TOPIC 2
PRIMARY ATOMIZATION (NEAR-NOZZLE MIXING)

Presenter: Michele Battistoni, University of Perugia

Valencia, September 10th, 2018

Contributors (list of groups):

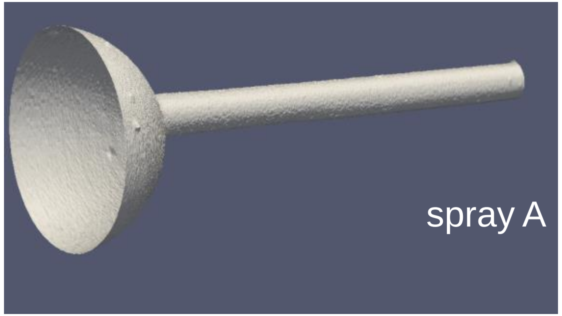
Experiments:

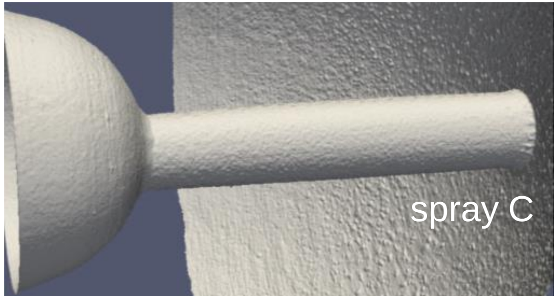
- Shane Daly, *Oregon State, -* Scott Skeen, Emre Cenker, Lyle Pickett, *Sandia National Laboratories* - Cyril Crua, *Univ. Brighton* - Fredrik Westlye, *Tech Univ. Denmark* - Julien Manin, *Artium*
- Brandon Sforzo, Alan Kastengren, Katie Matusik, Chris Powell, *Argonne National Laboratory,*

Simulations:

- Marco Arienti, Joonsik Hwang, *Sandia National Laboratories*
- Michele Battistoni, *University of Perugia*
- Mathis Bode, *Aachen University*
- José M. Pastor, *CMT* - Adrian Pandal, *University of Oviedo,* - Bertrand Naud, *CIEMAT*
- Aqeel Ahmed, François-Xavier Demoulin, *Coria*
- Julien Manin, *SANDIA, Artium*
- Peetak Mitra, David Schmidt, *University of Massachusetts*

NOTES





- More and more simulations consider both nozzle internal flow and near-field flow and how this affects spray characteristics
  - This allows proper boundary conditions
  - Transient effects can be tackled
  - Focusing on either nozzle internal flow or near-field flow only seems questionable (possibly, same simulation for two topics)

- Three different nozzles available: Spray A, C, D
  - With known boundary conditions:
    real geometries, needle tip motion, wall temperatures

OBJECTIVES

- Focus on the near-nozzle region: **<u>within first ~10 mm</u>**
  - Spray A
  - Spray C / D
- Capture spray physics under nominal ECN conditions and under cold conditions
- Study and comparison of different modeling approaches, from RANS to LES, to DNS, and Lagrangian-Eulerian, Eulerian-Eulerian
- Encourage high-fidelity simulations of fuel sprays to understand the physics of the primary atomization
- Provide a robust database for model validation and for physics understanding
  - mass distribution
  - phase interfacial area
  - droplet sizing

CONTRIBUTORS – EXPERIMENTS

Group		Spray A	Spray C	Spray D	Data & Conditions
ANL (US)	Brandon Sforzo Katarzyna Matusik Christopher Powell Alan Kastengren	✔	✔	✔	Radiography - spray A #675 ref. case + parametric variations - spray C #37 ref. case - spray D #133 ref. case + parametric variations - spray D #134 ref. case
			✔	✔	Tomography - spray C #37 ref. case - spray D #134 ref. case
		✔	✔	✔	USAXS - spray A #675 ref. case + parametric variations - spray C #37 ref. case + parametric variations - spray D #133 ref. case - spray D #134 ref. case
SANDIA (US)	Shane Daly, Oregon State Scott Skeen, Emre Cenker, Lyle Pickett, Sandia National Laboratories Cyril Crua, Univ. Brighton Fredrik Westlye, Tech Univ. Denmark Julien Manin, Artium		✔	✔	Optical long-distance microscopy Measurement of liquid envelope for Spray C and Spray D with different fuel and ambient temperatures

CONTRIBUTORS – CFD MODELERS

Institution/Group		Spray			Conditions: Steady state/Transient/…
		A	C	D	
Aachen RWTH (Germany)	Mathis Bode Marco Davidovic Heinz Pitsch		✔	✔	Reference Transient
CMT-UniOvi-CIEMAT (Spain)	José M. Pastor Adrian Pandal Blanco Bertrand Naud	✔			Reference + parametric variations Transient
CORIA (France)	Aqeel Ahmed François-Xavier Demoulin	✔			Reference + parametric variations Transient
Perugia (Italy)	Michele Battistoni		✔	✔	Reference Steady
SANDIA (US)	Marco Arienti Joonsik Hwang		✔		Reference Steady
SANDIA-Artium (US)	Julien Manin	✔			Reference Steady
UMass (US)	Peetak Mitra Declan Gwynne Eli Baldwin David Schmidt		✔	✔	Reference Steady Transient SOI/EOI & multiple-injection

MODEL DESCRIPTION

Institution/Group	approach	CFD code	Compressibility and EOS	Turbulence model
Aachen RWTH, Mathis Bode Marco Davidovic Heinz Pitsch	In-nozzle: LES/ Atomiz.: DNS	CIAO (in-house)	Compressible code with HEM with (SG/PR EOS) Low-Mach	LES - Dynamic Smagorinsky, with Lagrangian averaging backward in time
CMT-UniOvi-CIEMAT, José M. Pastor Adrian Pandal Blanco Bertrand Naud	Diffuse interface (mixture) + Σ-Y Eulerian single fluid	OpenFOAM	Barotropic liquid Ideal gas	LES eddy viscosity based SIGMA model (Nicoud et al. POF, 2011)
CORIA, Aqeel Ahmed François-Xavier Demoulin	Diffuse interface (mixture) + Σ-Y and ELSA model	OpenFOAM	Incompressible	LES WALE
Perugia, Michele Battistoni	1) Diffuse interface (mixture) 2) Sharp interface VOF	CONVERGE	1) barotropic liquid + ideal gas 2) incompressible	LES Dynamic Structure
SANDIA, Marco Arienti, Hwang	Diffuse interface (mixture)	CONVERGE	barotropic liquid + RK gas	RANS RNG k-e
SANDIA-Artium, Julien Manin	VOF	Gerris	Incompressible	DNS no model
UMass, Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt	Diffuse interface (mixture) + Σ-Y Homogeneous Relaxation Model Eulerian single fluid	HRMFoam	Compressible Refprop (NIST database)	RANS $\kappa-\omega$

MODEL DESCRIPTION

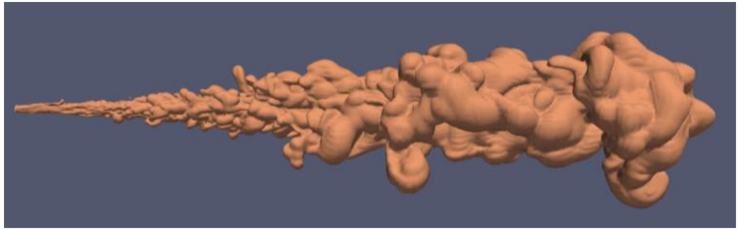
Institution/Group	min-max mesh resolution (within the 0-10 mm range)	Needle motion	Internal nozzle included	Dimensionality and domain extension
Aachen RWTH, Mathis Bode Marco Davidovic Heinz Pitsch	1 µm - 60 µm	Moving needle	1-way coupling interface at nozzle exit	3D
CMT-UniOvi-CIEMAT, José M. Pastor Adrian Pandal Blanco Bertrand Naud	3 µm – 90 µm	Fixed – high lift	Not included (educated ROI + synthetic turbulent fluctuations)	3D (chamber L = 20 mm)
CORIA, Aqeel Ahmed François-Xavier Demoulin	1 µm – 15 µm (axisymmetric) 2 µm – 80 µm (STL)	Fixed – high lift	Yes	3D (chamber L = 10 mm)
Perugia, Michele Battistoni	2.5 µm – 40 µm (with AMR)	Fixed – high lift	Yes	3D (chamber L = 15 mm)
SANDIA, Marco Arienti, Hwang	7.81µm - 250µm (with embedded refinements and AMR)	Fixed – high lift	Yes	3D (chamber L = 24 mm)
SANDIA-Artium, Julien Manin	0.9 µm (0 to 20 diam.) 1.8 µm (0 to 40 diam.) 3.6 µm (0 to 80 diam.)	Fixed – high lift	No internal flow (fixed velocity profile)	3D (20, 40 and 80 diameters long domains)
UMass, Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt	1.1 µm – 25 µm (Pacman mesh motion Library)	C) Fixed – high lift D) Moving needle	Yes	3D (chamber L= 3 mm)

MODEL DESCRIPTION

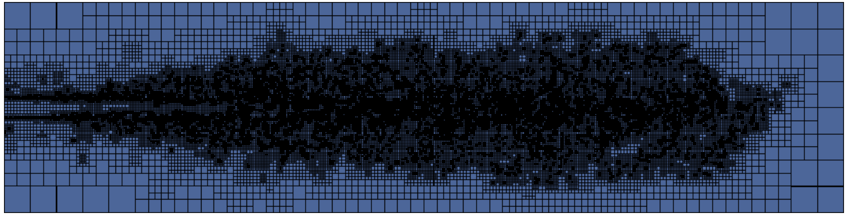
Institution/Group	nozzle surface	Cell type	Cell count	Spatial discretization	Temporal discretization
Aachen RWTH, Mathis Bode Marco Davidovic Heinz Pitsch	A #675 C #37 D #134	hex (structured Cartesian)	800 M	Hybrid (2nd/4th CD & WENO 3rd/5th)	2nd order Runge-Kutta
CMT-UniOvi-CIEMAT, José M. Pastor Adrian Pandal Blanco Bertrand Naud	A #675	hex	7 M	2nd order Gamma NVD	2nd order backward
CORIA, Aqeel Ahmed François-Xavier Demoulin	A #675 – axisymmetric A #675 – high resolution STL	hex (dominant)	32 M 5 M	2nd order linear 2nd order linear	2nd order backward for U 1st order Euler for volume fraction (MULES) with 3 sub-cyles
Perugia, Michele Battistoni	C #37 – high resolution STL D #134 – high resolution STL	hex	50 M	1) 2nd order CD for all (with flux limiter), except for turbulence, 2) VOF-LES 1st order	1st order Euler Dt ~ 1.0 ns
SANDIA, Marco Arienti, Hwang	C #37 – high resolution STL	hex	1 M	1st order upwind, except for turbulence. Rhie-Chow and strictly conservative	1st order Euler
SANDIA-Artium, Julien Manin	A #675	hex (Octree with ARM)	max 540 M	-	-
UMass, Peetak Mitra, Declan Gwynne, Eli Baldwin, David Schmidt	C #37 – Wireframe (axisym.) D #134 – high resolution STL	Polydehra	0.7 M	2nd order	1St order Euler

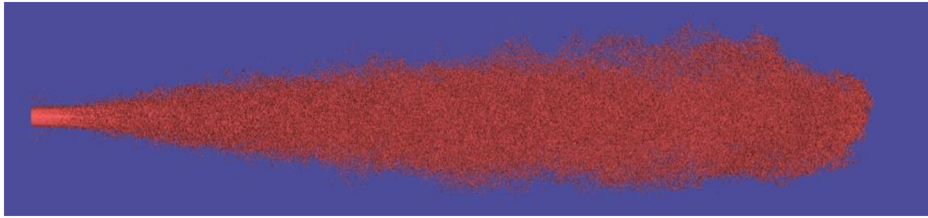
SPRAY A

CMT-UniOvi-CIEMAT (OpenFOAM – LES)

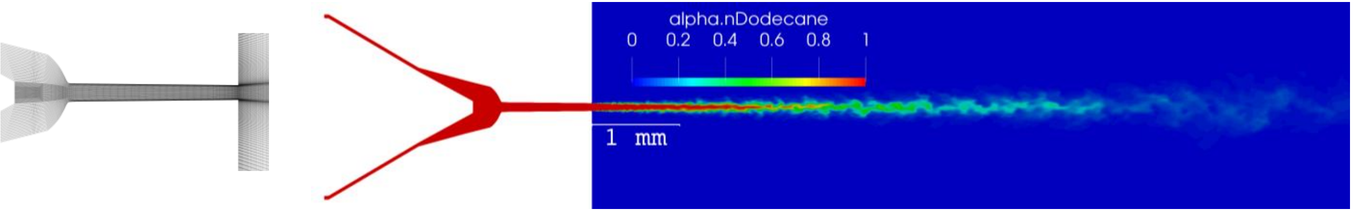


SANDIA-Artium (Gerris – DNS)





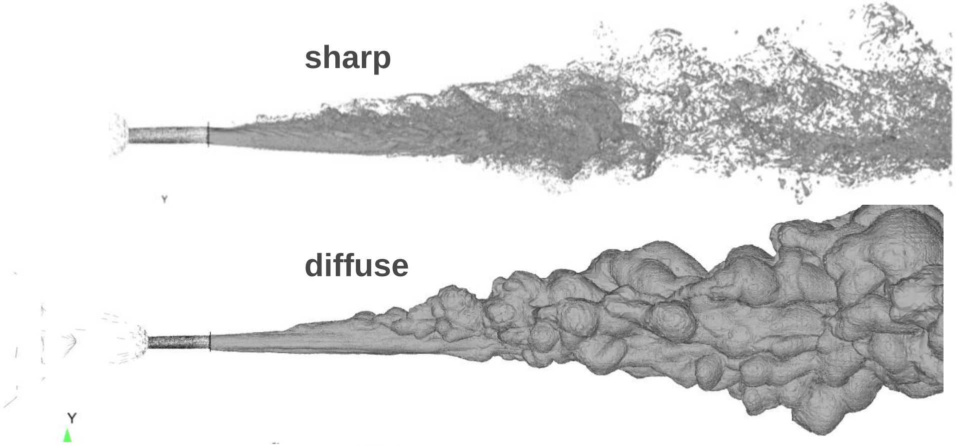
CORIA (OpenFOAM – LES)



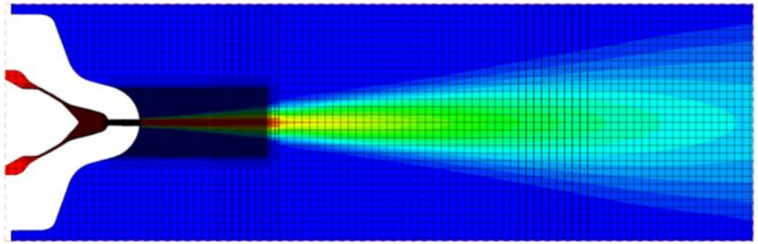
SPRAY C/D

Aachen (CIAO – DNS)

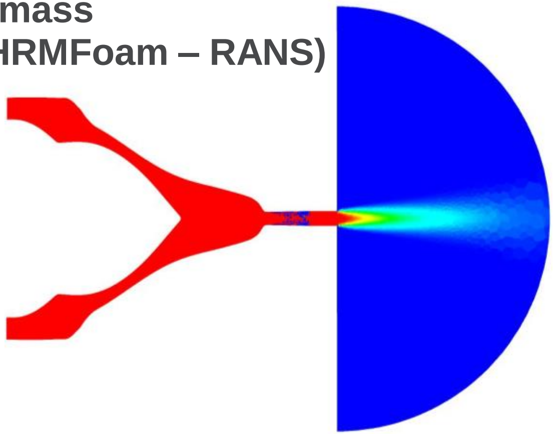
Perugia (CONVERGE – LES)



SANDIA (CONVERGE – RANS)

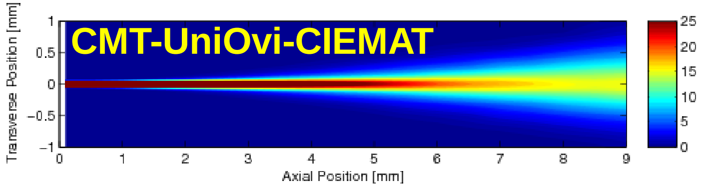


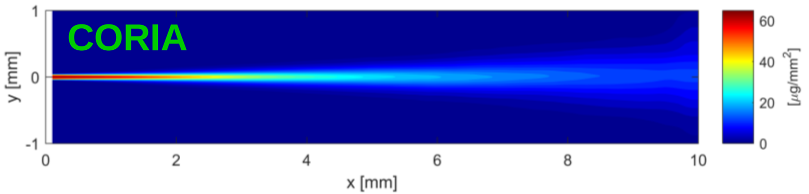
Umass (HRMFoam – RANS)

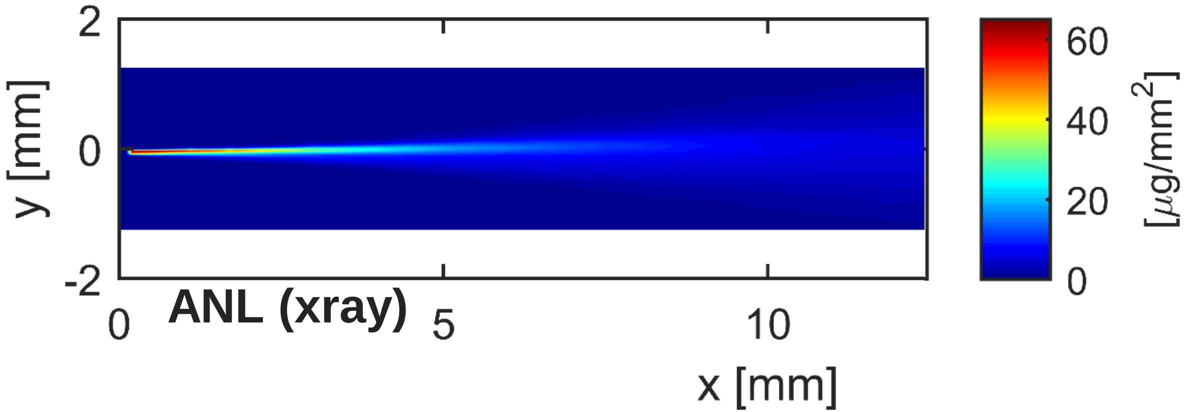


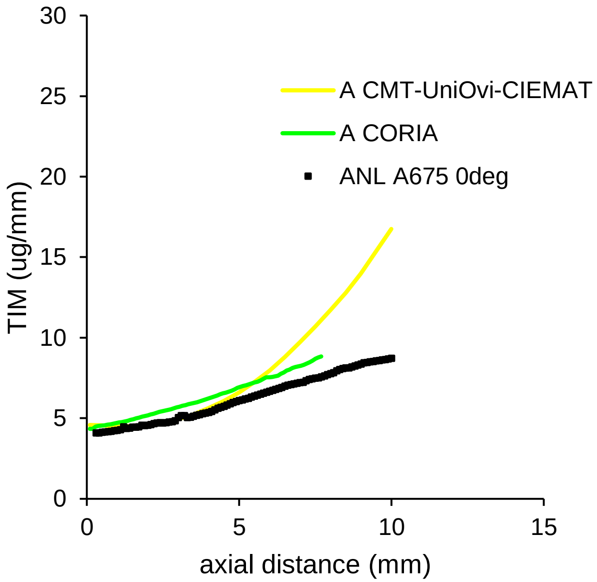
SPRAY A – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP VS. SIM)

LES calculations:
Single realization + time-averaging



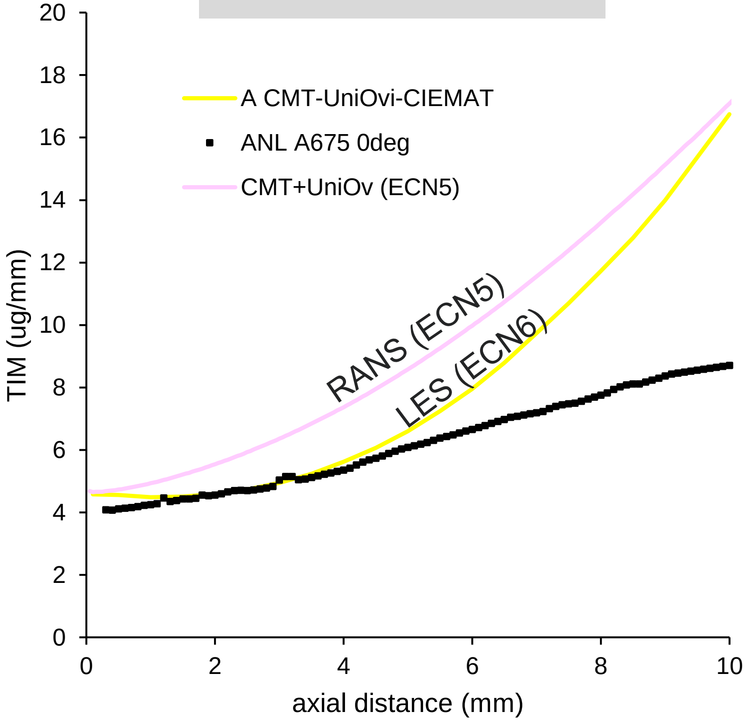




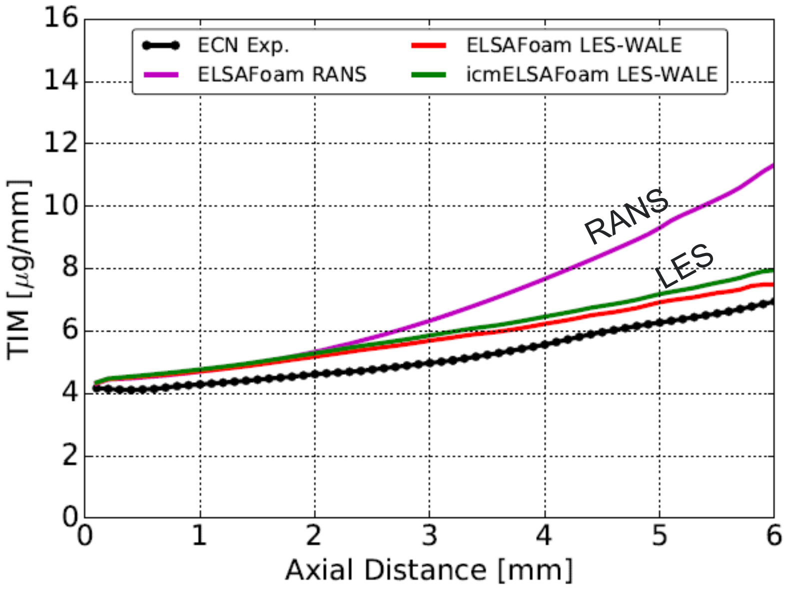


SPRAY A – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP VS. SIM)

CMT-UniOvi-CIEMAT



CORIA

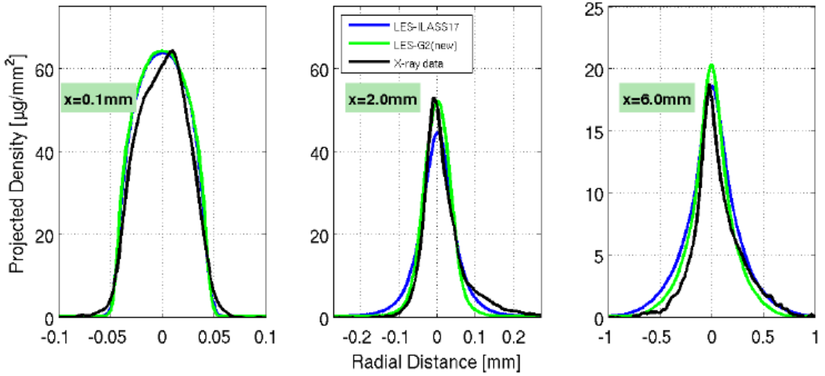


Improvements up to 5-6 mm, with LES:

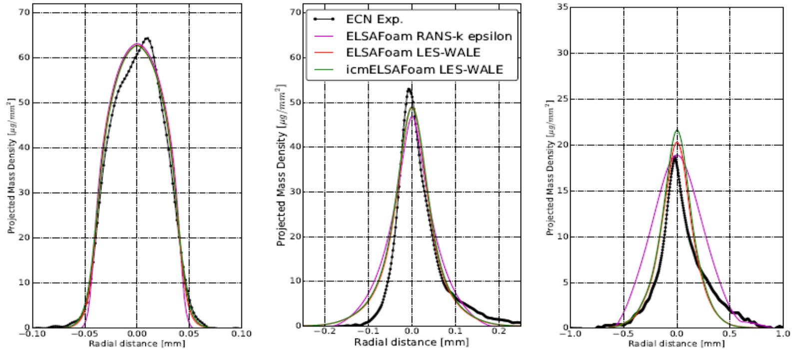
…..lack of resolution in the far field? (under-resolved LES?)

SPRAY A – PROJECTED FUEL MASS PROFILES

CMT-UniOvi-CIEMAT



CORIA



Improvements up to 5-6 mm, with LES:

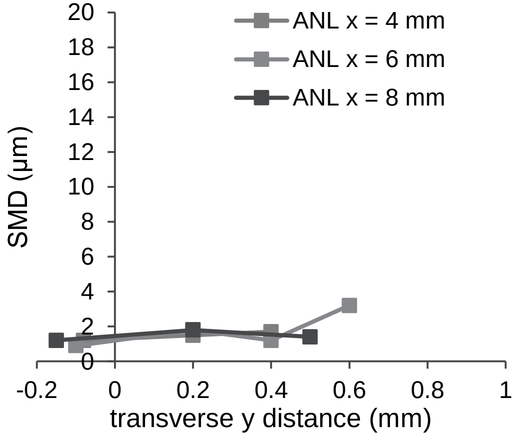
…..lack of resolution in the far field? (under-resolved LES?)

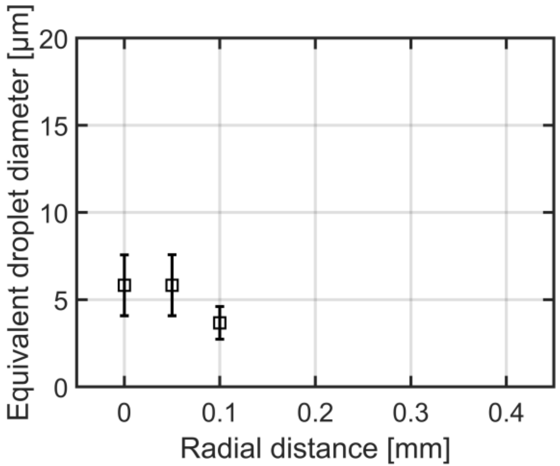
SPRAY A – DROPLET SIZE

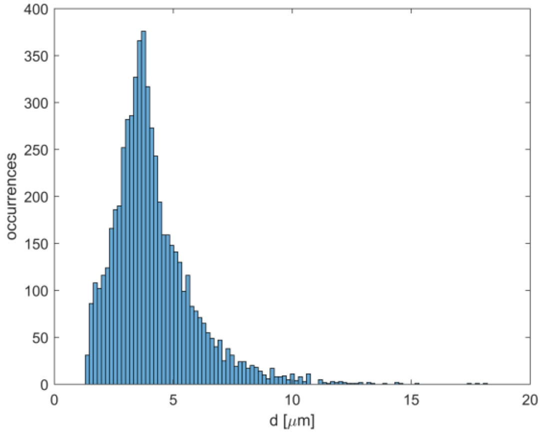
drop statistics (from DNS in the very early stage – Gerris code)

ANL (USAXS)

SANDIA-Artium



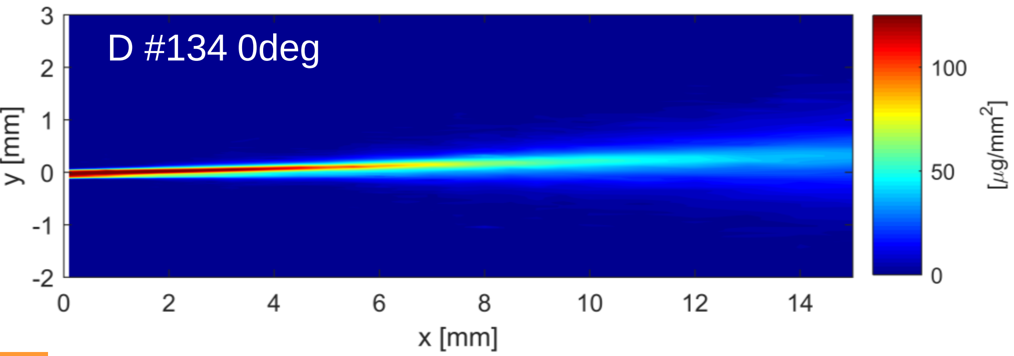


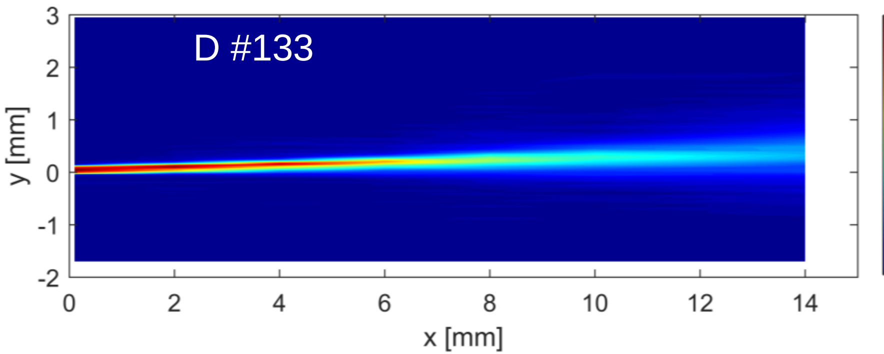


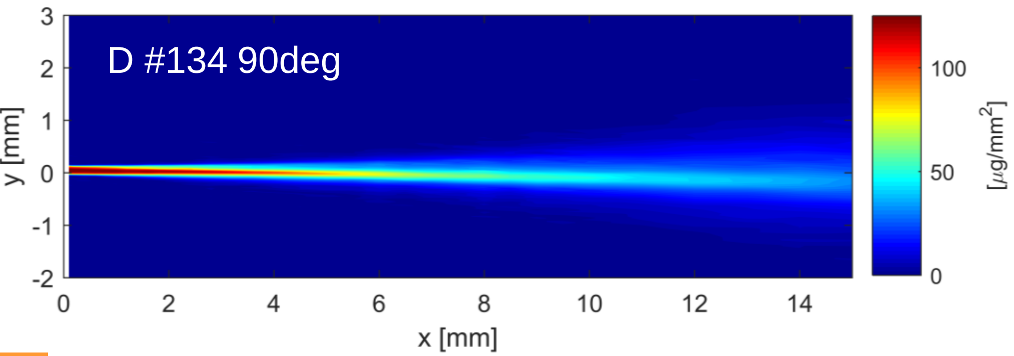
- pdf of diameters are still not available from experiments in the dense core for comparison

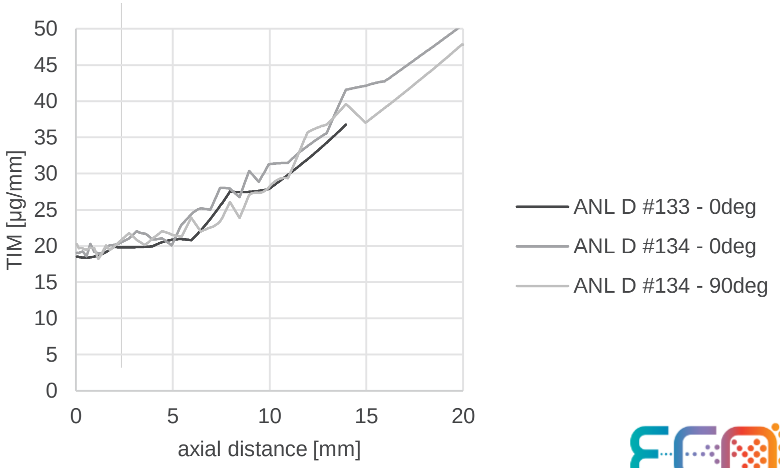
SMD from DNS is still over-estimated by a factor of about 4X (resolution used was 1um)

SPRAY D – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP)

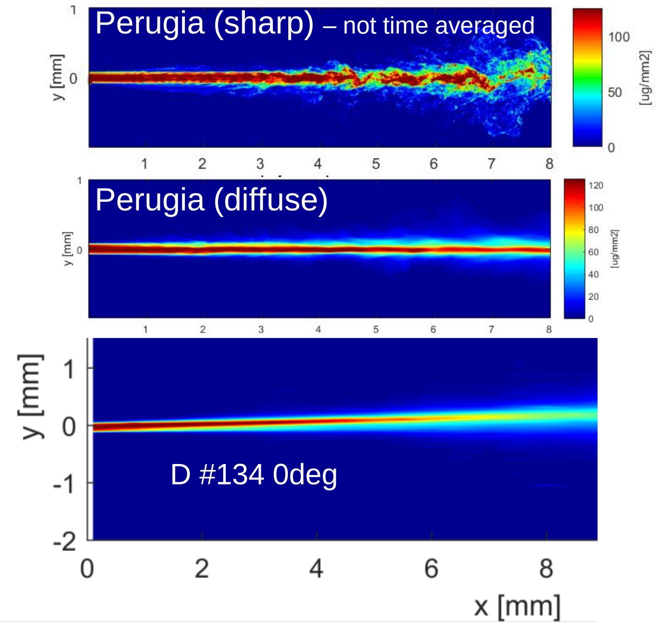


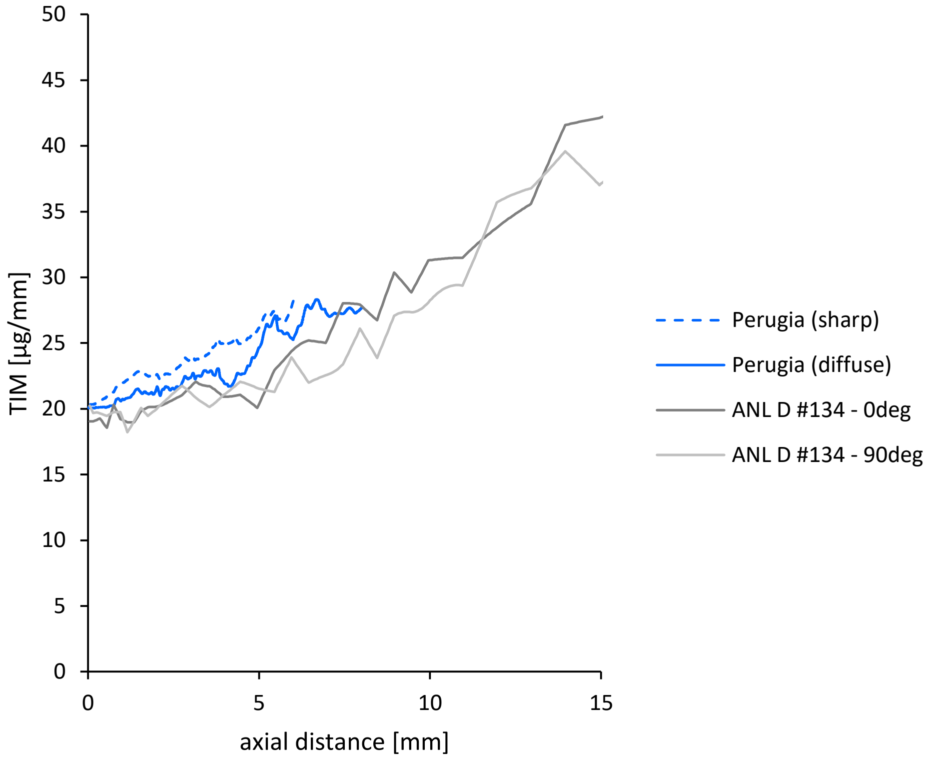




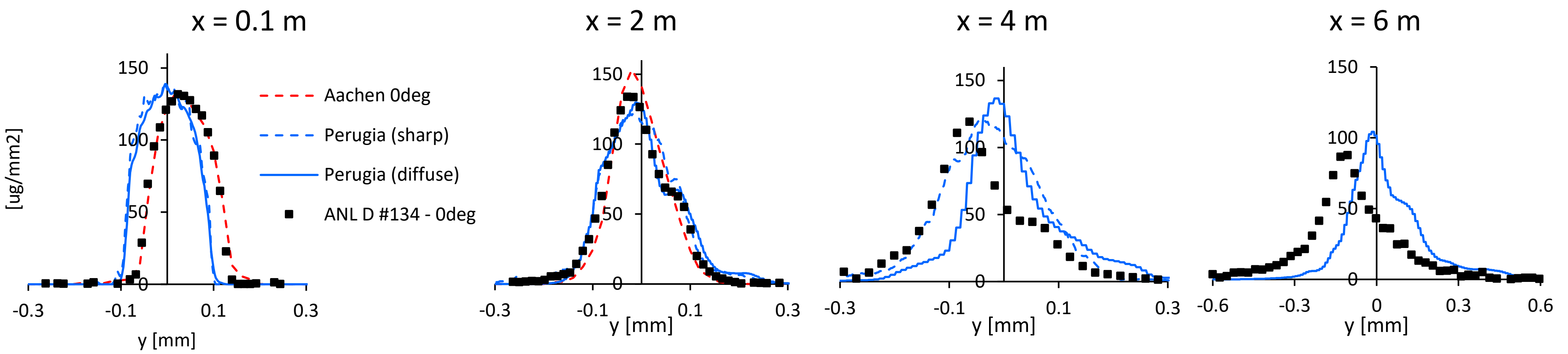


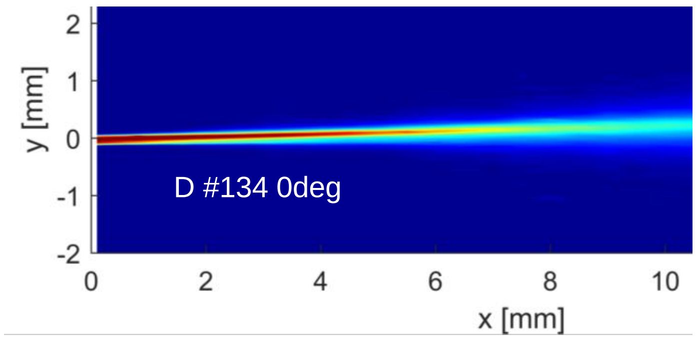
SPRAY D – PROJECTED MASS & TRANSV. INTEGRATED MASS (EXP VS. SIM)





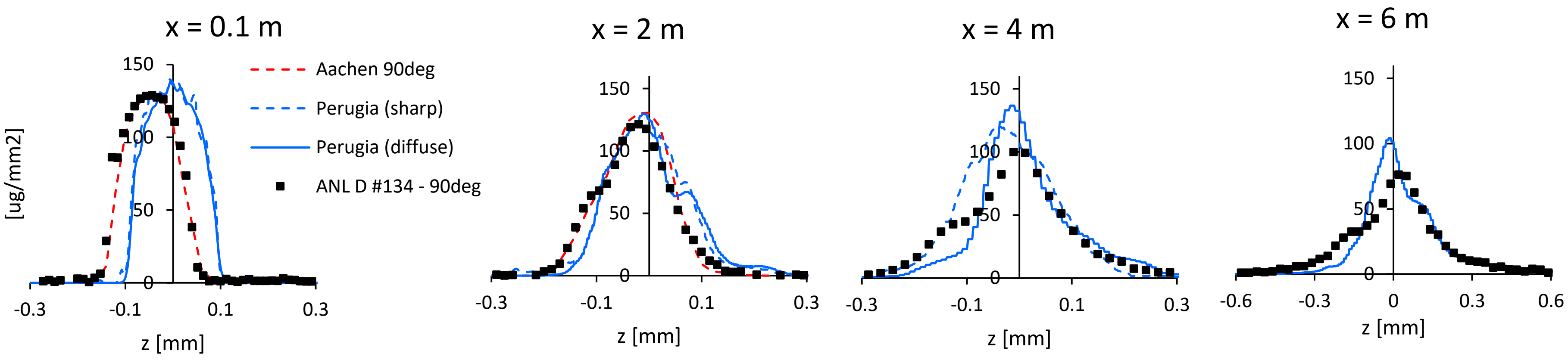
SPRAY D – PROJECTED FUEL MASS PROFILES (STEADY)

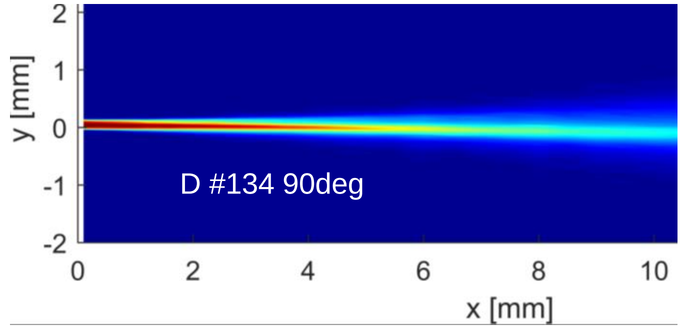




- Spray D #134 jet deviates substantially from the axis
- Models tend to capture the distribution, if a transv. offset is applied

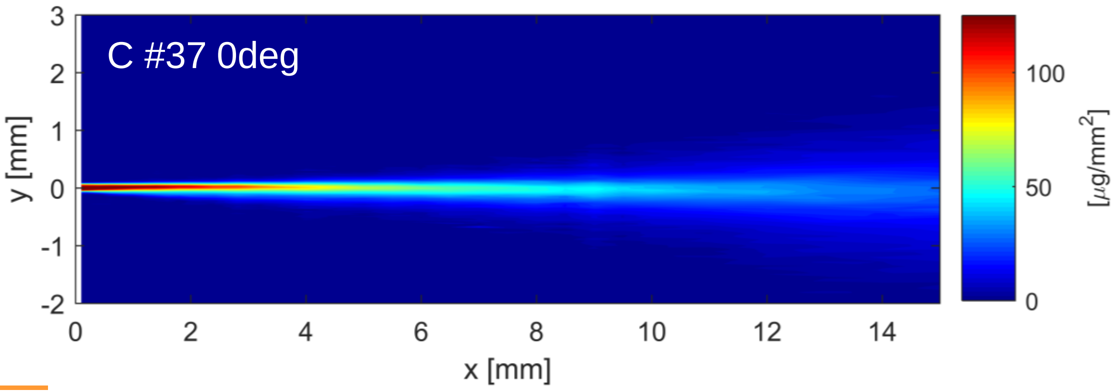
SPRAY D – PROJECTED FUEL MASS PROFILES (STEADY)

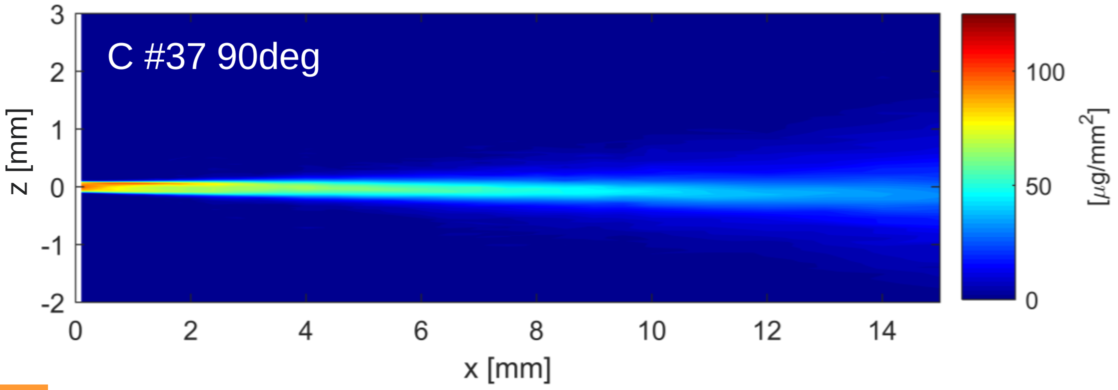


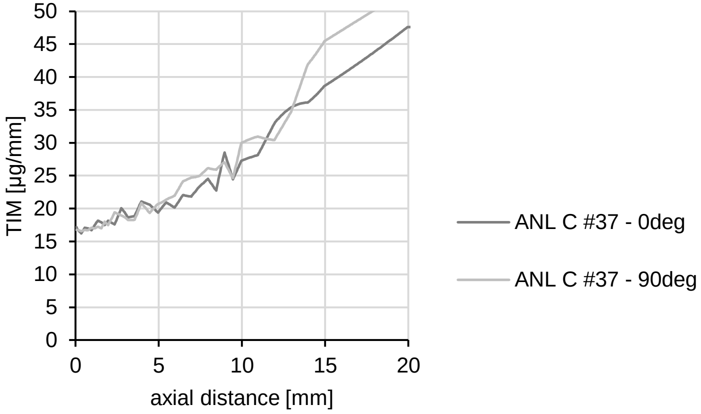


- Re-centering is needed for better comparison, maybe about the FWHM
- Models tend to capture the distribution and details of asymmetries

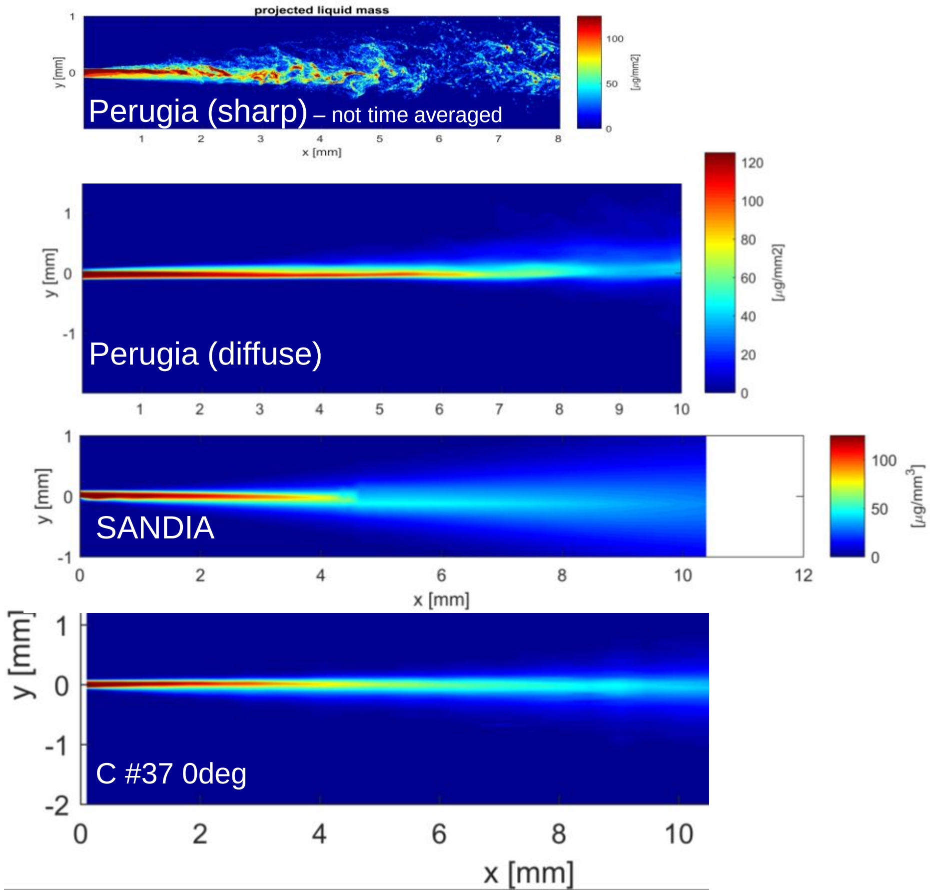
SPRAY C – PROJECTED FUEL MASS & TRANSVERSE INTEGRATED MASS (EXP)

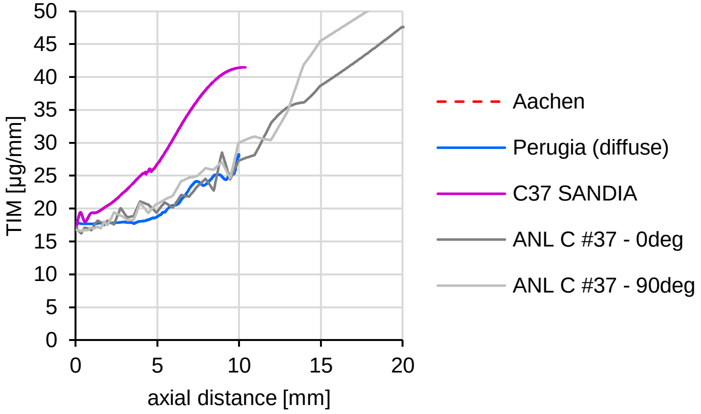




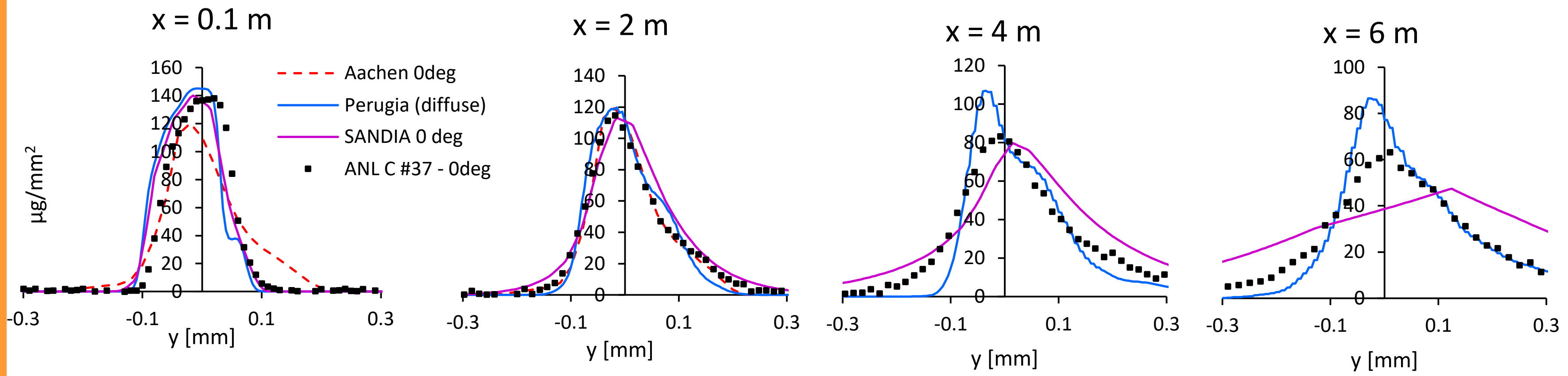


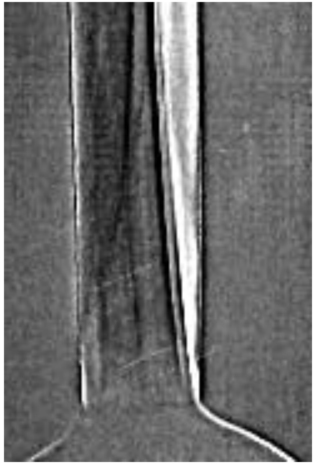
SPRAY C – PROJECTED FUEL MASS & TRANSVERSE INTEGRATED MASS (EXP VS. SIM)

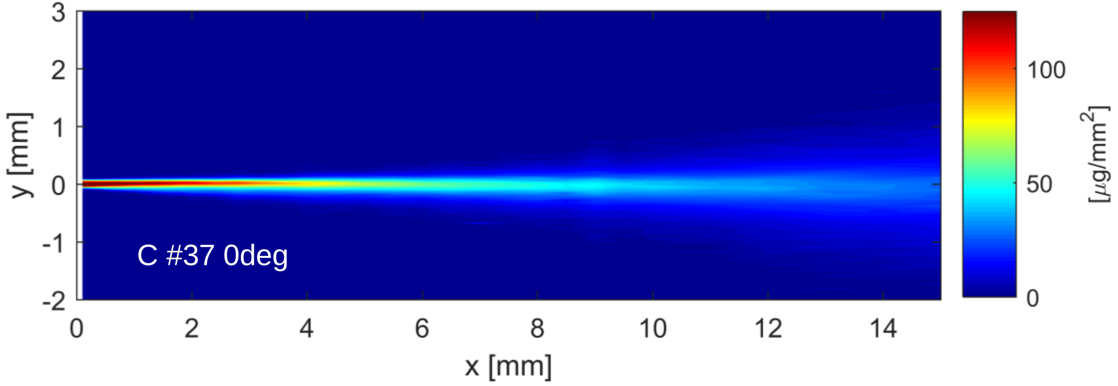




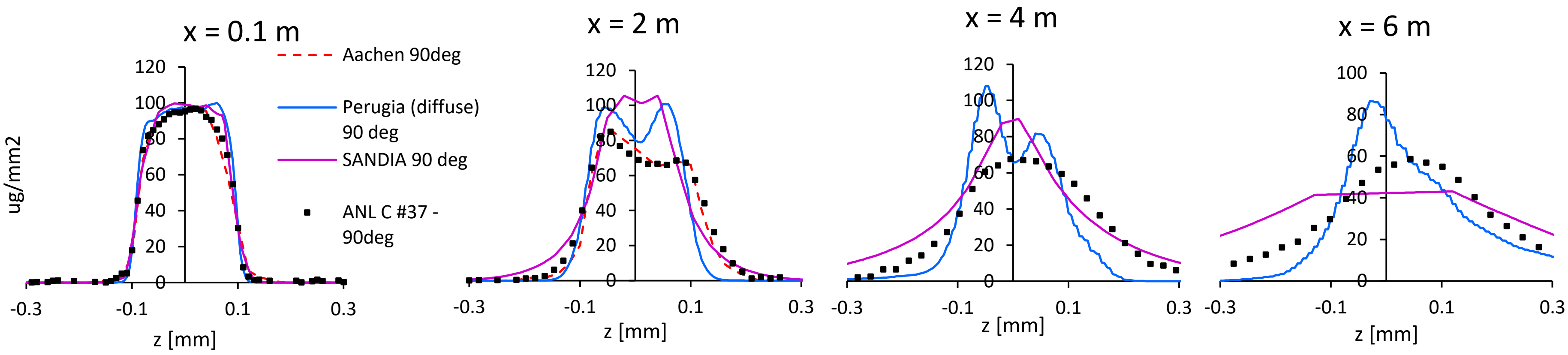
SPRAY C – PROJECTED FUEL MASS PROFILES (STEADY)

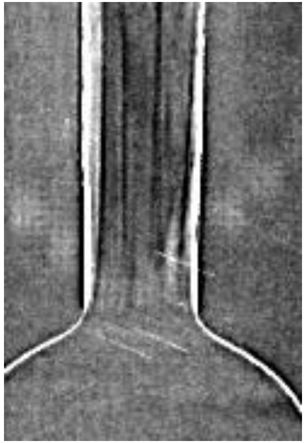


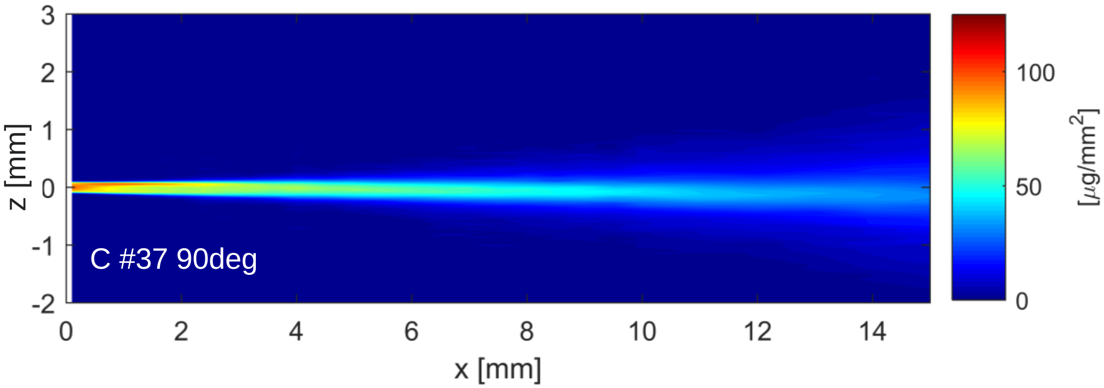




SPRAY C – PROJECTED FUEL MASS PROFILES (STEADY)







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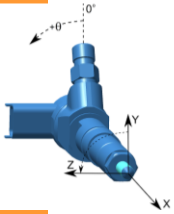
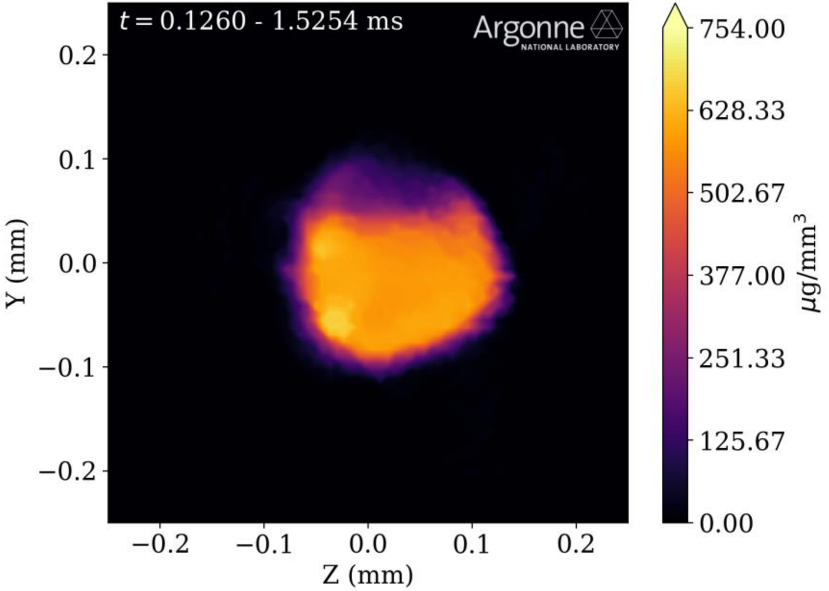
SPRAY D_134 vs. C_37: FUEL DENSITY FIELD at x = 0.1 mm

ANL reconstructed fuel density field (μg/mm³)

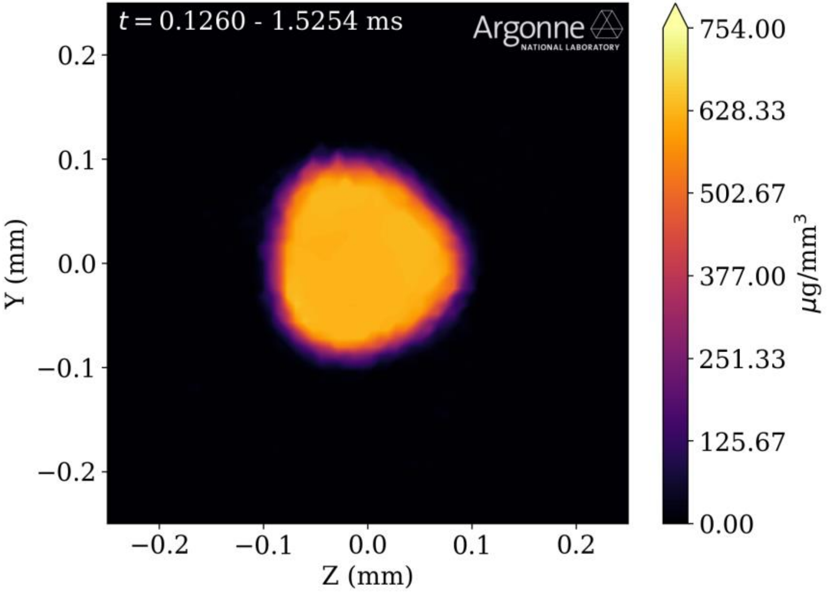
Time averaged in the steady state part



C_37



D_134



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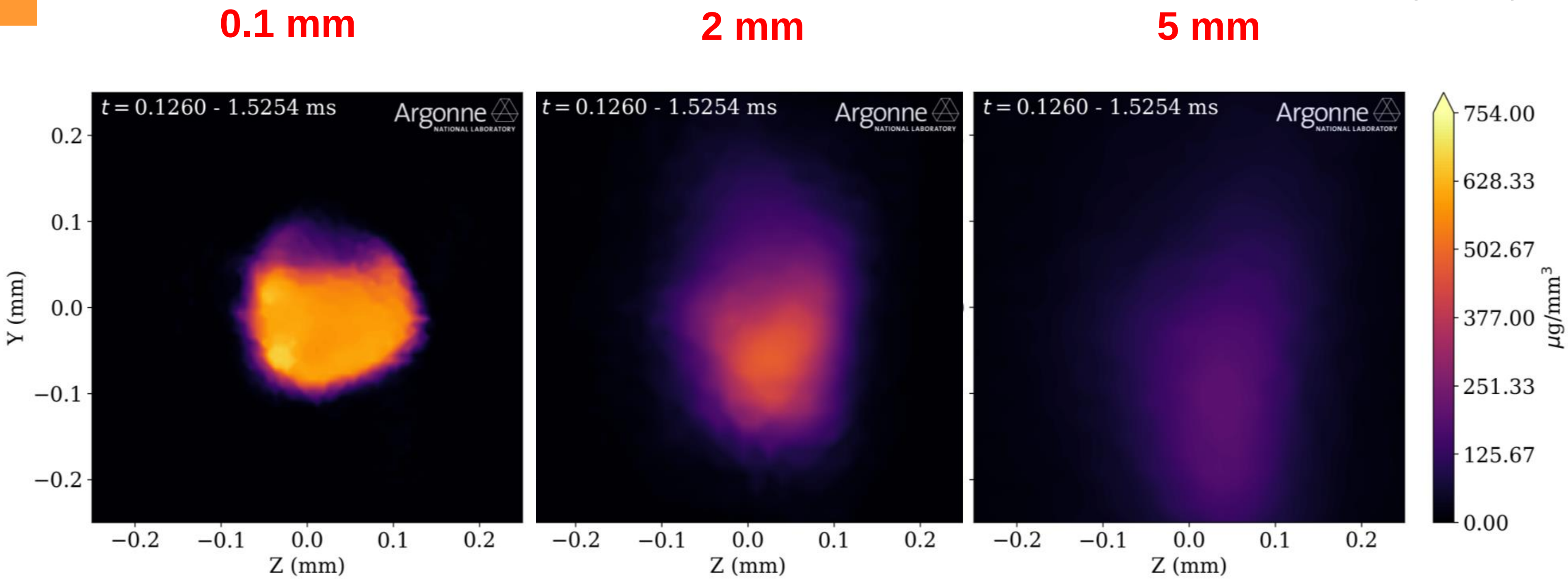
SPRAY C_37: FUEL DENSITY FIELD at x = 0.1, 2, 5 mm

ANL reconstructed fuel density field ($\mu g/mm^3$)

Time averaged in the steady state part



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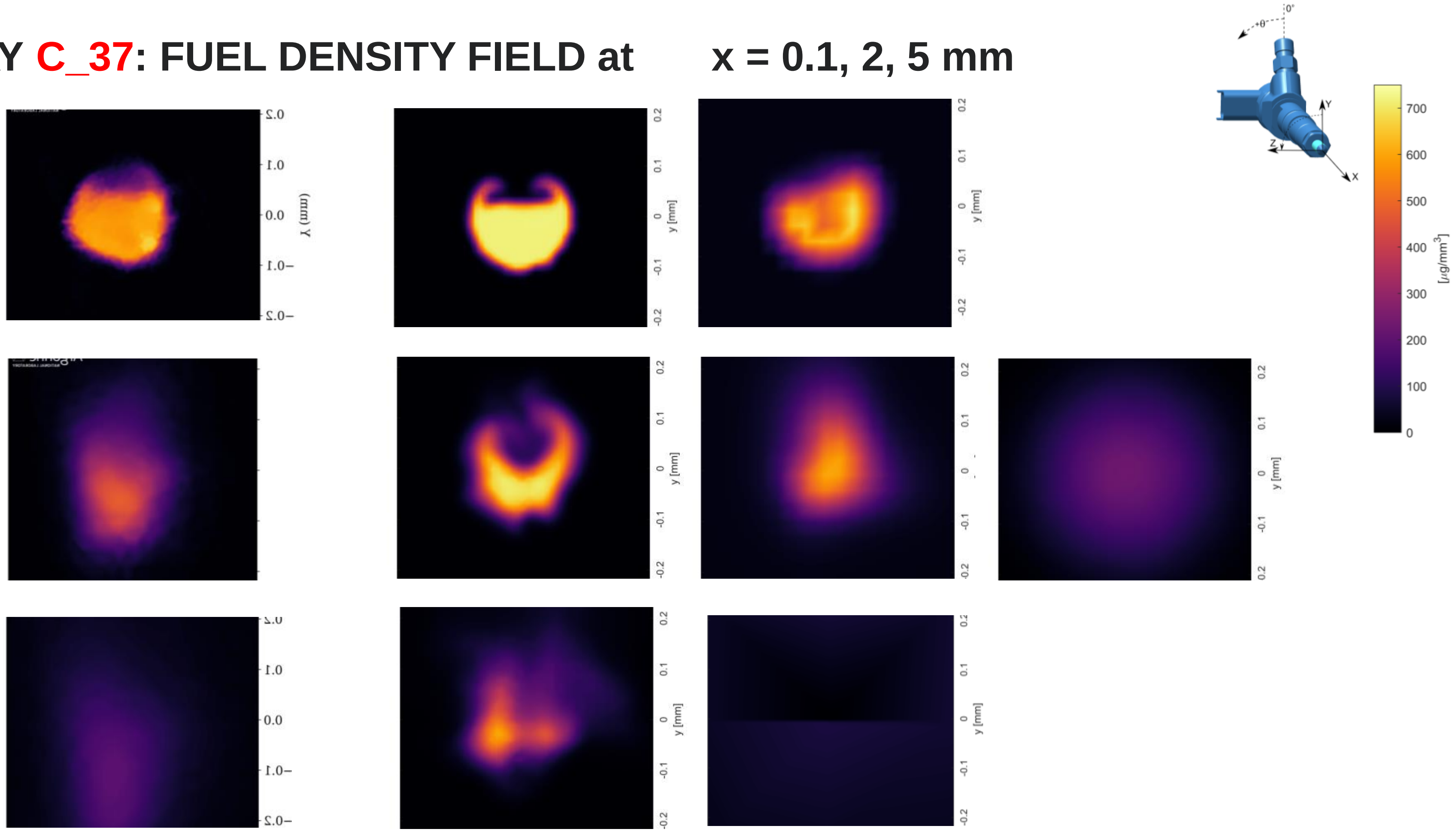
SPRAY C_37: FUEL DENSITY FIELD at x = 0.1, 2, 5 mm



0.1 mm

2 mm

5 mm

ANL

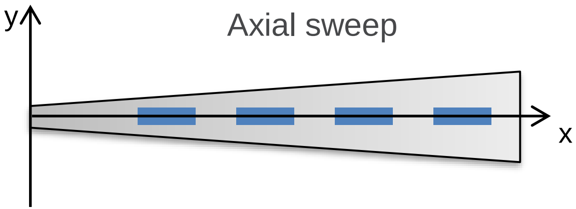
Perugia

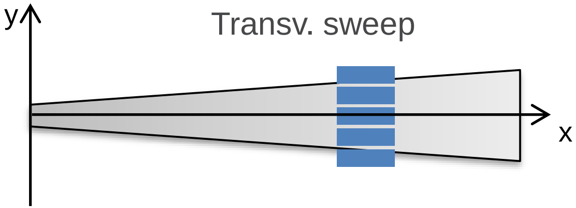
SANDIA

UMass

SPRAY C/D – INTERFACIAL AREA

Experiments: USAXS
(Ultra Small Angle Xray Scattering)

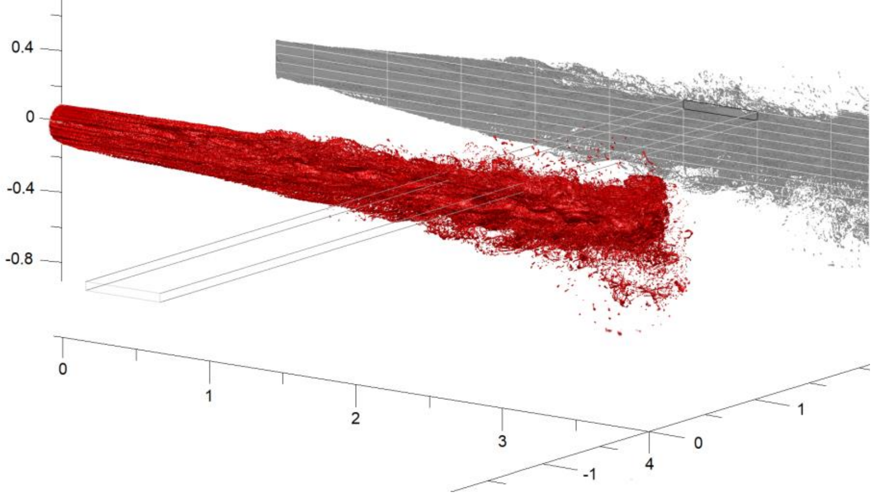




Bin size in the USAXS
experiments: 50 µm × 500 µm

Matusik et. al. ICLASS 2018
Kastengren et al., IJMF 2017

In order to compare "apple-to-apple":
Simulation postprocessing that <u>mimicks</u>
USAXS method



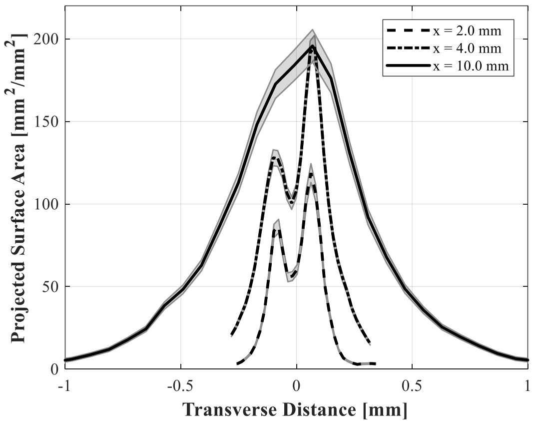
Total area of phase interface, A, and the total volume, V
with "USAXS-like" method: V/V_{box} & A/V_{box}
Line-of-sight box, moving along X and Y, to collect info on each structure, <u>including core</u>
On each box, collection of:
- liquid volume V
- interface area A

$$SMD = 6\frac{V/V_{box}}{A/V_{box}}$$

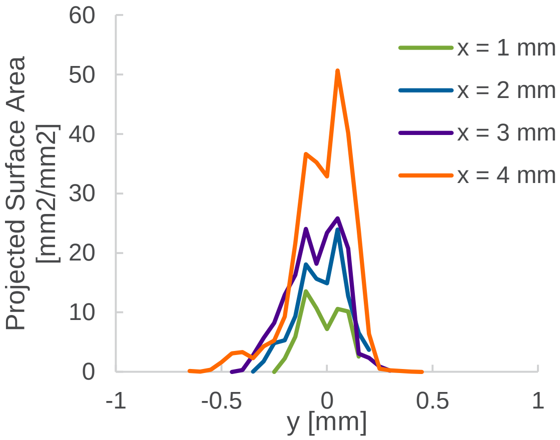
Battistoni, Magnotti, et al., SAE 2018

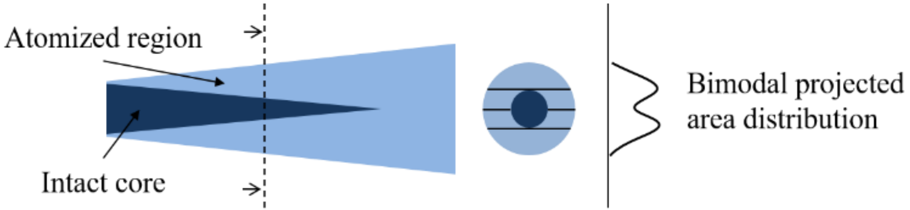
SPRAY D – PHASE INTERFACE AREA

ANL (USAXS data)



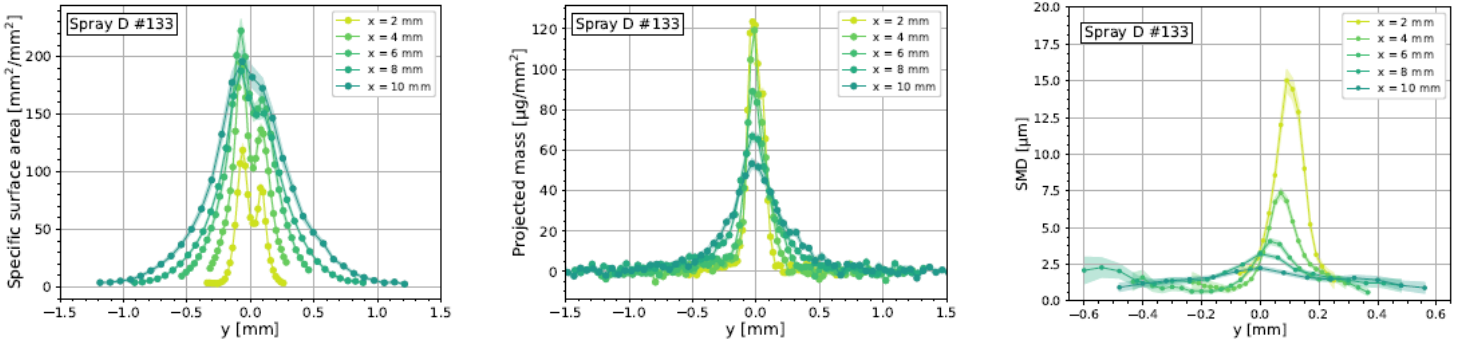
Perugia





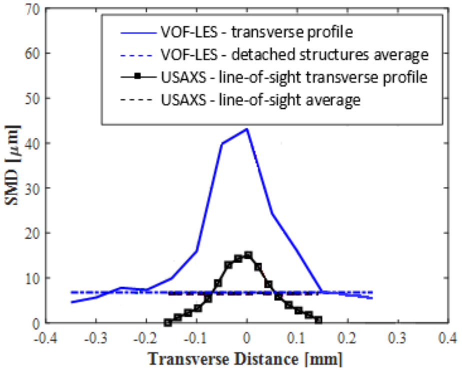
- The double peak in the projected area distribution is due to the intact core.
- It is therefore possible to identify the liquid core length. In this case about 5-6 mm

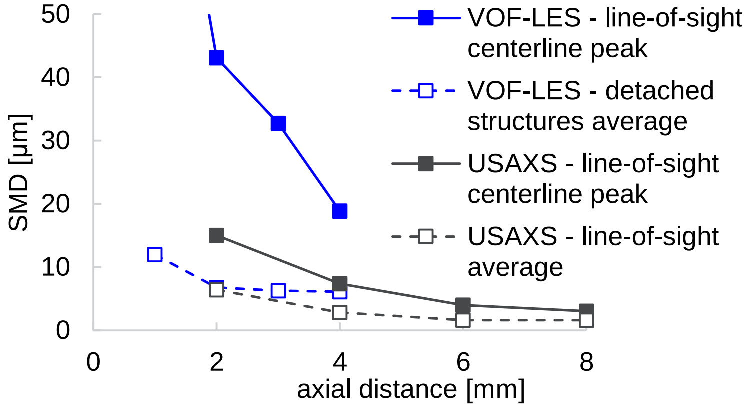
SPRAY D – SAUTER MEAN DIAMETER



Matusik et. al. ICLASS 2018

- Model captures the SMD trend
- Actual droplet size (detached structures) is insensitive to the axial distance
- Room for improvement: more resolution still required to be fully predictive at diesel spray conditions
- USAXS data include the liquid core: USAXS provide an apparent SMD in the centerline



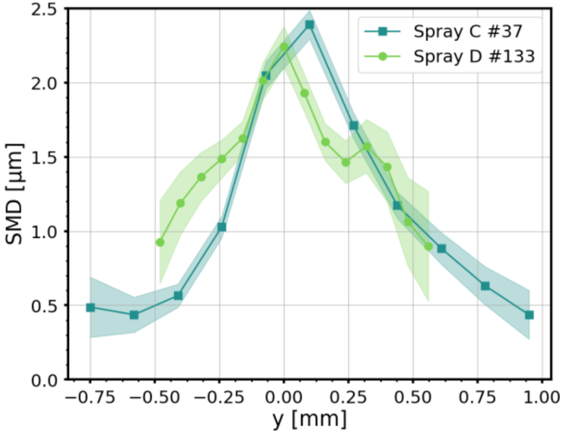


Battistoni, Magnotti, et al., SAE 2018

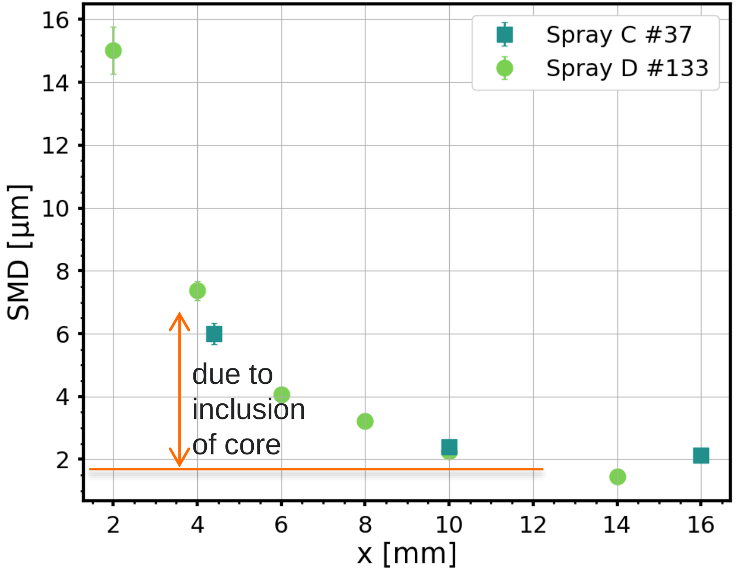
SPRAY C VS. D – SAUTER MEAN DIAMETER

x = 10 mm

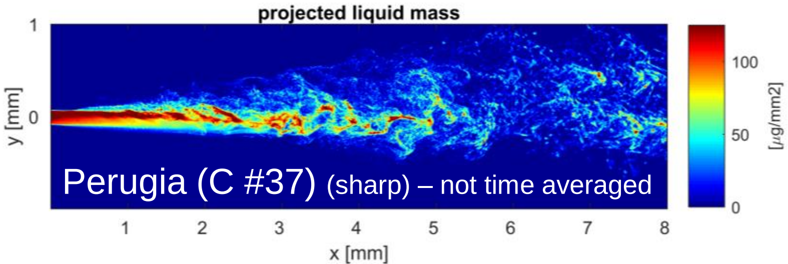
0 deg
(view 1)

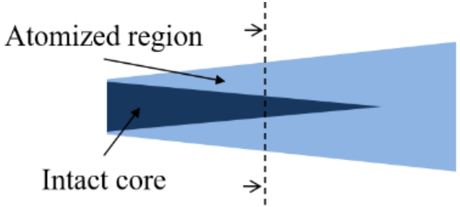


Spray centerline (y=0 mm)



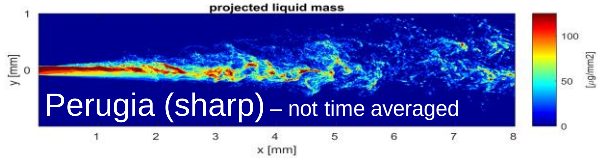
- C has finer structures in the periphery
- C is much more spread along y-dir

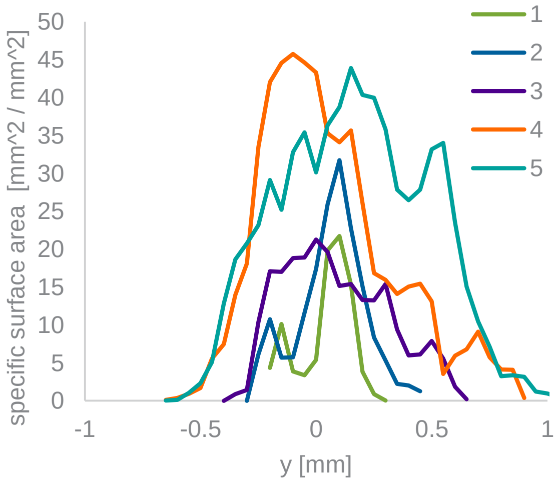


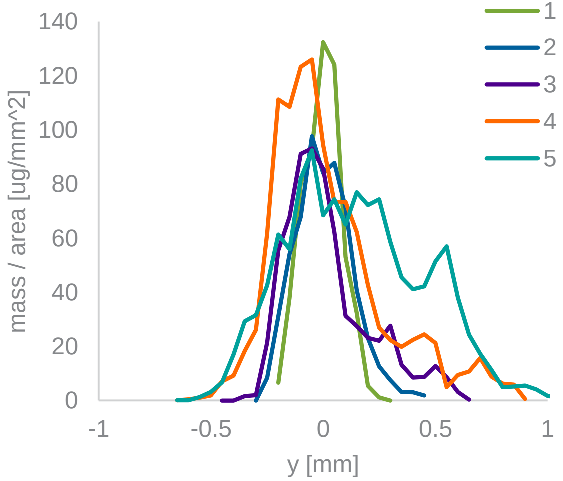


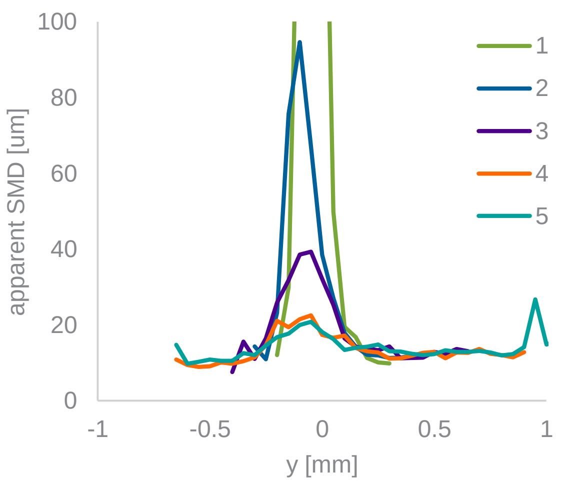
SPRAY C – PROJECTED AREA, MASS, AND SAUTER MEAN DIAMETER

0 deg view









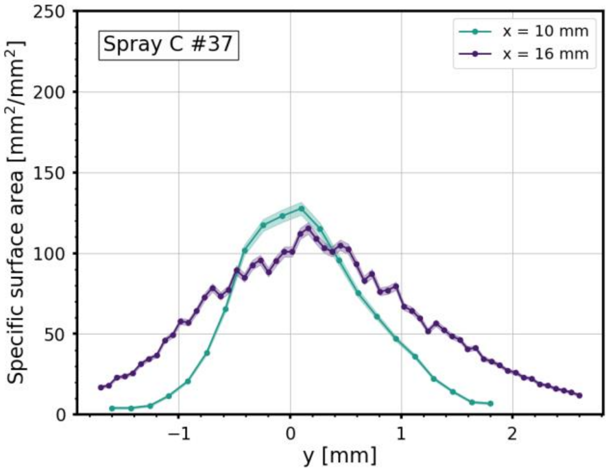
- Area is underestimated, so SMD overestimated, because of grid resolution limit
- The spreading of spray C is larger in y-dir, in accordance with x-ray experiments

ENGINE COMBUSTION NETWORK

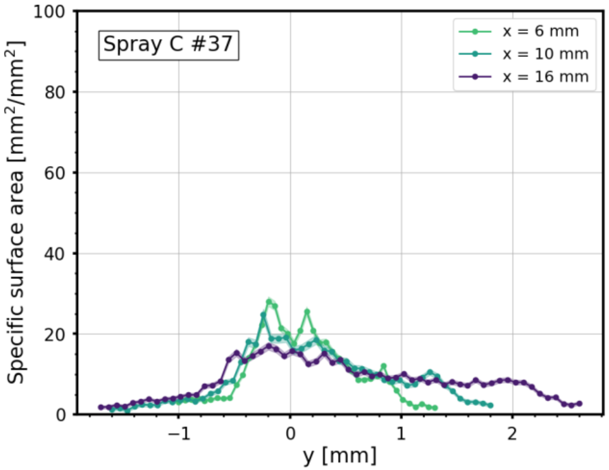
SPRAY C – INTERFACIAL AREA PARAMETRIC VARIATIONS

0 deg
(view 1)

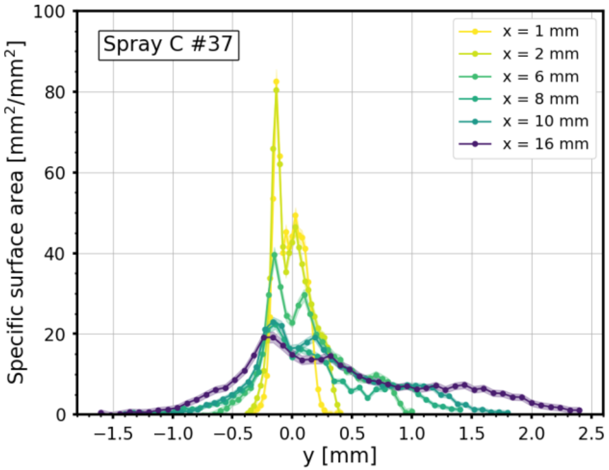
1500 - 20 bar



1500 -1 bar



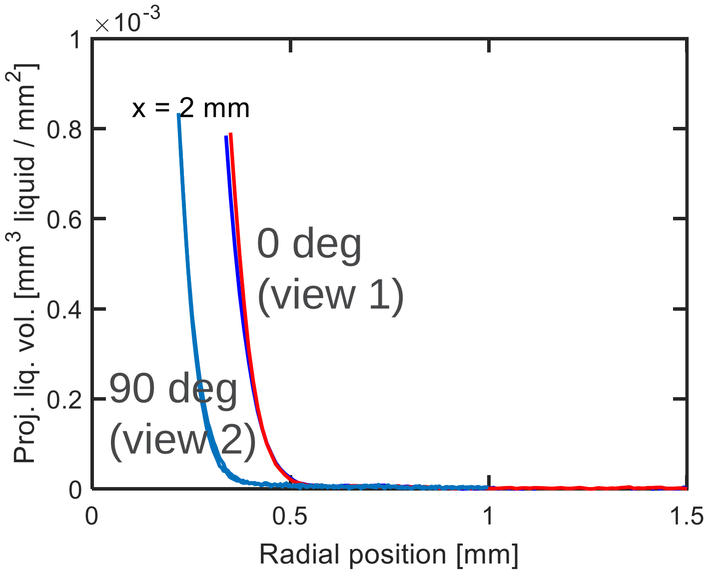
500 -1 bar



SPRAY C, 900 K AMBIENT, 440 K FUEL T

SANDIA

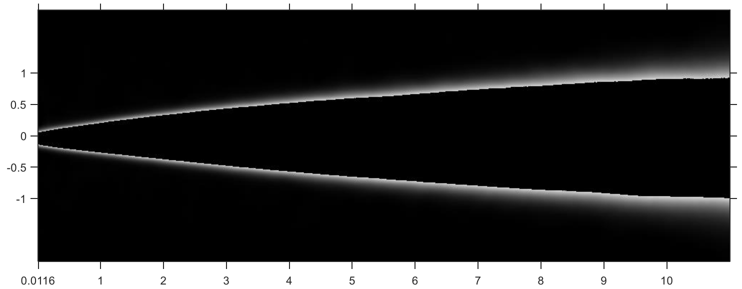
- View 2 much more narrow for Spray C
- Spray D the same
- Due to cavitation that causes a large disturbance that creates growth in the View 1 direction



SPRAY C, 900 K AMBIENT, 363 K FUEL T

SANDIA

Center plume and plot data at 2 and 8 mm

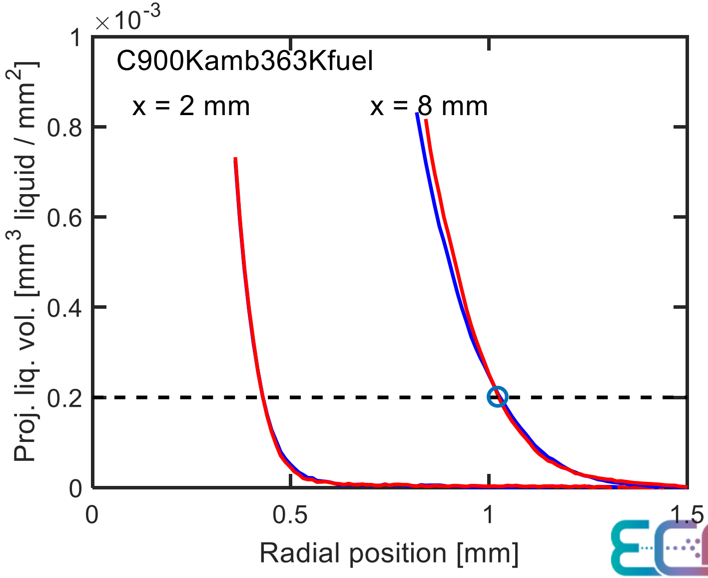


Recommendation for CFD comparison

Best estimate for a liquid length threshold, preserving past assumptions:

$\tau = 0.37$ estimated assuming about 2 μm droplet

$$\tau \frac{\pi\, d^3/6}{C_{ext}} = \int_{-y_\infty}^{y_\infty} LVF \cdot dy = \mathbf{0.2} \cdot 10^{-3}\ \frac{mm^3 liquid}{mm^2}$$



- Need to test Eulerian models with this criteria
- Assess the assumptions, like 2 μm? at different p,T

SOME FUTURE DIRECTIONS

- Need to validate liquid dispersion and atomization (like Σ-Y, or other models) on C/D, rather than on A. There is more knowledge now and more spatially varying dataset available on C/D.
- Need to check better the phase interaction (drag,…) in Eulerian formulation, with reference to turbulence models, and atomization (bi-directional effects should be included)
- Focus on the core and detached structures, being aware of the value interpretation.
- Test projected liquid volume (PLV) criterion to detect spray boundary (angle or penetration): compare models vs. optical measurements and mass-based measurements.
- Temperature of the fuel, temperature of the chamber
- Since most of the model development (or tuning) is based on mass-based measurements, it would be very important to quantify uncertainties (error bars) or define specific known test cases.