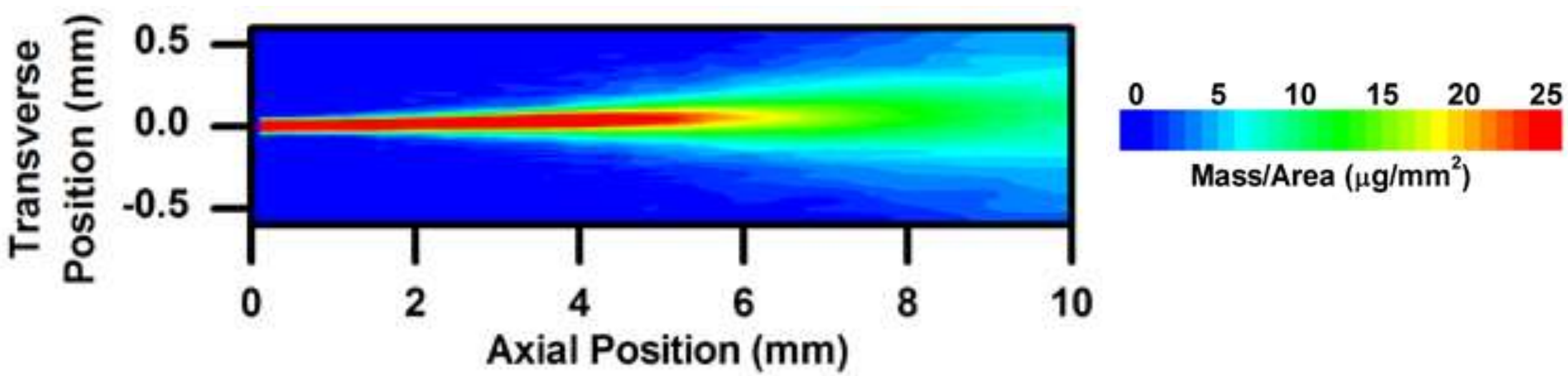
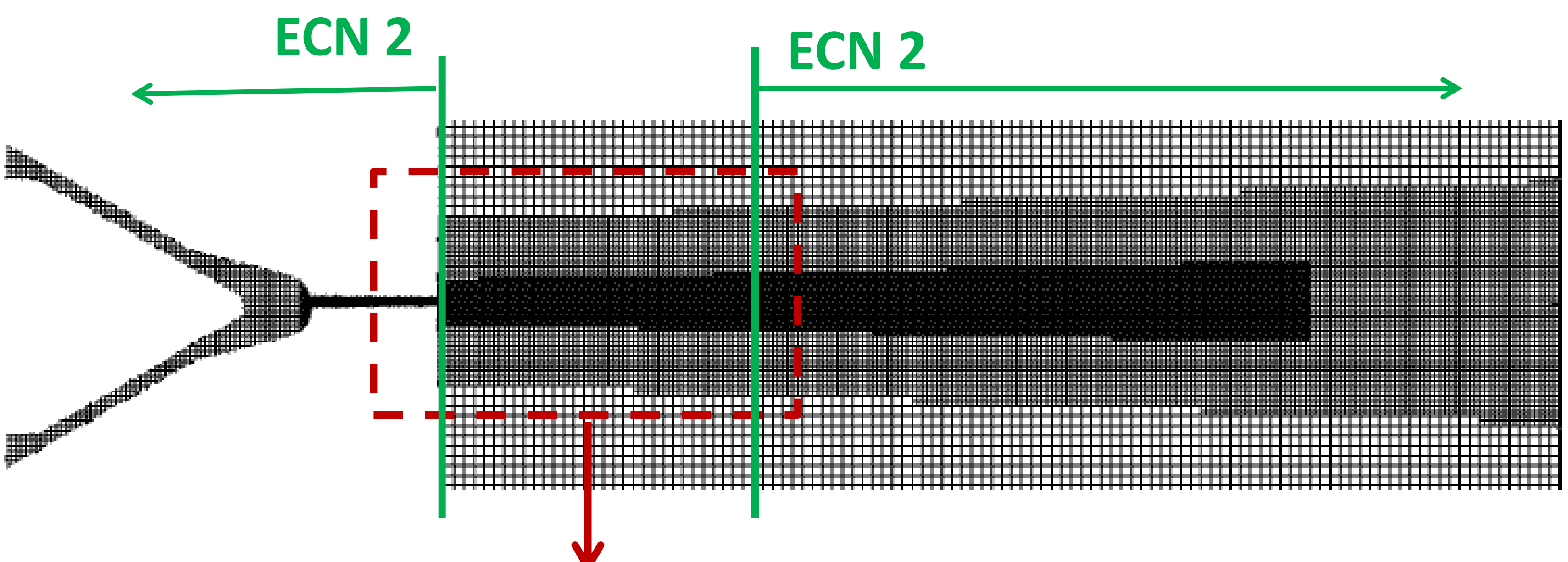
ECN 2 and ECN 3: Grand Challenge

Reproduce the near nozzle fuel spray structure from simulations



X-ray image by Chris Powell, ANL



Focus of ECN 3: Topic 1

Topic 1: Introduction

8:50	Introduction, Sibendu Som (Argonne)
8:55	Topic 1.1 In-nozzle experiments and simulations
	Chris Powell* (Argonne), David Schmidt (UMass)
9:45	Topic 1.2 Near field fuel structure and coupled nozzle flow and spray simulations
	Alan Kastengren* (Argonne), Qingluan Xue (Argonne) Julien Manin (Sandia), Chawki Habchi (IFPEN)
10:35	**Break**
11:05	Topic 1.2 Evaporation and Parametrics
	Tommaso Lucchini* (POLIMI), Alessandro Montanaro (CNR)
11:55	Synthesis of Topic 1 (Sibendu Som)
12:20	Panel Discussion (Raul Payri)
	Main Participants in Topic 1
12:50	**Lunch (50 minutes)**

Synthesis of Topic 1

Diesel Spray: Internal Flow, Near-nozzle Break-up, Mixing and Evaporation

Sibendu Som
Argonne National Laboratory

April 4th, 2014

The Contributors

Experiments

- ANL
- CMT
- IFPEN
- KAIST
- MTU/CNR
- SANDIA
- TU/E

Simulations

- ANL
- CHALMERS
- CMT
- IFPEN
- POLIMI
- SANDIA
- UMass

With different modeling approaches such as EE, LE, dense fluids together with x-ray and optical techniques, understanding of the near nozzle flow region was significantly enhanced!

Of course, this motivates further research – towards ECN 4

Modeling Objectives

- Define level of confidence of internal flow simulations by validating, where possible, with experimental data
- Quantify internal flow dynamics that are likely to affect spray characteristics of primary atomization
- **Facilitate dynamic coupling of in-nozzle flow and external spray approaches. Encourage high-fidelity simulations of jet atomization**
- Study the capability of the different modeling approaches (Lagrangian-Eulerian, Eulerian-Eulerian) and CFD frameworks (RANS, LES, DNS) for the simulation of the primary atomization and the cavitation
- Understand the influence of: compressibility, turbulence model, spatial resolution, geometric asymmetries on simulation results
- **Motivate the development of a consistent modeling approach for near-field and far-field spray and combustion modeling**

Experimental Objectives

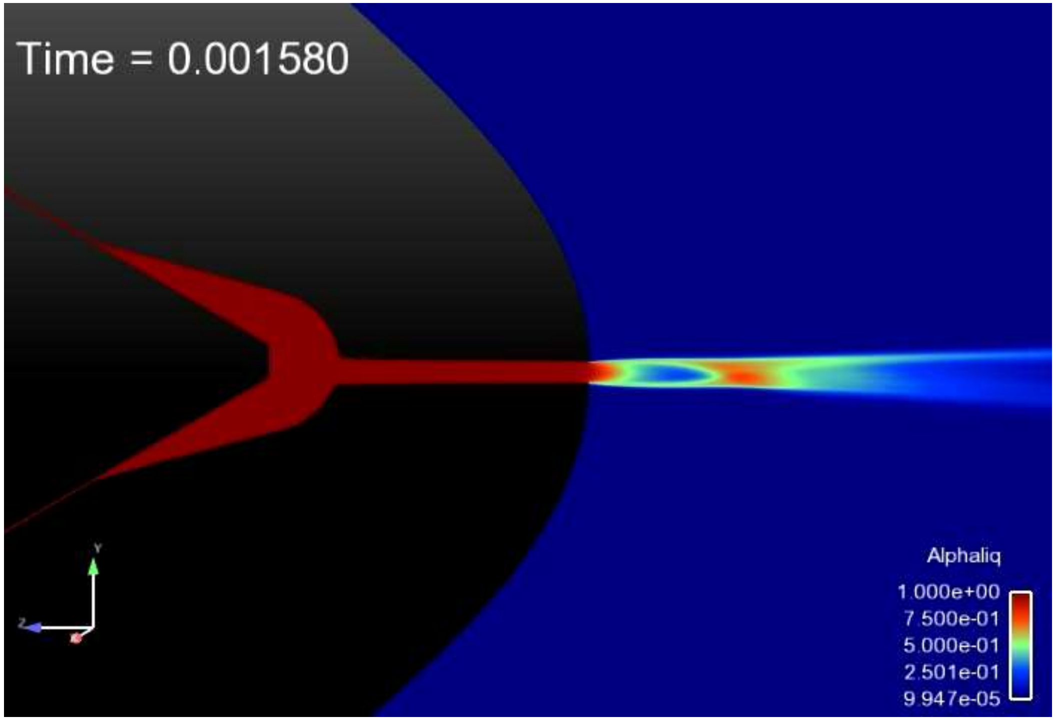
- Focus on the near nozzle region within first 10 mm
- **Obtain quantitative (fuel concentration, droplet size, etc.) and qualitative (macroscopic parameters, optical/x-ray relationship, etc.) information about the breakup process of sprays**
- Provide high-fidelity measurements of liquid penetration, liquid mass distribution, and droplet size in the nozzle near field and far field
- **Spray A single hole injector performance vs. Spray B multi-hole injector performance**
- Understanding how results are repeatable in different institutions (Spray A and Spray B).
- Understanding influence of different nozzle serial numbers on spray evolution (Spray A and Spray B).

Spray A

Spray A: Evidence for Gas in Sac at SOI

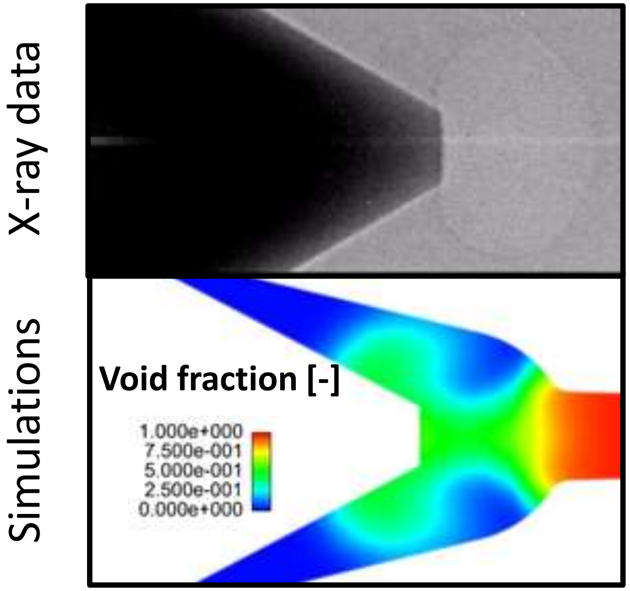
- At EOI, gas is pulled from the orifice into the sac
- Simulations from IFPEN and Argonne can capture this trend quite well
- Submerged nozzle flow simulations may not be accurate

At the end-of-injection, gas is being ingested into the sac and orifice for Spray A



Courtesy: C. Habchi, IFPEN

Clear Evidence of Gas in the Sac at the end of injection

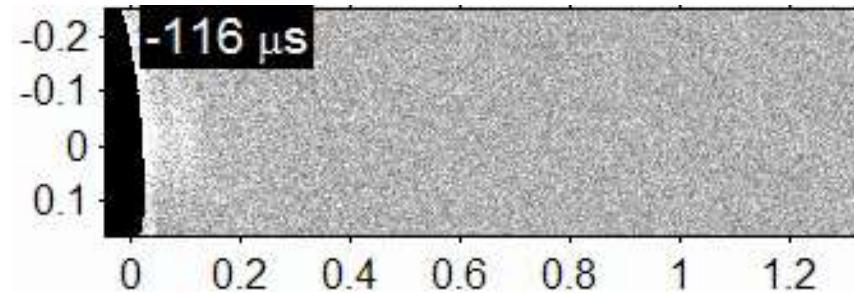


Courtesy: C. Powell, M. Battistoni
Note: This is not a ECN Injector

- Likely to have an effect on SOI transient
- Important to simulate this, particularly for Spray B Multi-Hole

Coupled Spray A Simulations with Gas In the Sac

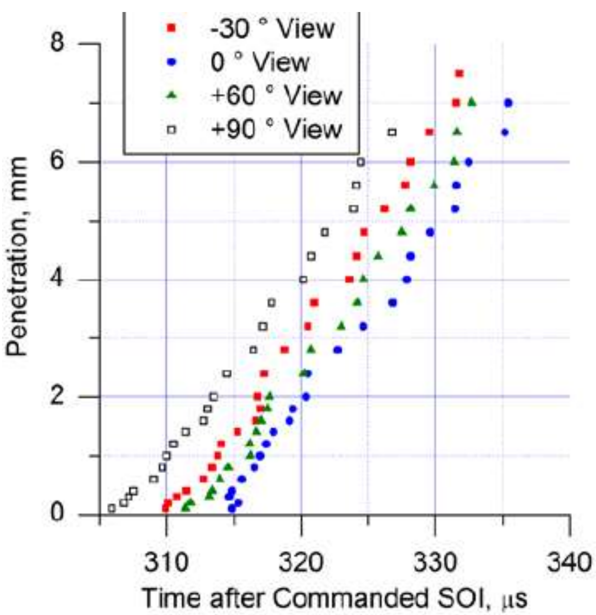
- Ingested gas at the end-of-injection is first injected
- Simulations by Sandia and Argonne
  - show low pressure in sac at needle closure
  - Can predict the time when spray first comes out of the nozzle



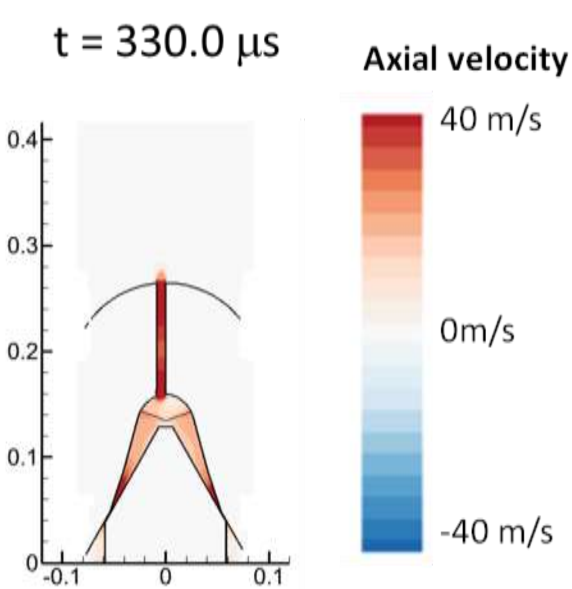
X-ray data: 310 μs
Argonne: 305 μs
Sandia: 330 μs

Courtesy of Lyle Pickett

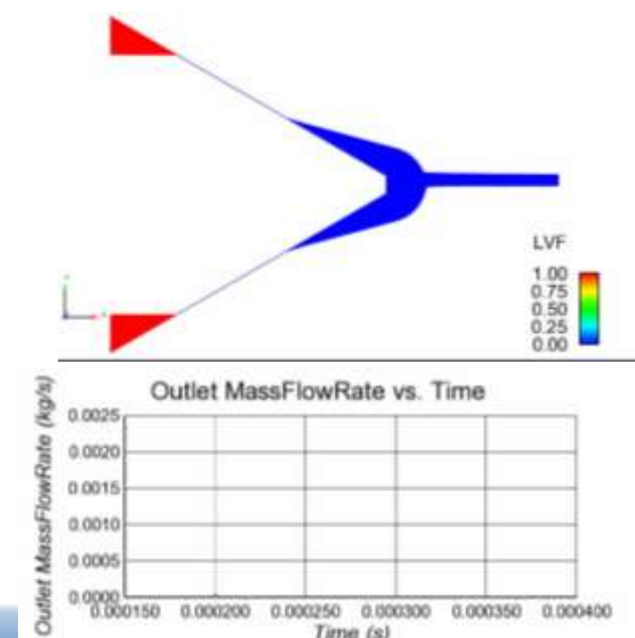
Argonne: X-ray data



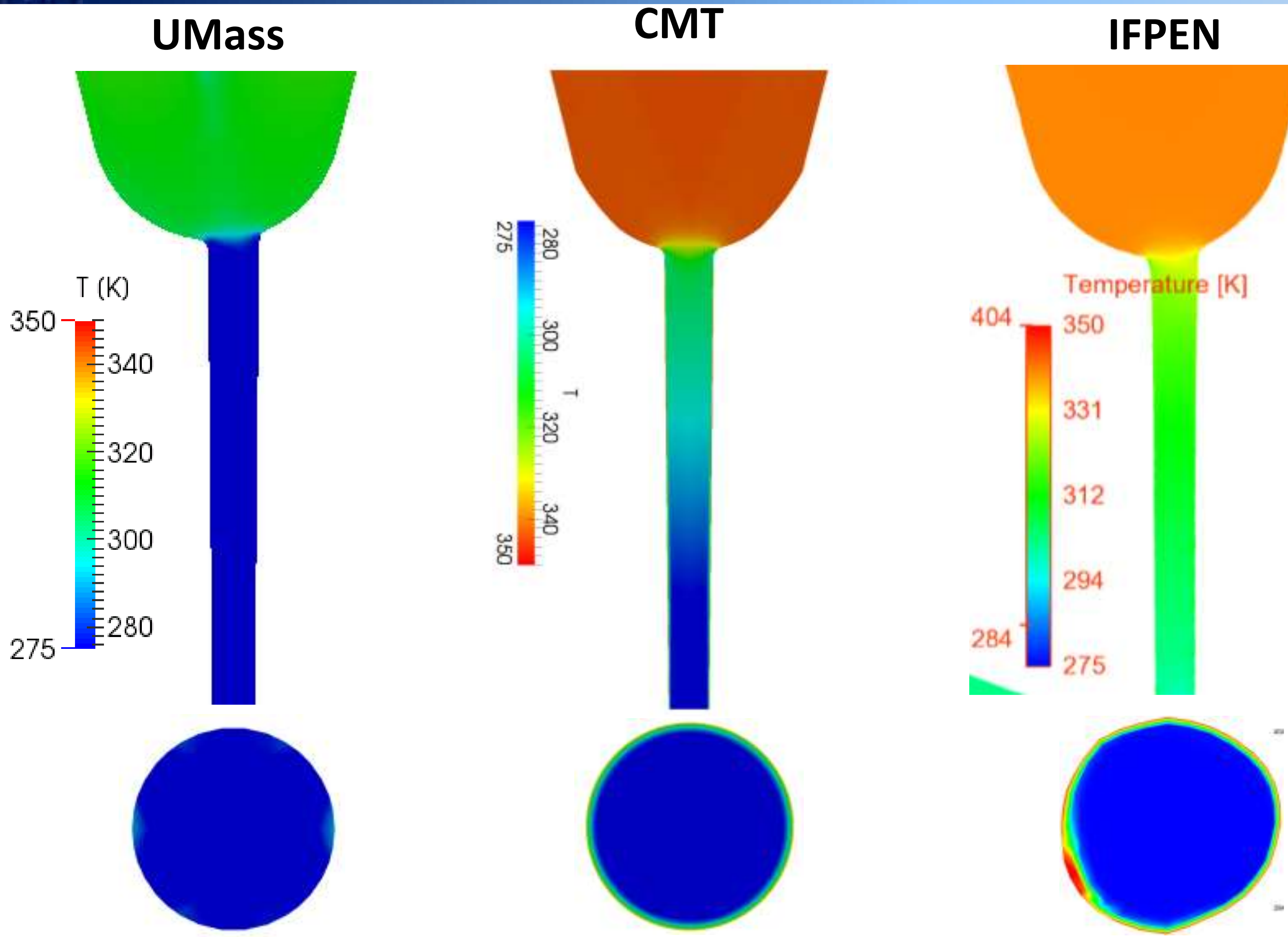
Sandia: Arienti



Argonne: Battistoni



Significant Temperature Gradients In-Nozzle

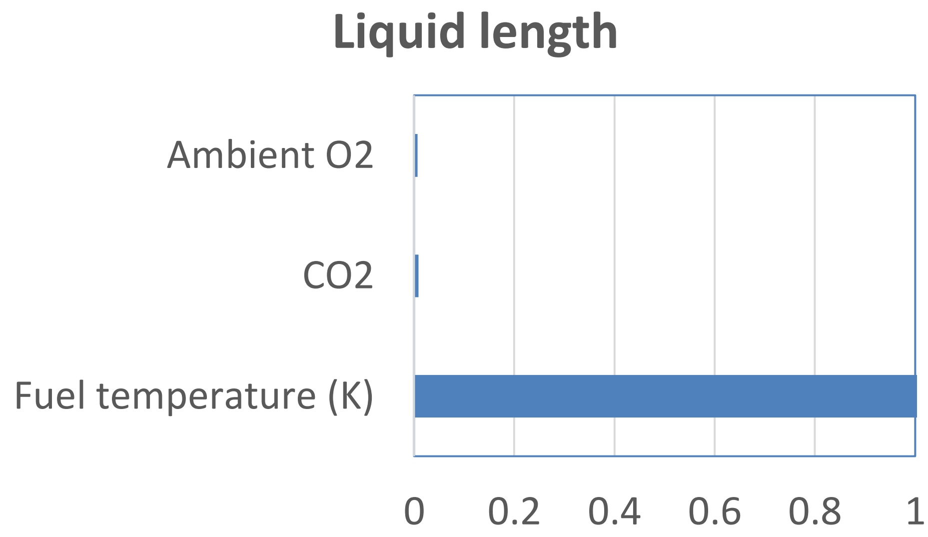


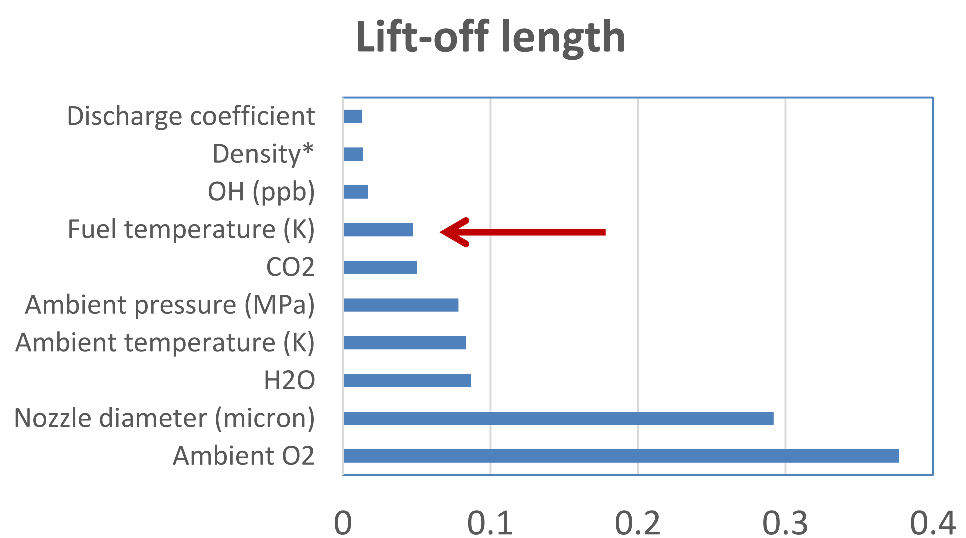
Density at the nozzle exit should be higher than what is being used for calculations of parameters at the nozzle exit!

Uncertainty Quantification*

	Parameters	Min	Max
Boundaries	Vessel wall temperature (K)	400	800
	Initial gas velocity fluctuation (m/s)	0.01	1
	Ambient temperature (K)	887.5	915.1
	Ambient pressure (MPa)	5.91	6.09
	Ambient O2	14.9	15.1
	OH (ppb)	0	16
	CO2	0	6.4
	H2O	0	11.6
	Duration of injection (ms)	1.49	1.65
	Fuel temperature (K)	343	403
	Discharge coefficient	0.88	0.92
	Nozzle diameter (micron)	83.7	90.8
Fuel properties	Critical temp (K)	645	659
	Density*	0.98	1.02
	Heat of vopoization*	0.98	1.02
	Vapor pressure*	0.98	1.02
	Viscosity*	0.98	1.02

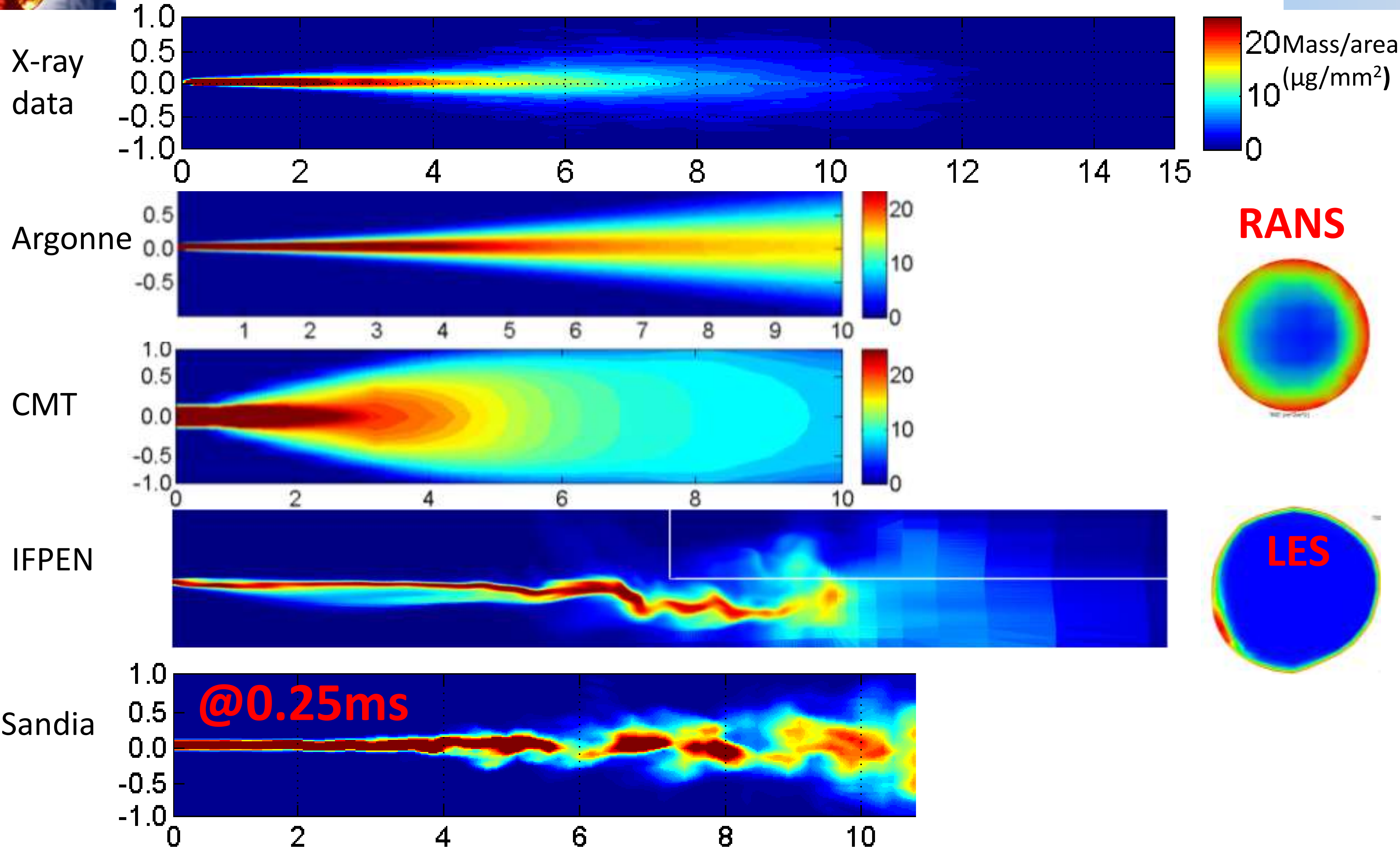
Ambient Temperature = 900 K





*** Dr. Y. Pei's presentation on April 5th**

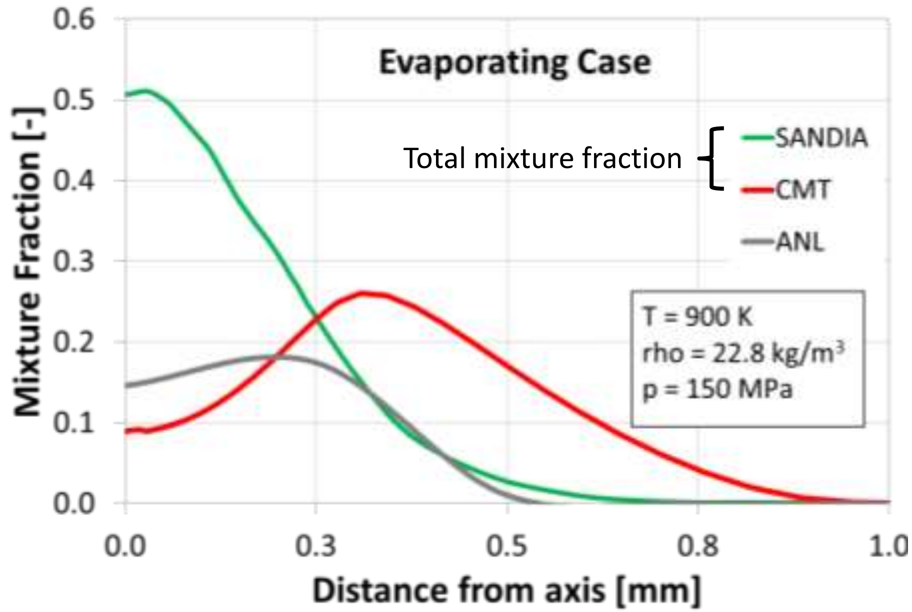
Spray A: projected mass density – 0.1ms ASOI

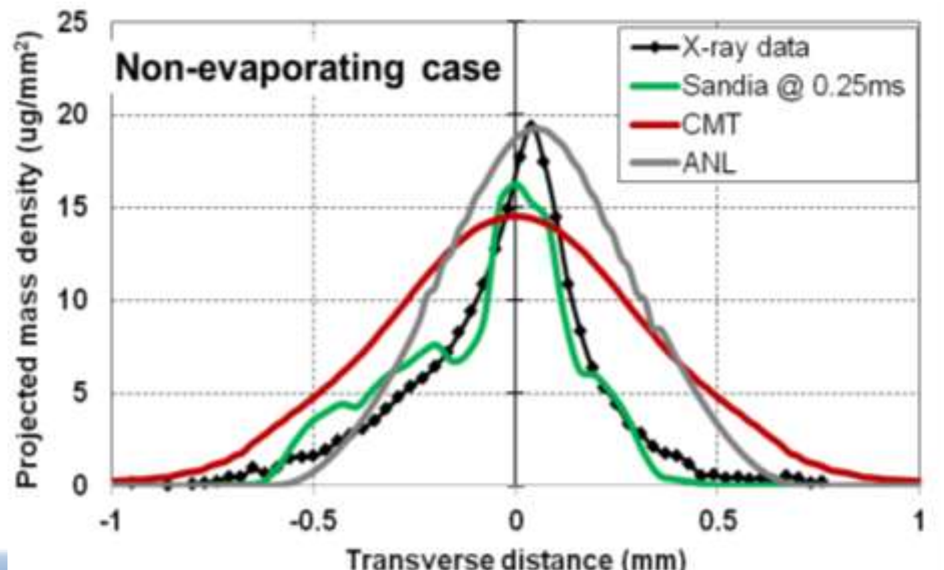


- **Significant qualitative and quantitative differences in the near nozzle region. Room for significant improvements!**
- **High-fidelity simulations can guide the choice of turbulence model constants and Schmidt number etc.**

Spray A Baseline condition: Radial Distributions

@ steady state, 6 mm

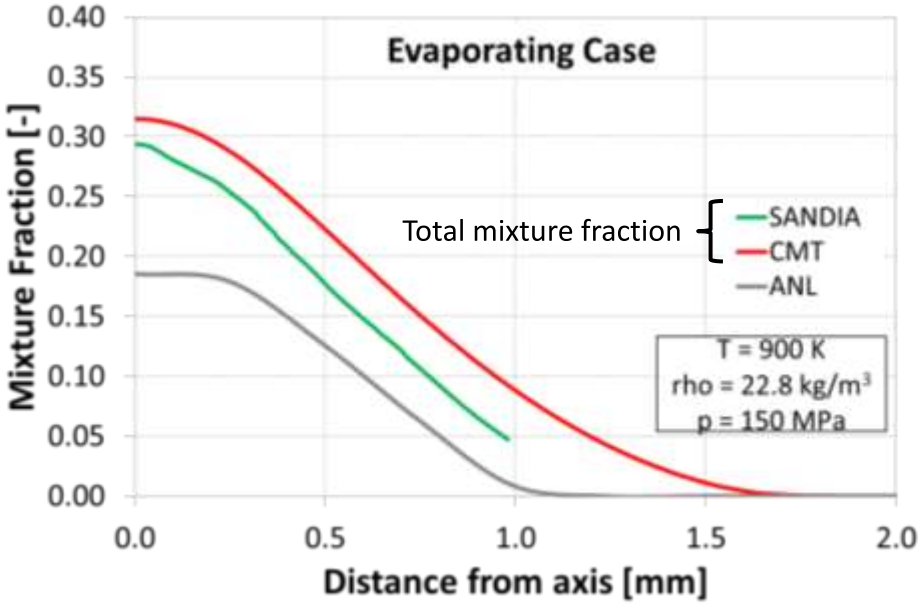




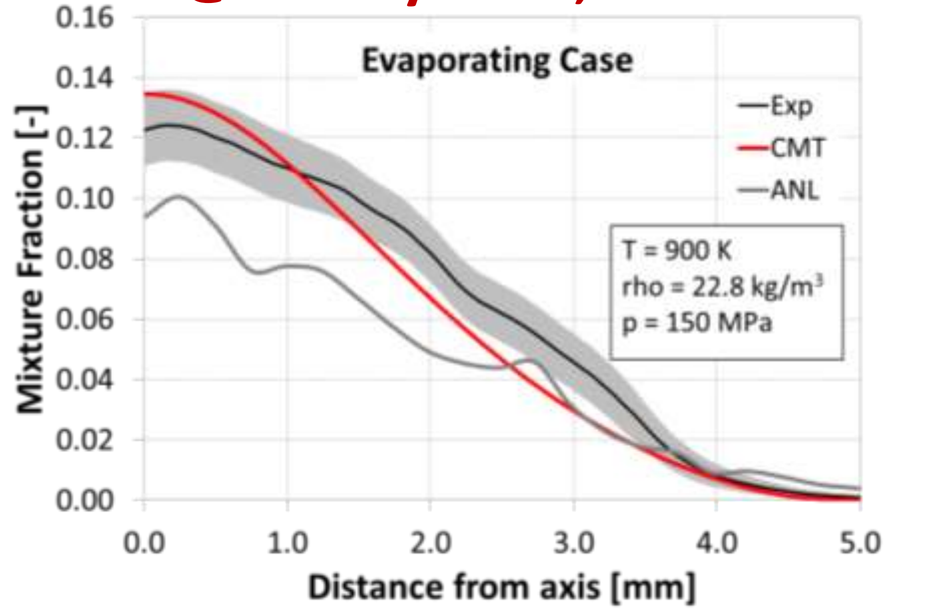
- ANL simulations for evaporating conditions are using LES (averaged over 20 realizations) and Lagrangian model
- CMT and Sandia simulations are using the single fluid model and a single realization
- Sandia performed a single simulation under evaporating conditions and some of this data was extracted in the near nozzle region for comparing against the non-reacting data
- No clear trends between evaporating and non-evaporating simulations
- Non-evaporating cases: at least simulations show consistent Gaussian like profiles similar to experiments

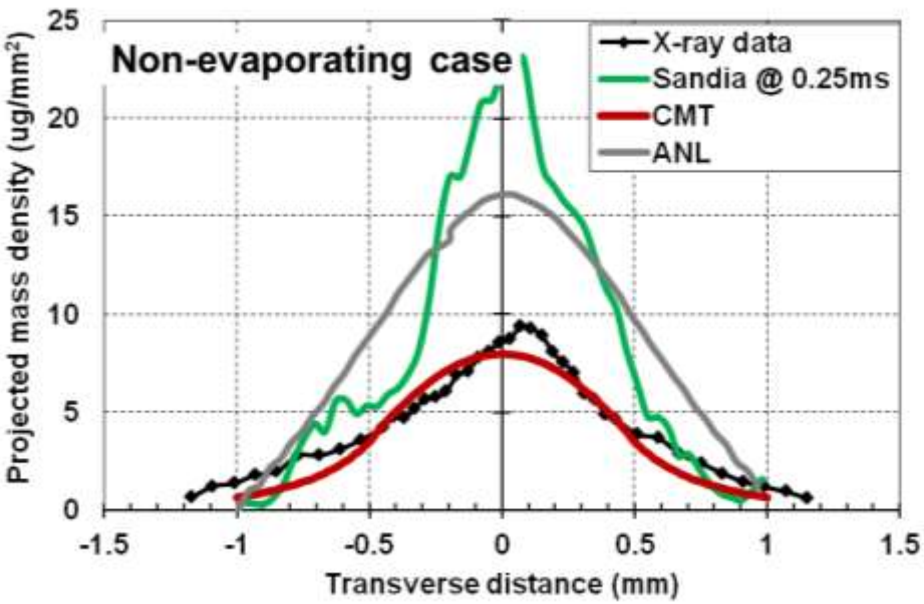
Spray A Baseline condition: Radial Distributions

@ steady state, 10 mm



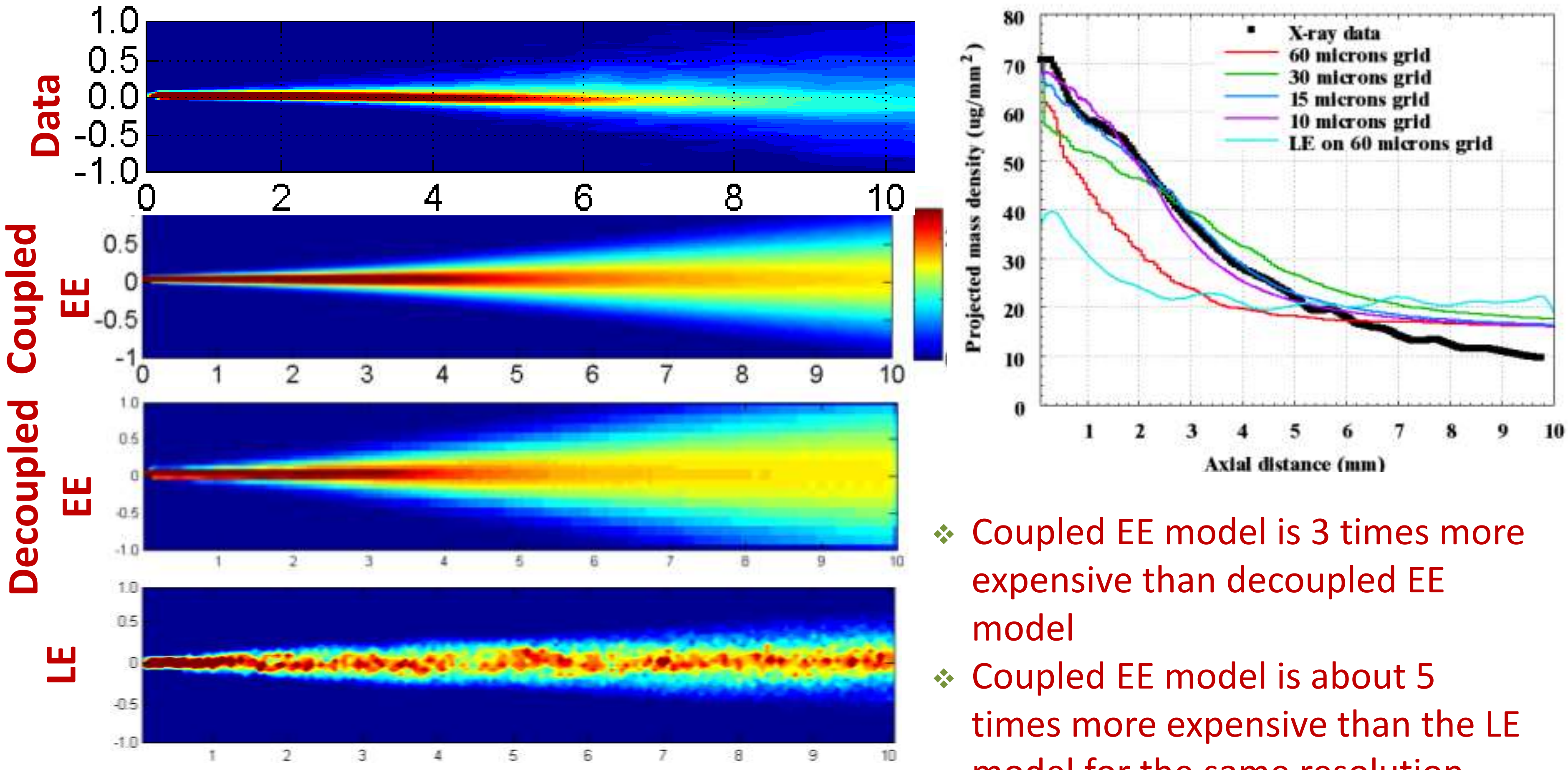
@ steady state, 25 mm





- Sandia simulations are not yet at steady state
- ANL simulations for evaporating conditions are using LES and Lagrangian model
- Based on evidence, CMT predictions are probably most accurate at 10 mm
- Non-evaporating case: ANL, Sandia ,over-predict projected density
- Evaporating conditions: ANL, Sandia predict lower mixture fractions compared to CMT

Spray A: EE vs. LE at Argonne

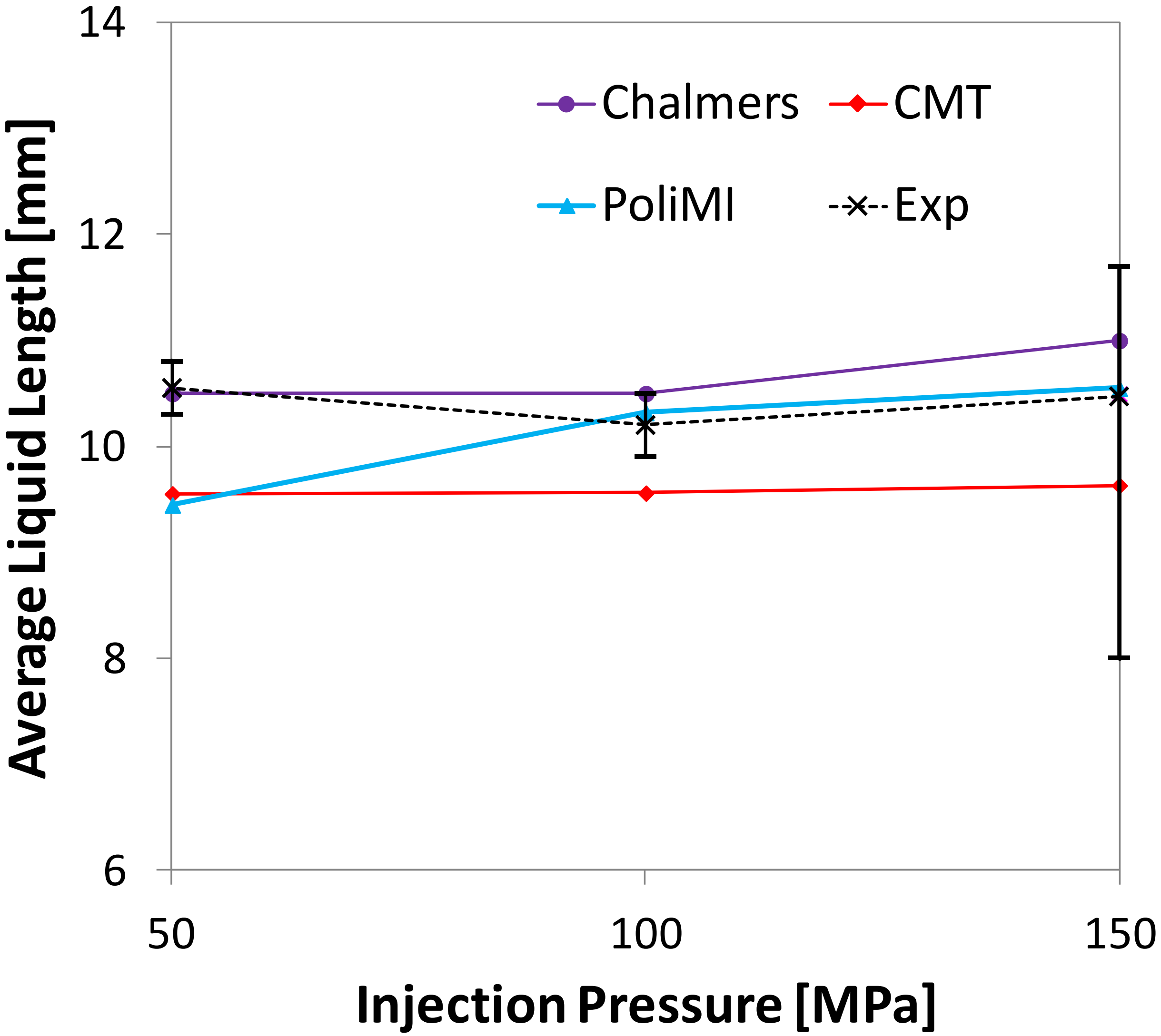


- Coupled EE model is 3 times more expensive than decoupled EE model
- Coupled EE model is about 5 times more expensive than the LE model for the same resolution

- Eulerian model is better than traditional Lagrangian approach in the near nozzle region
- Lagrangian simulations: 62.5µm minimum resolution, blob injection model, 300,000 parcels
- Decoupled EE simulations perform as well as coupled EE model for this case. This shows that if the ROI is good, perhaps decoupled EE model is sufficient.

Spray A: Injection pressure effect

Parametric variations : Liquid length

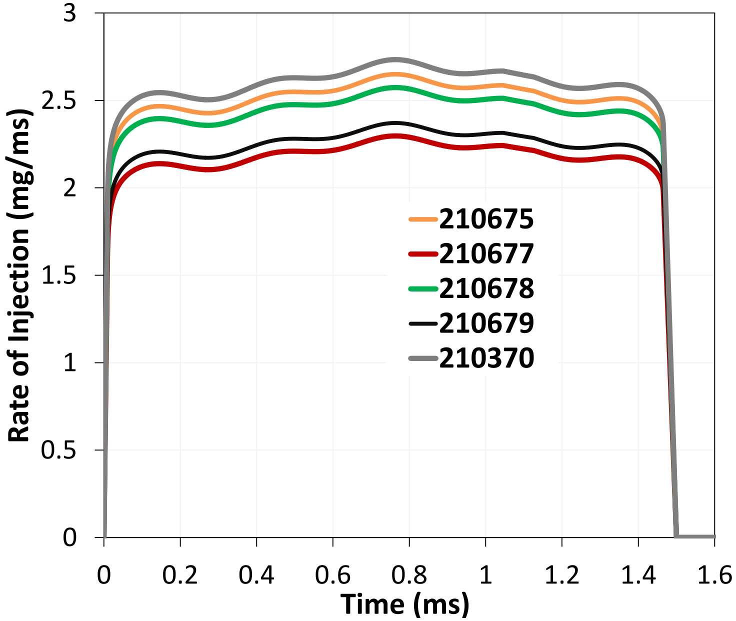


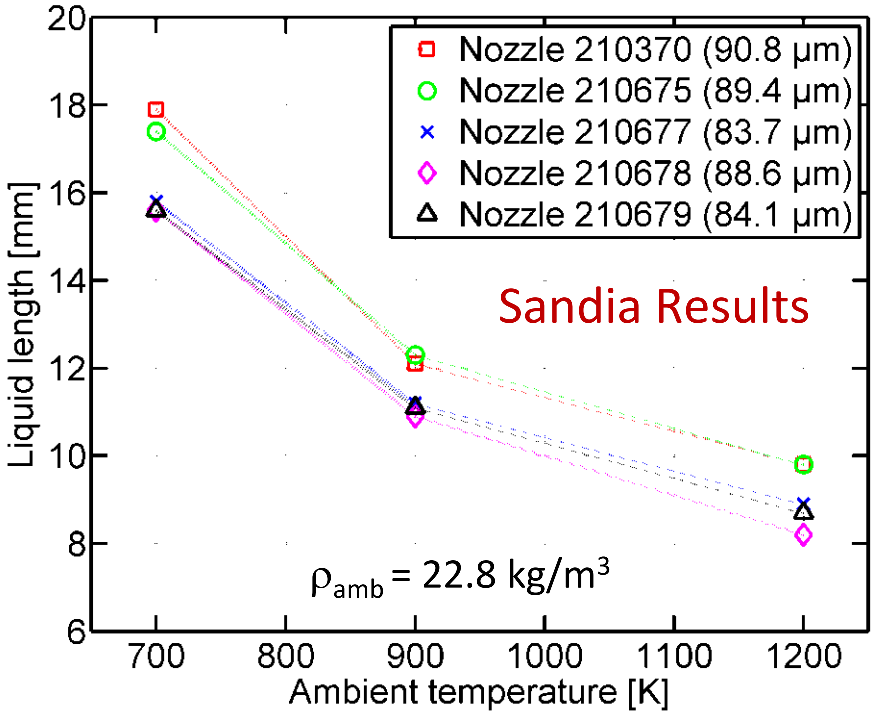
#	T [K]	ρ [kg/m³]	p_{inj} [Mpa]
1	900	22.8	150
2	900	22.8	100
3	900	22.8	50

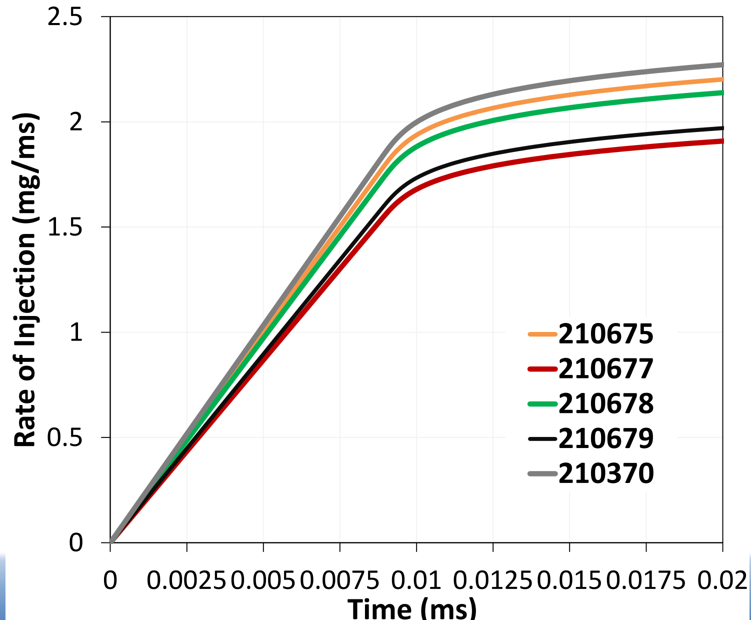
- From Topic 1.1, in-nozzle flow simulations were requested to serve as boundary conditions for topic 1.3
- Appropriate ROI was used as boundary conditions for the simulations in 1.3
- We know that Spray A does not cavitate. Is this due to the **influence of difference turbulence levels at the nozzle exit at different injection pressures**?

Differences between Spray A injectors

CMT Virtual Rate Generator

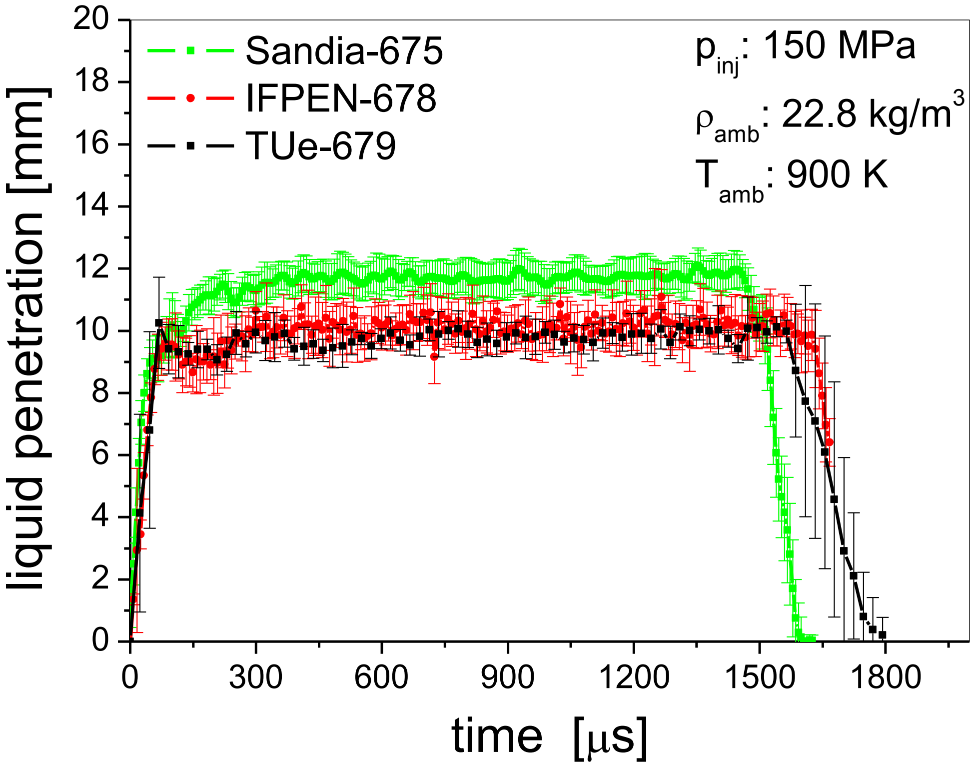


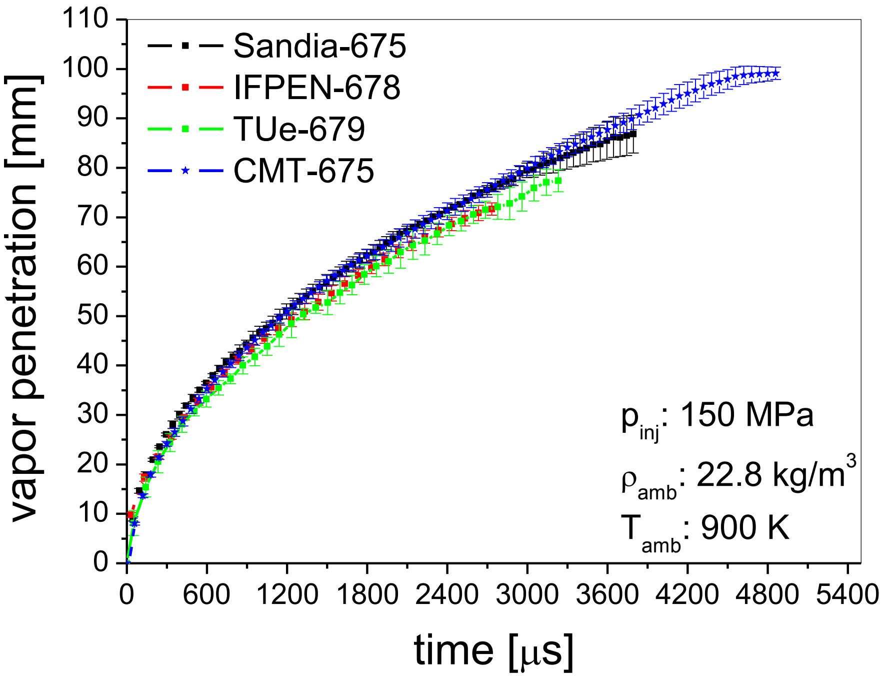




- Mass flow rate scales with the diameter of the nozzle. Significant differences!
- Initial transients also quite different.
  - ECN 4: Can simulations accurately predict the initial transients for different geometries?
- Nozzle 210675 shows longer liquid-phase penetration than the others (≈1 mm) due to the largest hole diameter

Institutions comparison: penetration –Spray A





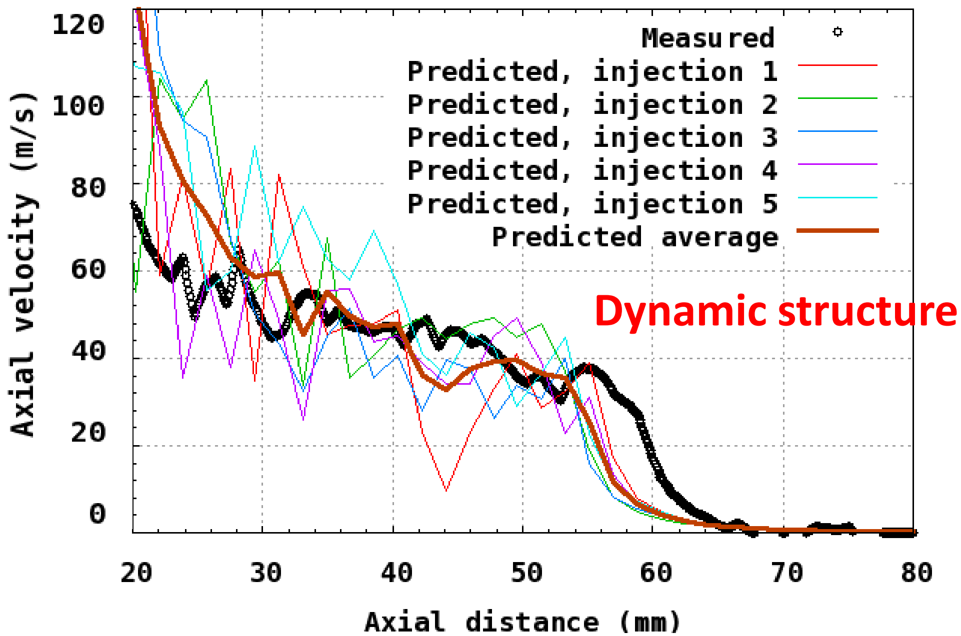
Steady-state liquid length			
Sandia	CMT	IFPEN	TUe
11.7	9.74	10.54	10.33

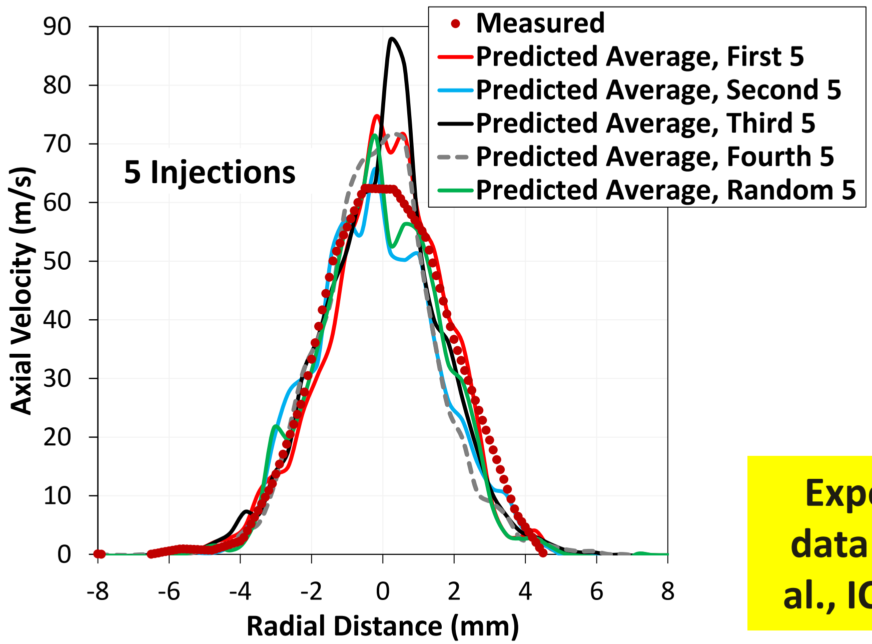
- The SNL one is higher than the others (≈10%)
- Good agreement beetwen IFPEN, TUe and CMT in terms of steady-state liquid value

- Although liquid penetrations were difference, Sandia and CMT measured almost identical penetration with the same injector
- Slight differences with other institutions, in agreement with the different ROI

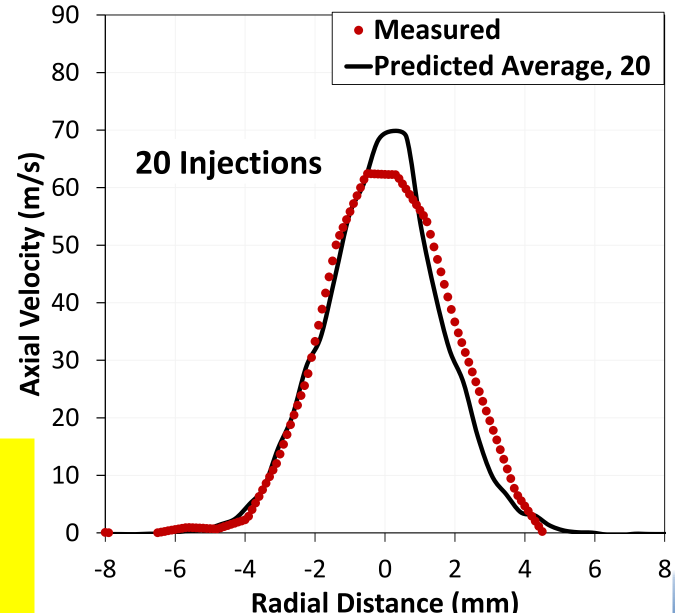
Need for Ensemble Averaged LES Calculations

- Any single realization of LES does not represent ensemble averaged experimental data
- Averaging over 20 realizations can capture the experimental trends
- Results from Xue et al. (AAS 2013) and Senecal et al. (JEGTP 2014)
- Similar results were also reported by Habchi et al. (ICLASS 2012), and Wehrfritz et al. (AAS 2013)





Experimental data: Meijer et al., ICLASS 2012

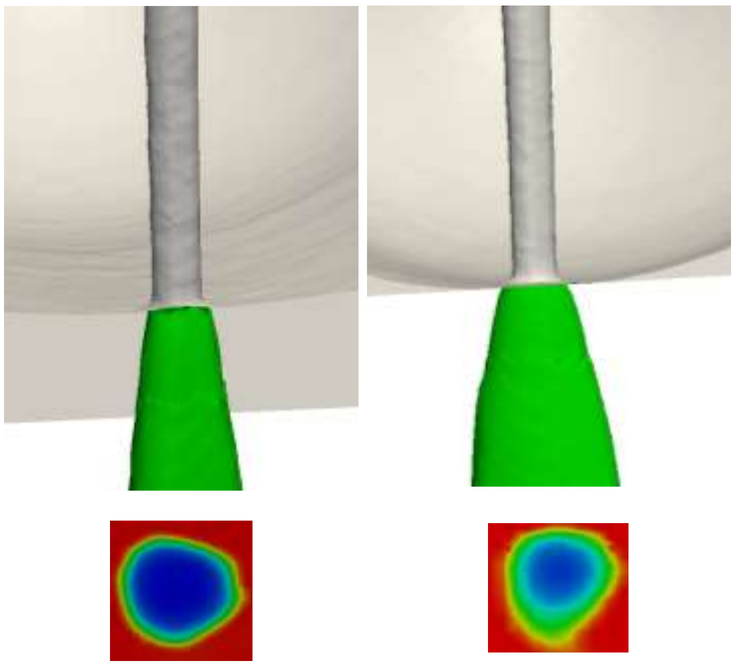


Spray B

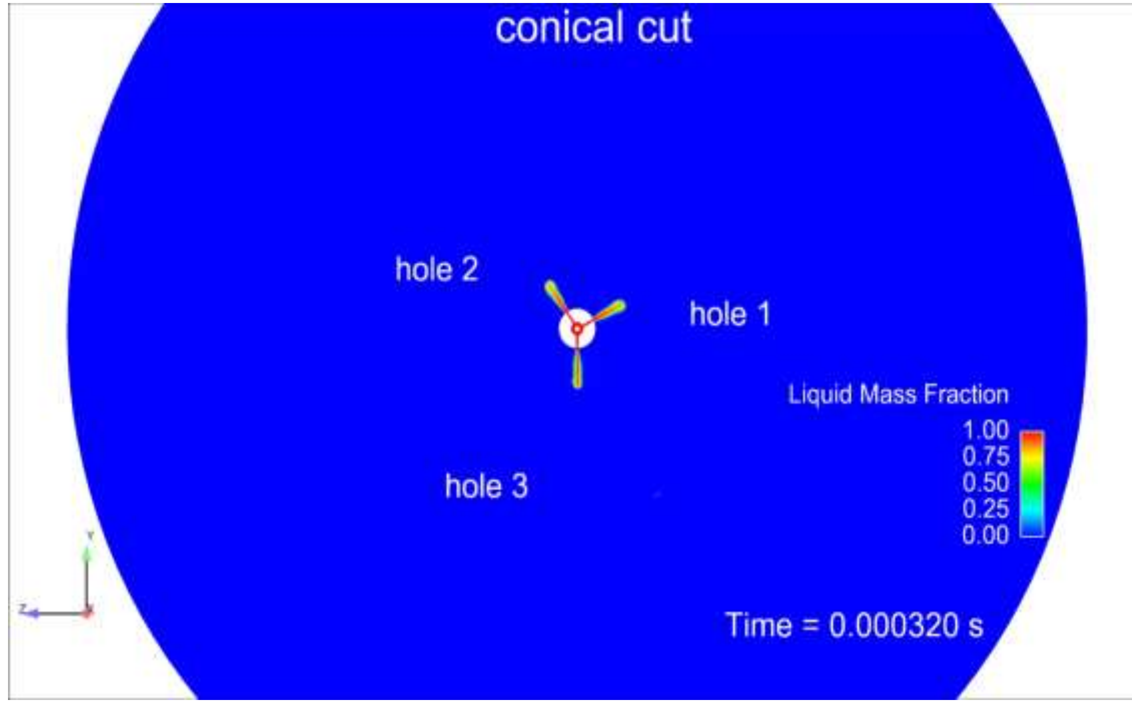
Spray B: Plume-to-Plume Variations

UMass

Hole 2 **Hole 3**

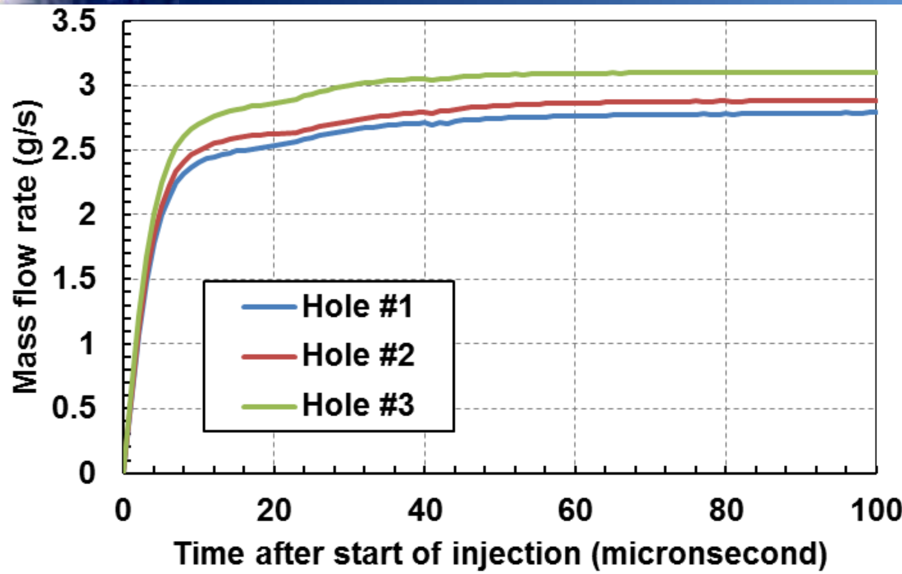


Argonne

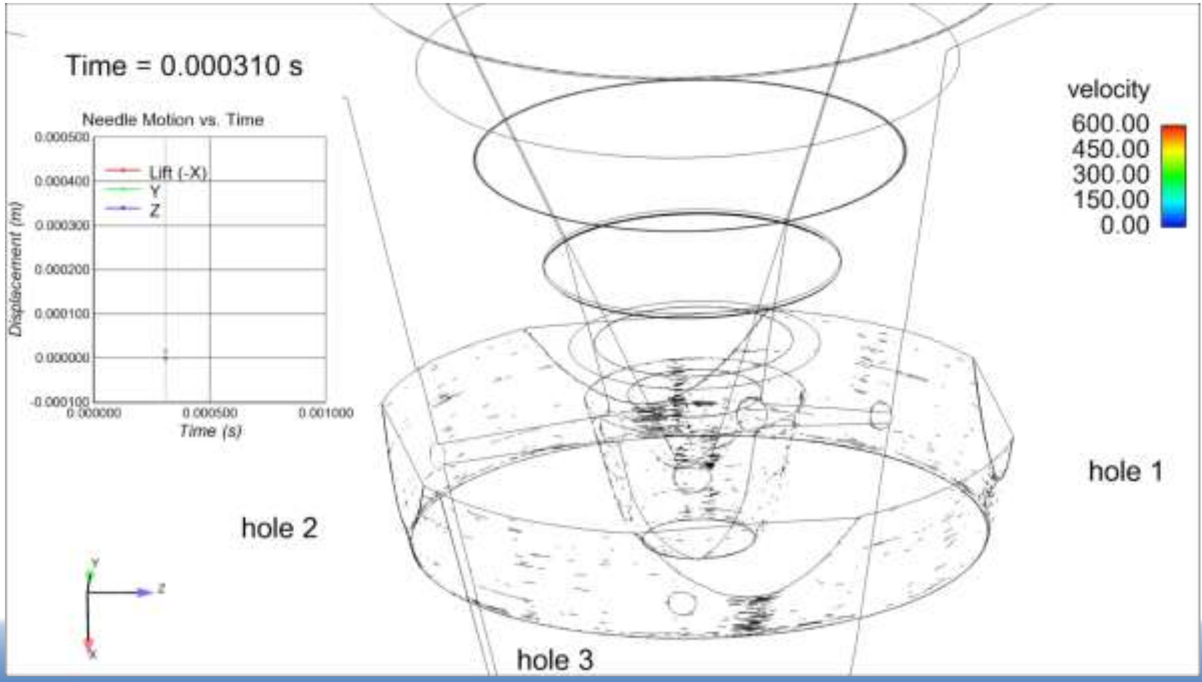


- Difficult to make any quantitative comparisons since grid-sizes, needle transients simulated were quite different
- For both UMass and Argonne, plume # 3 is aligned with the Cartesian mesh
- Plume-to-plume differences may be due to:
  - Gridding strategies
  - Needle wobble (Spray B has significantly higher wobble than Spray A)
  - Geometrical differences between different holes

Spray B: Plume-to-Plume Variations - Argonne



- Mass flow rate seems to scale with the diameter of the nozzle. This is consistent with CMT's virtual rate generator predictions
- Discharge coefficient of each hole is quite similar since it is obtained by normalizing with the nozzle exit diameter
- The influence of wobble on flow development not yet quantified
- **Sac volume is probably too large for just 3 holes**
- **Future work: Comparing simulations with and without wobble**

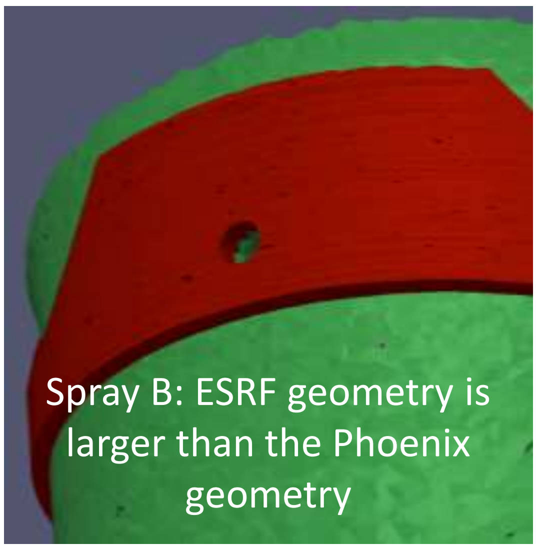


Courtesy:
M. Battistoni

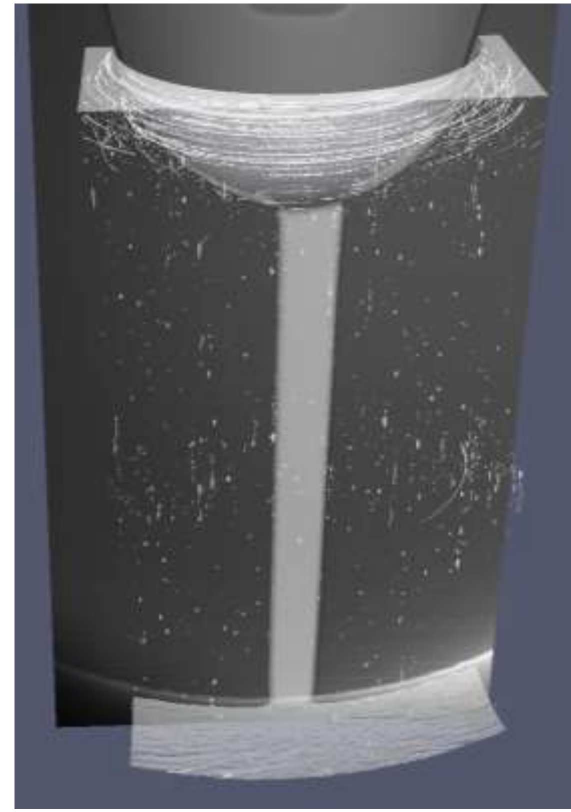
Spray A vs. Spray B

Geometry Analysis Synopsis

- Spray A: we do not have a good geometry yet for 675 which was the recommended injector for Topics 1 (Phoenix and CNRS geometries currently used in simulations)
- Spray B: CONVERGE geometry is accurate and sufficient enough for CFD meshing

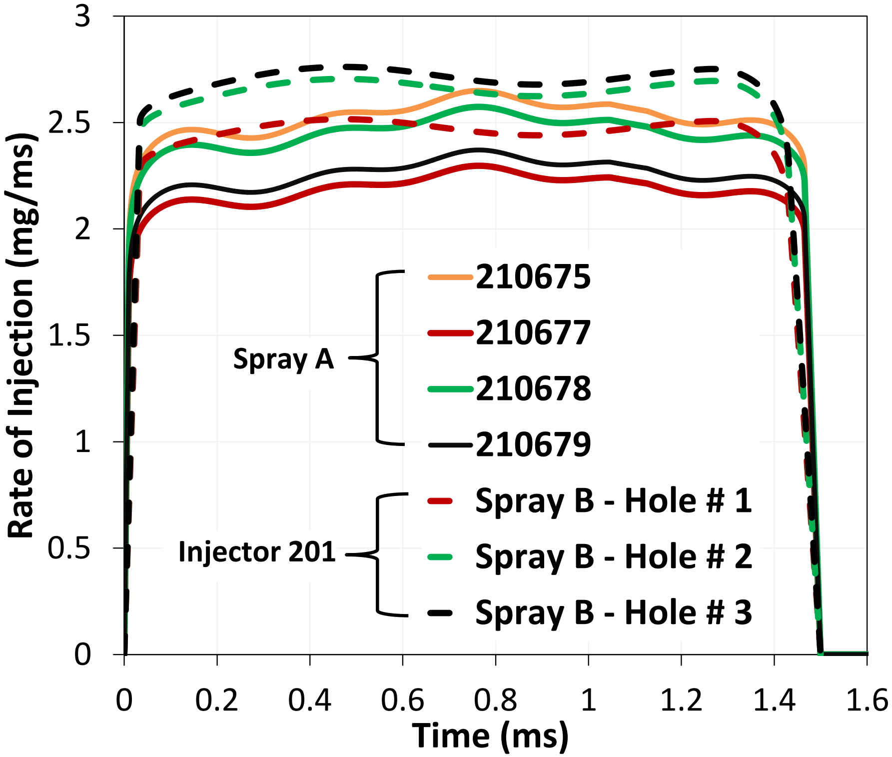


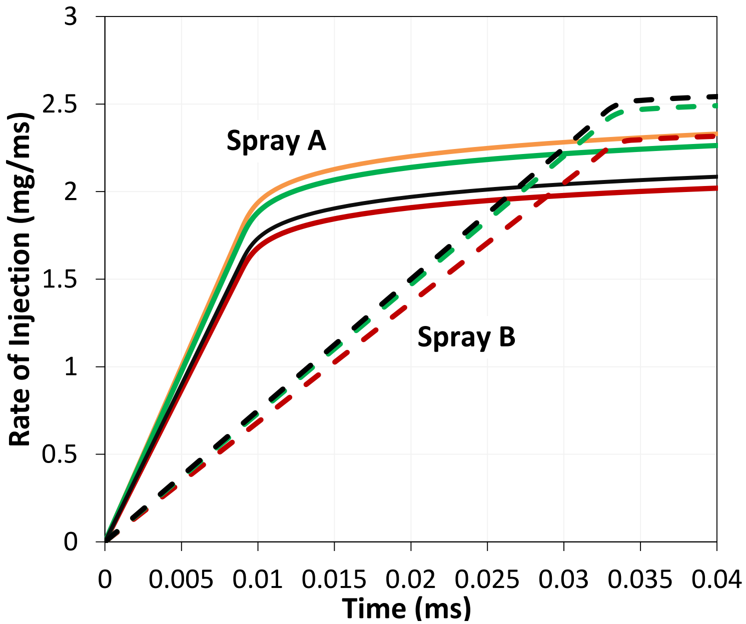
Spray A: ESRF mesh aligns very well with phase contrast data



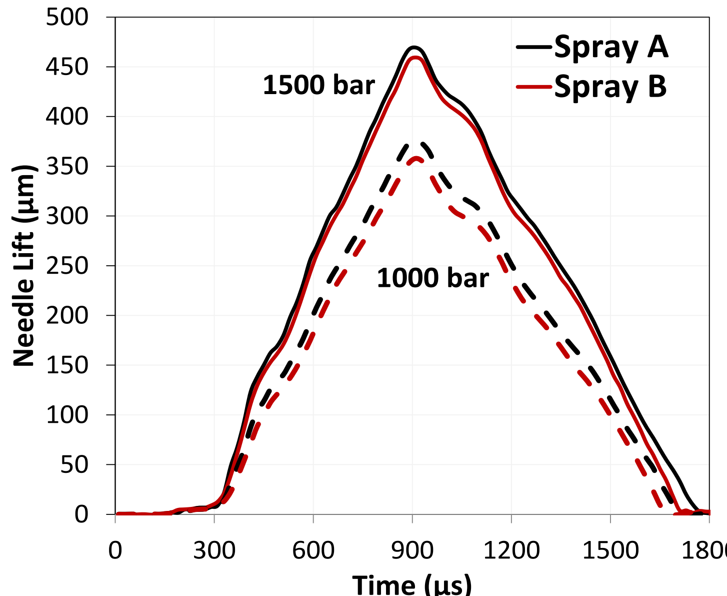
Name	Supplier	Size (MB)	Num. Points	Resolution
Phoenix	Caterpillar	31	260 k	16 μm
ESRF	Infineum, ESRF	4128	34 million	1.5 μm
Converge	Convergent Science (ESRF)	23	290 k	≥ 10 μm

Comparison of Spray A and Spray B: ROI





Spray A: 675; Spray B: 201

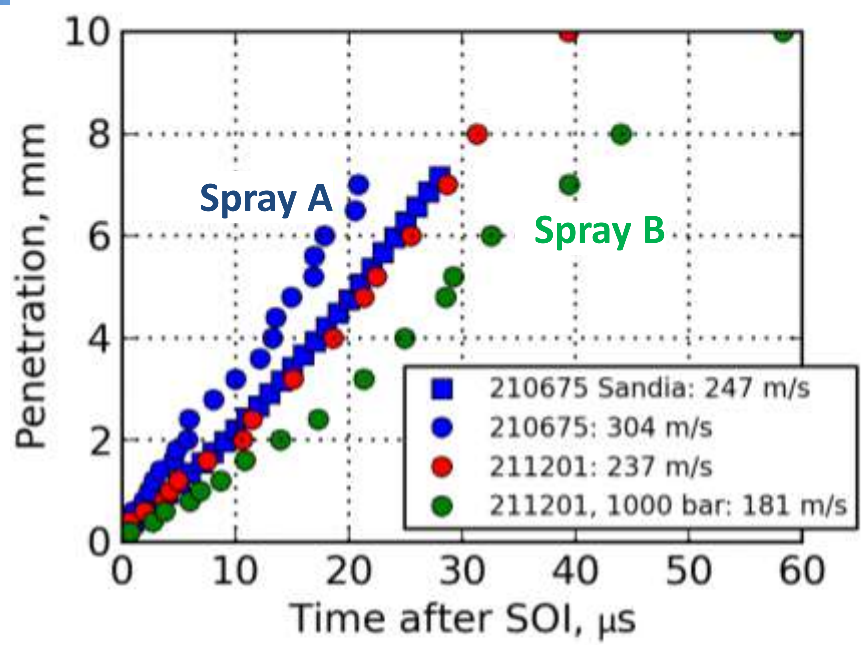


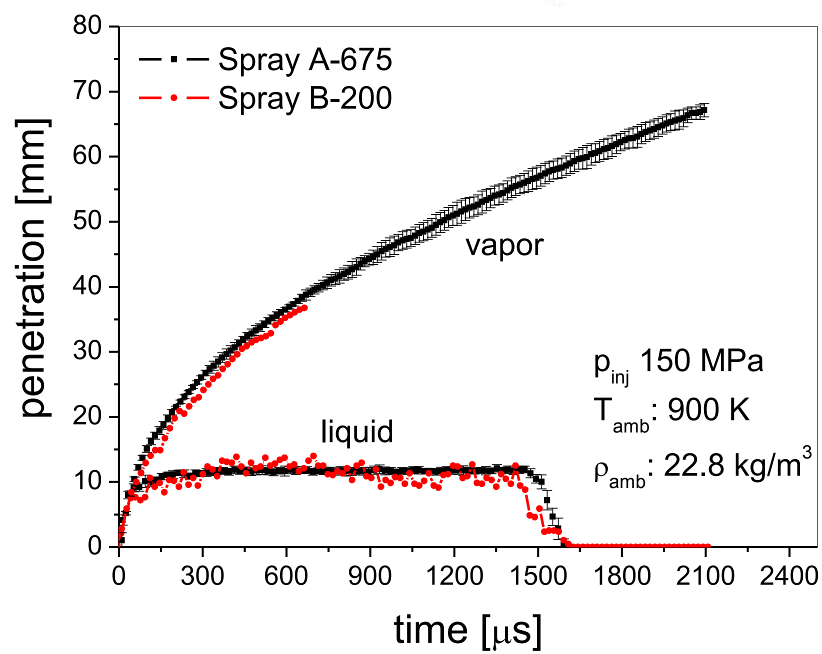
- Mass flow rate through each plume for Spray B is significantly different from one another and different from Spray A also
- Spray A shows faster rise than Spray B
  - Possibly due to the dynamics in the sac
- Needle lift profiles are quite similar for Spray A and Spray B for different injection pressures

Spray A vs. Spray B: Penetration

- Same orifice specifications for Spray A and Spray B injectors
- **Penetration is significantly faster for Spray A than Spray B in the near nozzle region**
  - Initial ROI ramp is faster for Spray A compared to Spray B
  - Lower sac pressure due to throttling at needle seat for Spray A
  - Perhaps more turbulence inside the sac due to higher wobble for Spray B
- **Fairly good agreement in terms of liquid and vapor penetration trends in the far-field regions for Spray A and Spray B**
  - **Vapor penetration of Spray A is marginally higher than Spray B**

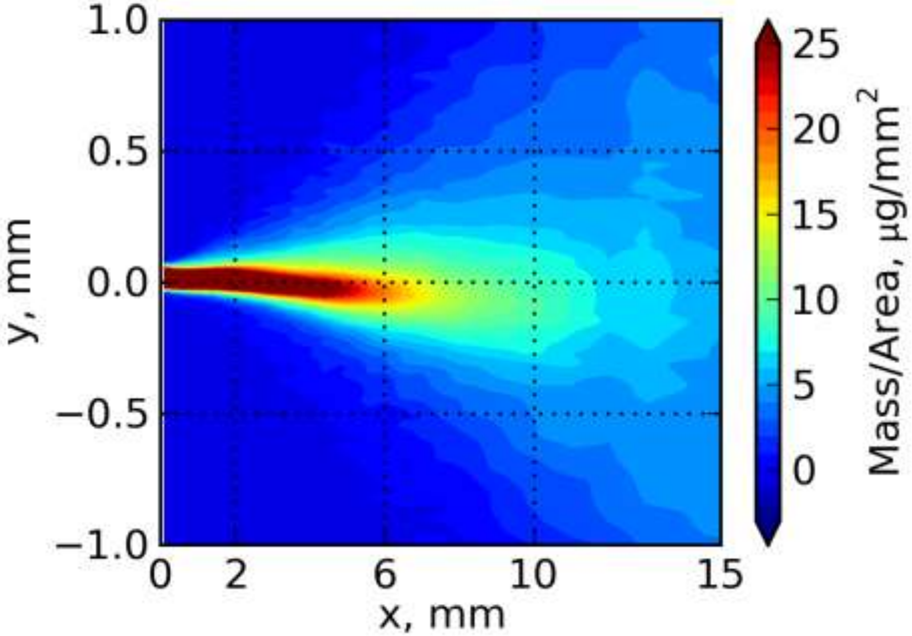
Spray A: 675; Spray B: 200, 201



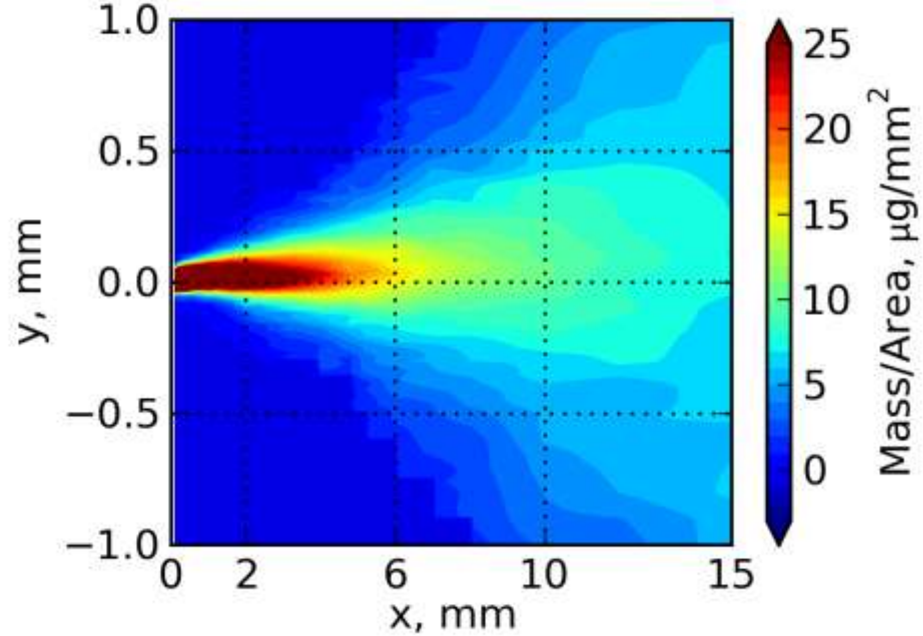


Spray A vs. Spray B: X-ray Data - 2D Mass Distribution

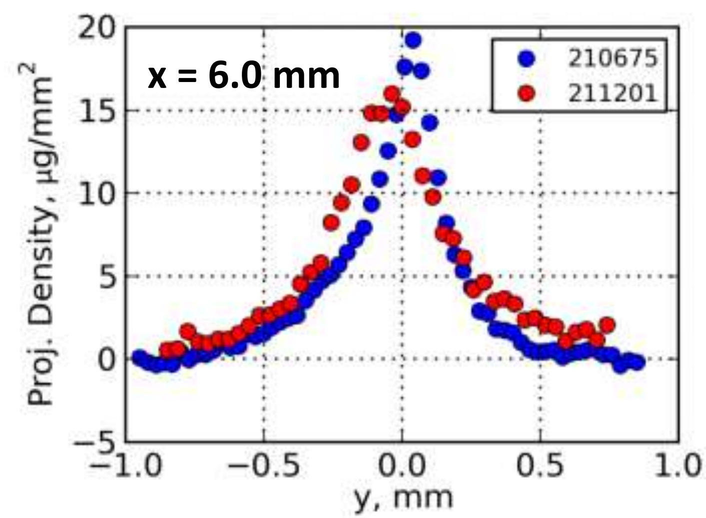
Spray A - 675



Spray B - 201



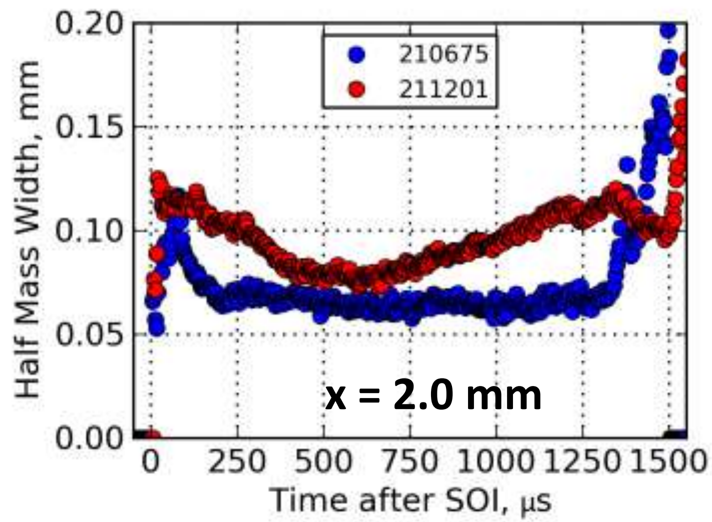
- Overall spray shape similar between two sprays
- **Spray B wider, but less dense along spray axis x = 6 – 10 mm**
- For most points, Spray B wider than Spray A
- Spray B more dense for x > 10 mm, but this is transient. Density lower at later times

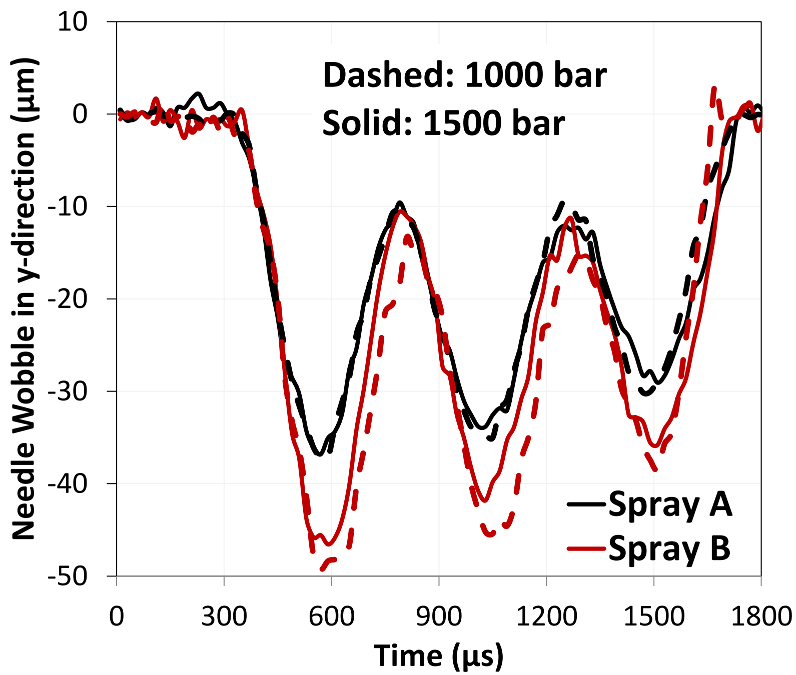


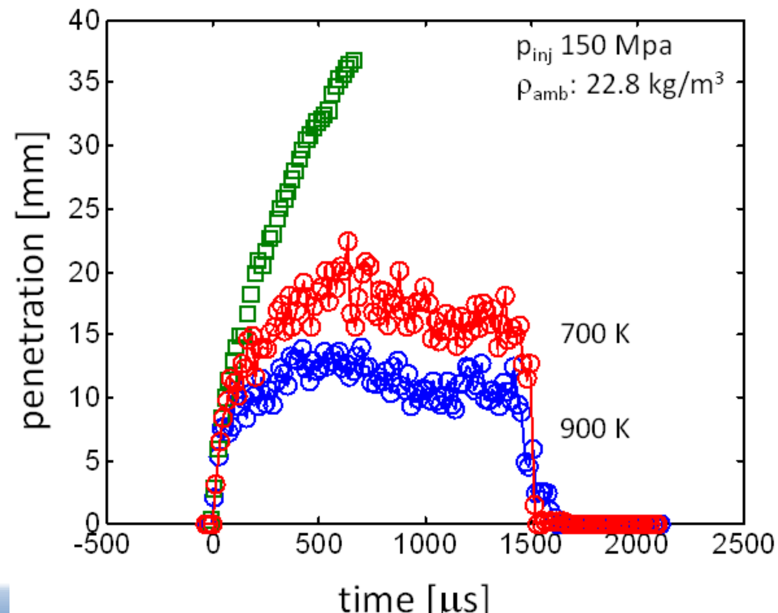
Spray A vs. Spray B: Dynamics

- Spray B is more dynamic than Spray A; Spray B never really at steady-state
- Liquid penetration does not stabilize for Spray B, while it does for Spray A
- Spray B has higher off-axis motion (wobble) compared to Spray A. Perhaps this can be the reason for more dynamic Spray B behavior

Spray A: 675; Spray B: 201



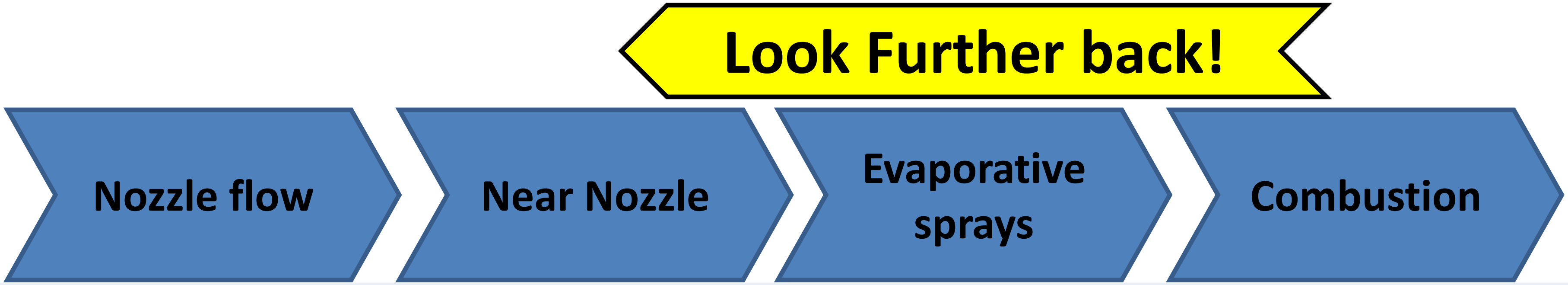




Is there a Consistent Modeling Approach?

Probably obvious, but the answer is "NO"

- **Argonne**: Needs a transition model from EE to LE for combustion
- **CMT**: Needs to couple their simulation strategy with a combustion model
- **IFPEN**: Probably has the code in place to perform coupled simulations between topics 1 and 2
- **POLIMI, Chalmers**: Needs to simulate and couple in-nozzle flows with downstream calculations
- **Sandia**: Two modeling approaches presented. Plan to develop a consistent approach to couple with combustion modeling



Recommendation for Simulations

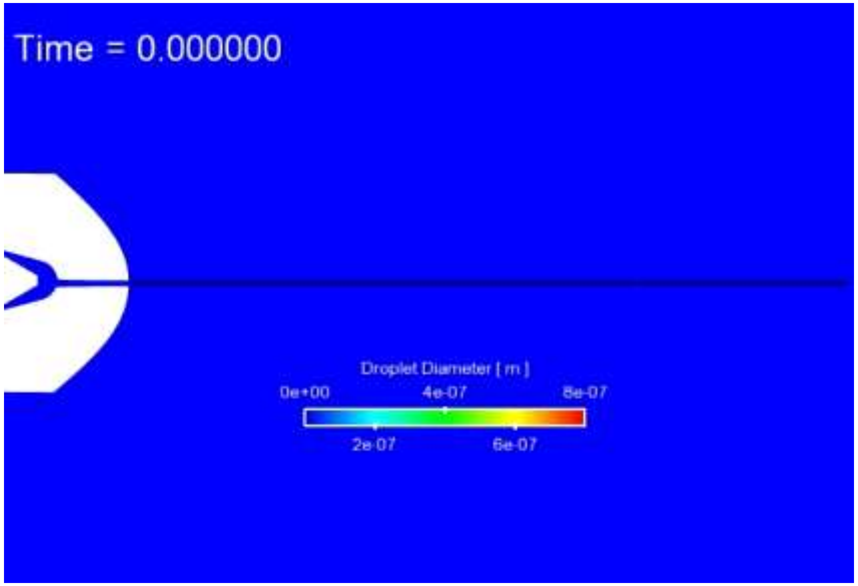
- EE models need a primary breakup model, since the turbulence mixing based models only capture mixing but not spray breakup
- Simulations with high needle lifts need to reduce the initial lift values, otherwise they run the risk of completely missing the initial transients. At 20 μm min. lift, injection velocity is already quite high for Spray A
- Is Spray A supercritical?
  - Yes/No/Unsure
  - What are the implications to modeling these sprays if they are indeed supercritical?
- Simulations need to account of liquid compressibility and temperature variations
- There is a clear evidence of the gas in the sac. Sub-merged nozzle flow simulations are not accurate
- Need more Grid resolution!
- 2-D results are good and computationally cheap, needle off-axis motion and geometric asymmetries necessitate 3-D simulations

Recommendation for Experiments

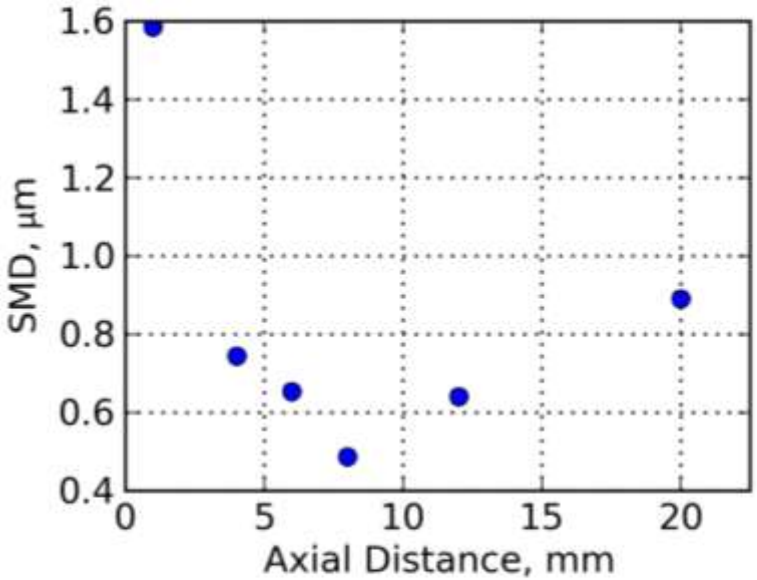
- Data not reliable in some cases due to injector coking issues. Some guidelines developed on how to handle the injectors under the reacting environments.
  - ECN requirement is to measure flow rate before and after tests
  - There are also other storage and handling requirements
- Radial mixture fraction and velocity distributions were available beyond 20 mm. Possible to perform these measurements in the near nozzle region using optical techniques?
- Simulations predict significant temperature drop as the fuel exits the nozzle. Density reconstruction at the nozzle exit possible?
- Similar to Spray A: (1) quantification of differences between Spray B injectors, (2) Robust parametric variations

ECN 4: Grand Challenge

- **Experiments and simulations to work together and identify means to transition from EE to LE models** (since topic 1.3 and topic 2 were mostly LE)
- This is not a new problem, researchers have attempted these transitions before, but the transitions seem rather empirical in nature and lose fidelity from the EE calculations
- Perhaps long-distance microscopy and droplet size measurements can aid in the development of such models



IFPEN Calculation



Argonne X-ray experiments

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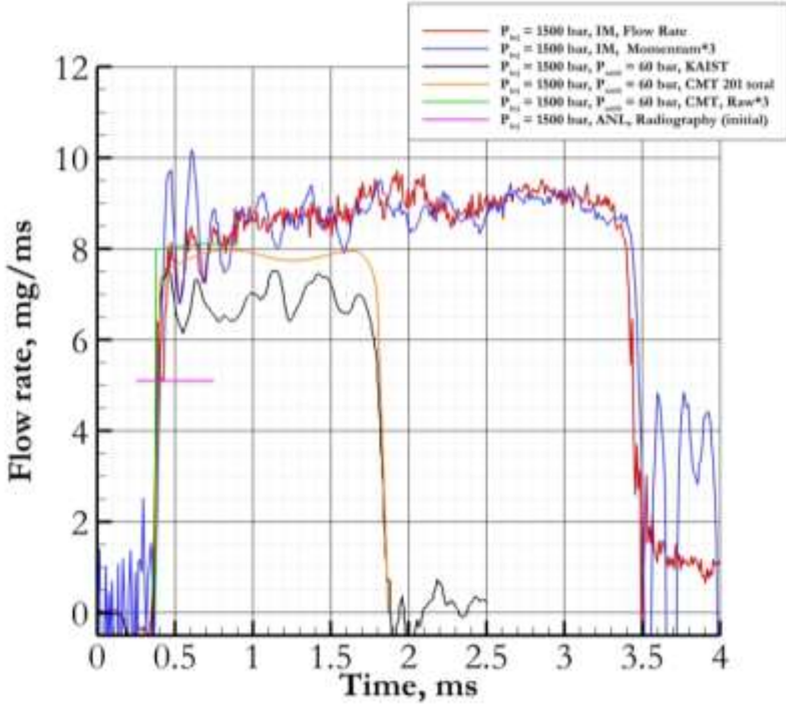
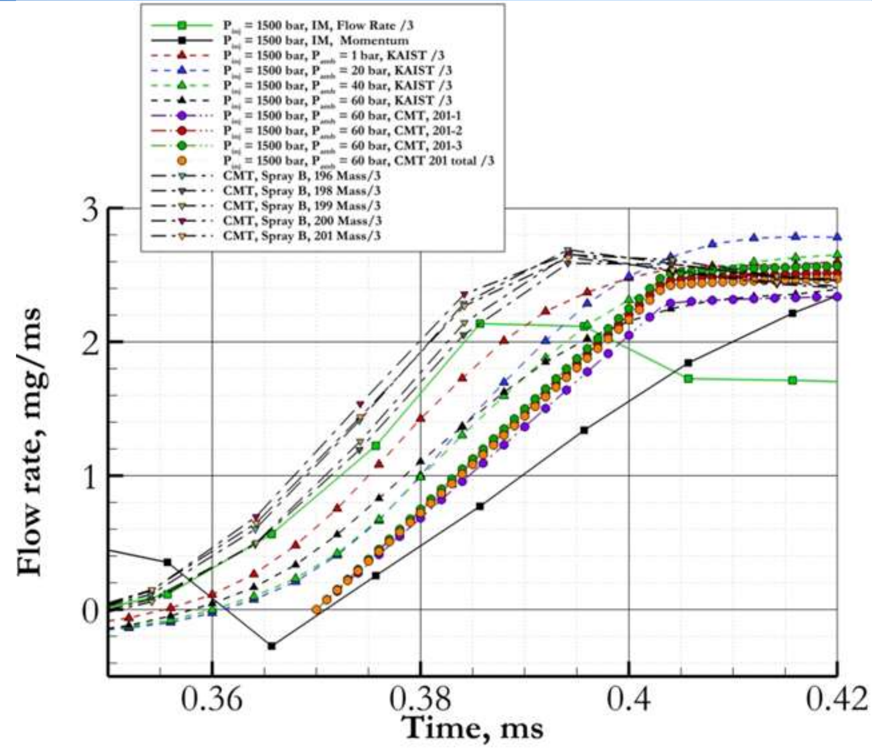
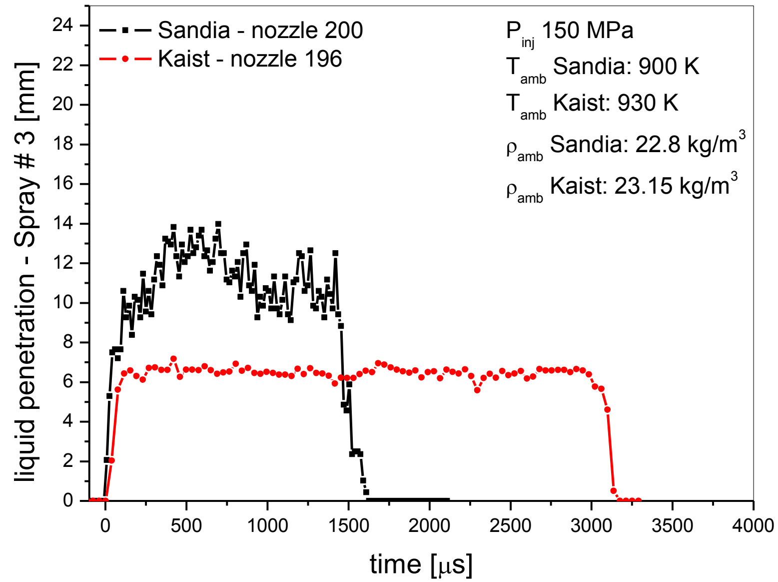
Spray B: Initial Transients, ROI, and Spray Penetration



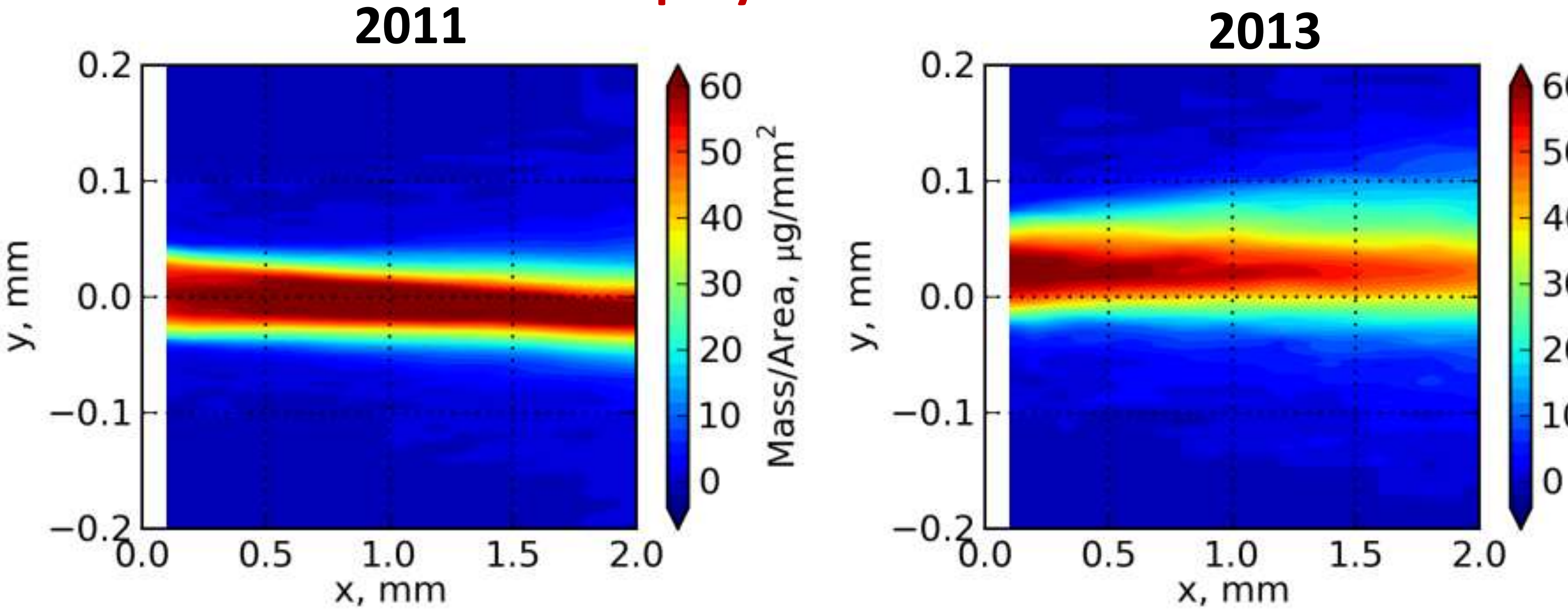




- Sandia ROI is expected to be similar to the virtual rate generator from CMT

Injector Ageing and Serious Damage

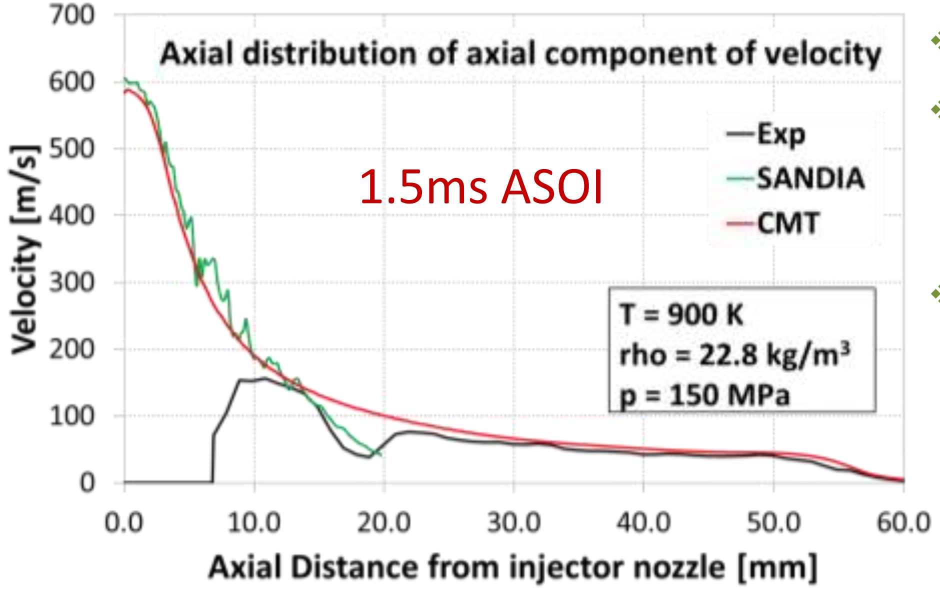
Spray A - 210679



- Nozzle ageing is a serious and growing problem. Causes both quantitative and qualitative changes in spray behavior
- Need to better understand how this occurs
- These nozzles run for thousands of hours on the road.
- Need to better adhere to guidelines for care and use of injectors
- Critical for new additions to the experimental campaign

211196

Spray A Baseline condition: Fuel Distribution



- Sandia simulations are not yet at steady state
- Near nozzle velocity fields i.e., < 10 mm match quite well between Sandia and CMT simulations
- Projected mass density profiles are very dissimilar between Sandia and CMT simulations.
  - Perhaps this is due to the cut-off of mixture fraction chosen for plotting for the Sandia simulations