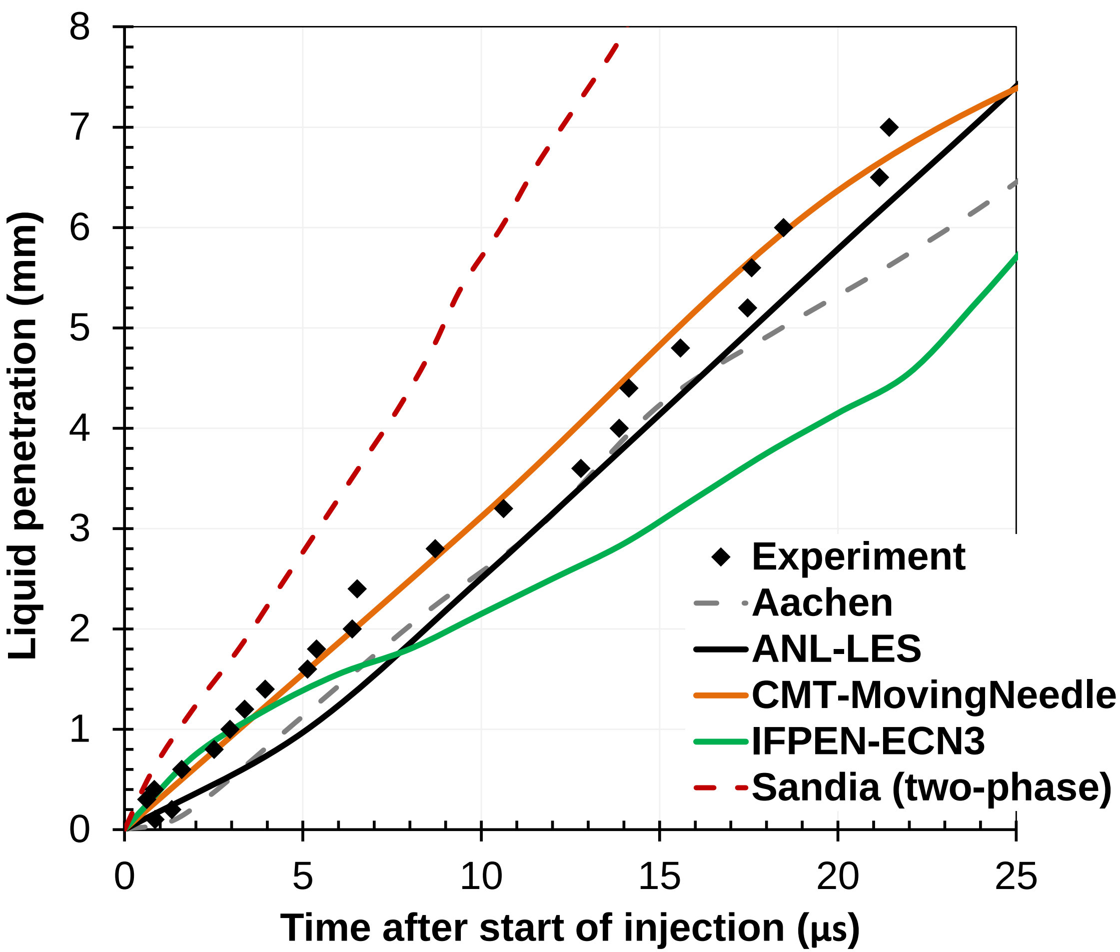
Mass Flow rate at nozzle exit





- In general, most groups are able to predict the mass flow rate quite well
- The initial transients are not well predicted by any approach. In some cases this might be due to the fact that fixed needle simulations are being performed
- Bosch results are under predicting mass flow rate due to the equation of state that they employed

Liquid Penetration

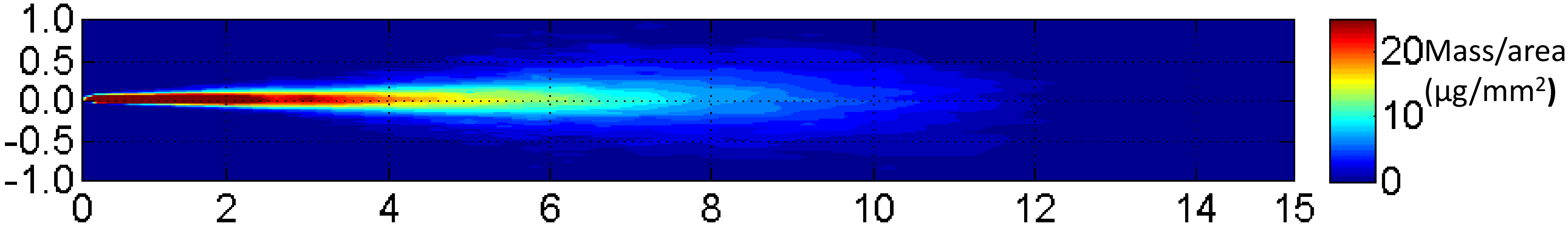


- Argonne and Aachen results compare quite well with the experimental data
- Bosch results not shown, since they performed simulations with a fixed lift and the initial liquid penetration is not well predicted although vapor penetration is well captured (not shown here)
- CMT simulations considering needle transients matches best with the experimental data

- Sandia simulations are over penetrating (note that the injection BC has no transient)
- IFPEN: ECN3 results are shown. ECN4 results may be able to better predict liquid penetration

Spray A: projected mass density – 0.1ms ASOI

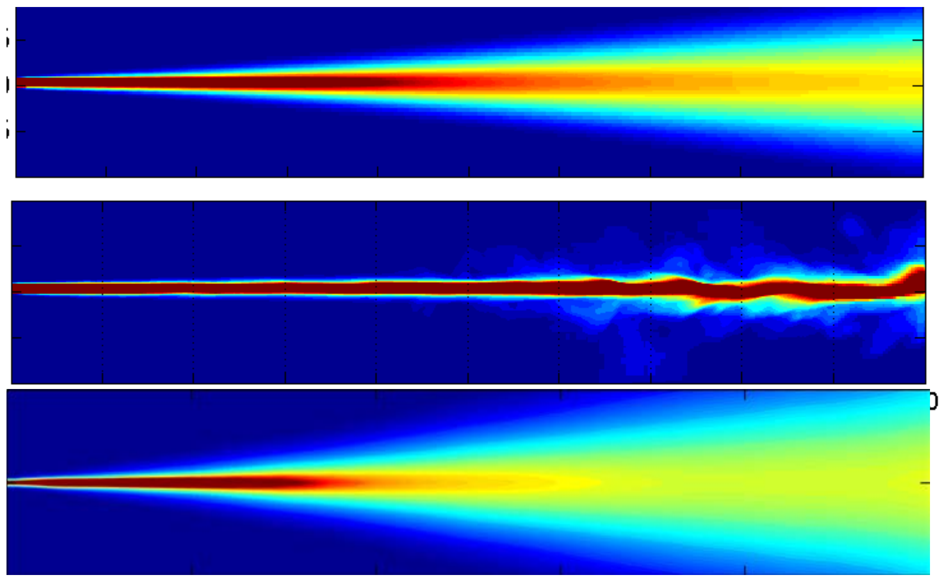
X-ray data



Argonne RANS

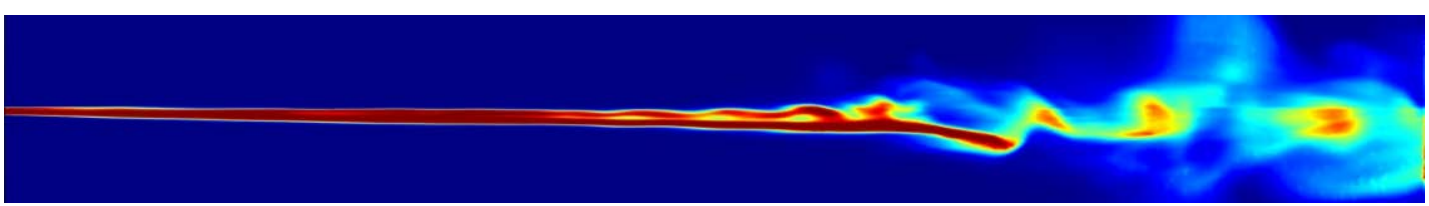
Argonne LES

CMT RANS



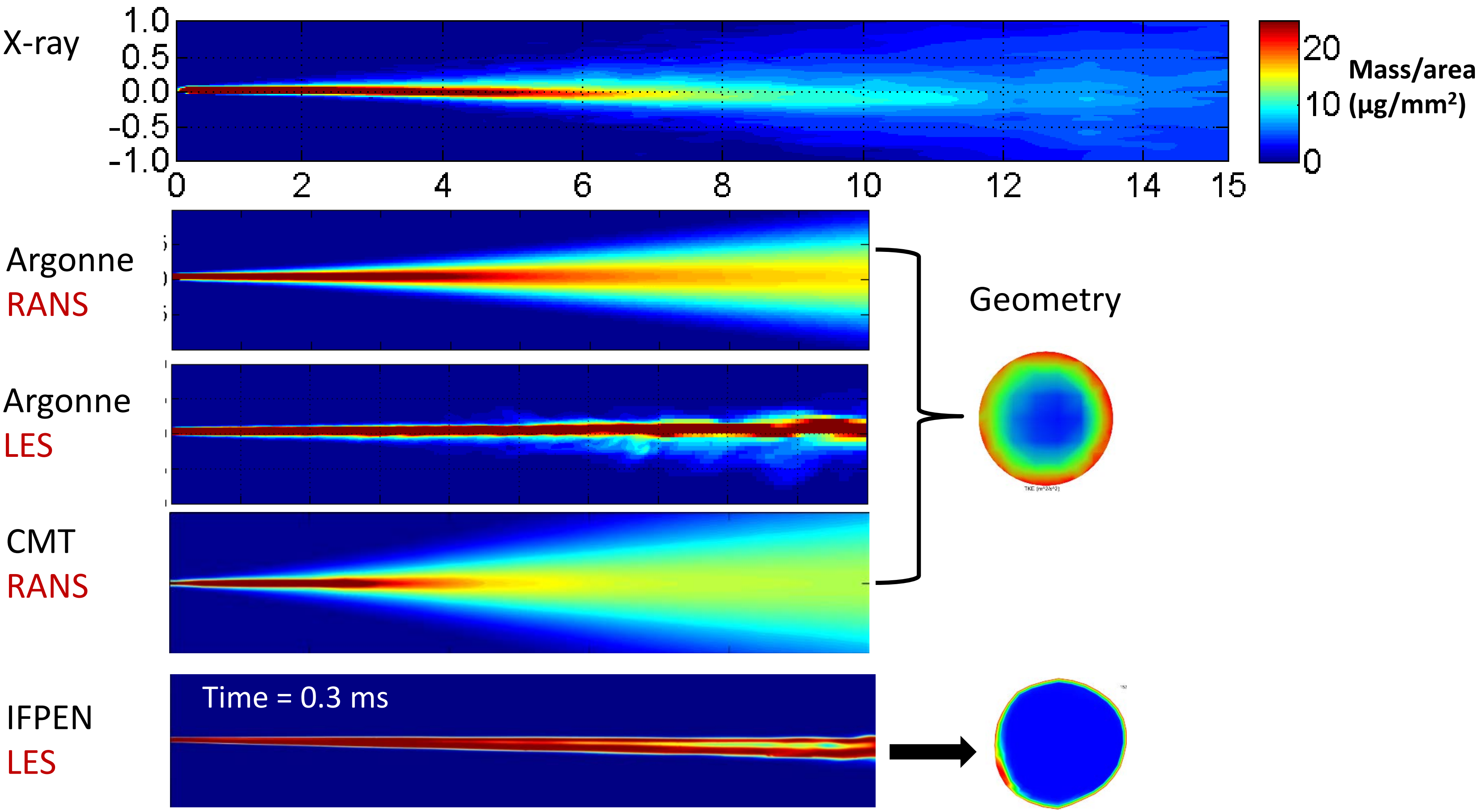
- All simulations predict similar mass flow rate at nozzle exit, however, quite different ensuing spray
- Qualitatively dense liquid core near nozzle region is captured by all simulations

IFPEN LES



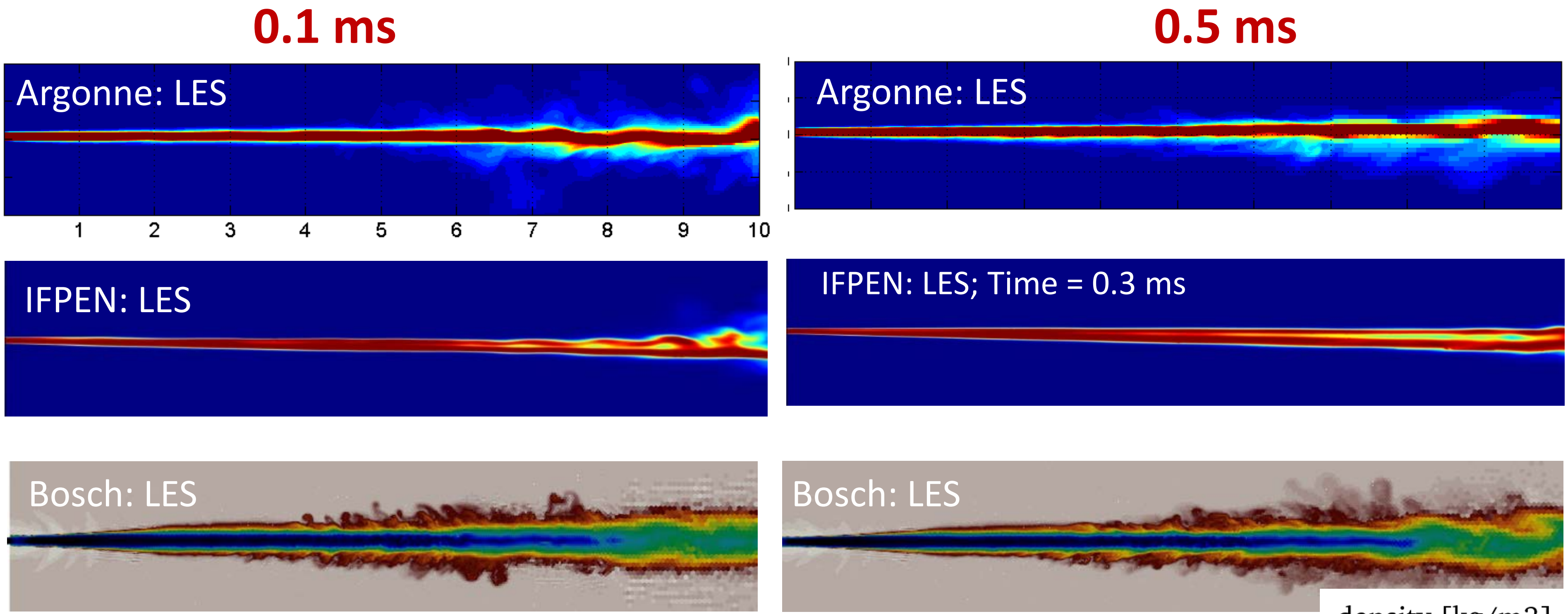
- RANS models tend to be overly diffusive compared to LES
- LES models tend to over-predict the core length and under predict spray dispersion

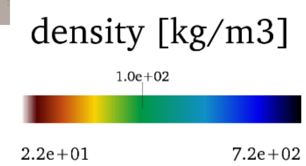
Spray A: projected mass density – 0.5ms ASOI



- At steady-state, the observations are consistent with earlier injection time (0.1 ms)

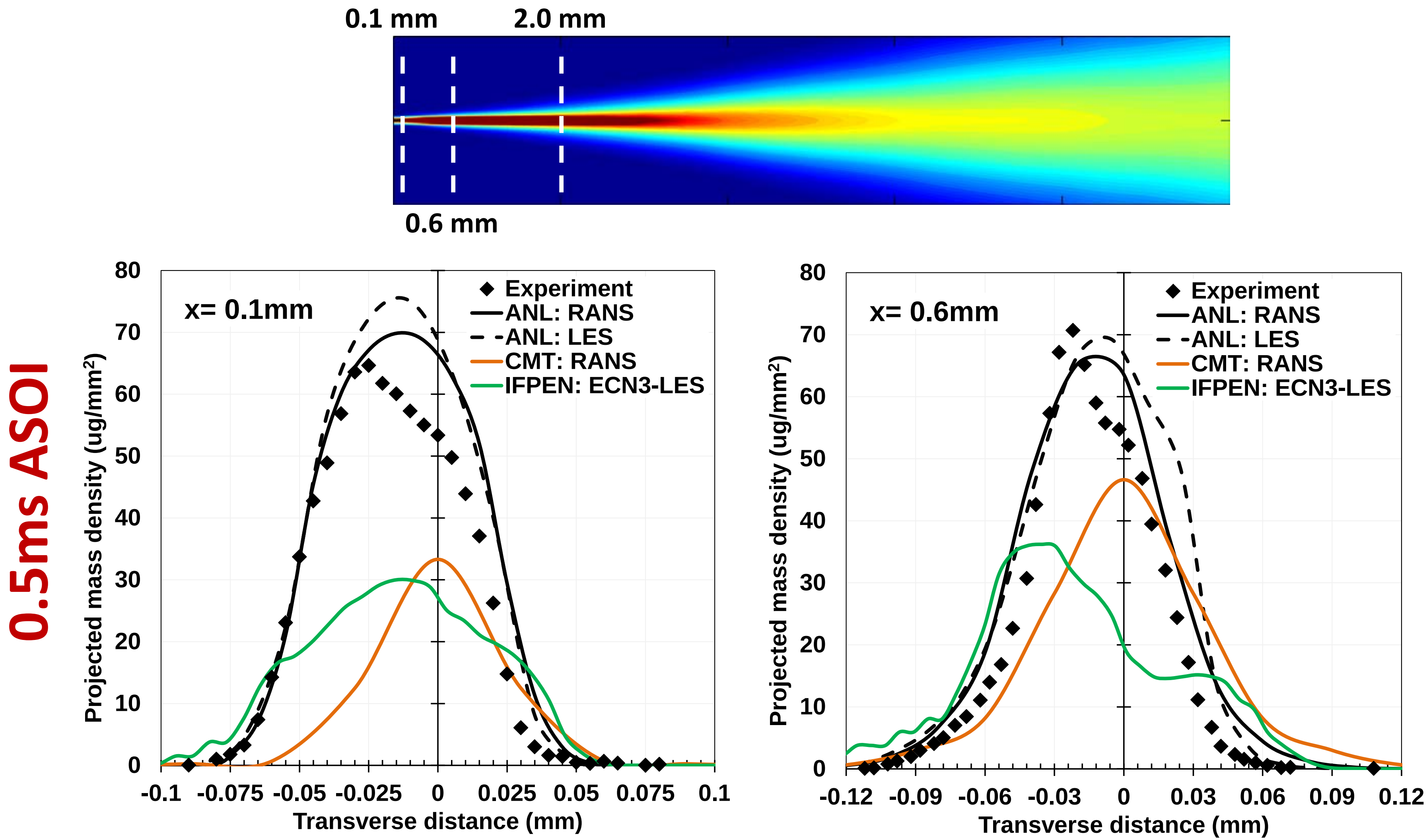
Projected mass density and fuel density - LES





- BOSCH results show liquid density on a cut-plane through jet center
- Argonne and IFPEN results show projected mass density, also shown in previous slides
- Bosch calculations show flow features like shock waves and capture flow structures
- Argonne and IFPEN result are line-of-sight averaged and hence do not show these features
- Argonne and BOSCH calculations seems to be broader than IFPEN results

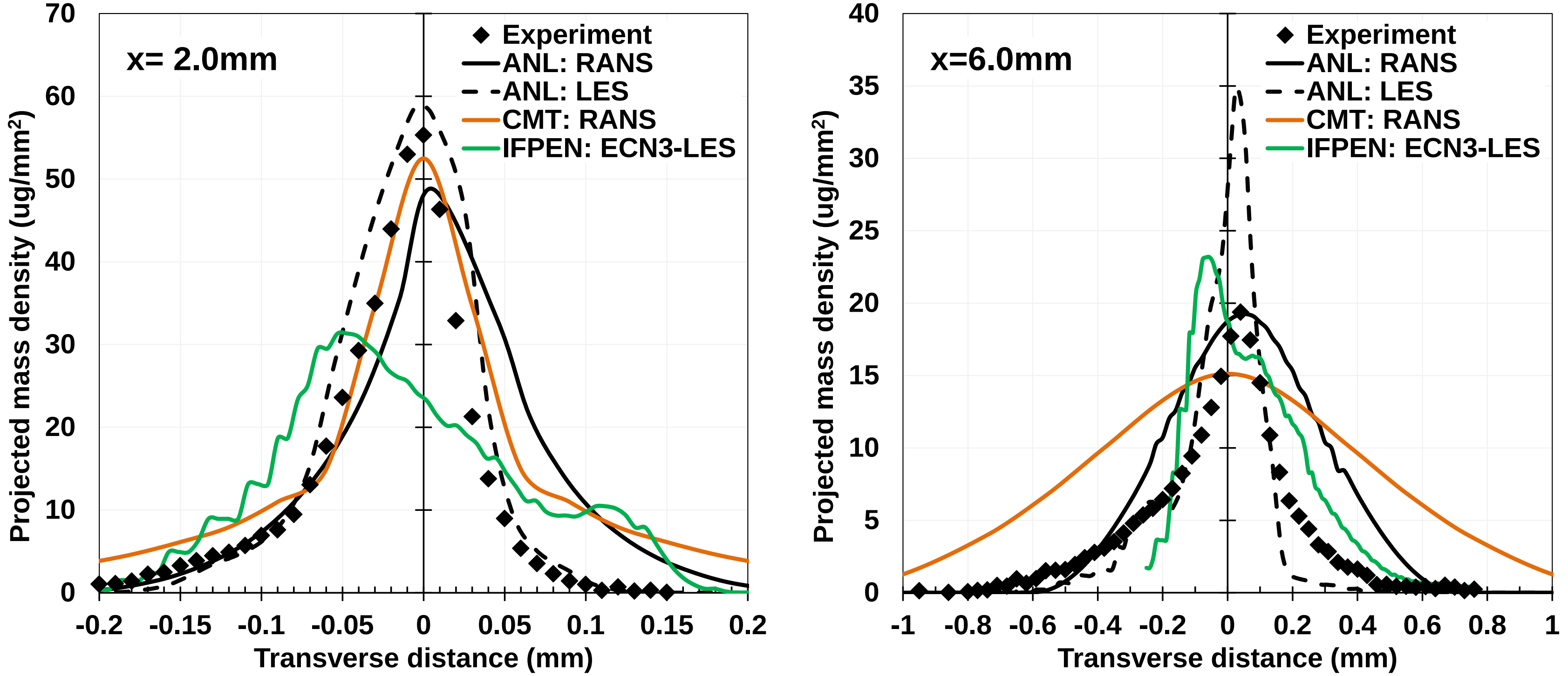
Spray A: Radial profiles of projected density



- All simulations capture the shape of the radial profile, however, significant differences in the peak values and tails
- The lower peak values from IFPEN (from ECN3) are possibly due to the choice of EOS

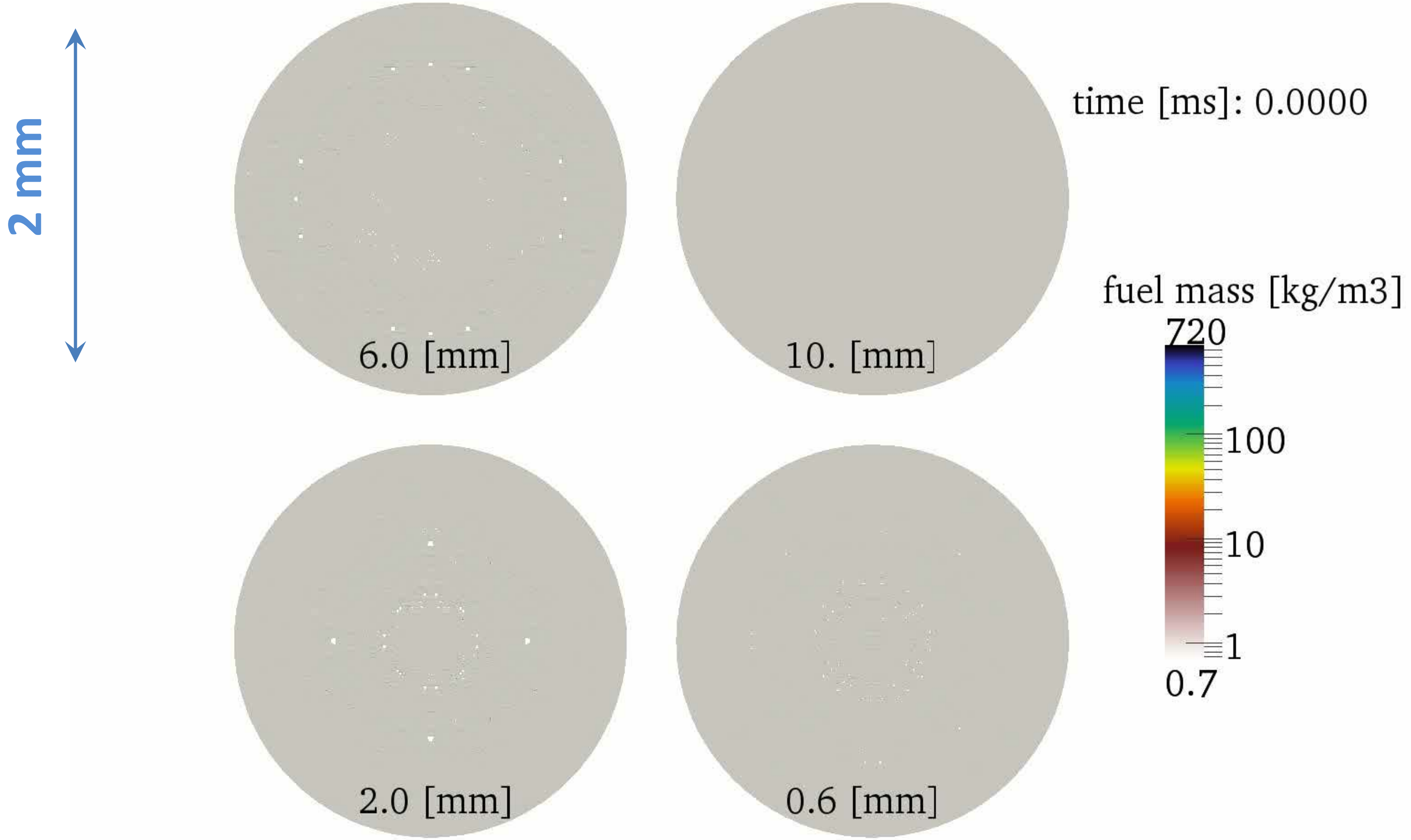
Spray A: Radial profiles of projected density

0.5ms ASOI



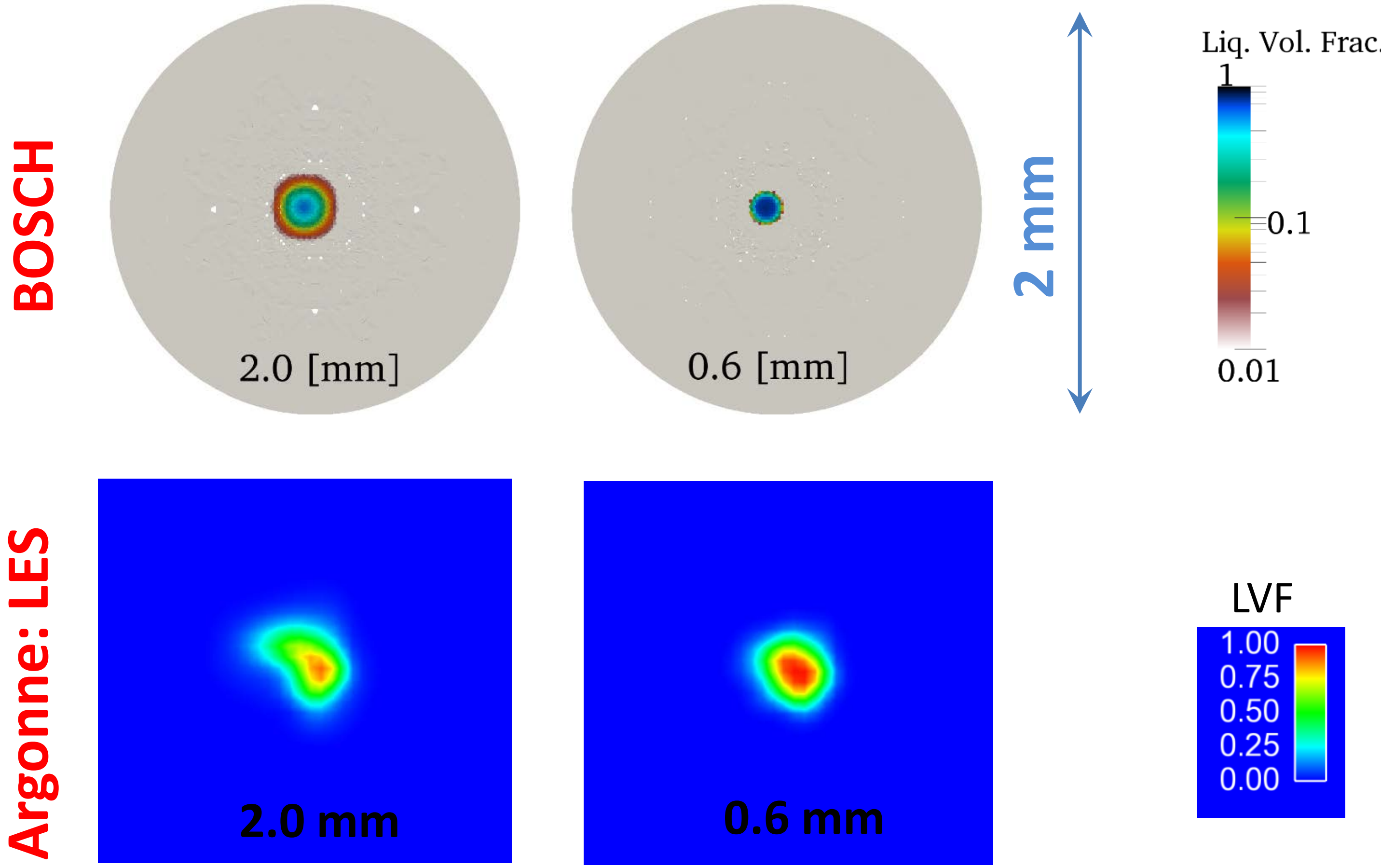
- @ 2mm, ANL and CMT calculations can predict the projected mass density contours fairly well
- @ 6 mm none of the modeling approaches can capture both the peak values and dispersion well. This may suggest that at these axial locations, transition to an Lagrangian approach may be necessary
  - Open question: What should be the criteria for transition from Eulerian to Lagrangian?
- Since projected density is already calculated by line of sight integration, perhaps multiple realizations are not necessary with LES to get smoother profiles

Bosch Contribution: LVF with LES



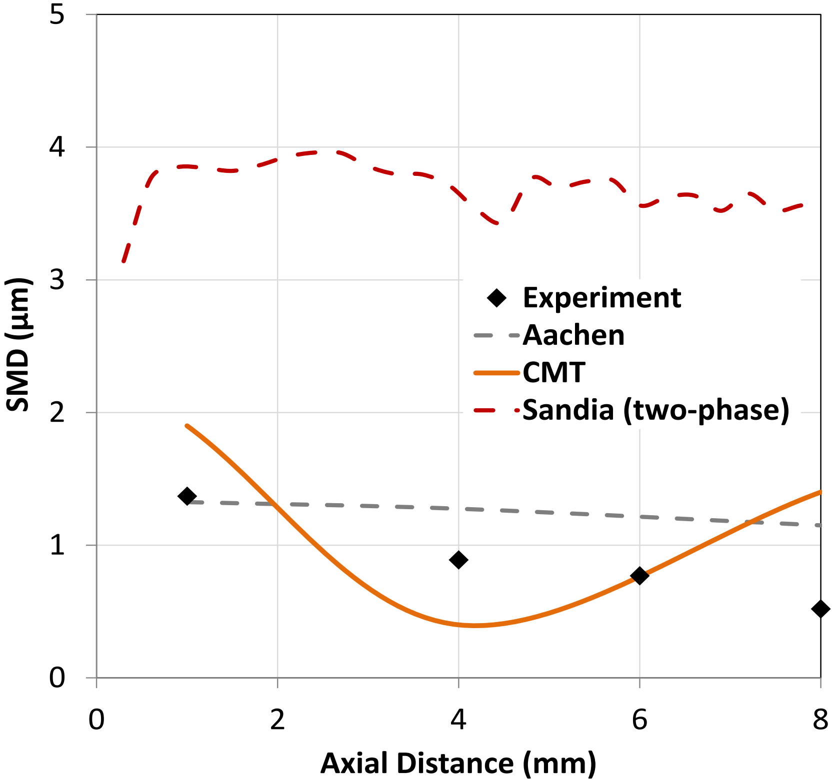
- No structures observed for 0.6 mm and 2 mm near nozzle regions
- At 6 mm, turbulent and transient structures are observed
- 10 mm location does not have enough resolution to show any structures

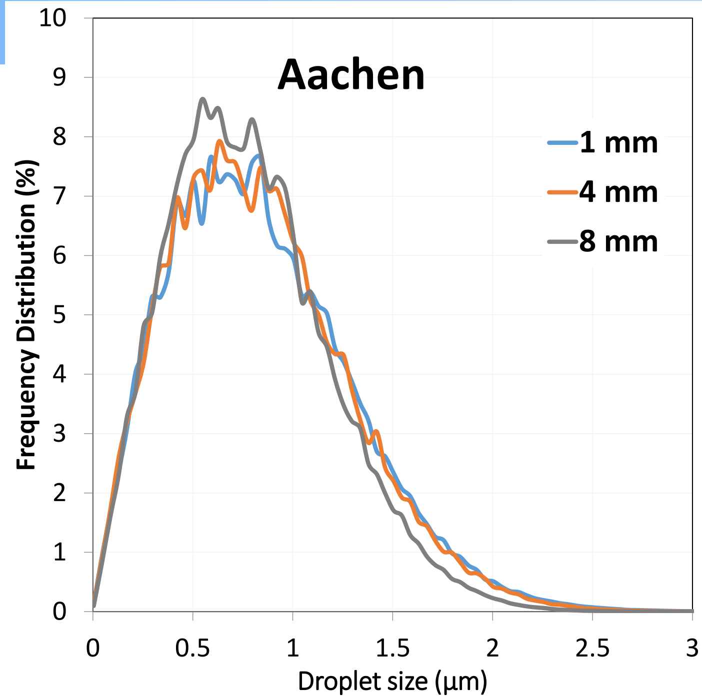
LVF with LES: Bosch and ANL

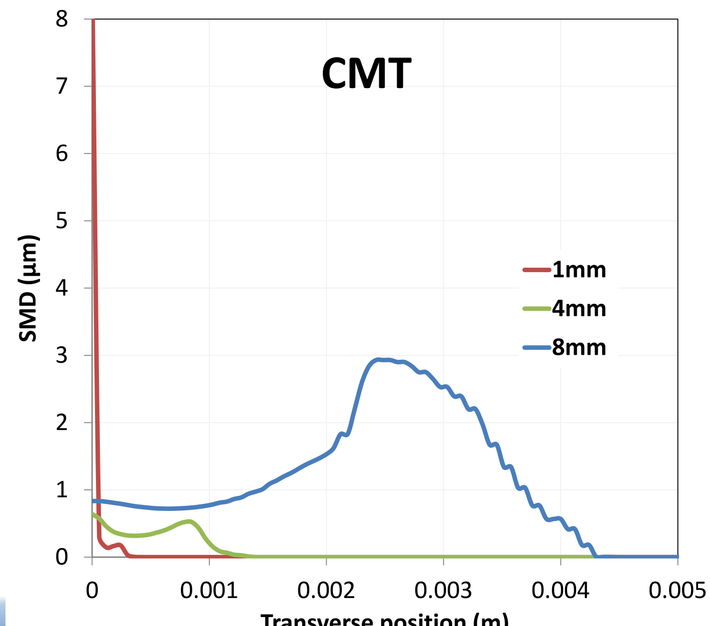


- 0.6 mm and 2 mm are axial distances from nozzle exit
- Comparison between ANL and Bosch is not apples-to-apples
- However, ANL LES results shows significant asymmetry
- BOSCH results seem to show asymmetry and turbulent structures at further downstream locations

SMD at different locations







- Aachen provided results in terms of a droplet size frequency distribution
- CMT provided radial distribution of SMD
- Sandia provided SMD as a function of axial distance
- Overall, SMD is over predicted by Sandia's approach which is still under development
- Experimental uncertainties may still persist

Parametric Studies

ECN RANS vs. LES

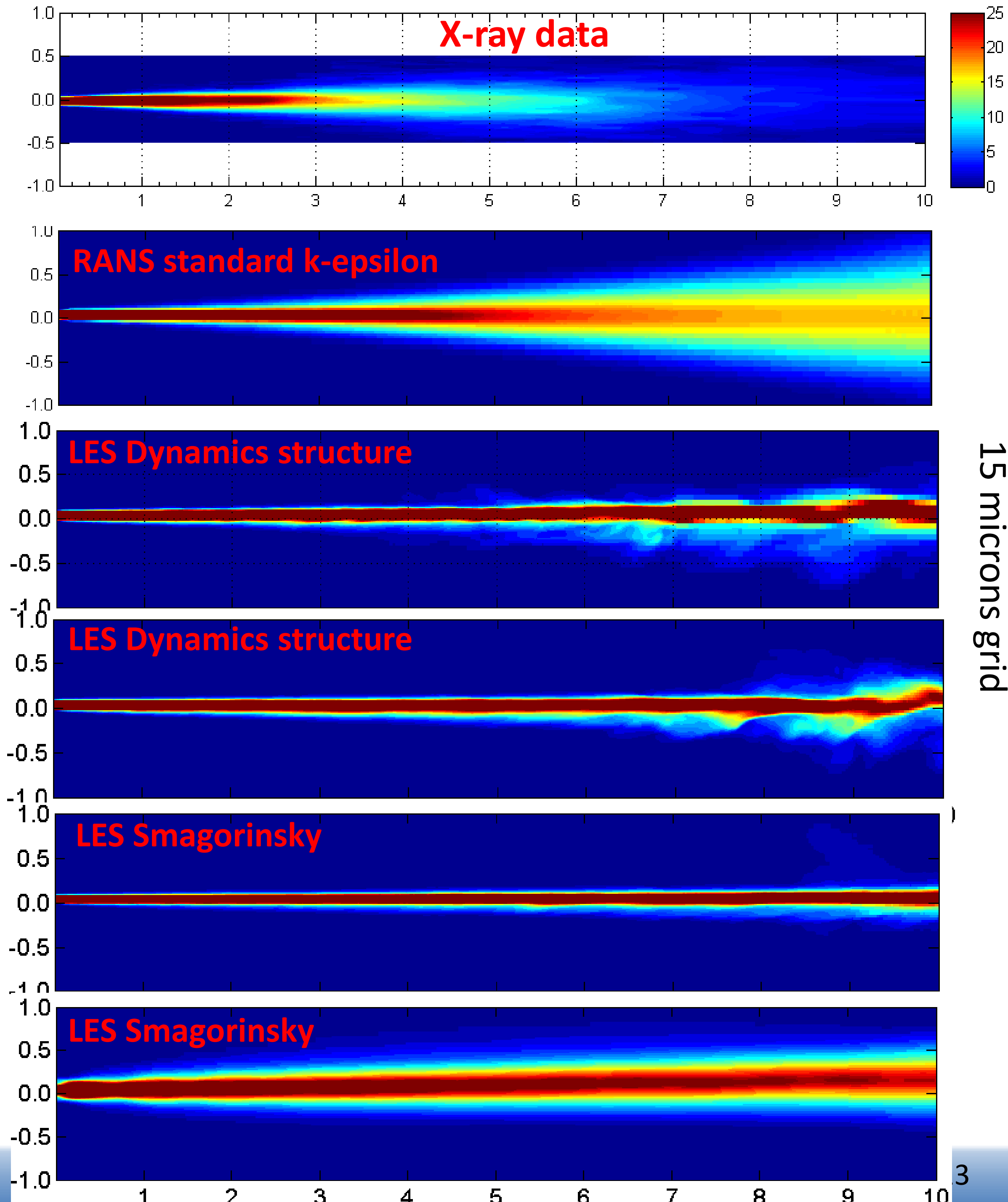
- ANL conducted a systematic study on the influence of turbulence model constants and Schmidt number of spray penetration and dispersion. The most promising results are shown here
- Smagorinsky model does not seem to show onset of turbulence structures
- Schmidt number seems to have a minor effect on the results
- In general, all turbulence models over predict the spray penetration

$Sc_t=0.7$

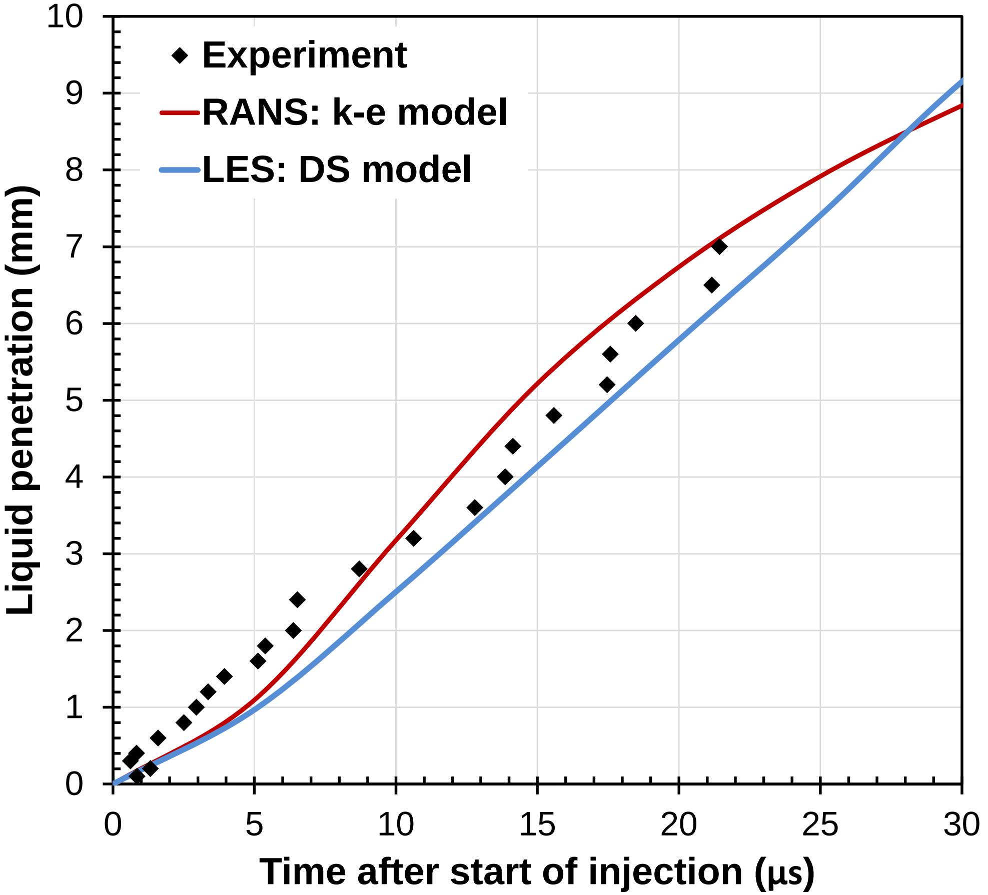
$Sc_t=0.5$

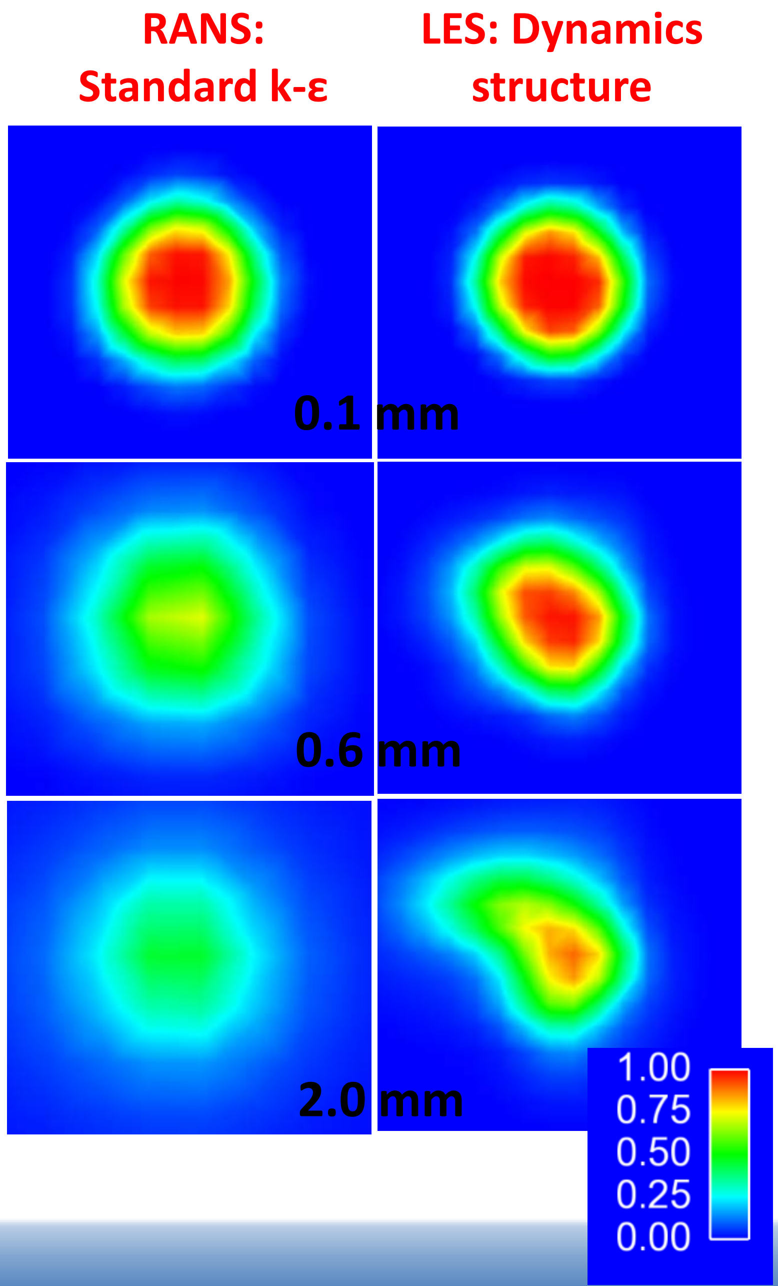
$Sc_t=0.7$
$Cs=0.05$

$Sc_t=0.7$
$Cs=1.0$



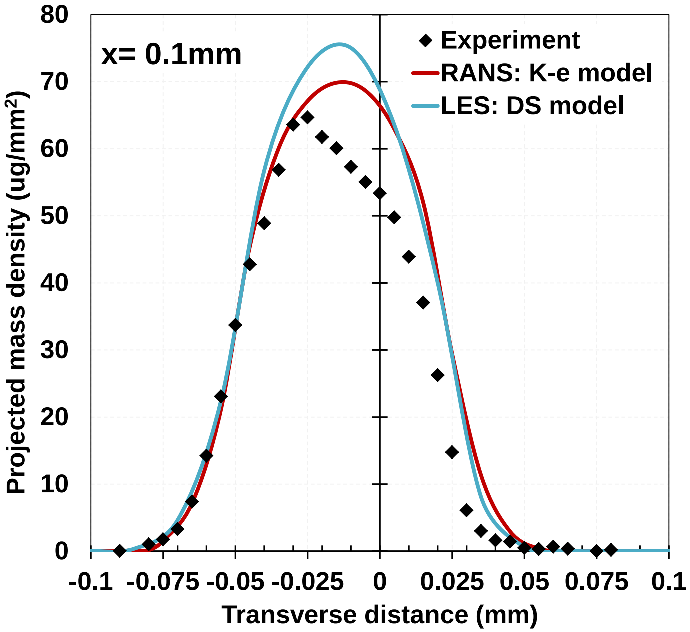
ANL Contribution: RANS vs. LES

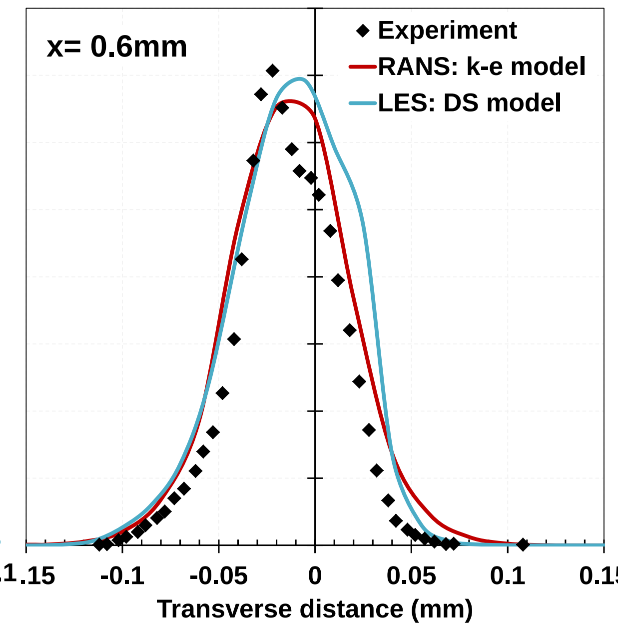


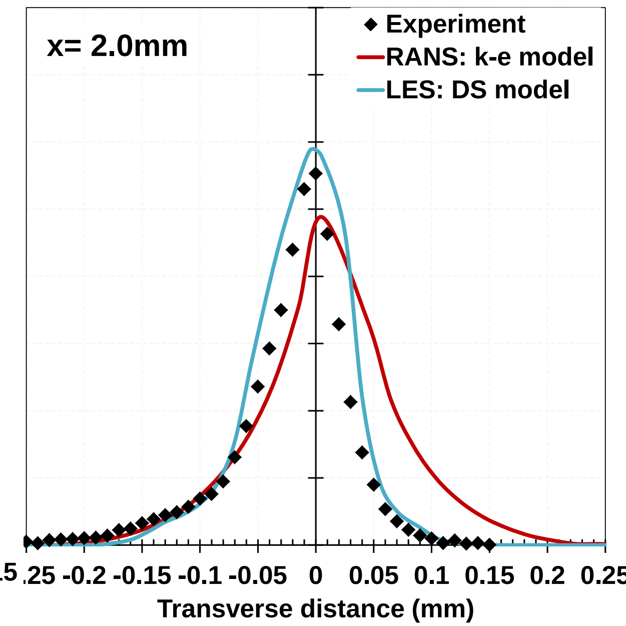


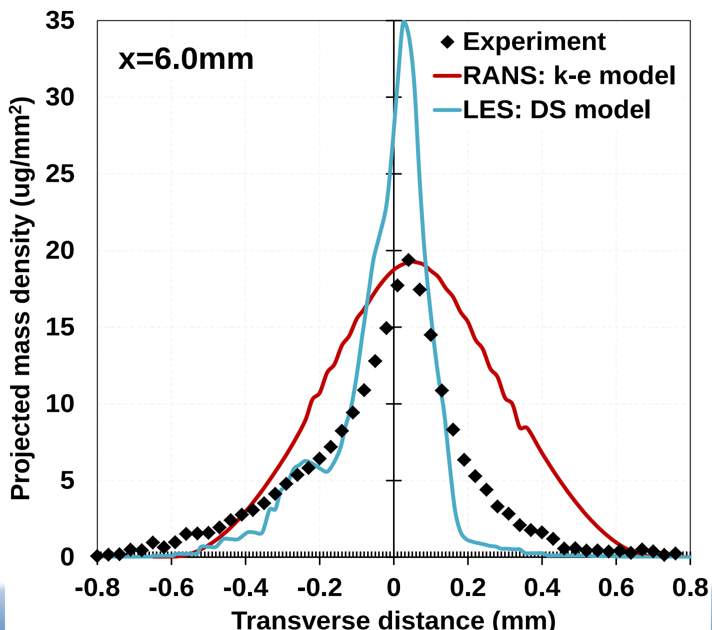
- Penetration is fairly well captured by both RANS and LES models
- Liquid volume fraction results with RANS are much more diffused compared to LES, which is expected
- Higher fuel density at the spray core is observed with LES calculations

ANL Contribution: RANS vs. LES









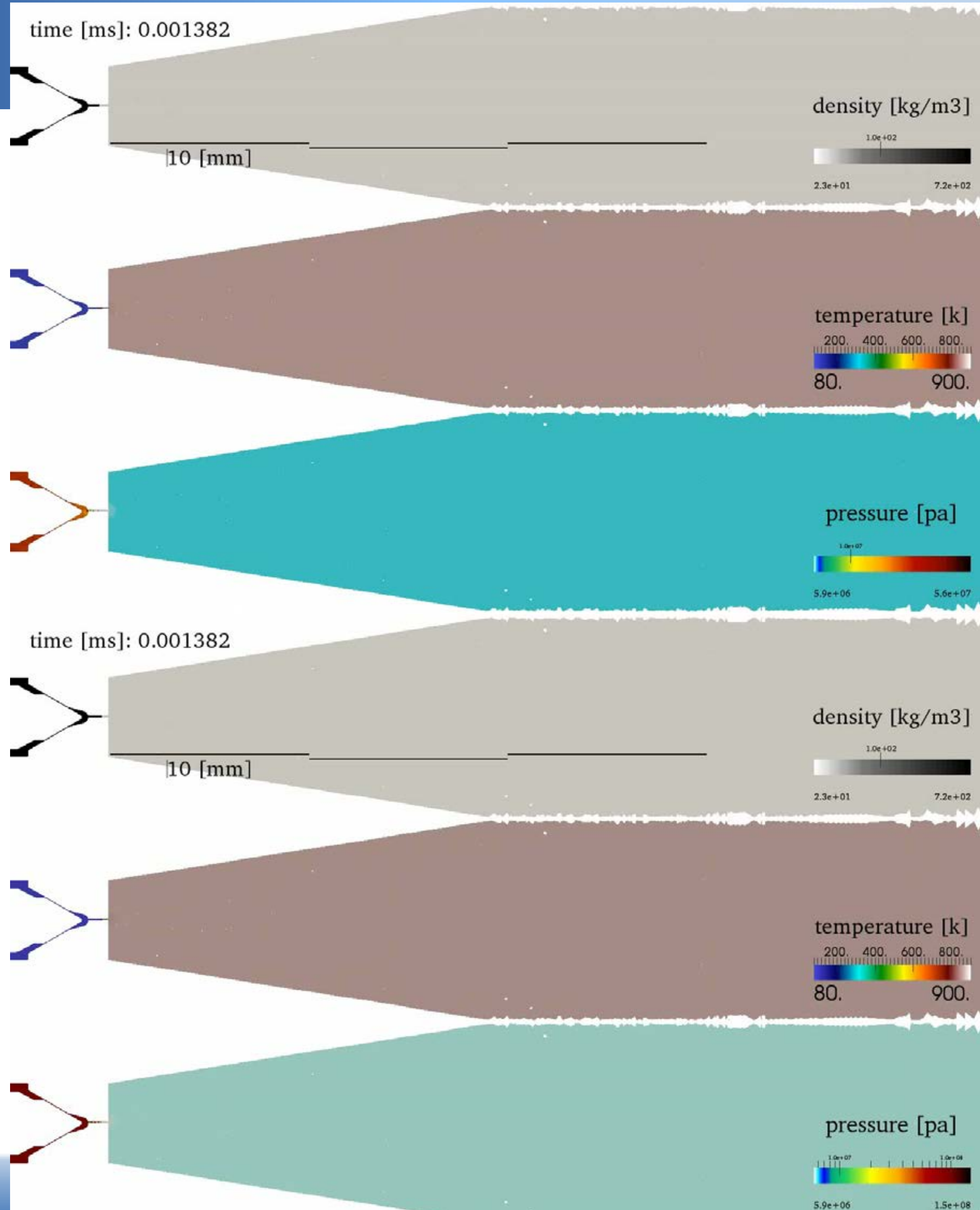
- In the near nozzle region (less than 2 mm), turbulence model effects seem to be minimal. LES with DS is perhaps performing better than RANS
- Based on previous studies at Argonne, resolution seems to influence the results more significantly rather than the choice of turbulence models
- Beyond 2 mm, LES seems to capture the dispersion well while RANS does a better job in capturing the peak values

Bosch Contribution: Effect of Injection Pressure

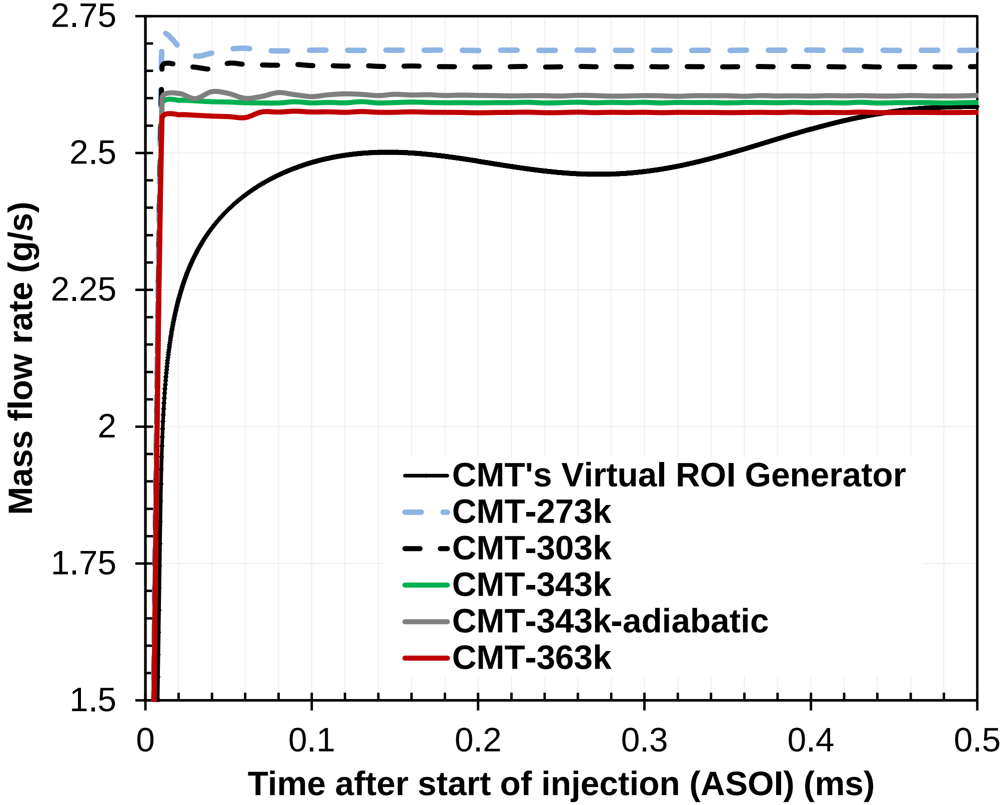
- Vapor penetration curves agreed well with experiments after initial transient
- Penetration scaled as expected with rail pressure

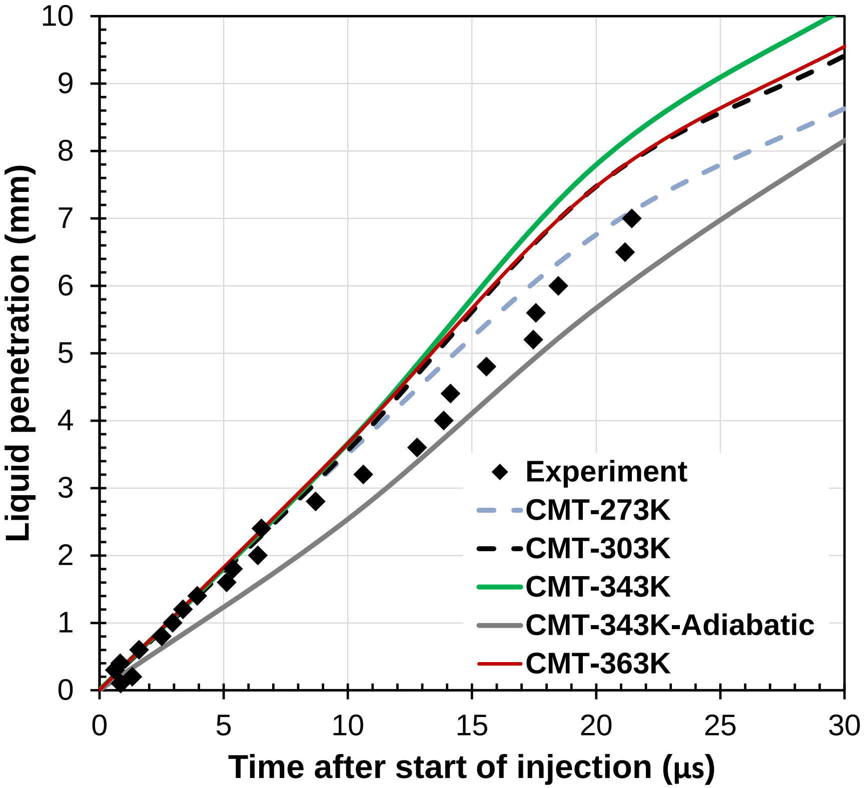
560 bar

1560 bar



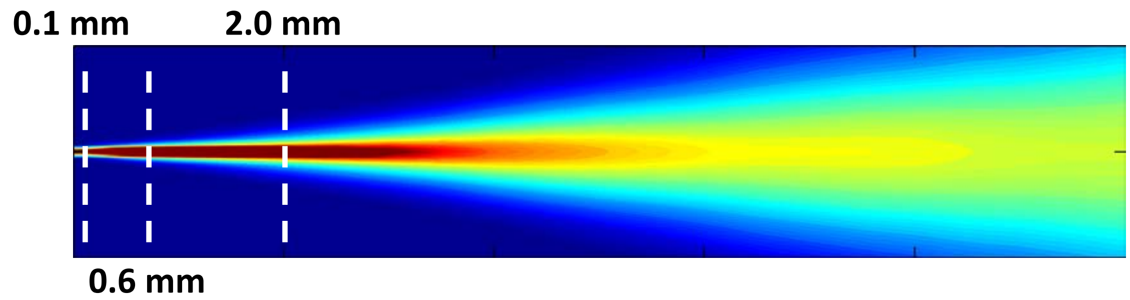
CMT contribution: Effect of Wall Temperature

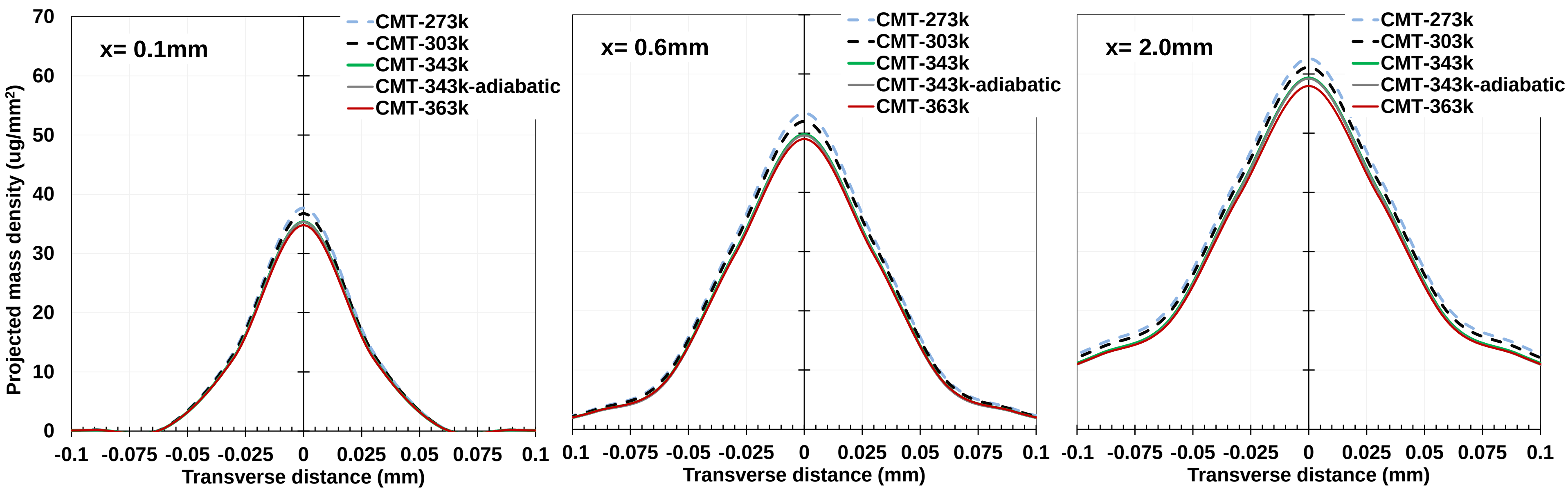




- All results with fixed needle lift
- Wall temperature:
  - Influences the mass flow rate as expected (density effect)
  - Has a relatively small and non-linear effect on near nozzle spray penetration
- Adiabatic wall influences spray penetration, although mass flow rate was not influenced

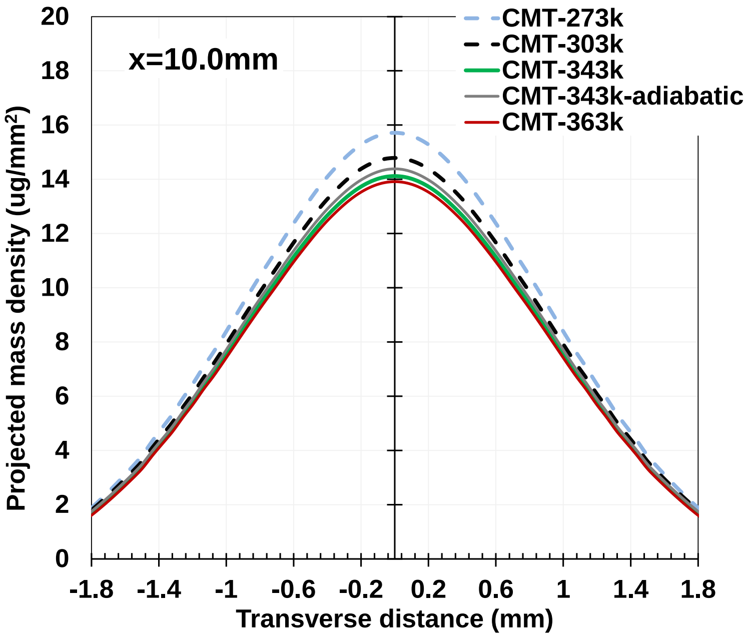
CMT: Effect of Wall Temperature (up to 2 mm)

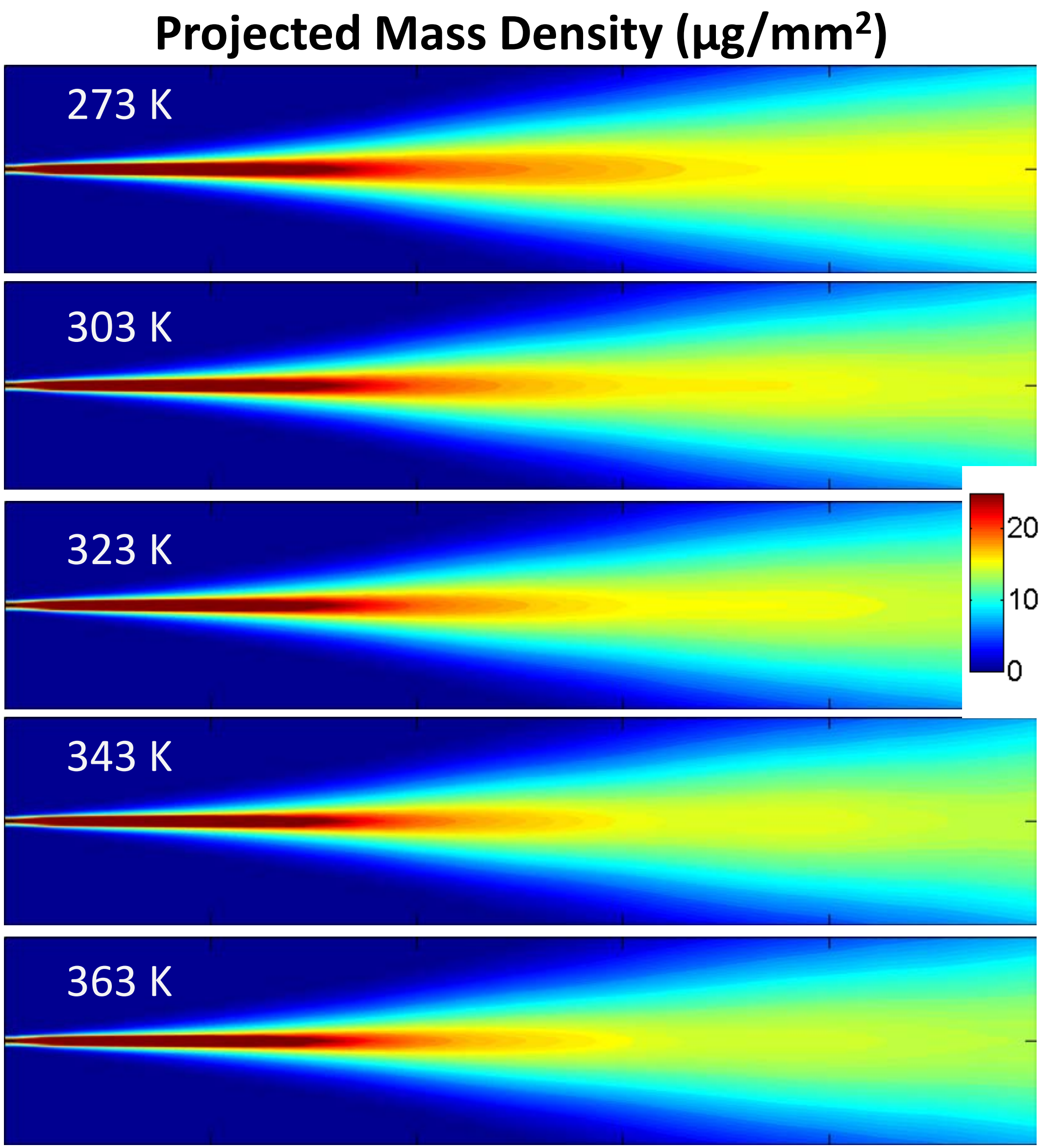




- All results with fixed needle lift
- Peaks are marginally different but dispersion is quite similar for all wall temperatures
- Adiabatic walls does not influence the projected density results

CMT: Effect of Wall Temperature

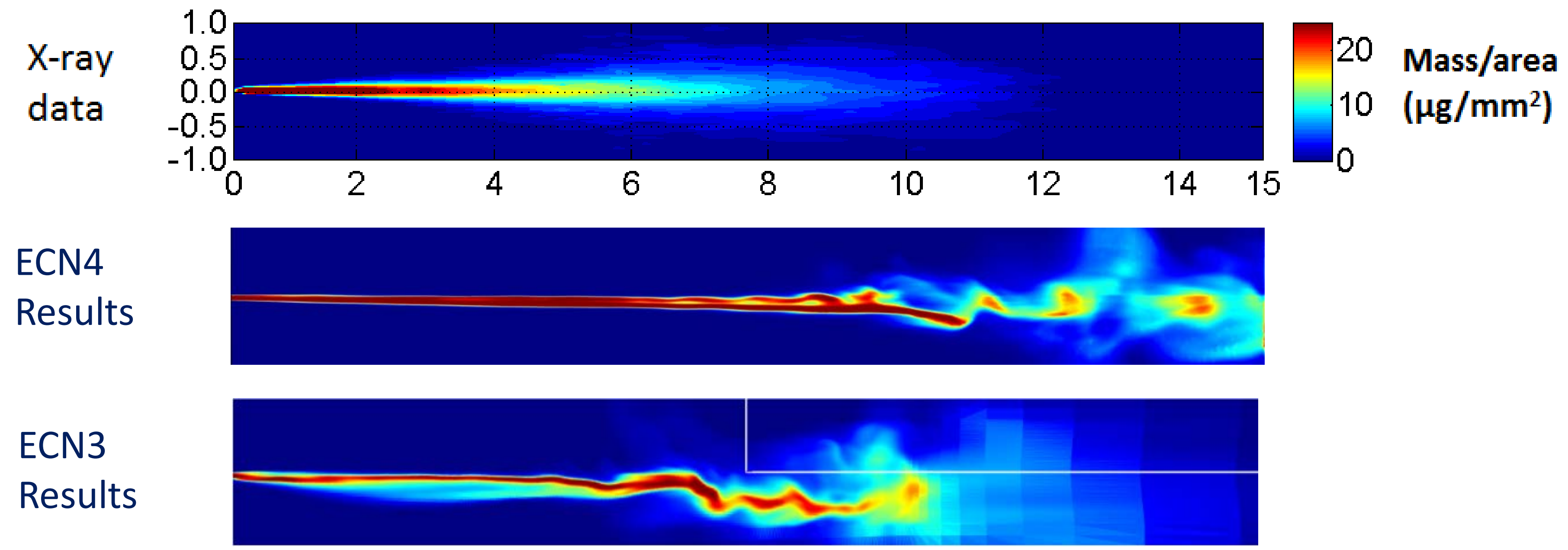




- Contour plots of projected mass density profiles looks quite similar for all temperatures
- Peaks are marginally different but dispersion is quite similar for all wall temperatures
- Adiabatic walls does not influence the projected density results

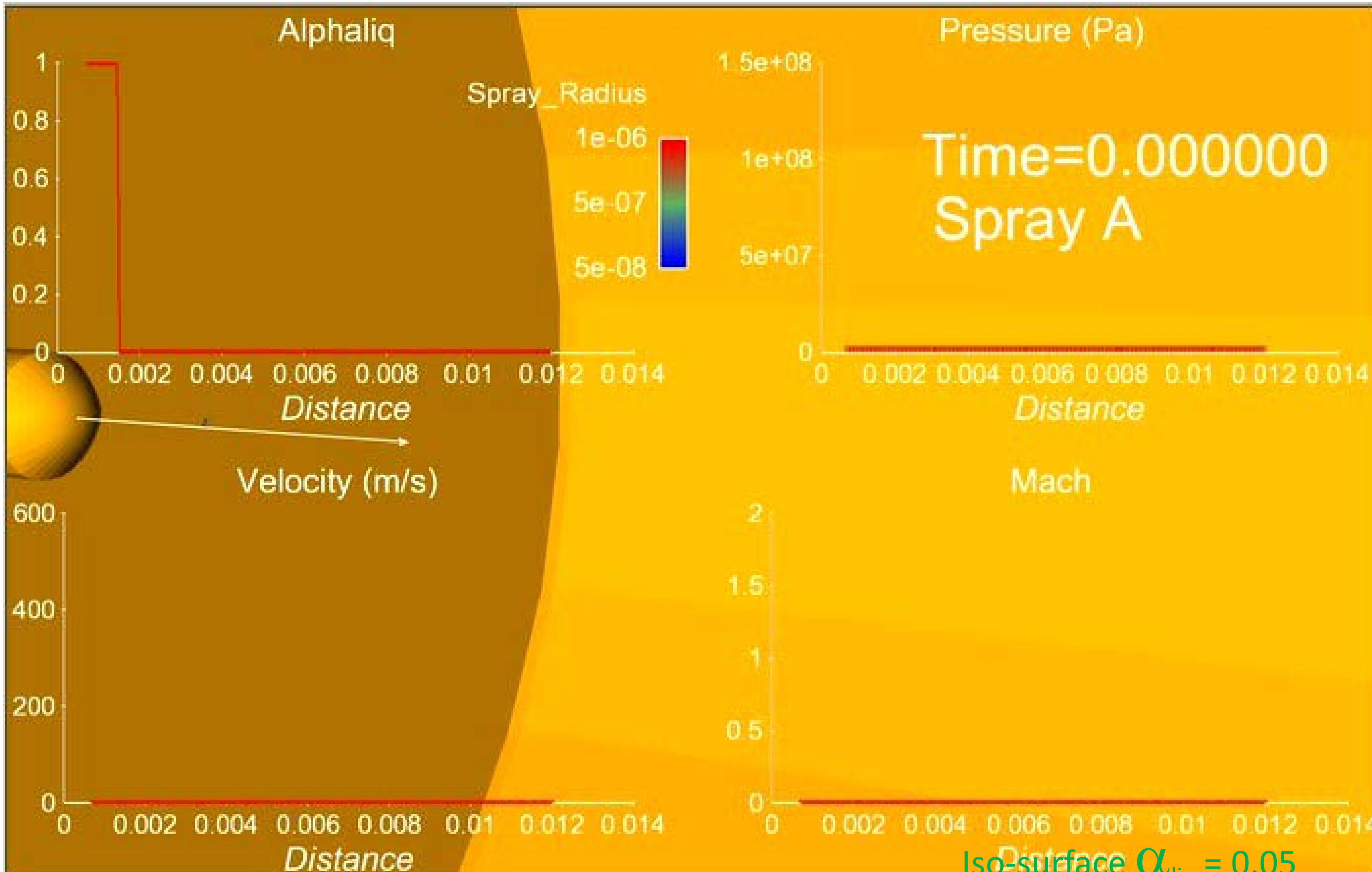
Primary atomization using Two-Surfaces density model and EE coupling with EL approach

IFPEN results from Chawki Habchi



- The liquid core length is overestimated, perhaps due to a lack of initial dispersion of droplets in the primary atomization model
- More work is needed for the primary atomization model

IFPEN: Spray A @ subcritical conditions



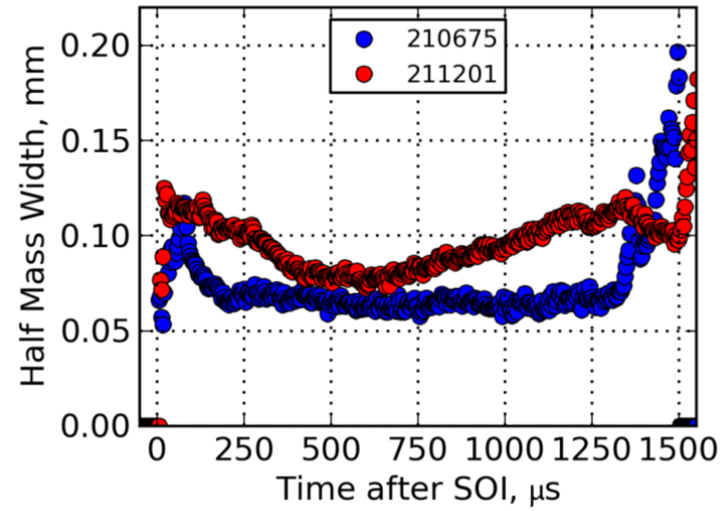
Iso-surface α_{liq} = 0.05

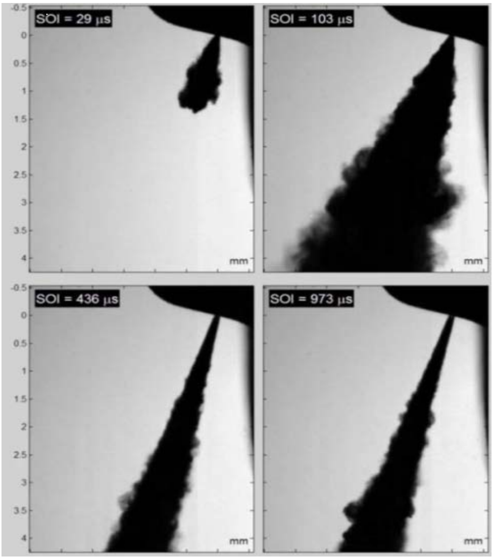
Spray A vs. Spray B Dynamics

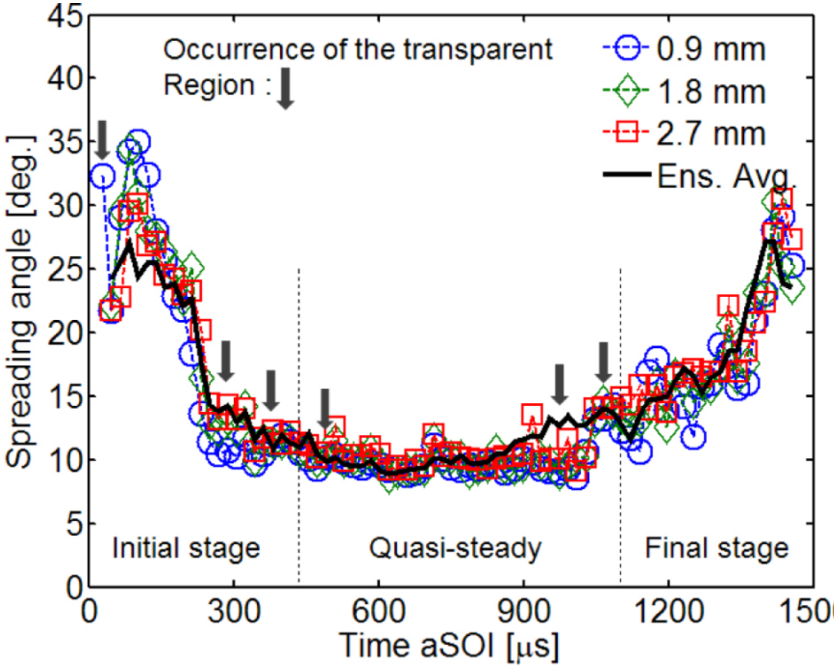
Experimental Observation:

Spray B dynamics

- Transient external spray for Spray B observed by experiments[1,2,3,4]
- Numerical simulation of injector to study the internal flow and near-field spray development



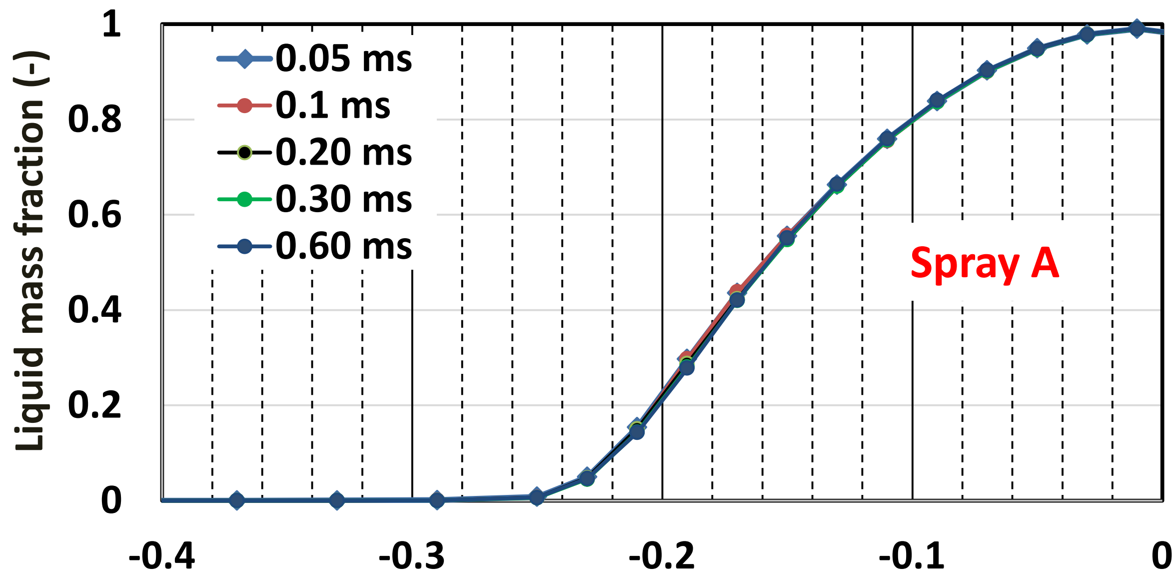


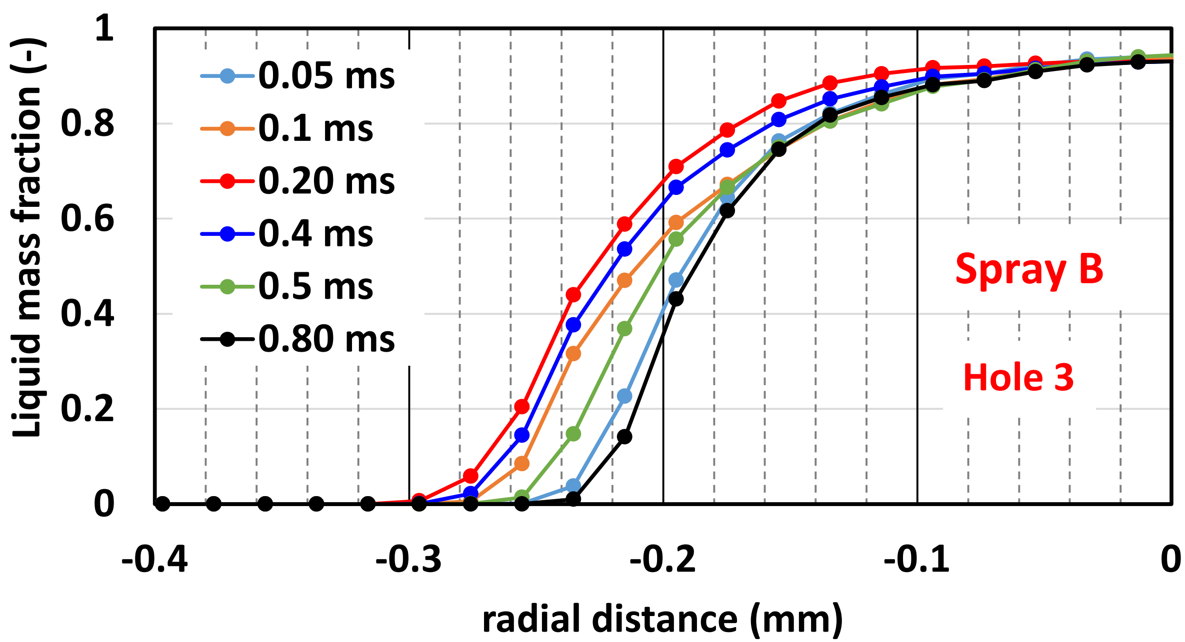


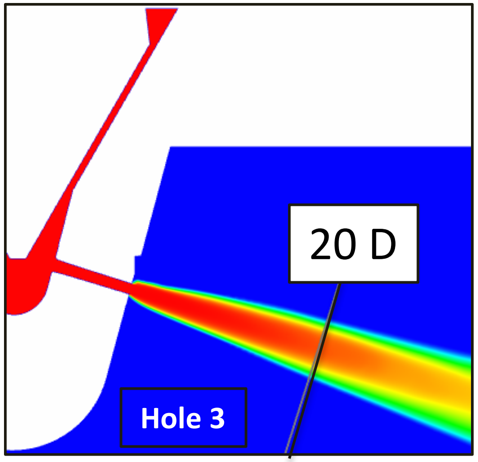
1. Jung Y., Manin J., Scott S., Pickett L.M., *SAE Technical Paper* No. 2015-01-0946, 2015
2. Kastengren A., Xue Q., Manin J., Habchi C., ECN3, 2014
3. Kastengren, A.L., Tilocco, F.Z., Duke, D., Powell, C.F., Moon, S., and Zhang, X., *ILCASS 2012, Heidelberg, September 2-6, 2012*
4. Engine Combustion Network (ECN), www.sandia.gov/ecn

ANL Contribution: Spray A vs. Spray B dynamics

At 20 D of downstream

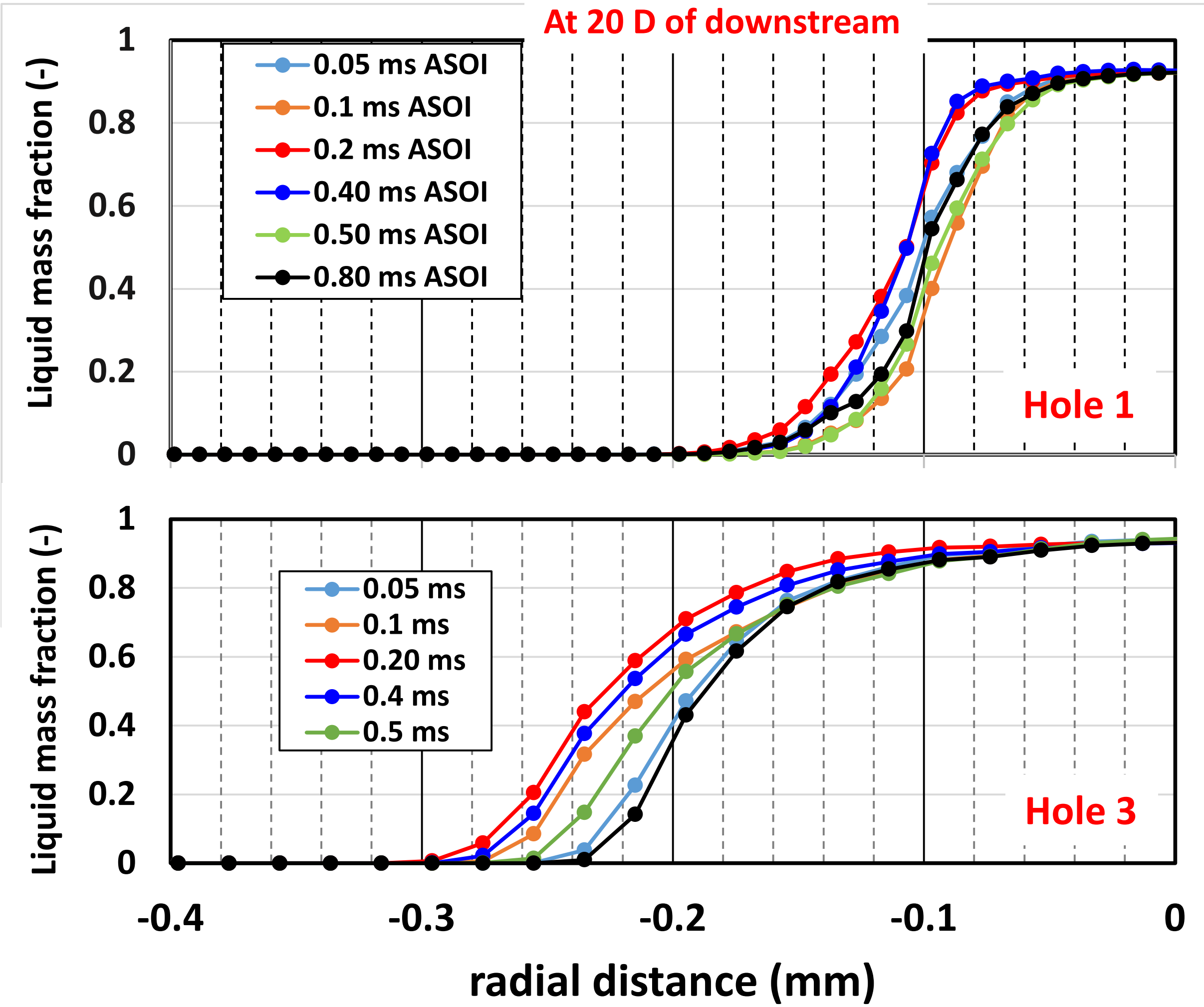


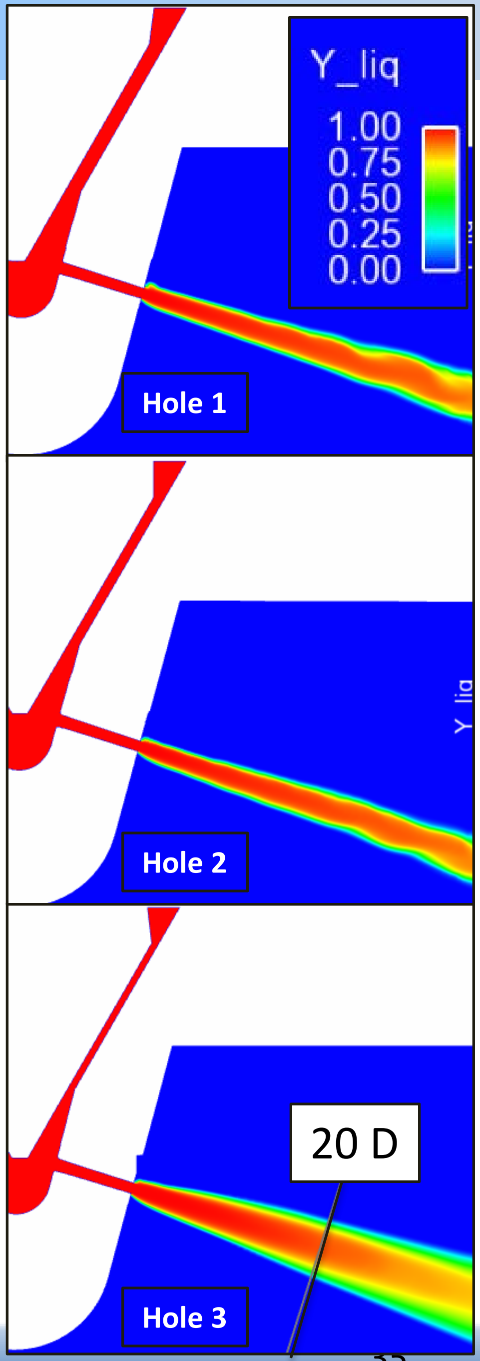




- Spray A has negligible variation in radial distribution at this axial location. It seems to have reached a quasi-steady state
- Spray B has significant radial spreading variation at different time instants. In fact, the variation in spreading is non-monotonic

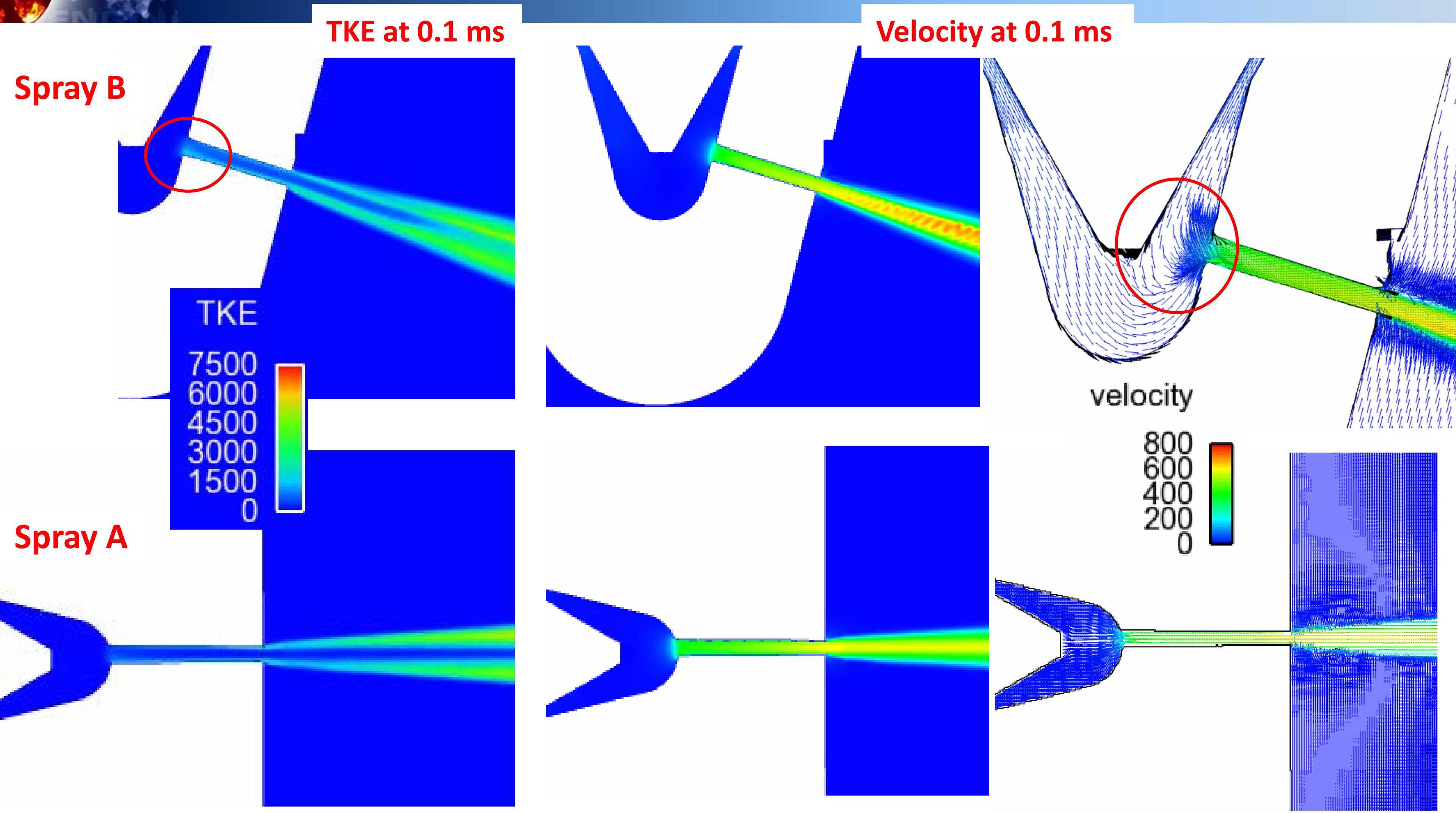
ANL contribution: Spray B dynamics





- Spray transient behavior observed for all holes
- Hole 3 has a larger spray radial spreading and variation
- Maximum variation of 60 microns for hole 3
- Overall variation in spreading from simulations smaller than that observed in the experiments

ANL Contribution: Spray A vs. Spray B dynamics



- Turbulent kinetic energy is higher for Spray B inside the hole than Spray A
- Velocity streamline shows flow turns at the inlet of the hole
- Flow is more transient for Spray B vs. Spray A

Concluding Remarks/Suggestions

- A well developed Eulerian-based 2D approach seems to work quite well in predicting the spray structure in the near nozzle region. The higher fidelity approaches still need further development
- In the near nozzle region, resolution seems to influence the results more than the choice of turbulence models
- Transitioning to an Lagrangian approach somewhere between 2 mm to 6 mm is necessary. Unfortunately, we do not have experimental data in this region
- Even with the Eulerian model, upstream of 2 mm, the need for a proper atomization model (to initiate the onset of instabilities) is imperative
    - Note: None of the models presented use phase interface tracking (apart from Aachen, with DNS), and hence liquid gas interface is not enforced. Most approaches instead, model small scale breakup as a turbulent diffusion process.
- Wall temperature has an appreciable influence on the spray behavior, especially on mass flow rate at nozzle exit and spray penetration. Projected density contours are minimally affected, at least with the temperature range investigated here
- Accounting for needle movement (and initial transient mass flow rate) can significantly improve the predictions, although for a single hole injector needle wobble does not have a profound influence on results

Future work/Suggestions

- RANS can capture some of the single vs. multi-hole dynamics. LES can probably better predict the transients observed with multi-hole injector compared to the single hole injector
- From Sandia: The uncertainty introduced by temperature via surface tension seems much more worrying. The liquid temperature gradient is very strong close to the dense region, merely stabilized by vaporization. We would like to insist on the relevance of trying to experimentally assess droplet temperature in the future.
- From IFPEN: . In future work, Chawki will use the ligament length in order to release the primary droplets farther from the liquid core, thus promote droplets dispersion. This kind of work need some special experimental data. Chawki would like to ask the experimentalists to measure ligament length/diameter in order to help for primary atomization modeling.