CURRENT STATE-OF-THE-ART IN FUEL INJECTION AND SPRAY MODELING FOR INTERNAL COMBUSTION ENGINE SIMULATIONS

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CONVERGE CFD SOFTWARE

Acknowledgements

- The organizing committee for inviting me
- My colleagues at Convergent Science
- Our collaborators at national laboratories, universities, and other research institutions
- Our clients, who motivate us to continue to push the envelope
- This is only a small set of all of the great spray work being done

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CMT motores térmicos

Collaborative research through the Engine Combustion Network accelerates CFD model development

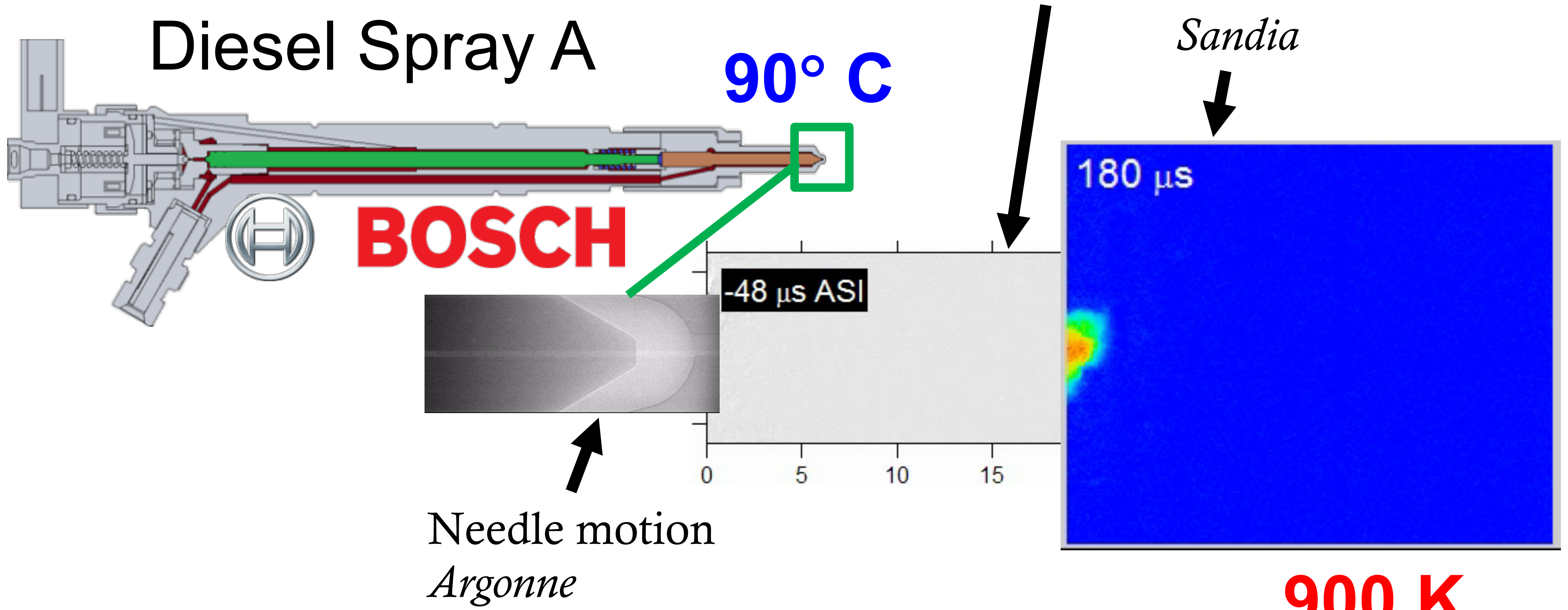
Approach

- Develop diesel and gasoline target conditions with emphasis on CFD modeling shortcomings
- Comprehensive experimental and modeling contributions
- Diesel Spray A, B, C, D
- Gasoline Spray G
- Results submitted to online archive with fields (like geometry and uncertainty) specifically tailored for CFD simulations

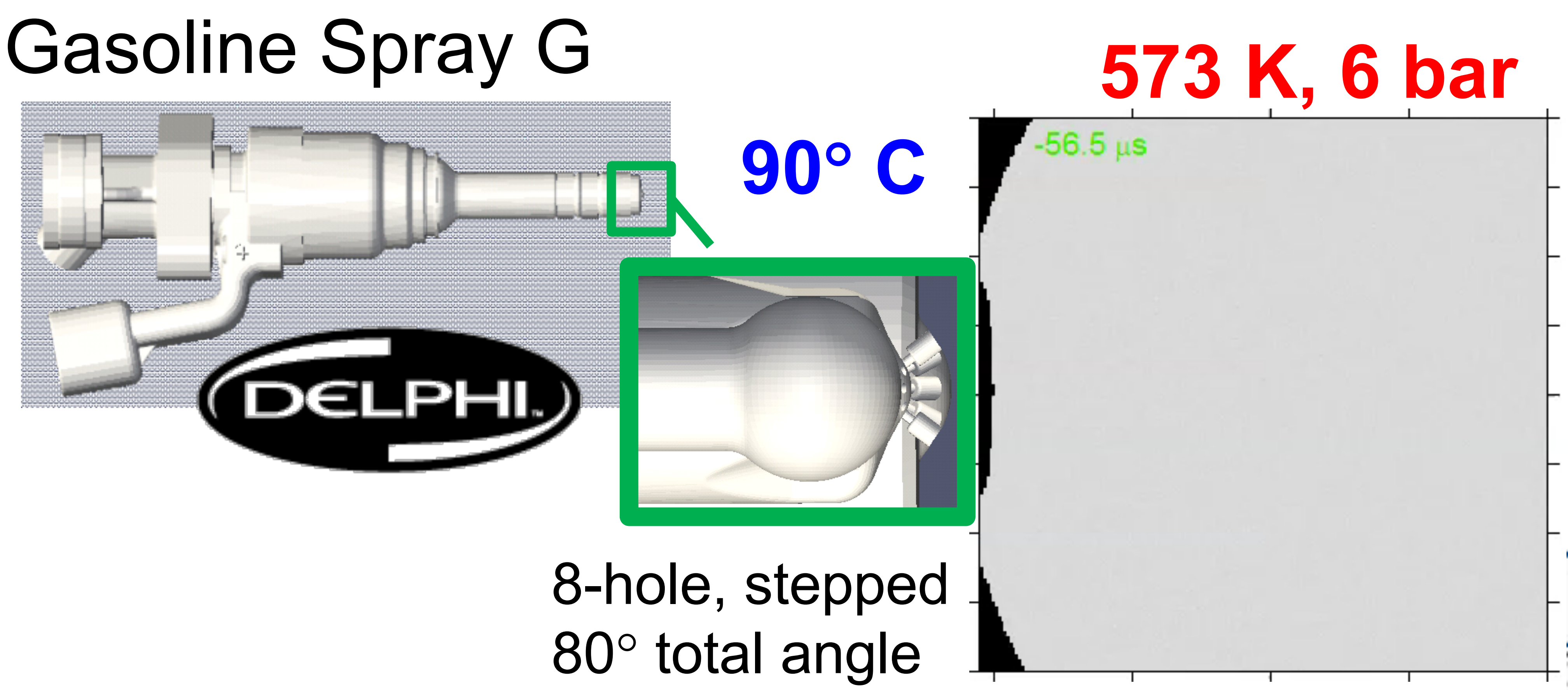
Impact

- Established in 2009, there are already 1400 citations of the ECN data archive
- Most automotive industry (light- and heavy-duty) use ECN archive to test their own CFD methods

ECN formed by Sandia in 2009



>65 measurements/diagnostics contributed from >15 institutions



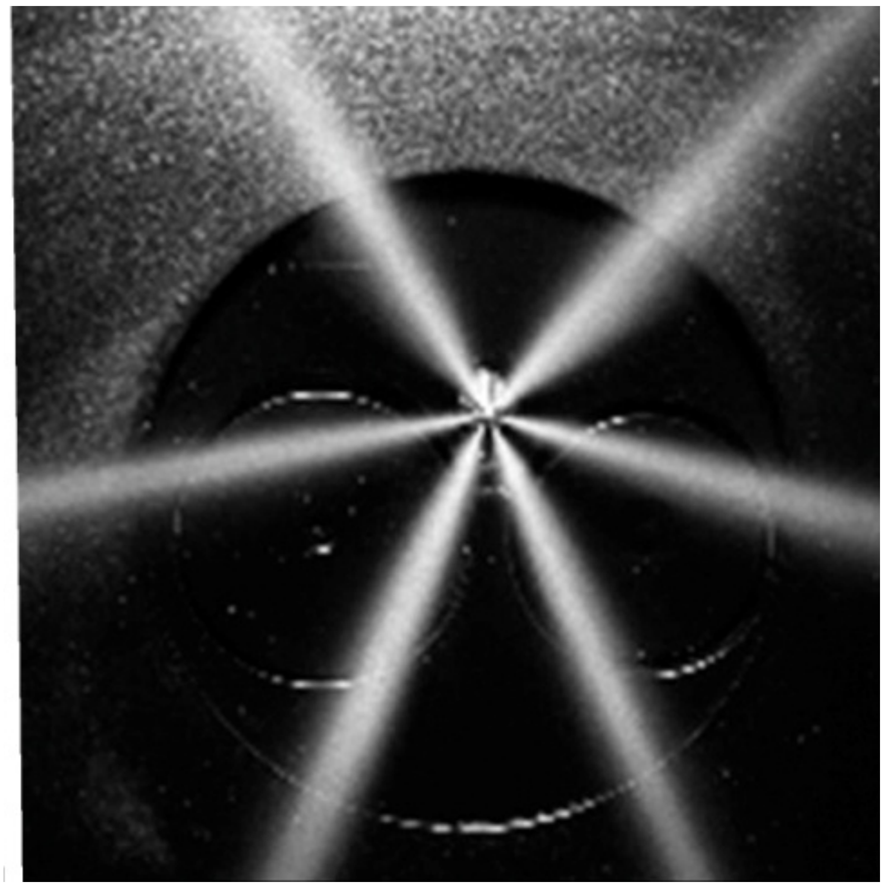
Presentation Outline

- Why model sprays?
- What are the physics?
- How do we model sprays?
  - ★ LE, EE, ELE methods
- How far have we come?
  - ★ Grid convergence
- LES
- Model assumptions
- What's next?

Why Model Sprays?

- Many practical applications involve sprays



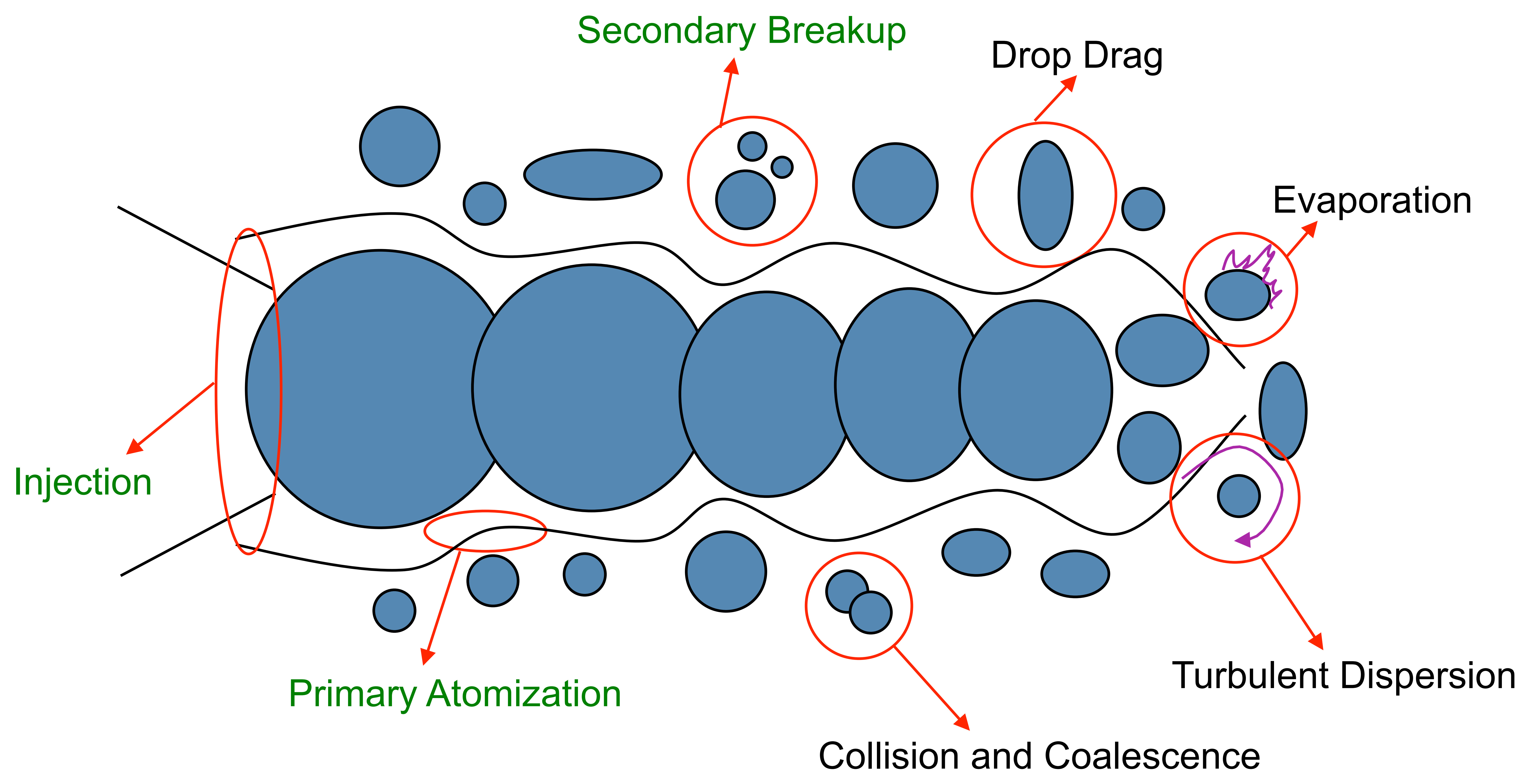



- Detailed modeling of spray processes may lead to substantial improvements in product performance
  - ★ Increased understanding of flow behavior
  - ★ Optimization
- In liquid-fueled IC engines, it’s how the fuel is delivered to the engine!

Why Model Sprays?

- CFD: "Chocolate Fluid Dynamics"

What are the Physics?



What are the Physics?

What are the Physics?

On the sheet breakup of liquid emanating from a garden nozzle

How Do We Model Sprays?

- Three major formulations
  - ★ Lagrangian (liquid) - Eulerian (gas): LE
  - ★ Eulerian (liquid) - Eulerian (gas): EE
  - ★ Eulerian-Lagrangian (liquid) - Eulerian (gas): ELE (aka ELSA)
- Turbulence modeling
  - ★ RANS
  - ★ LES
  - ★ DNS

Eulerian: fluid motion focusing on specific locations in space through which the fluid flows as time passes (think of a CFD mesh)

Lagrangian: fluid motion where the observer follows an individual fluid parcel as it travels through space and time

How Do We Model Sprays?

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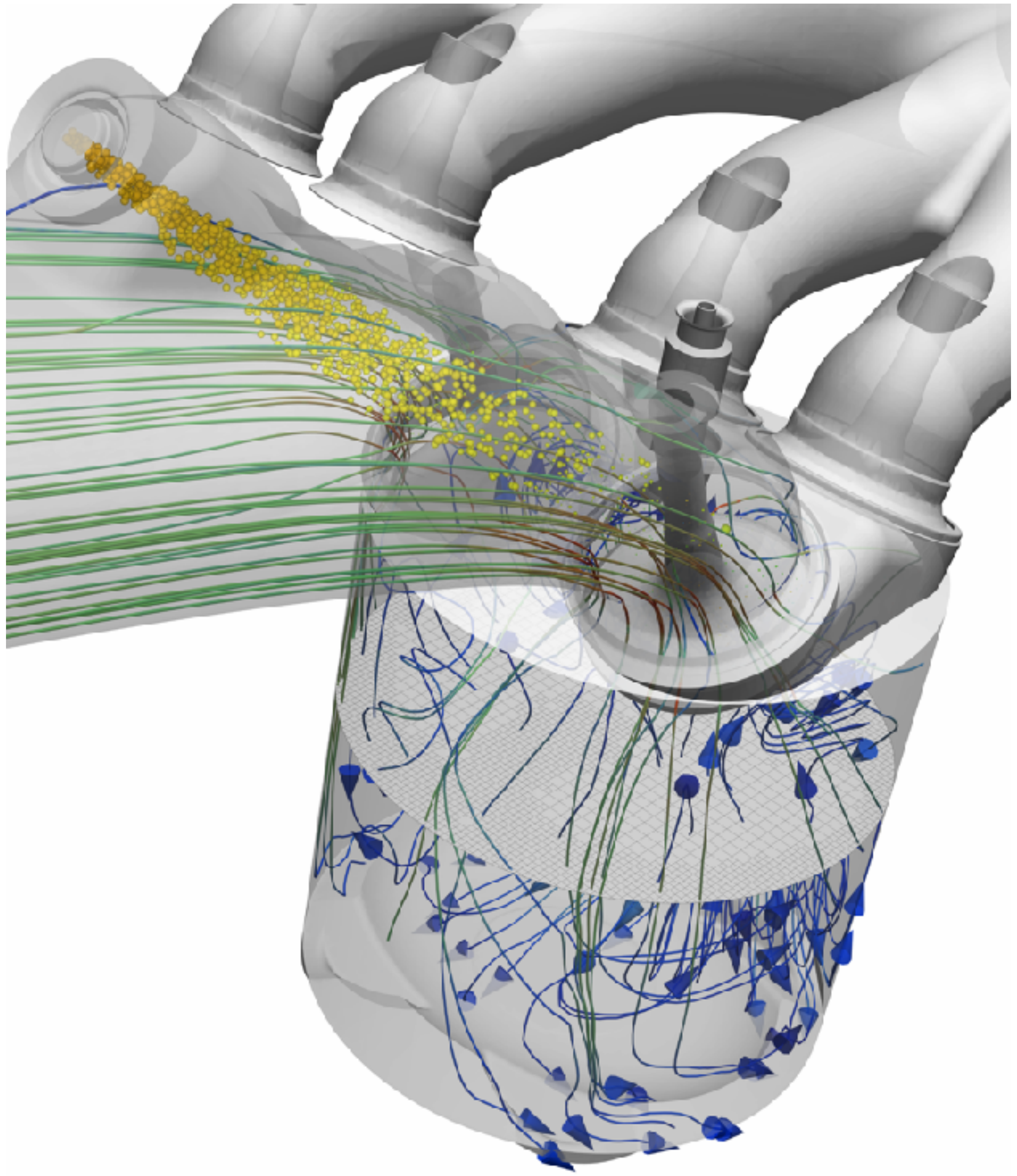
  - ★ **LES**
  - ★ DNS

Eulerian: fluid motion focusing on specific locations in space through which the fluid flows as time passes (think of a CFD mesh)

Lagrangian: fluid motion where the observer follows an individual fluid parcel as it travels through space and time

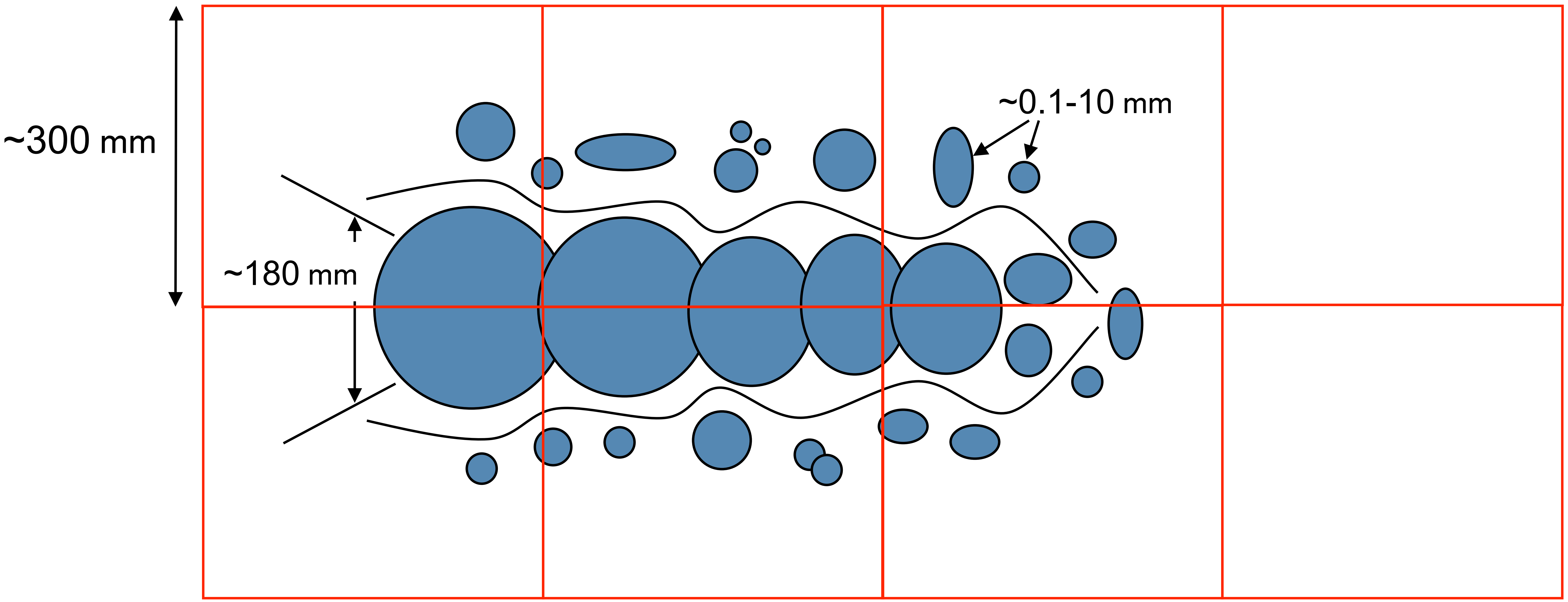
Lagrangian (liquid) - Eulerian (gas): LE

- The spray is represented by drops or “blobs” of liquid which are transported in the Lagrangian framework
- Drops with the same radius, velocity, temperature, etc. are grouped into “parcels” which are used to statistically represent the entire spray field
- The mass of each parcel is determined by the overall injected mass and the injected number of parcels
- The parcel concept can significantly reduce the computational time needed to calculate a spray
- It is important to note that there can be fewer than one drop per parcel
    - ★ This is critical when fine meshes are used



Lagrangian (liquid) - Eulerian (gas): LE

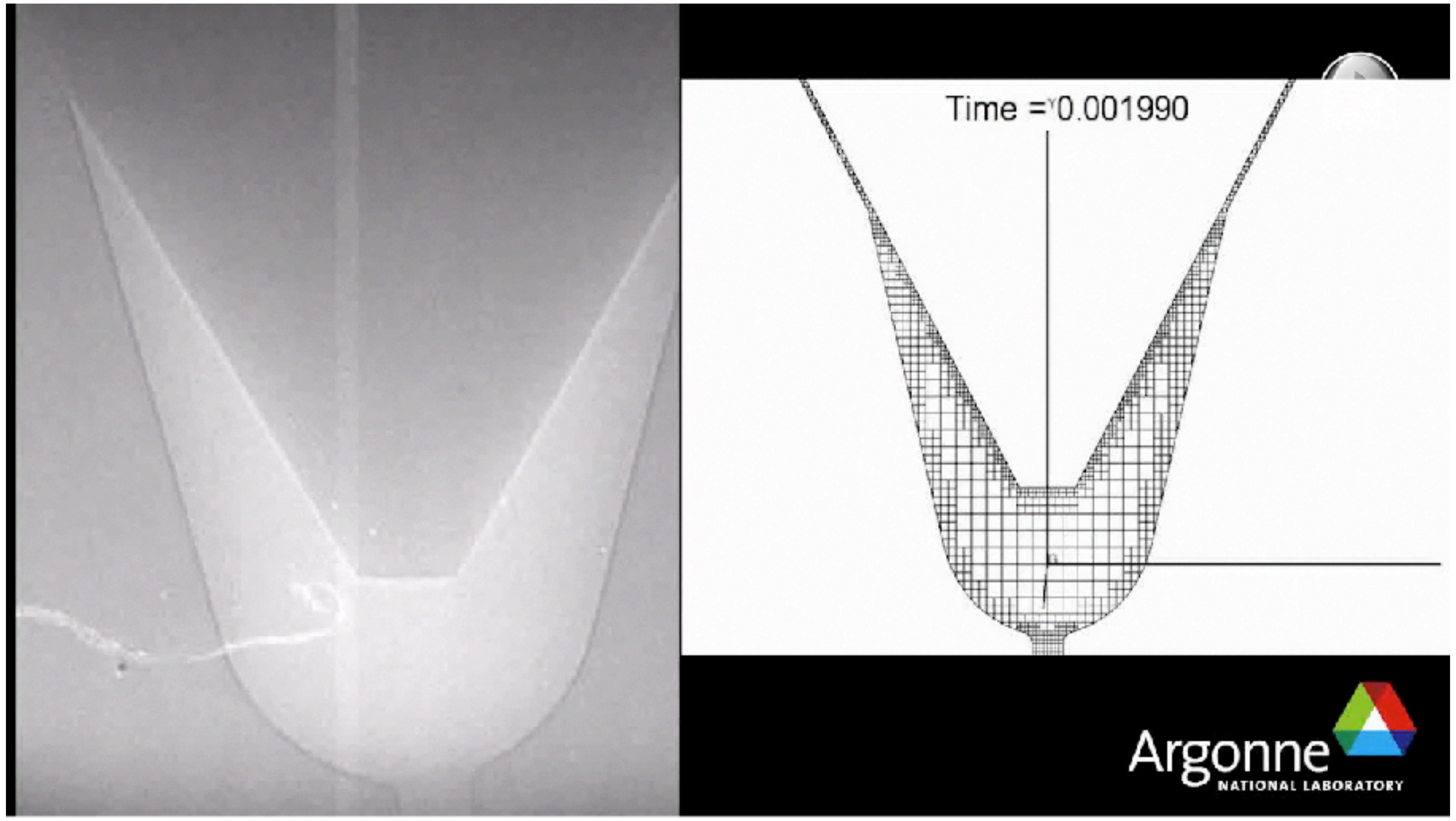
- Sub-grid models are needed for processes that occur on length scales that are too small to be resolved

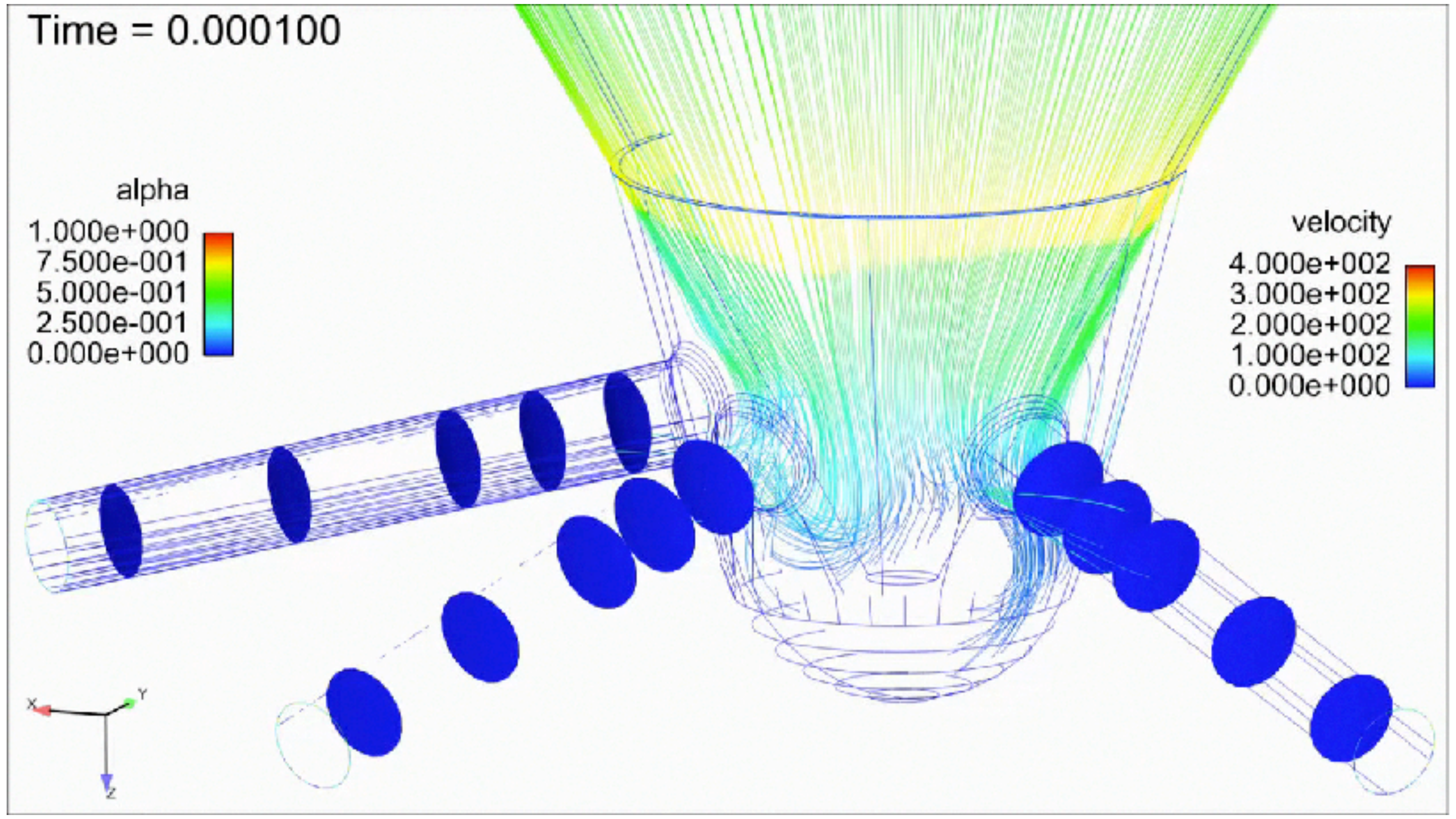


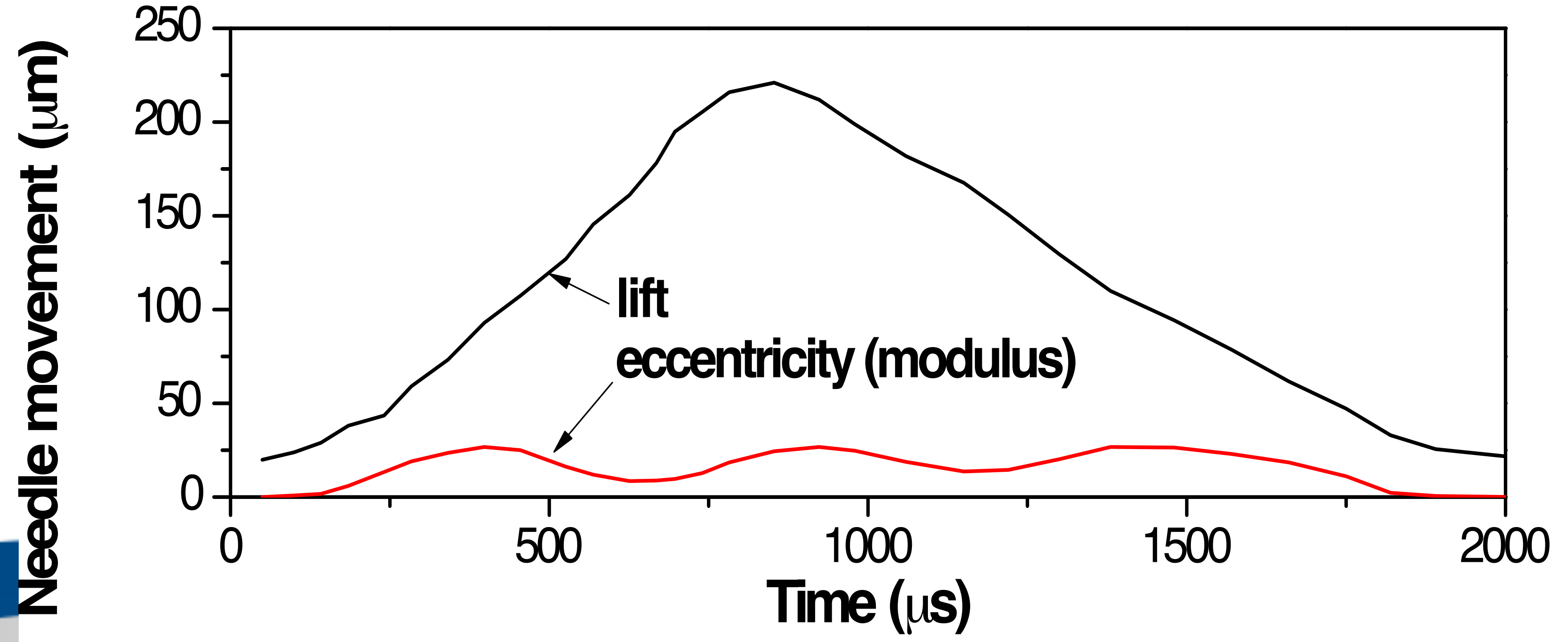
EE Modeling Allows Us to Capture More Physics

- Able to predict effects of needle wobble
- Able to account for needle off-axis motion effects on nozzle-flow development
- Able to predict hole-to-hole variations

X-ray Phase-Contrast Imaging Simulation







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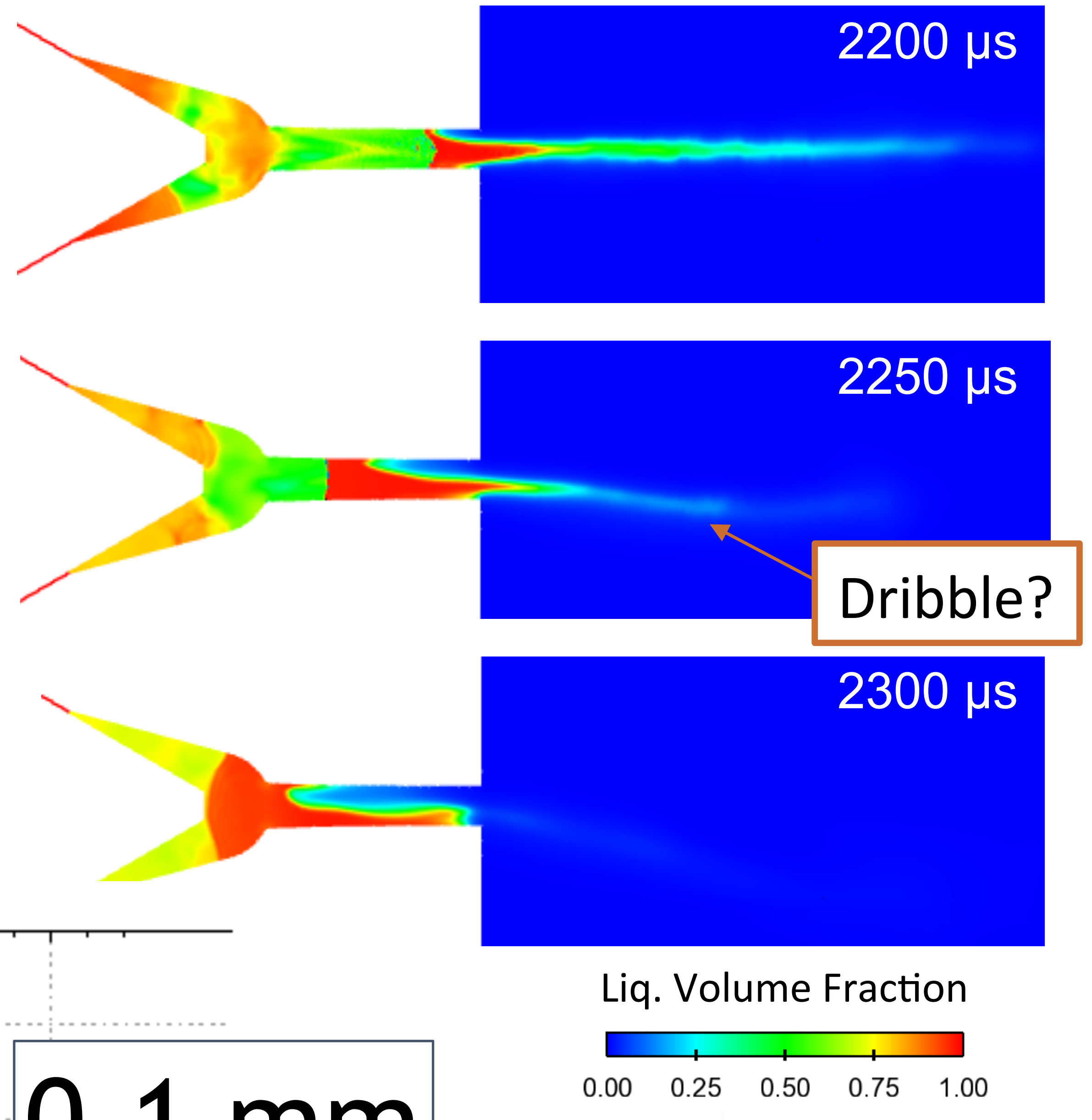
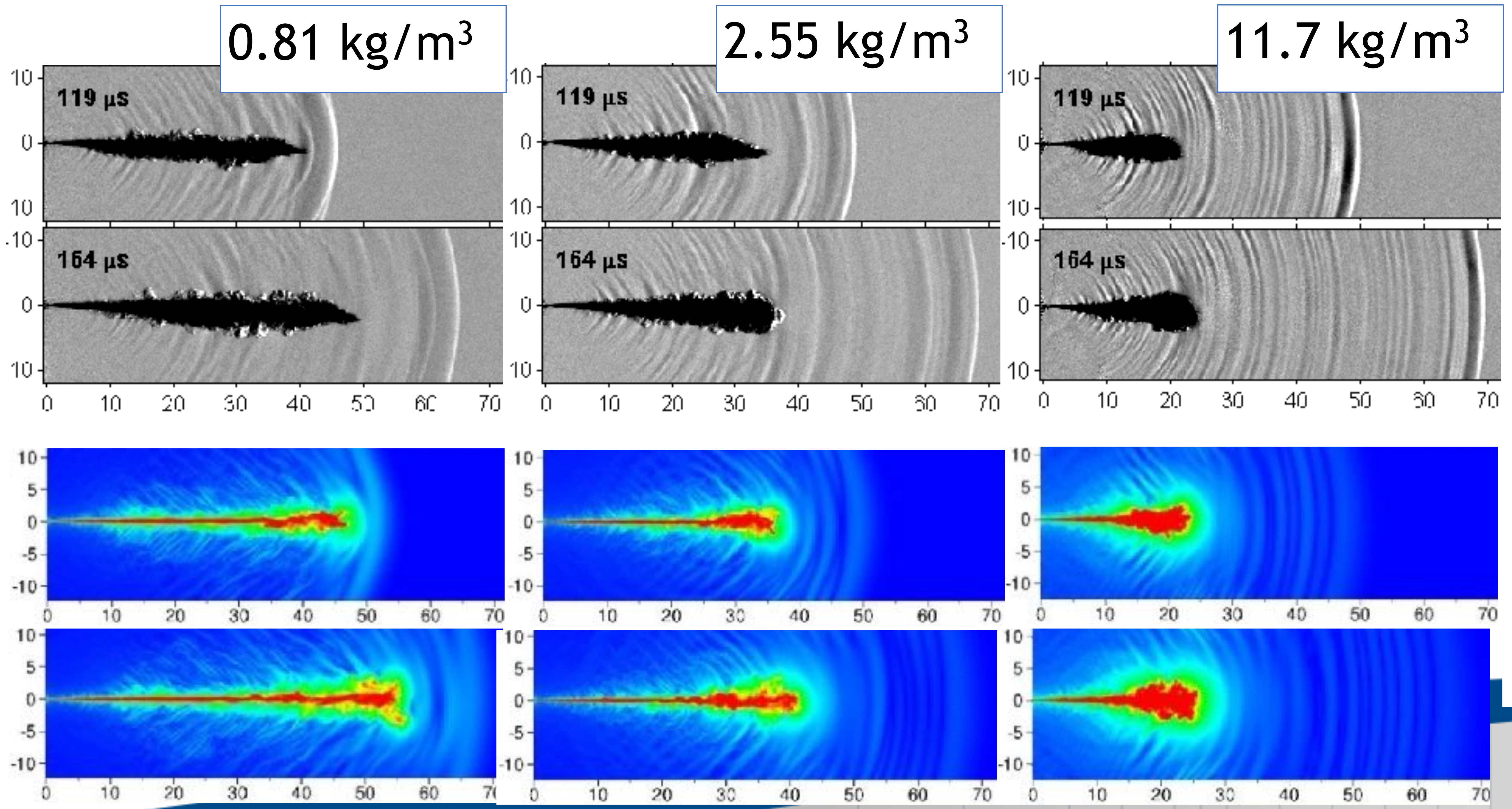
EE Modeling Allows Us to Capture More Physics

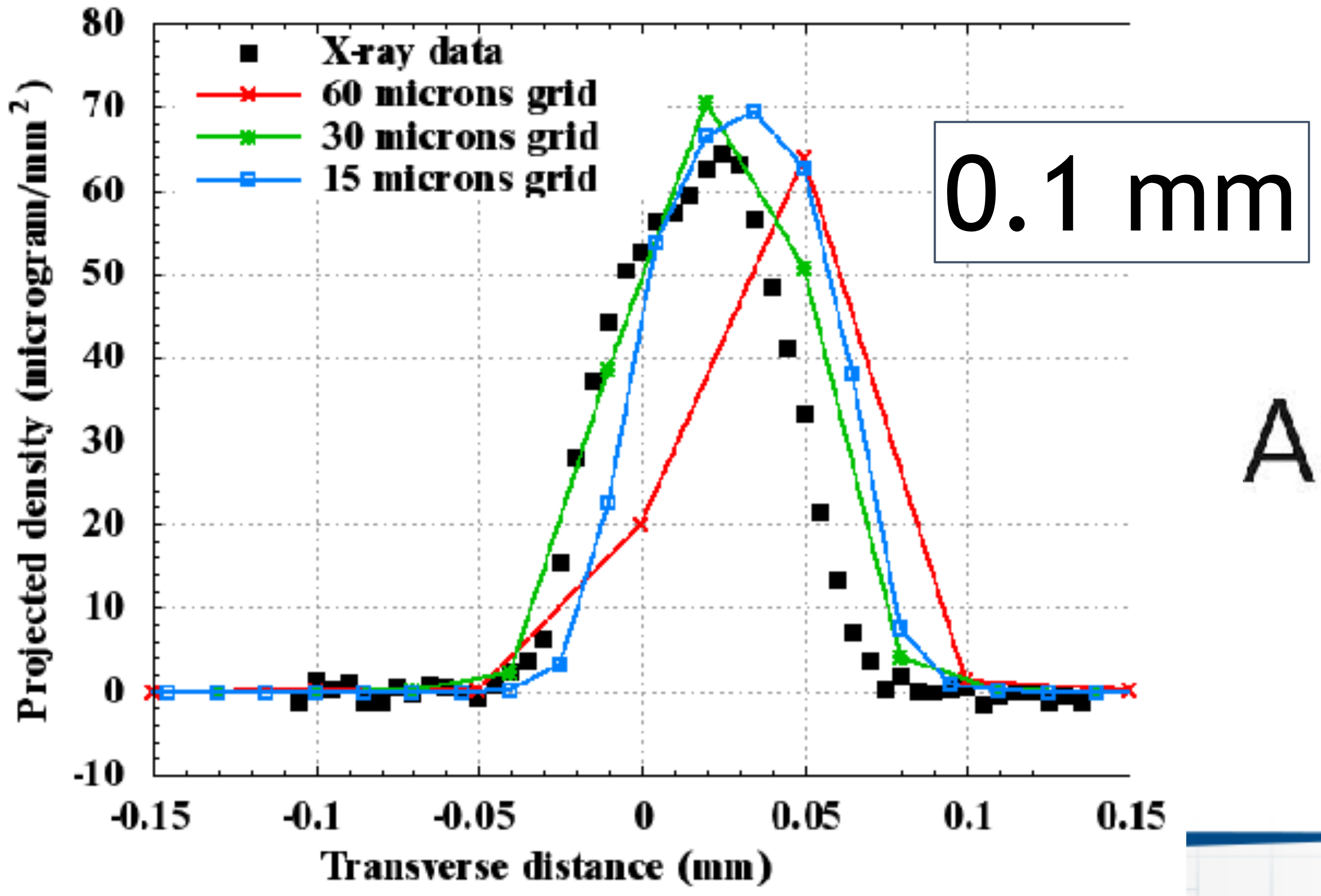
- Start of injection simulations show gas injection before liquid
- End of injection simulations show dribble and ingested gas in the sac

- Improved near nozzle comparisons with x-ray data
- Spray jet shock wave generation

End-of-Injection







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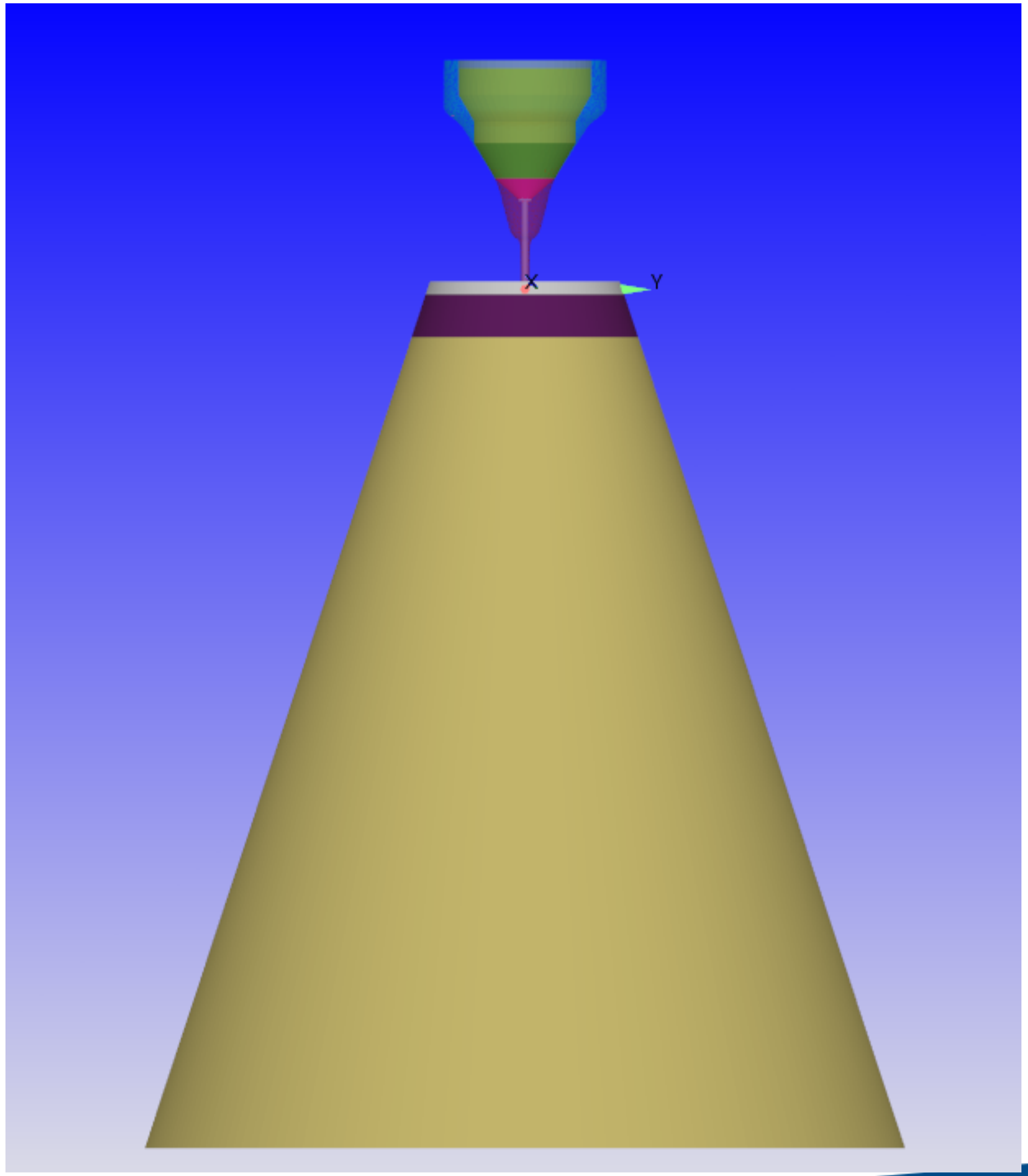
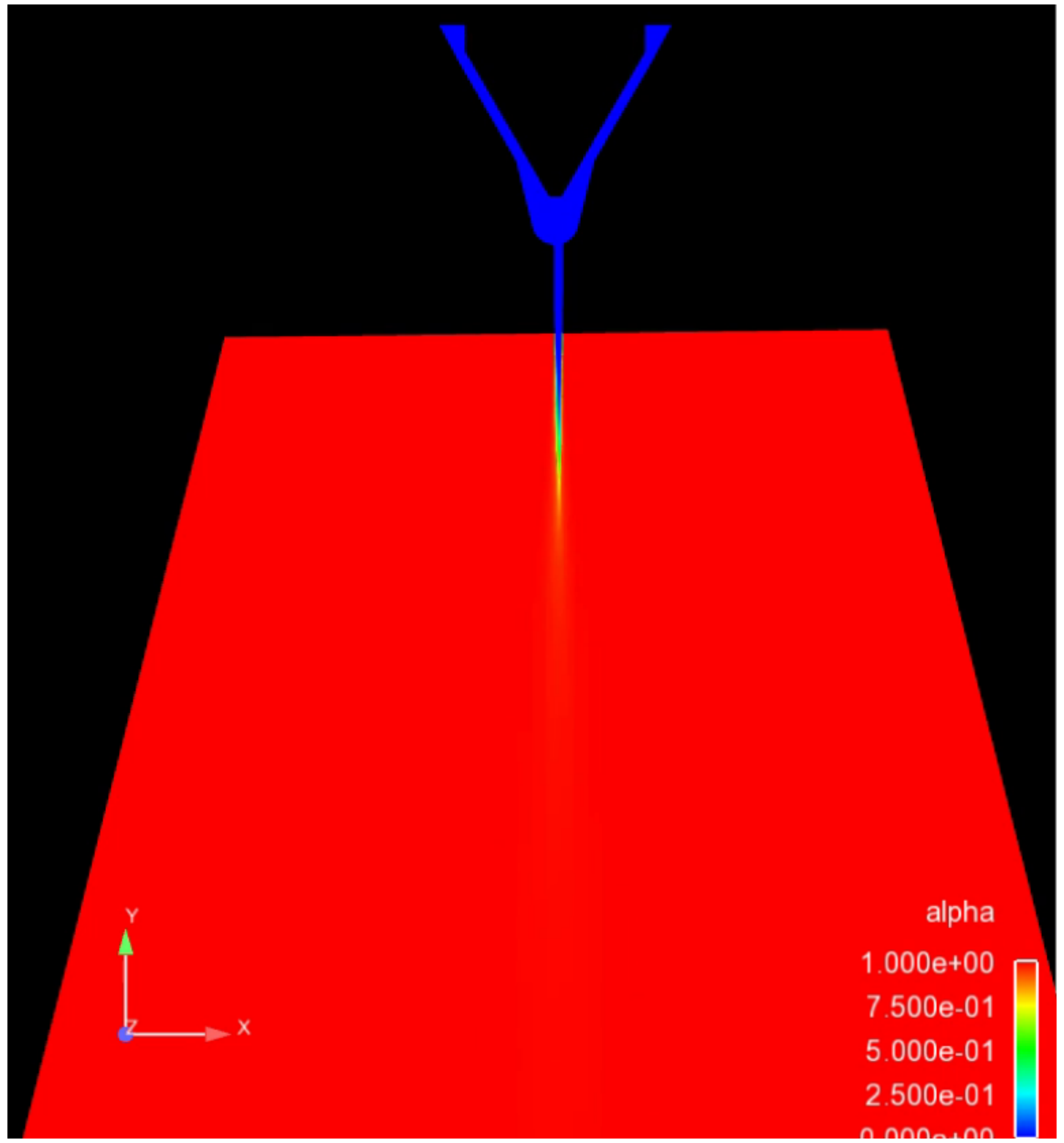
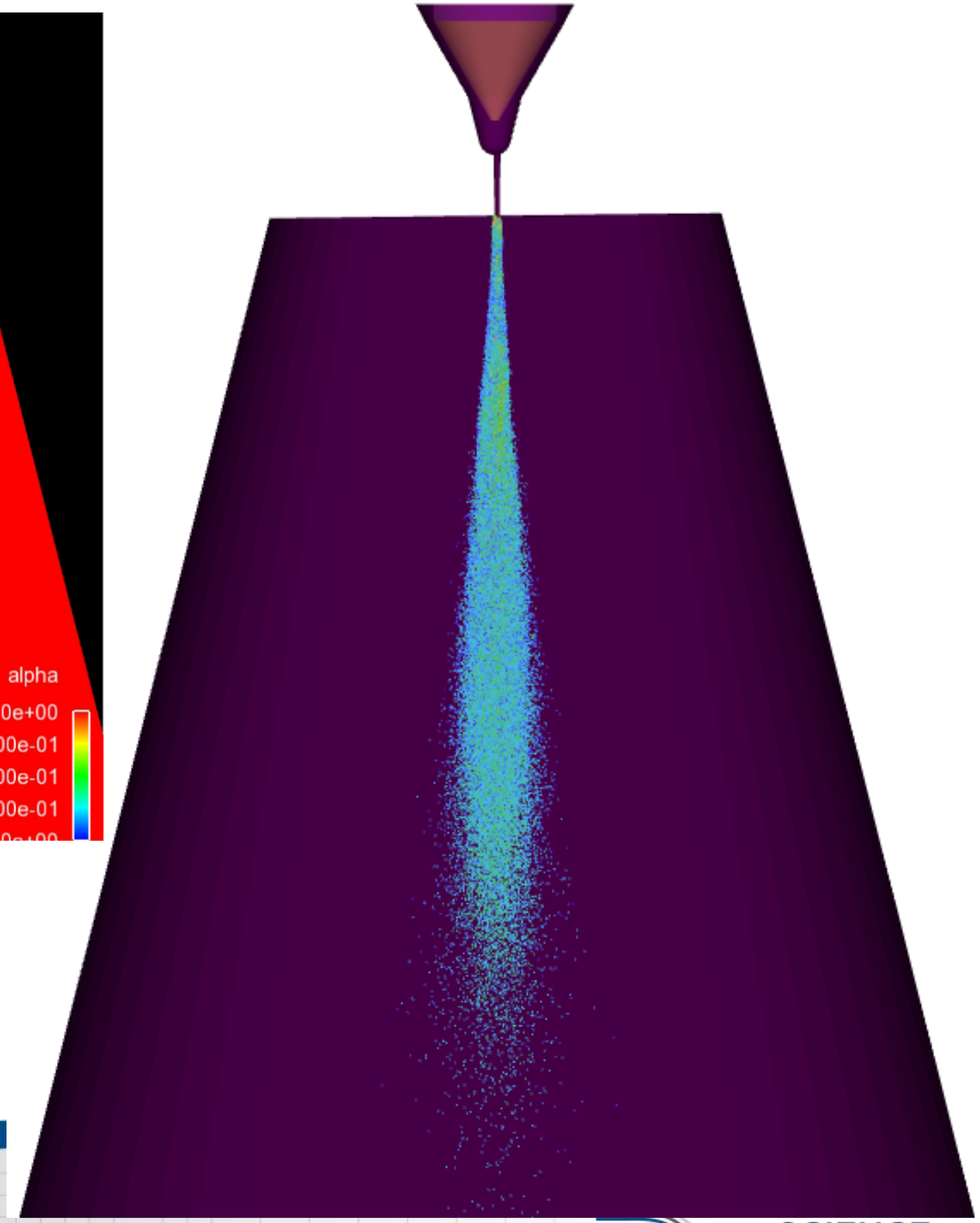
Eulerian-Lagrangian (liquid) - Eulerian (gas): ELE

- Hybrid of the previous two approaches where the liquid is represented by both Eulerian and Lagrangian phases
- The near nozzle, dense spray is modeled in the Eulerian phase
- The dilute spray downstream of the nozzle and at the spray edges is modeled in the Lagrangian phase
- Challenging to know when to transition from Eulerian to Lagrangian and how to initialize the Lagrangian parcels
- Requires finer mesh near the nozzle than LE methods
- Attractive for two-way coupling with the internal nozzle flow

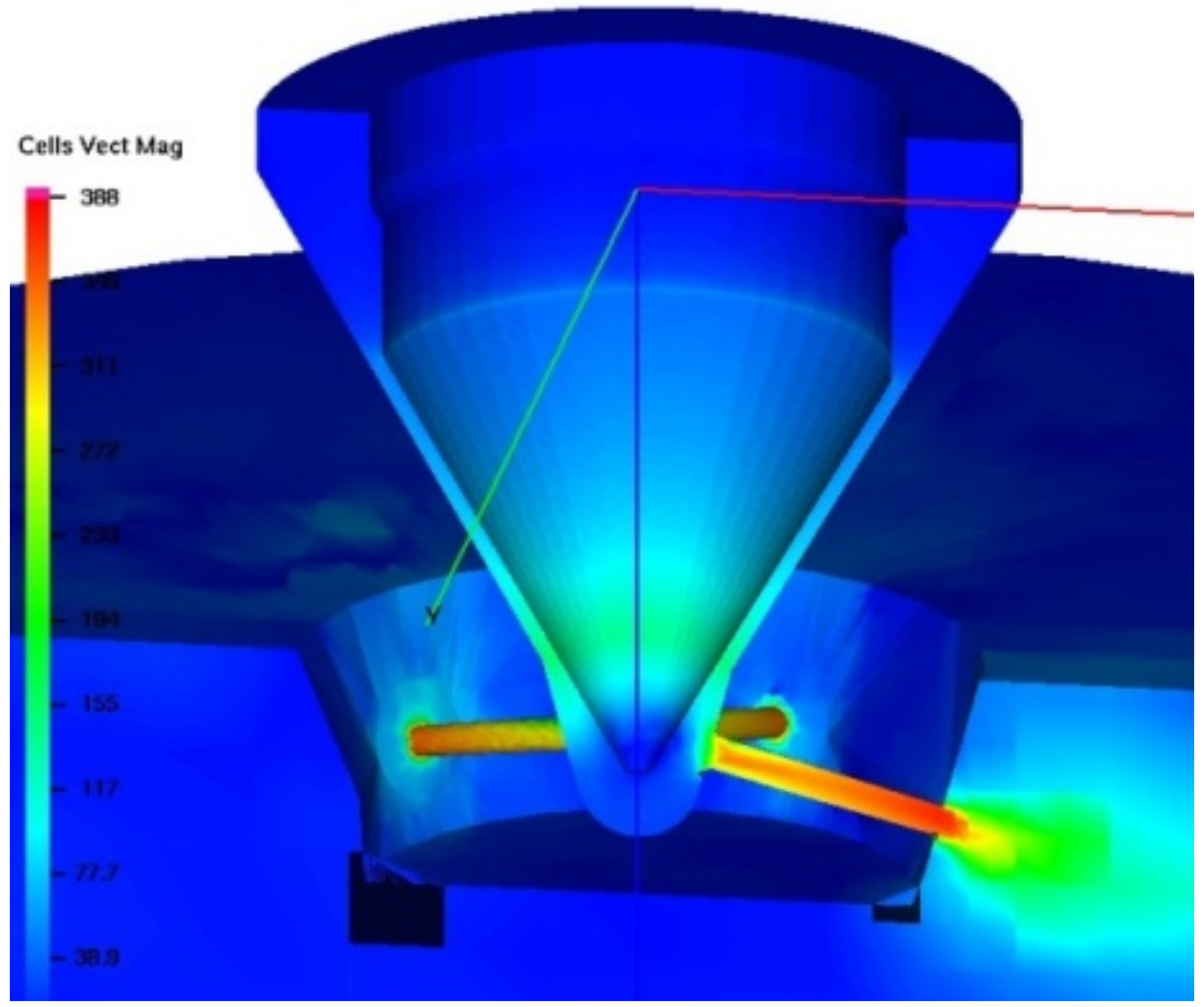
Eulerian-Lagrangian (liquid) - Eulerian (gas): ELE



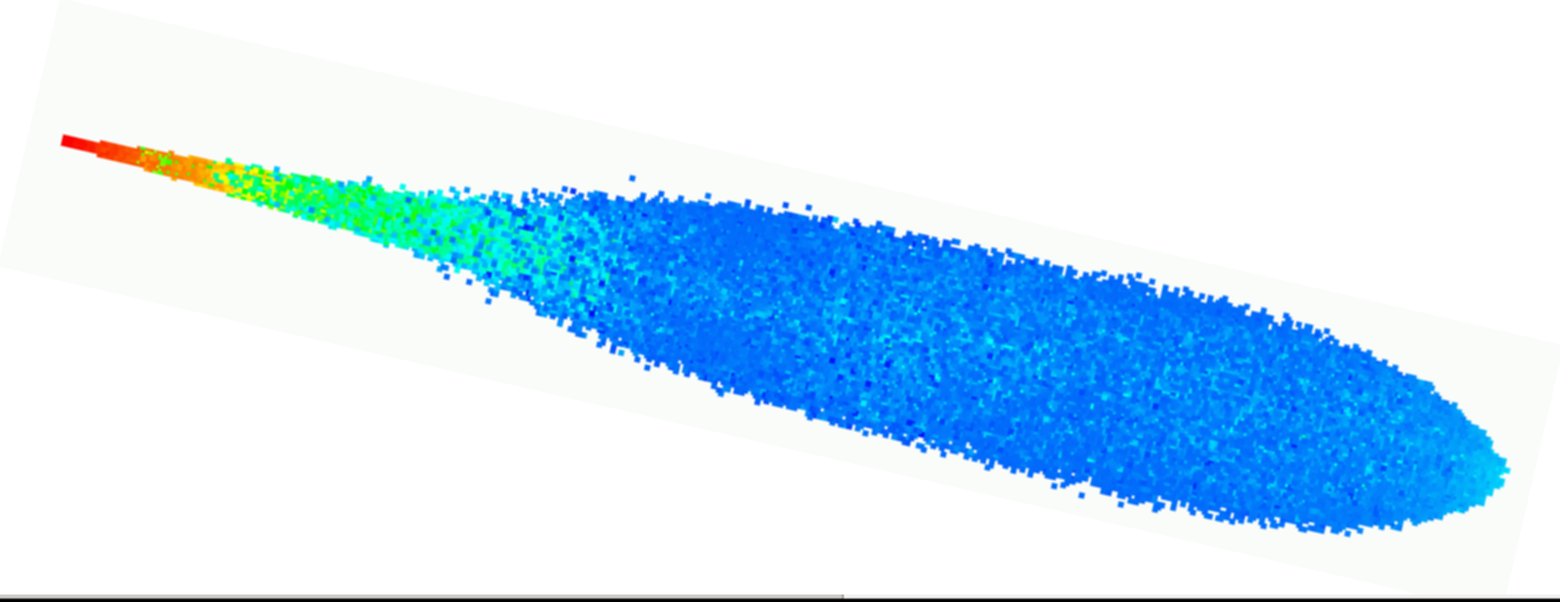


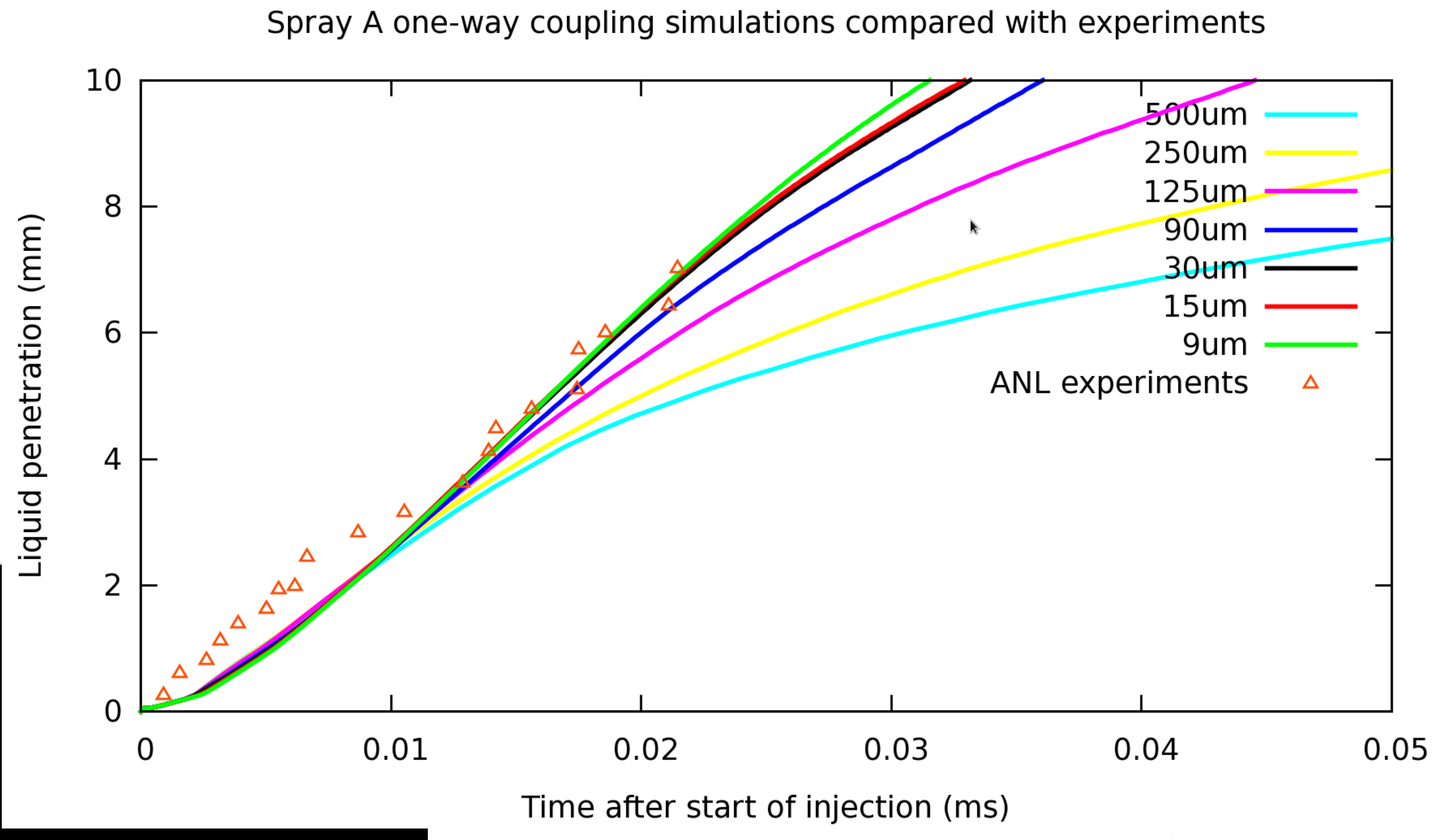


Combined EE-LE Approach



- Perform simulations with VOF and output a map file with detailed information of cells near the nozzle exit
- Setup a corresponding spray case
- Run the spray case with the map file by injecting parcels using the information in the map file






```
# CONVERGE Release 2.2.0/  Jul 16, 2010        Run Date:Thu Mar 12 16:00:32 2015
# VOF map data file.
Time                  0.0000001096868        (s)
Nozzle_Center         -2.8656697e-08   5.1912572e-08    -1.8247947e-03
Nozzle_ID             0                Region_IDs             2        0
Mass_Flow_Rate        1.8514582e-03    Mass_Flow_Rate_Liquid  1.6358705e-03
Total_Mass            2.0064526e-10    Total_Mass_Liquid      1.7955243e-10    Ca                    6.4355567e-01
TKE                   1.0556815e+03    EPS                    9.0046500e+07
Cell_Count            386
              X              Y               Z              U              V               W     Liquid VOF    Liquid Mass            TKE            EPS           TEMP
  7.0187500e-05  6.9692500e-05  -1.8167225e-03  2.3346437e+01  2.2094160e+01  -5.4717892e+01  6.5304106e-01  1.5273562e-12  9.0580598e+02  9.2937177e+07  2.9889935e+02
  7.0187500e-05  6.9692500e-05  -1.8323475e-03  7.2084868e+00  6.9568371e+00  -8.0779165e+01  3.0532000e-01  4.1810413e-13  9.3663589e+02  8.3568100e+07  2.9889935e+02
  6.9231037e-05  8.4223656e-05  -1.8167225e-03  1.0492458e+01  1.4409081e+01  -3.6957784e+01  9.1206852e-01  2.2499036e-12  1.7079816e+02  1.7769563e+08  3.0003529e+02
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```

How Far Have We Come (LE)?

- The models have not changed much in 30 years!
- Most breakup models are based on length and time scales derived from unstable waves growing on the liquid surface

$$\eta = \eta_0 \exp(ikx + \omega t)$$

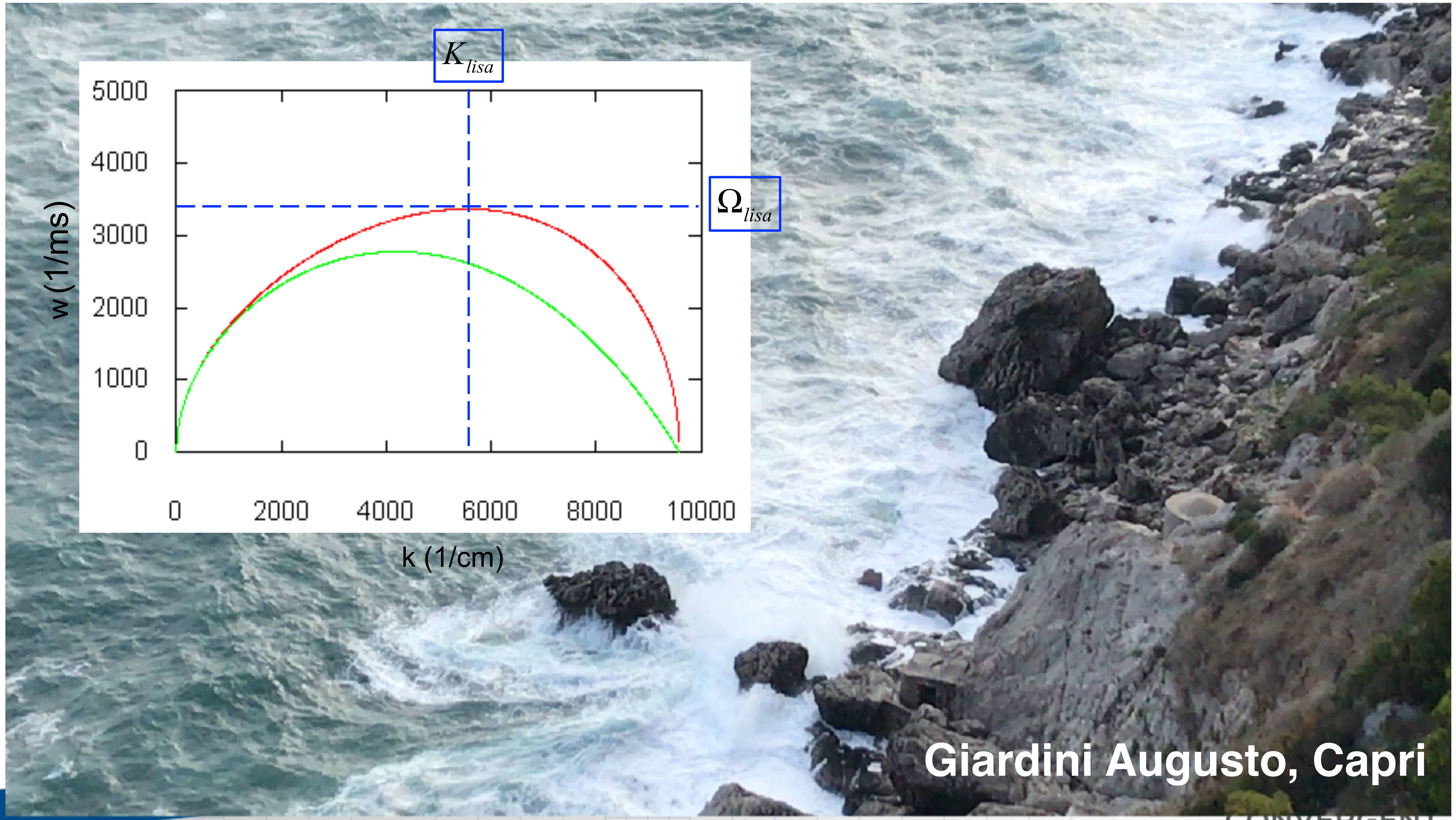
$$\omega = \omega(k)$$

$$\Omega_{lisa} = \text{ maximum value of } \omega$$

$$\Lambda_{lisa} = 2\pi / K_{lisa}$$

$$\omega^2 \left[\tanh(kh) + Q\right] + \omega\left[4\nu_1 k^2 \tanh(kh) + 2iQkU\right]$$
$$+4\nu_1^2 k^4 \tanh(kh) - 4\nu_1^2 k^3 L \tanh(Lh) - QU^2k^2 + \frac{\sigma k^3}{\rho_1} = 0$$

$$\omega_r = -2\nu_l k^2 + \sqrt{4\nu_l^2 k^4 + QU^2 k^2 - \sigma k^3 / \rho_l}$$



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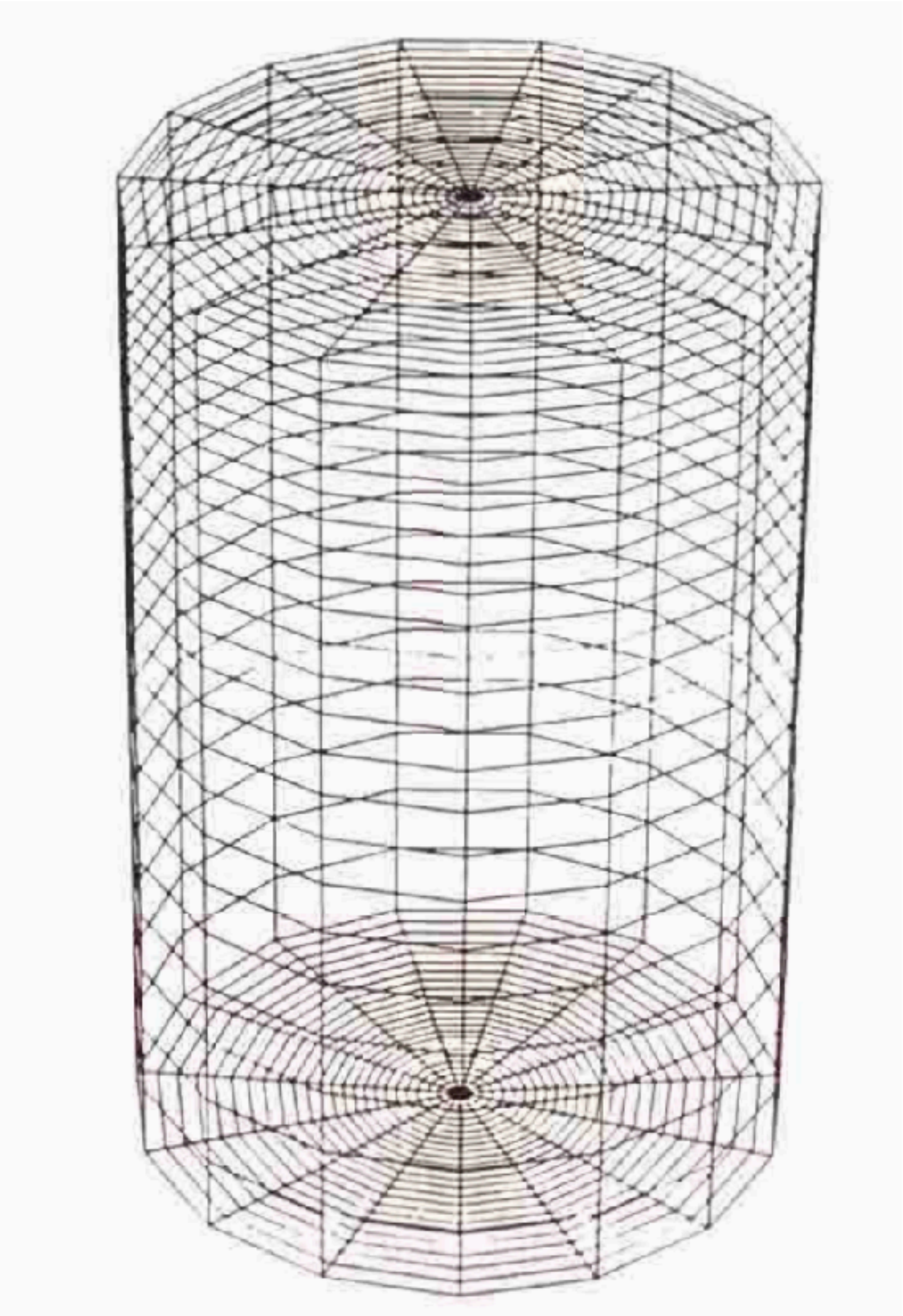
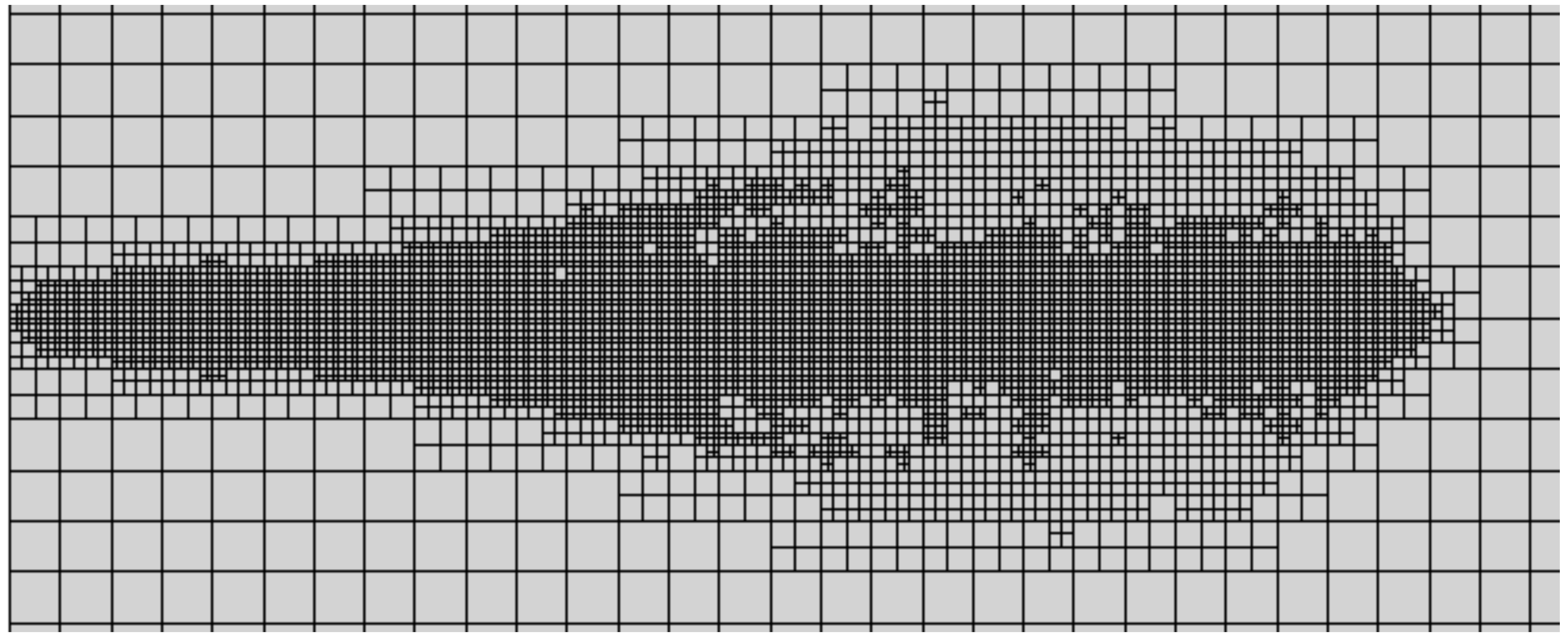
How Far Have We Come (LE)?

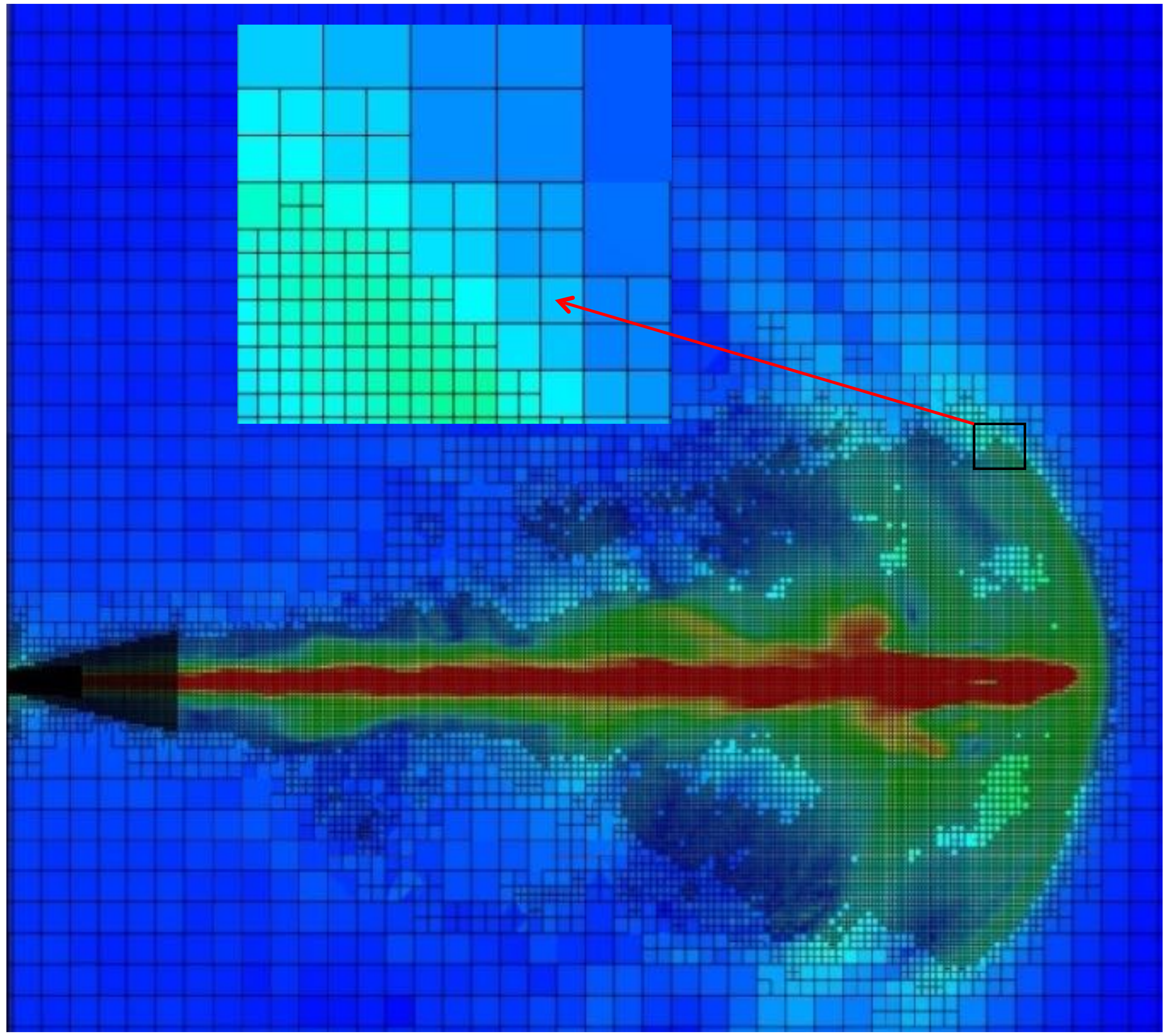
- 1987, original "wave" breakup model paper
- Cylinder of 30 mm radius and 100 mm length
- 24 radial, 15 azimuthal, 24 axial cells
- Smallest cell of 1 mm x 2 mm
- 4000 parcels
- "Numerical experiments with finer meshes and more drops confirmed that results are also grid- and timestep-independent."



How Far Have We Come (LE)?

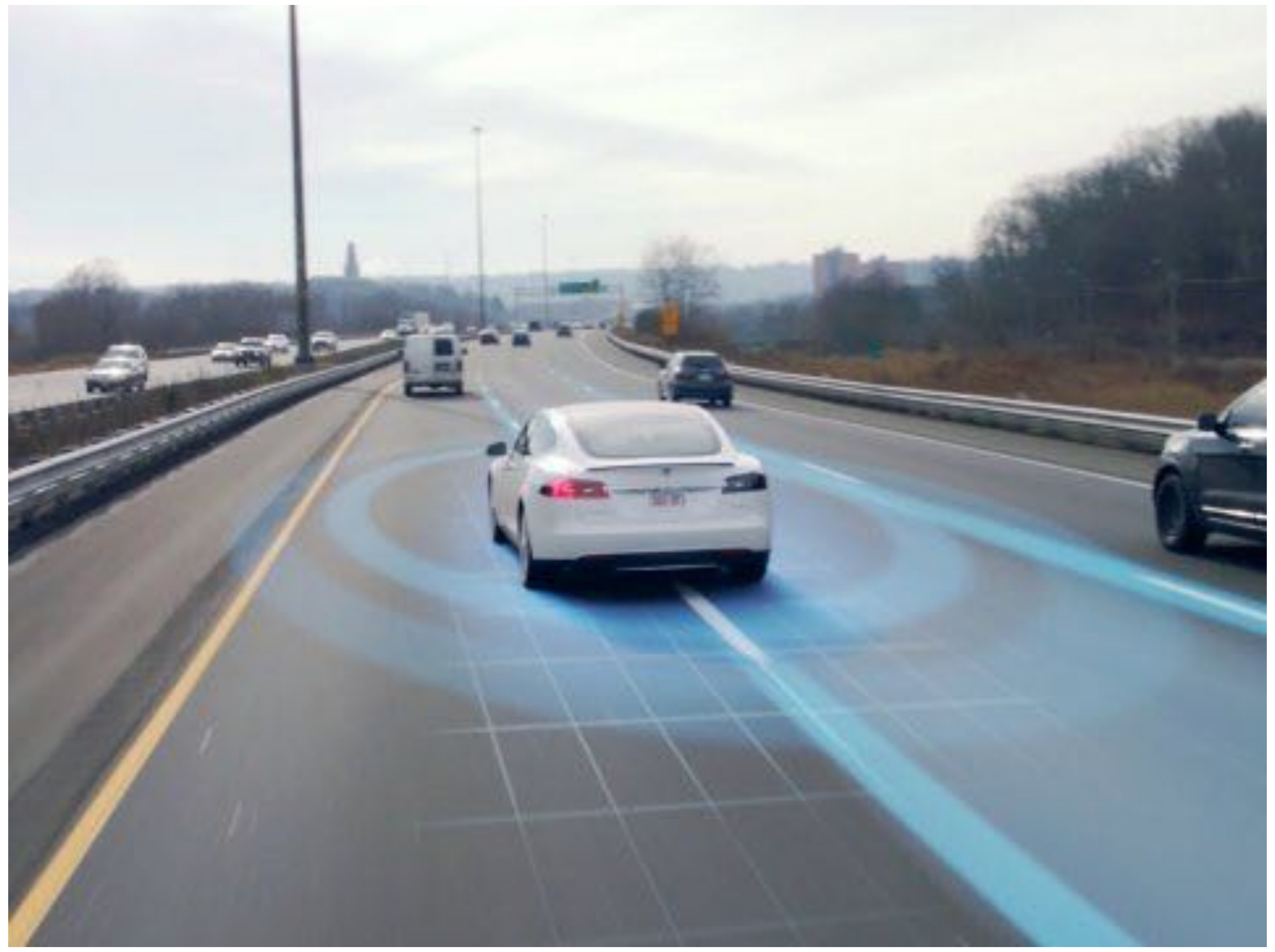
- We've come a long way in the last 30 years!





Enabling Technologies

- Autonomous Meshing
  - ★ Automatic (No User Meshing)
  - ★ Adaptive Mesh Refinement
  - ★ No more meshing by guessing
- Improved Accuracy
  - ★ Increased resolution
  - ★ Better models or even less modeling
  - ★ Small changes cannot be predicted if simulation is overly smeared
- High Performance Computing
  - ★ Capability Computing - use computing power to solve one large problem in the least amount of time
  - ★ Capacity Computing - spread the computing power amongst many smaller problems so they can be run simultaneously



http://www.businessinsider.com/autonomous-car-limitations-2016-8

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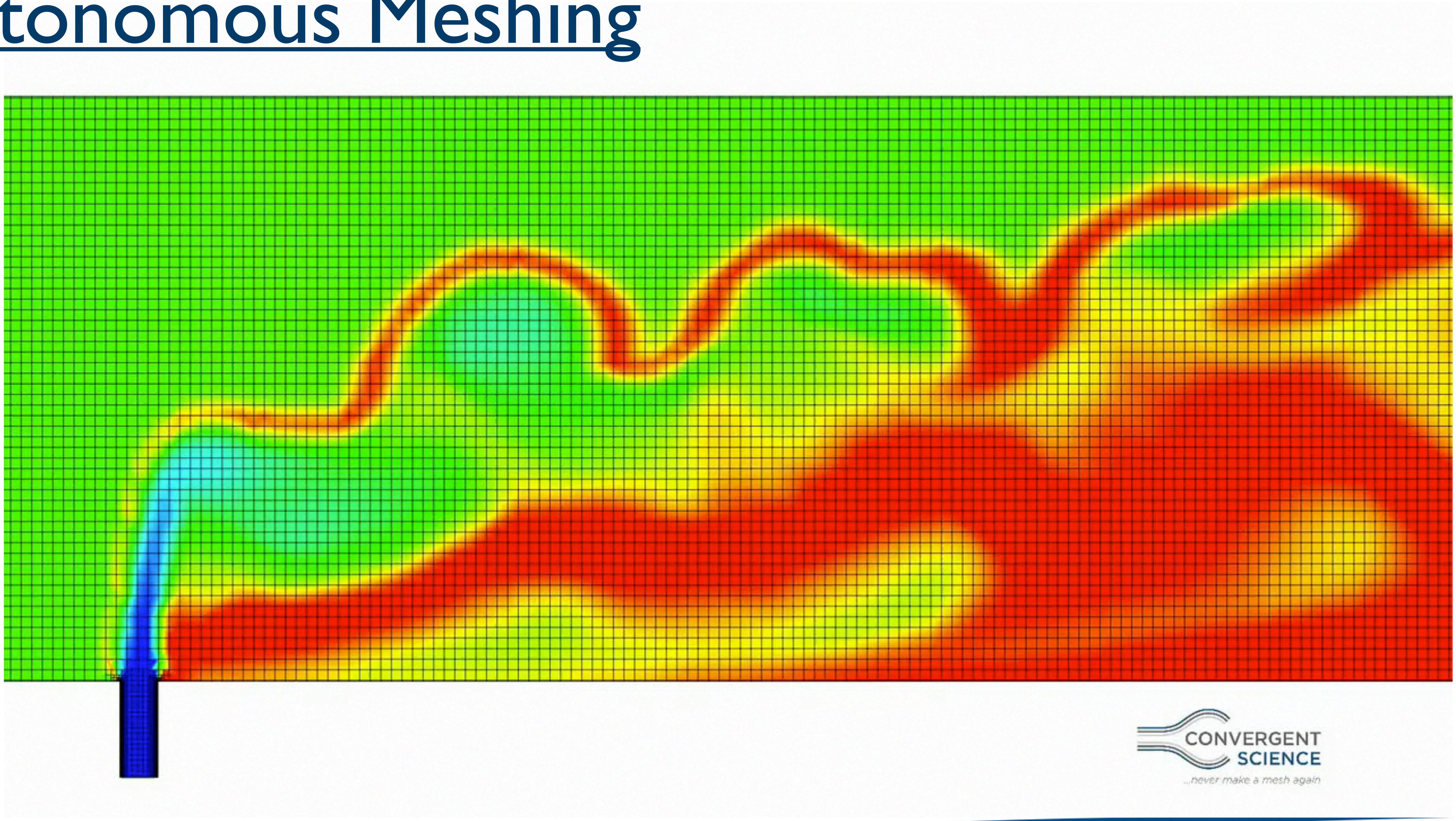
Autonomous Meshing

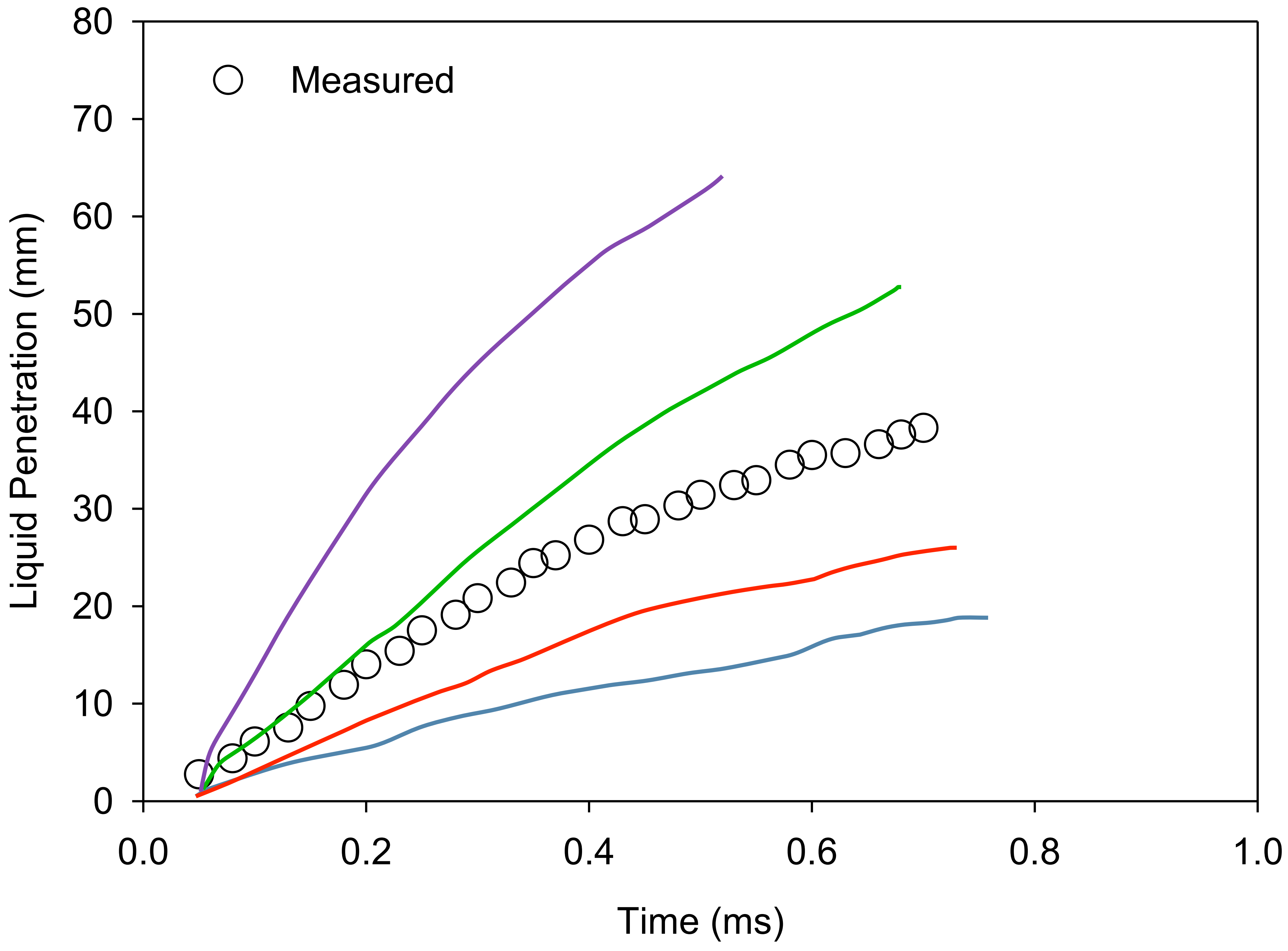


Grid Convergence

- Historically, grid convergence has been often overlooked
  - ★ Difficult to make one mesh, let alone a suite of meshes
  - ★ Fine meshes = long runtimes
- Errors from being under-resolved were swept away through sub-model constants
- Autonomous Meshing + HPC enable an ensemble of grids to be run for a simulation
- It is critical to make deliberate choices about mesh resolution from knowledge of the accuracy/speed tradeoff

Why is Grid Convergence Important?

- Lagrangian droplet models are extensively used to simulate IC Engine sprays
- Many researchers have reported a strong dependency of the spray on grid size
- What cell sizes should be used?
- What causes errors in simulations?
  - ★ input uncertainties?
  - ★ deficiencies in sub-models?
  - ★ under-resolved spray?



How Do We Overcome Grid Dependency?

- Use sub-models that are grid-convergent, not grid-independent
- As the mesh is refined the results approach a reasonably converged answer
- Adaptive Mesh Refinement (AMR) is a key component of this approach as it allows the use of very fine grids around the spray

Why?

- Model development and validation can be done with confidence as the results will not keep changing as the mesh is refined
- Recommendations on cell sizes to optimize the accuracy/runtime tradeoff can be made

Cases for Demonstrating Grid Convergence

Fuel	Diesel
Ambient Composition	SF_6
Ambient Temperature (K)	298
Ambient Density (kg/m³)	22
Injection Pressure (MPa)	80
Fuel Temperature (K)	363
Fuel Density (kg/m³)	806
Nozzle Diameter (mm)	0.14
Injection Duration (ms)	1.45

Non-evaporating data of Margot et al. (CMT)

Sandia National Laboratories

Engine Combustion Network
Average of 20-40 Spray Realizations

ECN Spray Case	Vaporizing Spray	Reacting Spray
Fuel	n-Dodecane	n-Heptane
Ambient Composition	0% O_2	10–21% O_2
Ambient Temperature (K)	900	800–1300
Ambient Density (kg/m³)	22.8	14.8, 30
Injection pressure (MPa)	150	150
Fuel Temperature (K)	363	373
Nozzle diameter (mm)	0.09	0.10
Injection Duration (ms)	1.5	6.8
Mass Injected (mg)	3.5	17.8

cmt motores térmicos

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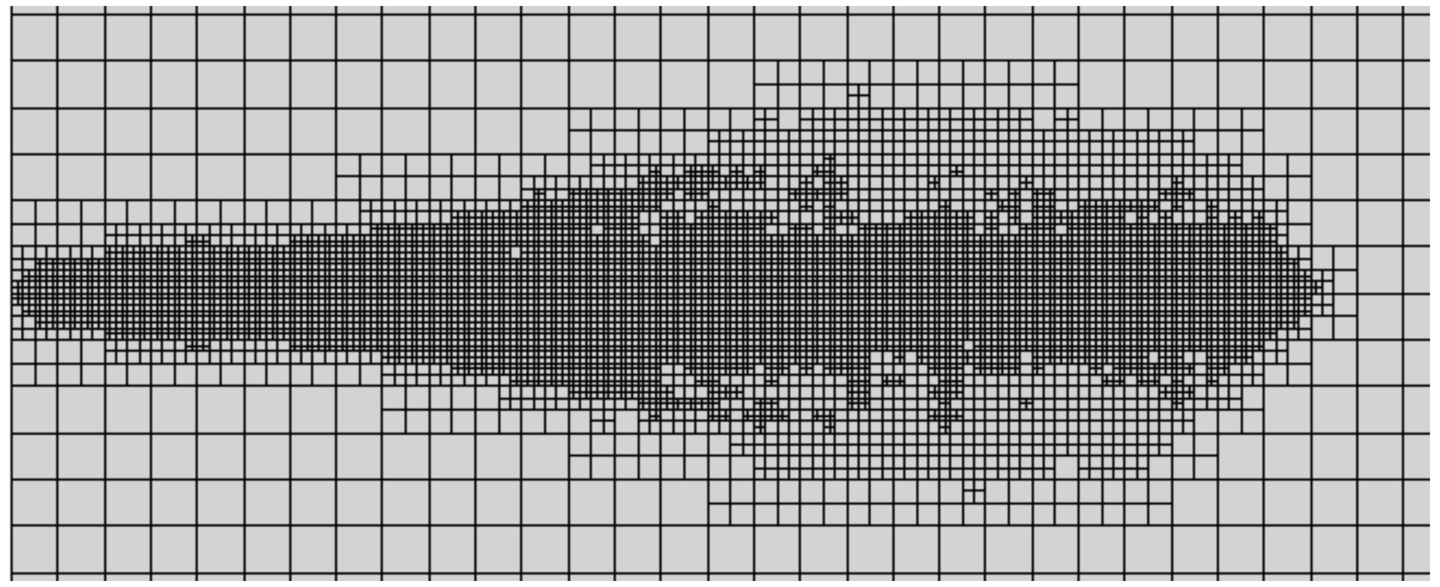
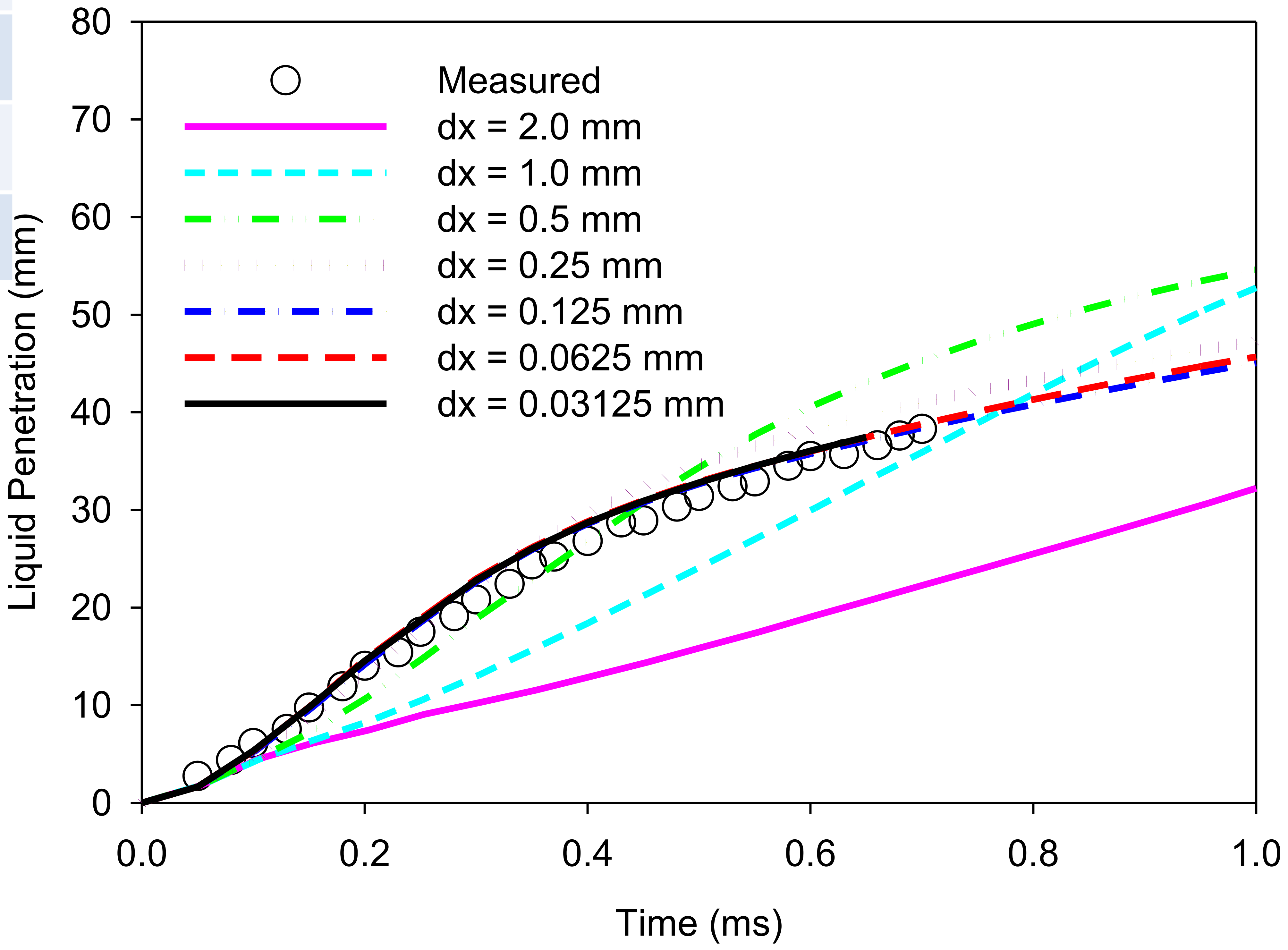
Results: Non-Evaporating Sprays

Embed Scale	Cell Size, dx (mm)	d_n / dx	Number of Injected Parcels
0	2.0	0.07	2,000
1	1.0	0.14	16,000
2	0.5	0.28	128,000
3	0.25	0.56	512,000
4	0.125	1.12	2,048,000
5	0.0625	2.24	8,192,000
6	0.03125	4.48	21,000,000



$$dx = dx_{base} \times 2^{-(embed\ scale)}$$

- Reasonable grid convergence achieved at 0.25 mm
- Similar cell sizes found for evaporating and reacting sprays



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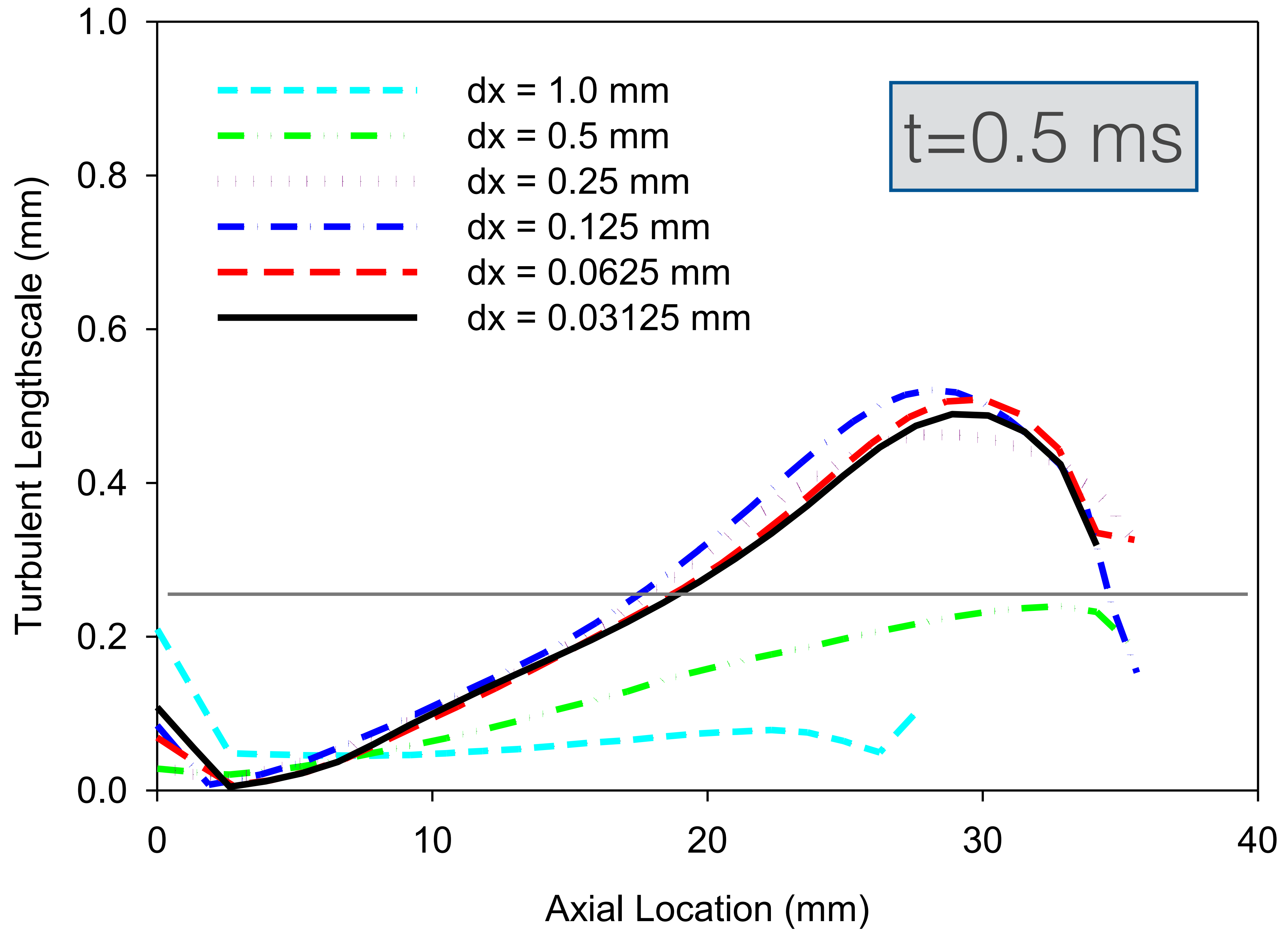
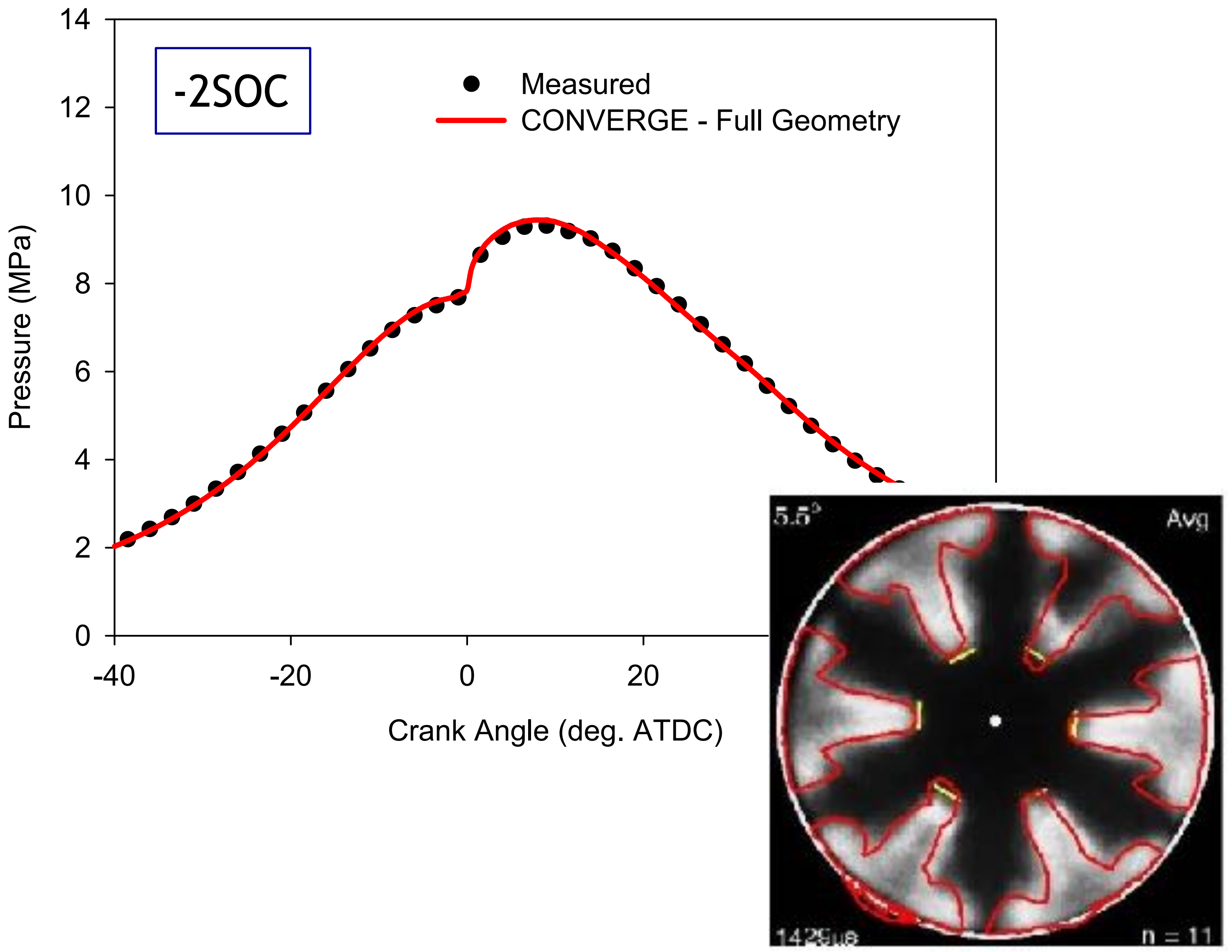
Results: Non-Evaporating Sprays

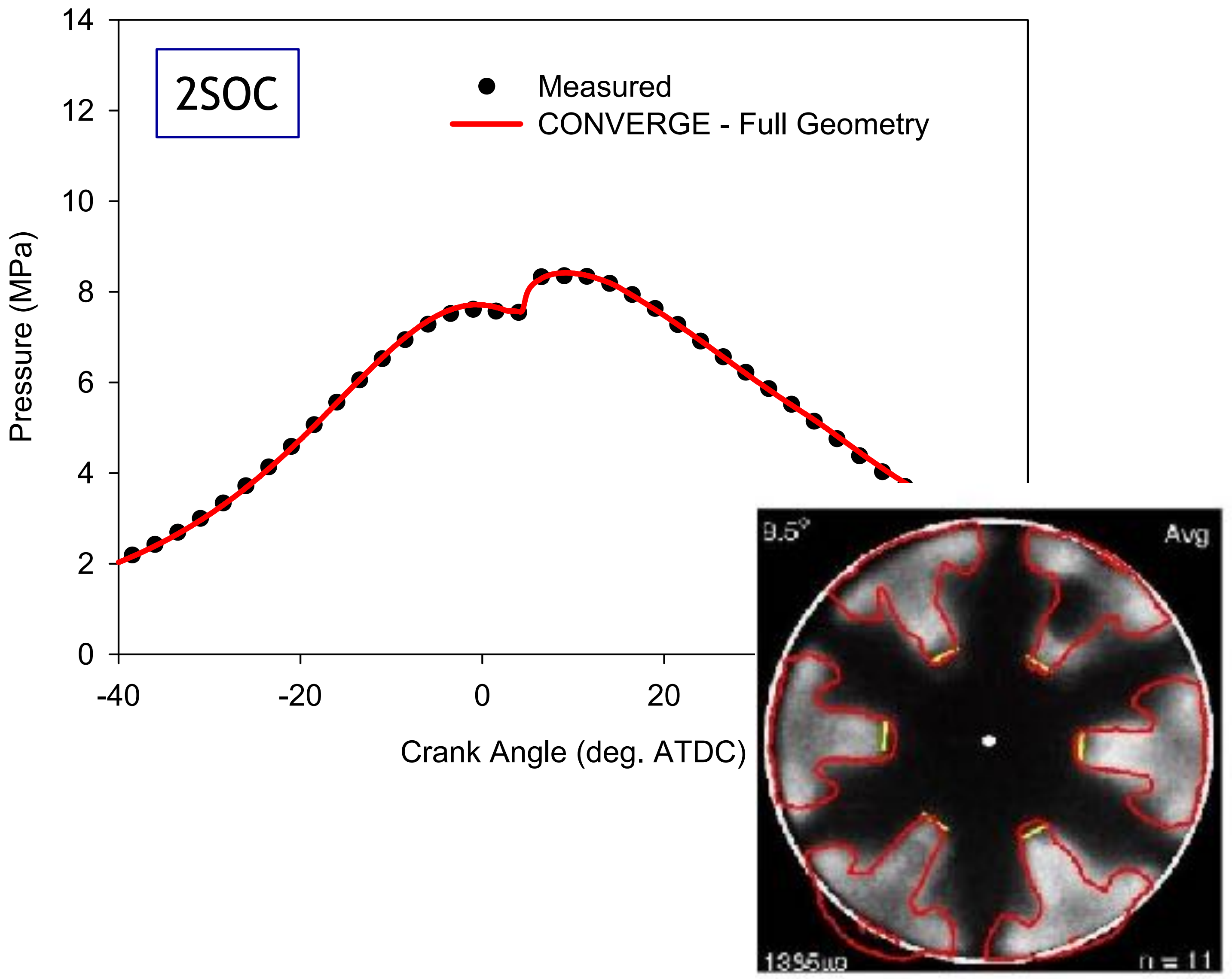


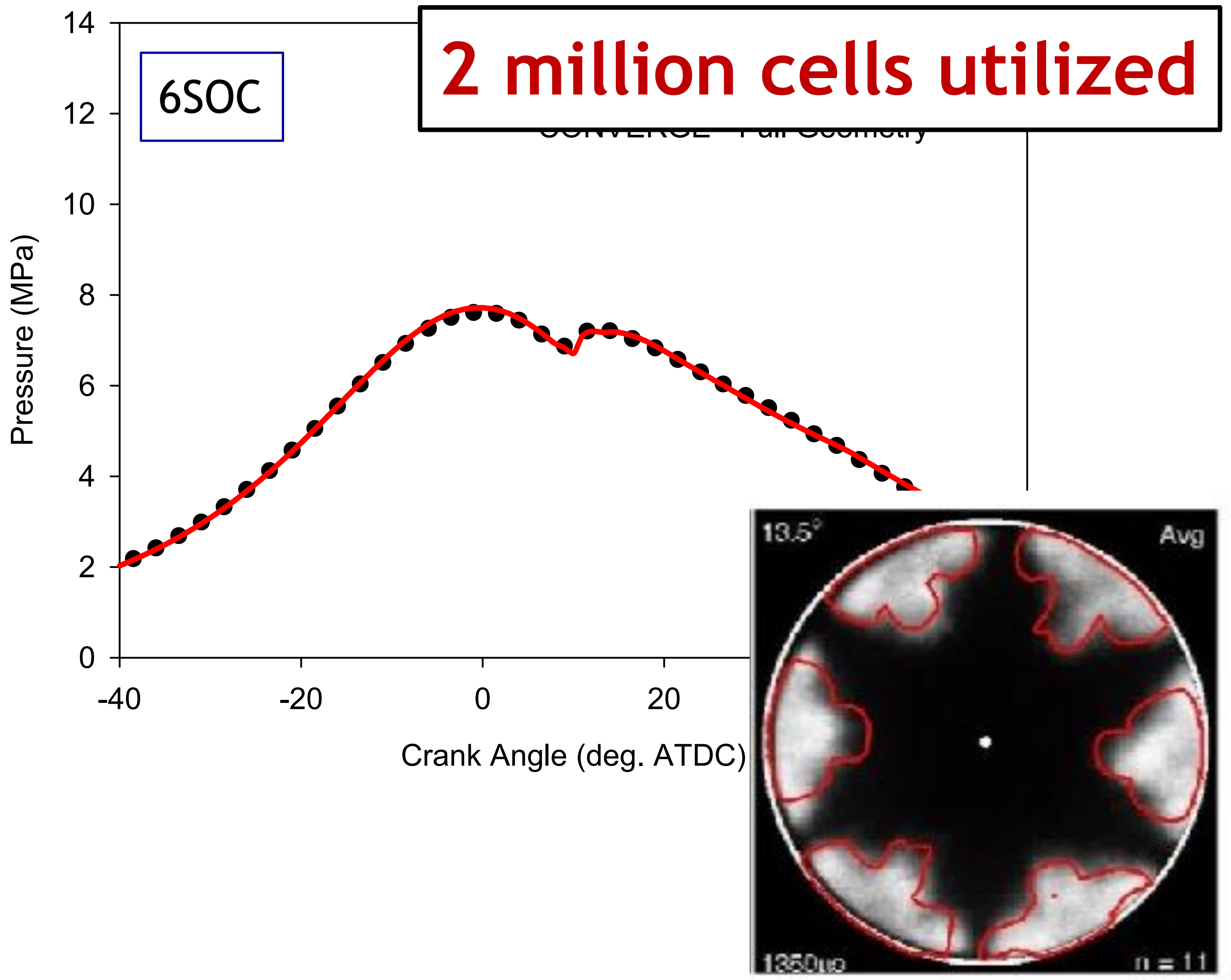
$$l_t = \left(\nu_t^{\,3} / \varepsilon \right)^{1/4} = C_\mu^{\,3/4} k^{3/2} / \varepsilon$$

- Turbulent length-scale shown is an indication of the smallest scales in the domain
- Length-scale achieves reasonable grid-convergence at 0.25 mm
- Length-scales predicted for coarse grids (1.0 mm and 0.5 mm) are significantly lower than the cell sizes
  - ★ Understandable that these simulations are not converged as they do not resolve the smallest scales
- Cells of 0.25 mm and smaller are below the size of the turbulent length-scales throughout much of the spray
  - ★ Important scales are resolved resulting in grid-convergence

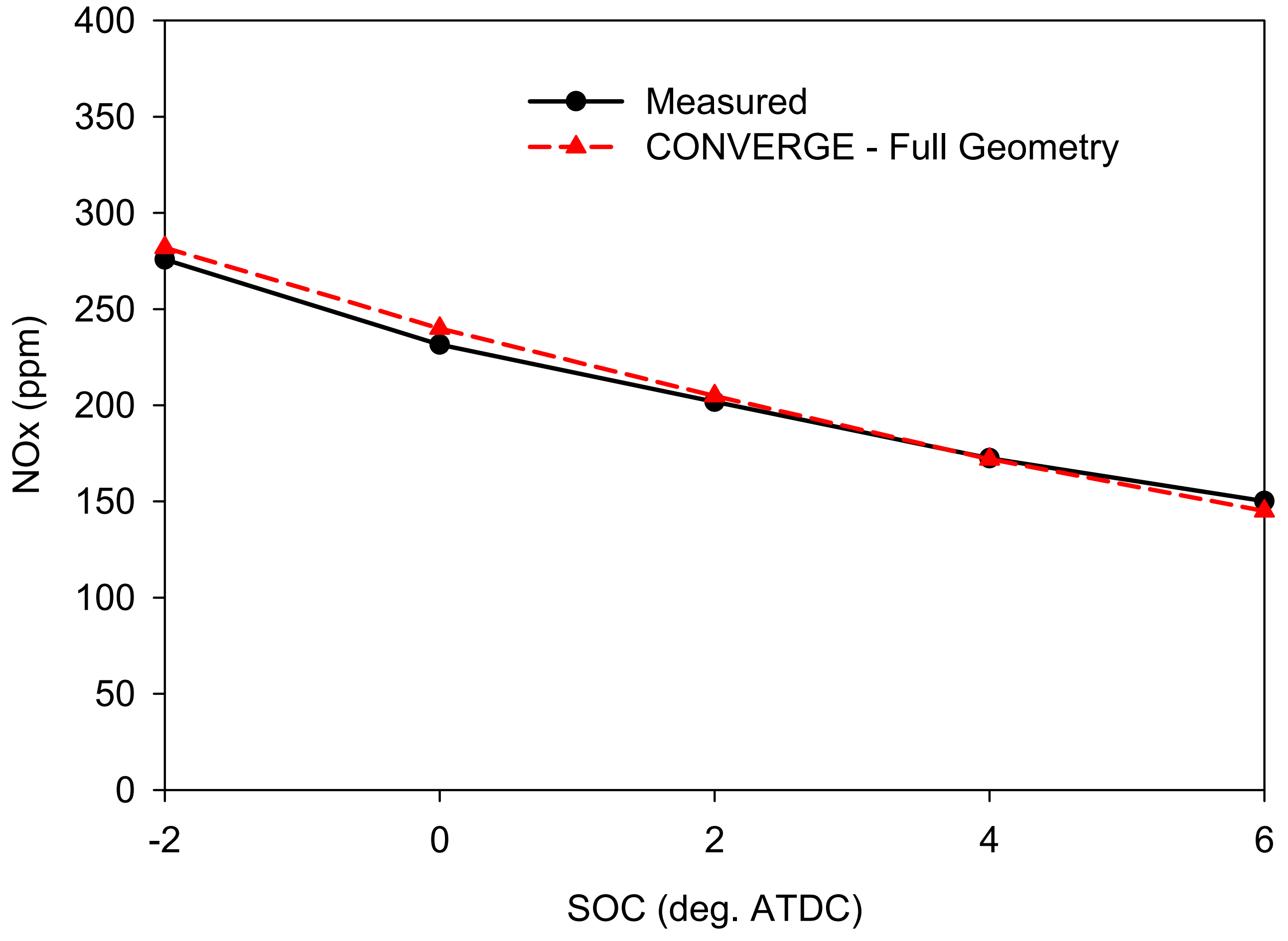
Results: Optical Diesel Engine



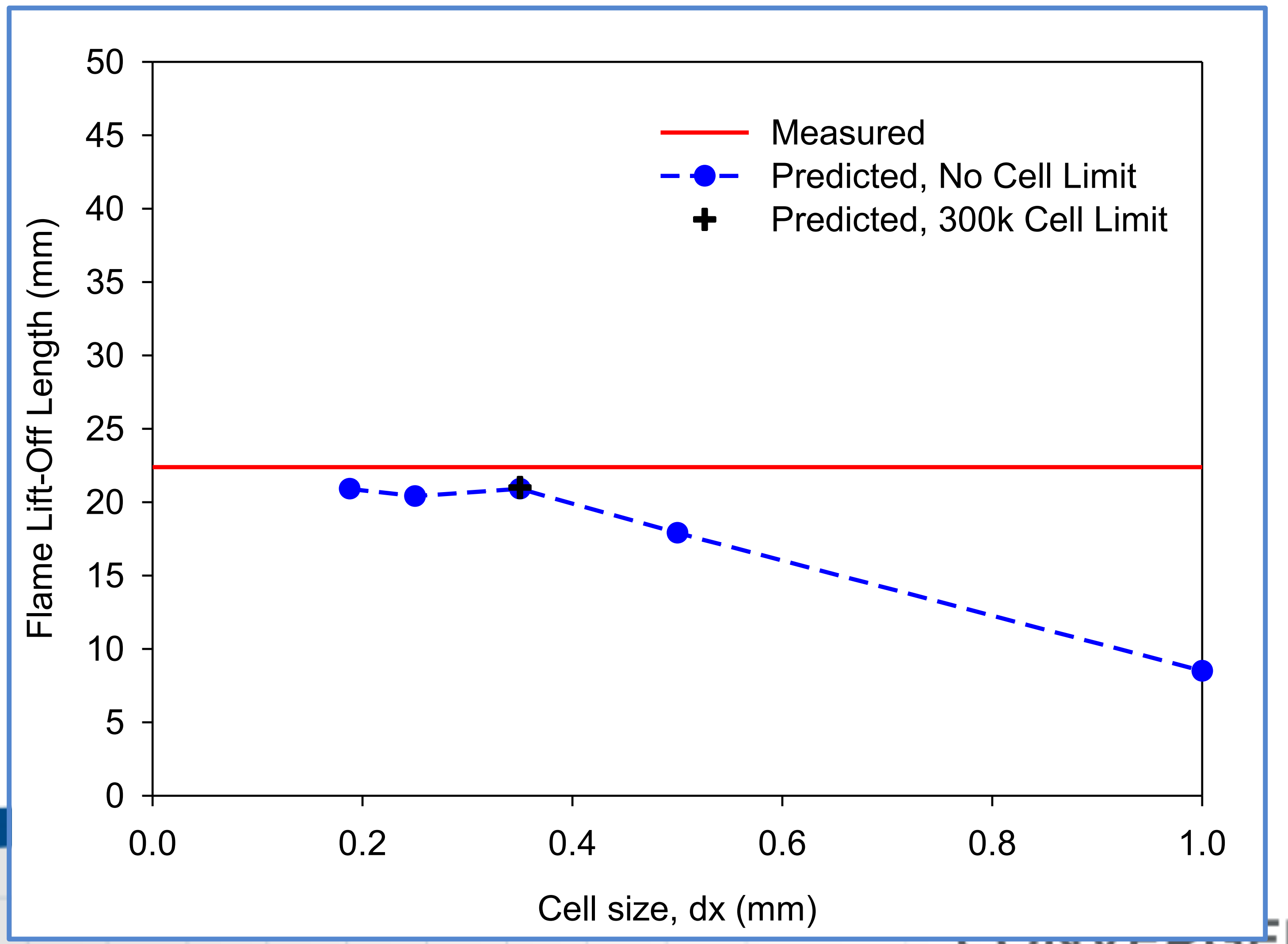




OH* Chemiluminescence vs. OH iso-surface, 7.5 degrees after SOC



The grid-convergent methodology results in excellent agreement with global combustion behavior as well as flame lift-off length and flame location



*Senecal et al., *J. Eng. Gas Turbines Power*, 2014

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CAT

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How Many Parcels?

Embed Scale	Cell Size, dx (mm)	d_n / dx	Number of Injected Parcels
0	2.0	0.07	2,000
1	1.0	0.14	16,000
2	0.5	0.28	128,000
3	0.25	0.56	512,000
4	0.125	1.12	2,048,000
5	0.0625	2.24	8,192,000
6	0.03125	4.48	21,000,000

8x

8x

4x

4x

4x

2.5x

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How Many Parcels?

UMASS AMHERST SIEMENS

$$n_{pc} \propto \frac{1}{\Delta x^{2c-1}}$$

- ILASS 2017 Paper
- n_{pc} is the number of parcels per cell
- c is the rate of convergence
- Keeping the number of parcels per cell constant, results in order 1/2 convergence
- For first-order, n_{pc} should be increased by a factor of 2
- For second-order, n_{pc} should be increased by a factor of 8
- Verifies results of Senecal et al. for grid convergence
- But still doesn't answer the question - how many parcels for a given cell size for a given amount of liquid mass?

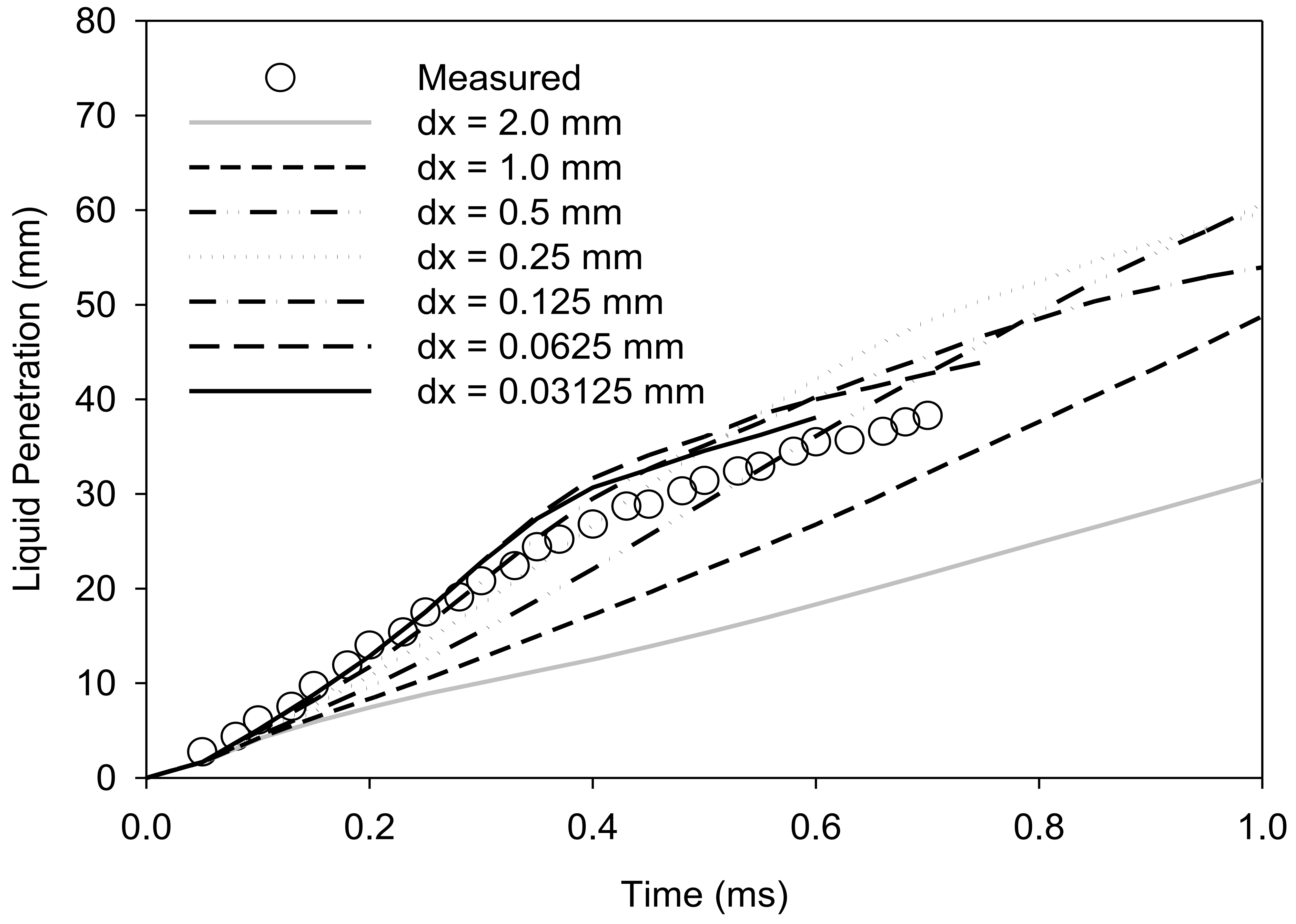
What About LES?

- With parallel processing and faster CPU speeds, Large Eddy Simulation (LES) is becoming an increasingly practical technique for IC engine modeling.
- Recently it has been shown that LES can provide good qualitative and quantitative comparisons to instantaneous engine spray measurements since it directly resolves the large scales in the flow field.
- The typical approach for RANS modeling is to simulate a single injection as RANS tends to dampen out small-scale perturbations through the turbulent viscosity.
- LES modeling does not dampen out these small-scale perturbations and is similar to a single-shot experimental injection.
- Two major questions when running LES: what is the grid resolution that should be used, and how many realizations need to be simulated?

LES Grid Convergence for Non-Evaporating Sprays

Embed Scale	Cell Size, dx (mm)	d_n / dx	Number of Injected Parcels	Cell Count at 0.6 ms
0	2.0	0.07	15,625	54,540
1	1.0	0.14	15,625	410,844
2	0.5	0.28	62,500	421,659
3	0.25	0.56	250,000	493,486
4	0.125	1.12	1,000,000	933,464
5	0.0625	2.24	2,000,000	3,731,098
6	0.03125	4.48	4,000,000	23,672,040

$$dx = dx_{base} \times 2^{-(embed\ scale)}$$



- Reasonable grid convergence between 0.0625 and 0.125 mm

motores térmicos

Non-evaporating data of Margot et al. (CMT)

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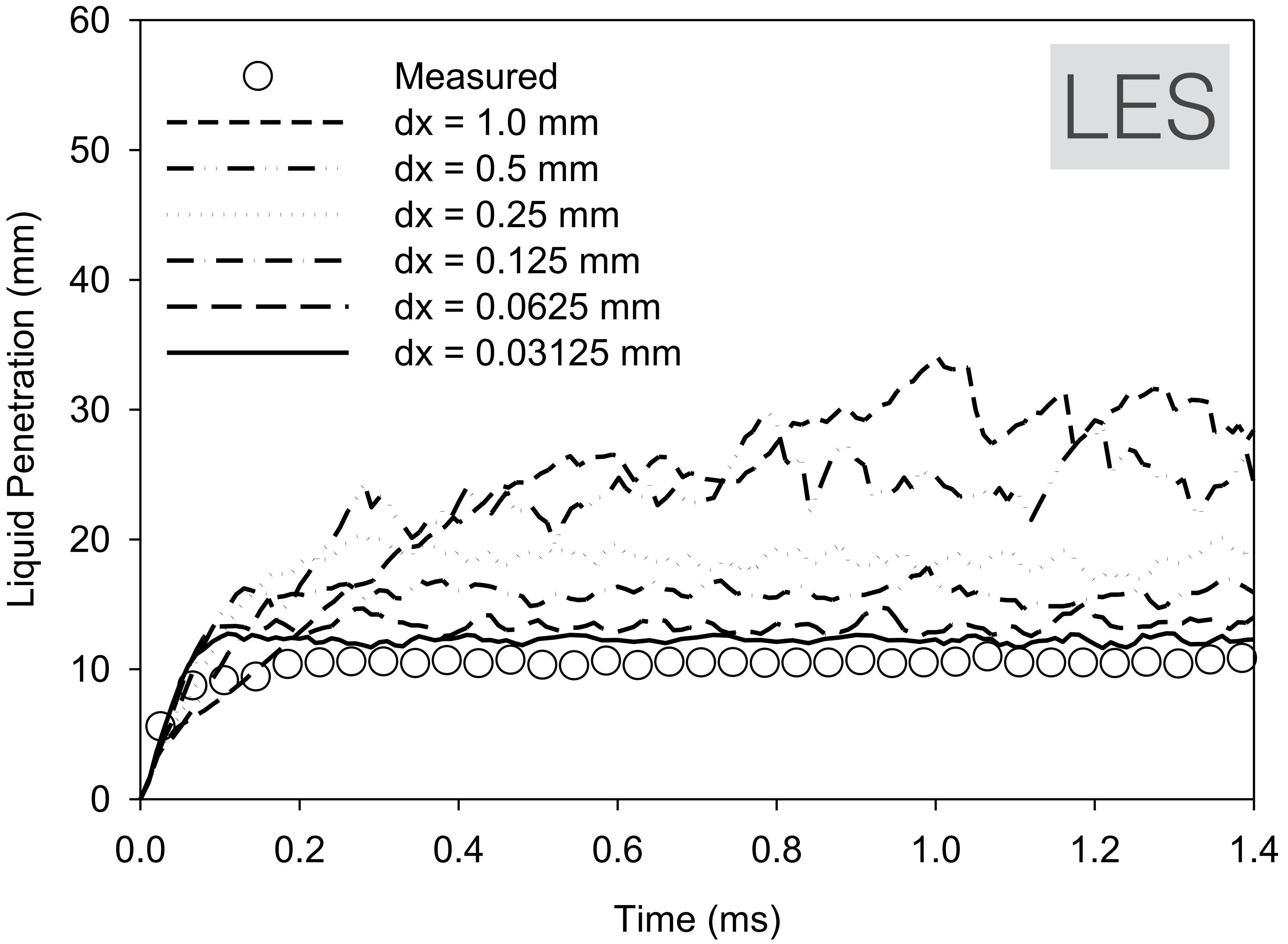
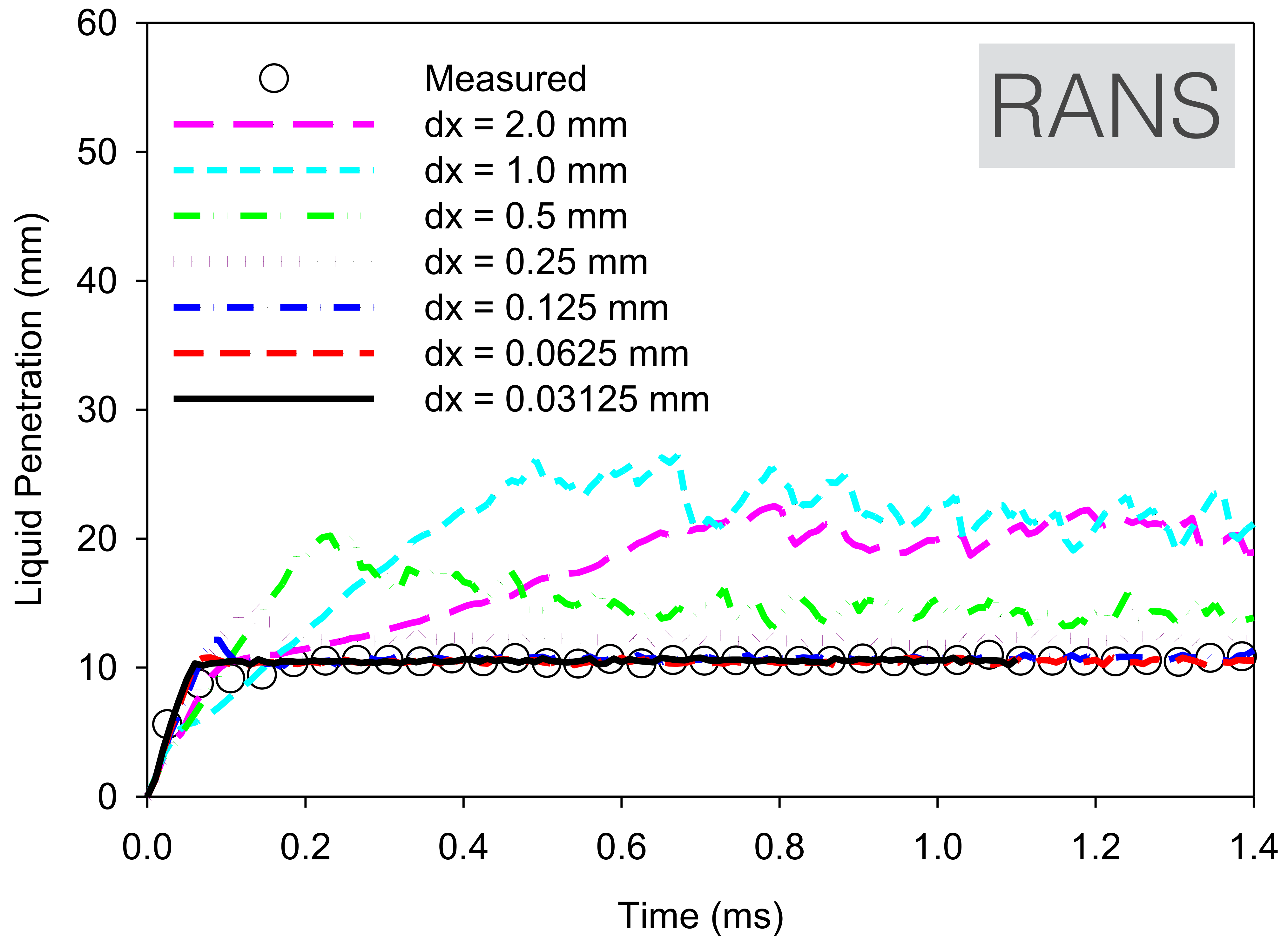
LES Grid Convergence for Evaporating Sprays

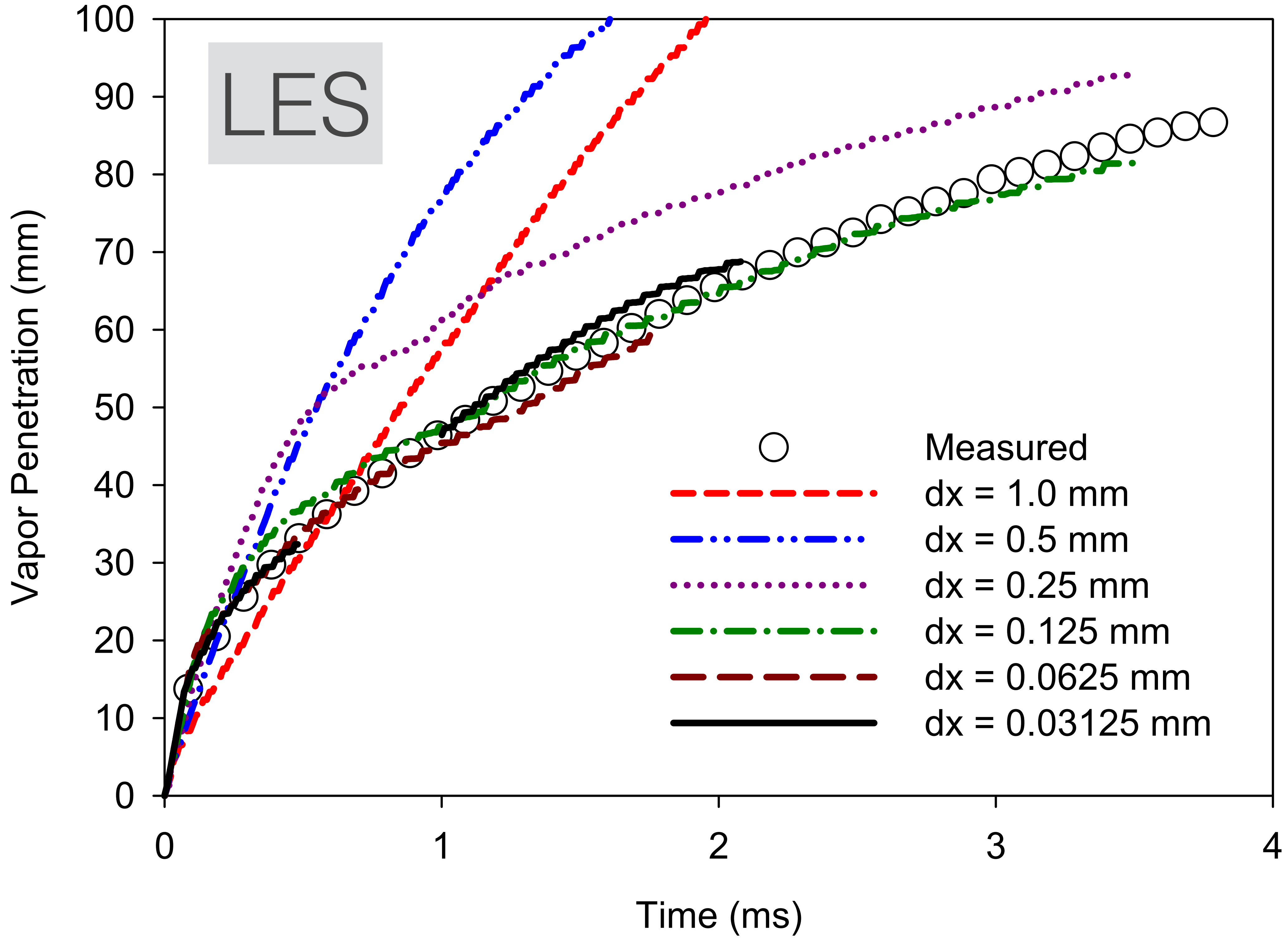


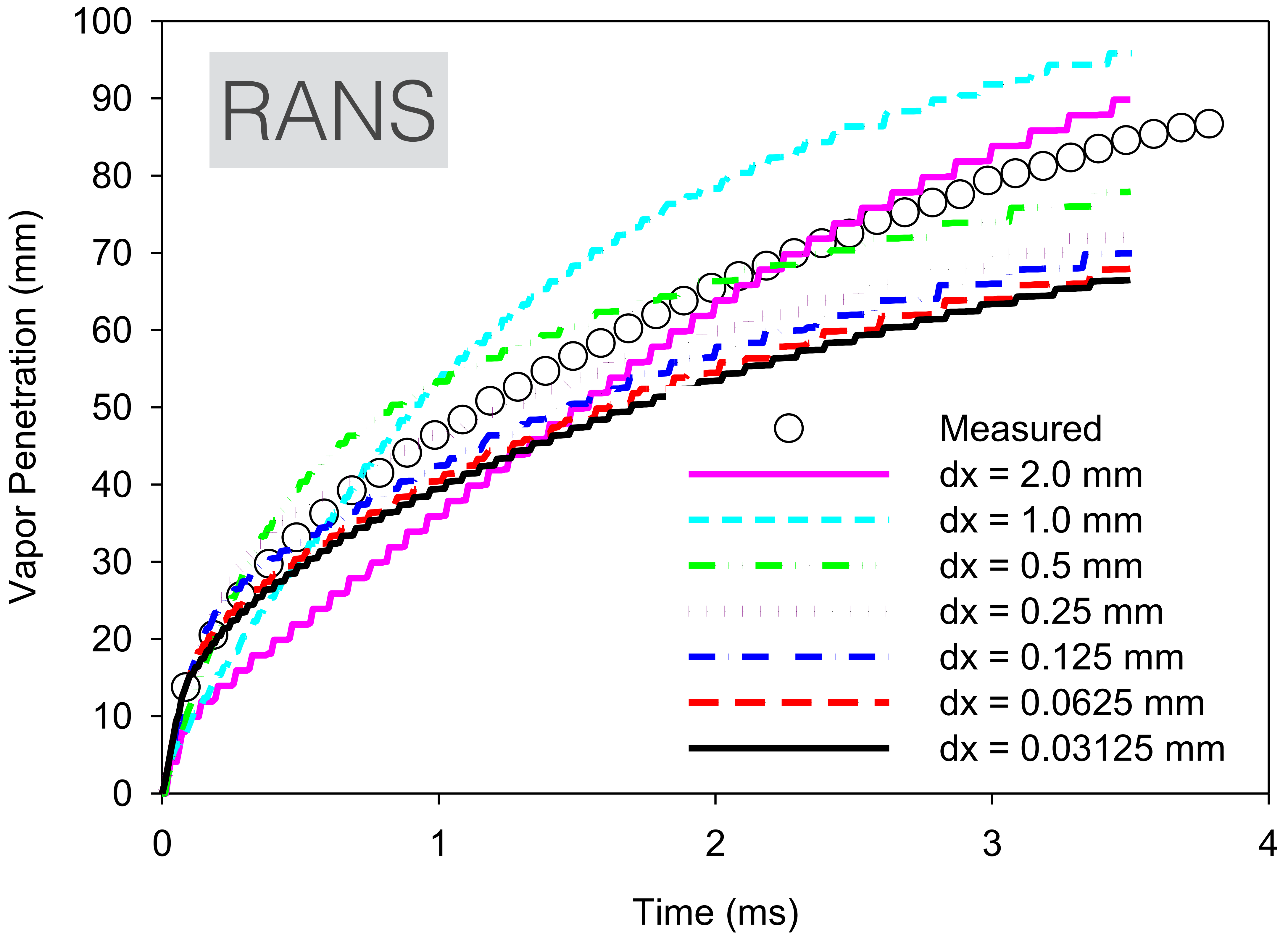


- Coarse grids significantly over-predict the liquid length (both LES and RANS)
- For LES, cell sizes of 0.0625 mm and finer are grid convergent
- For RANS, cell sizes of 0.25 mm and finer are grid convergent

Spray A

LES Grid Convergence for Evaporating Sprays





- LES vapor penetration exhibits grid-convergent behavior at 0.125 mm and agrees well with data
- RANS vapor penetration exhibits grid-convergent behavior at 0.25 mm but the later part converges to the wrong value
- Local instantaneous fuel-air mixing is better predicted with LES compared to RANS

Spray A

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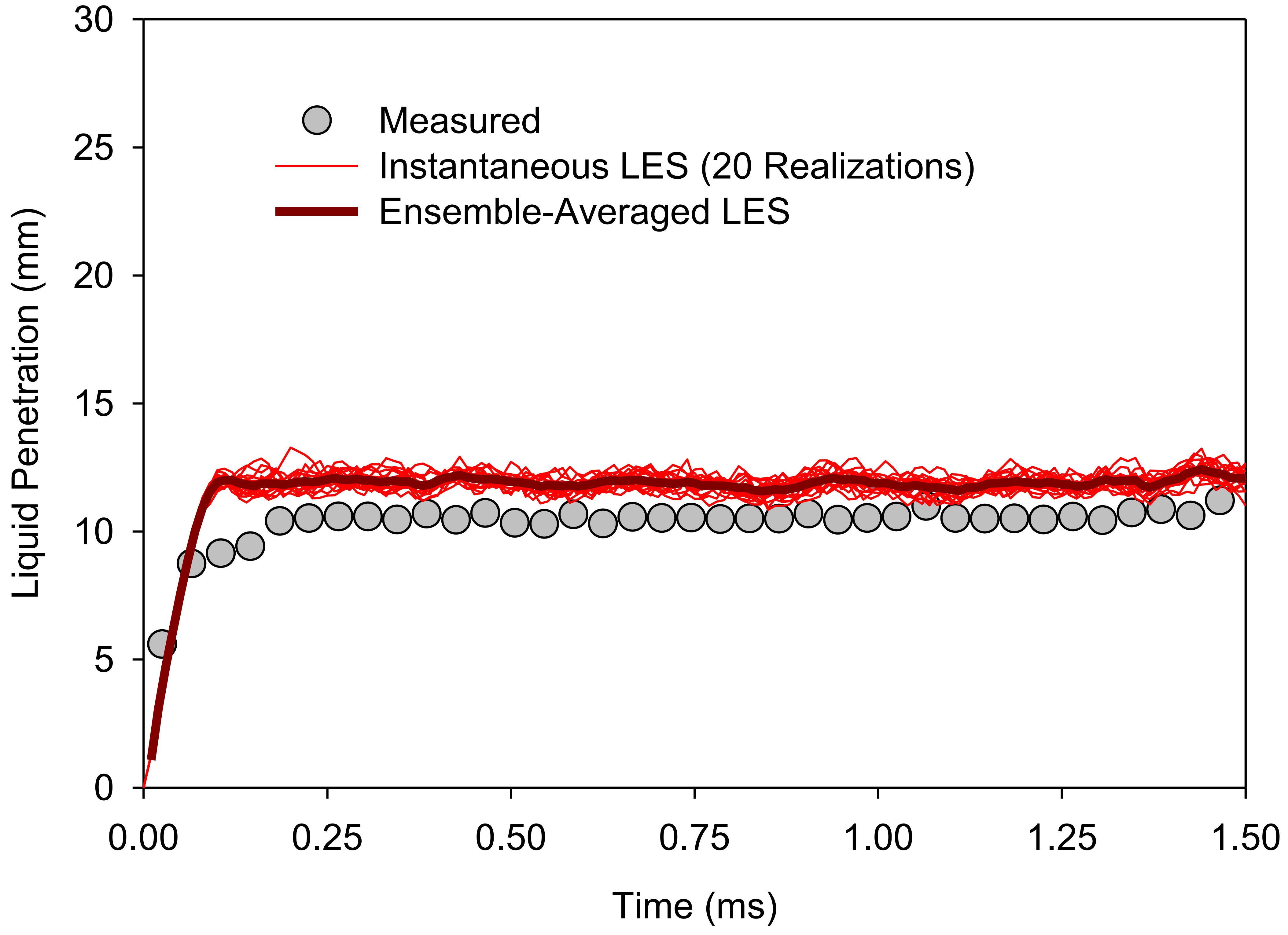
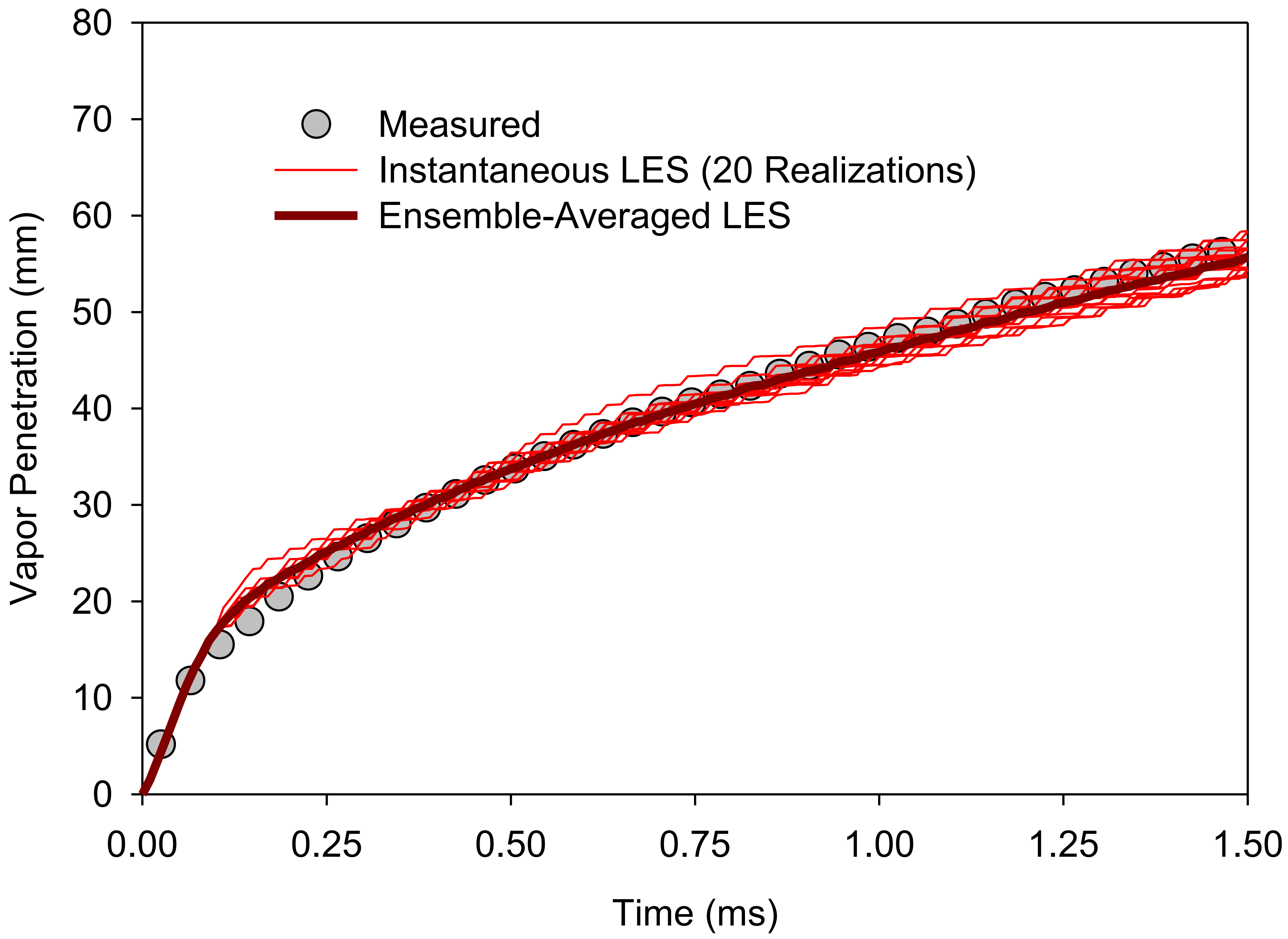
What About Multiple Realizations?





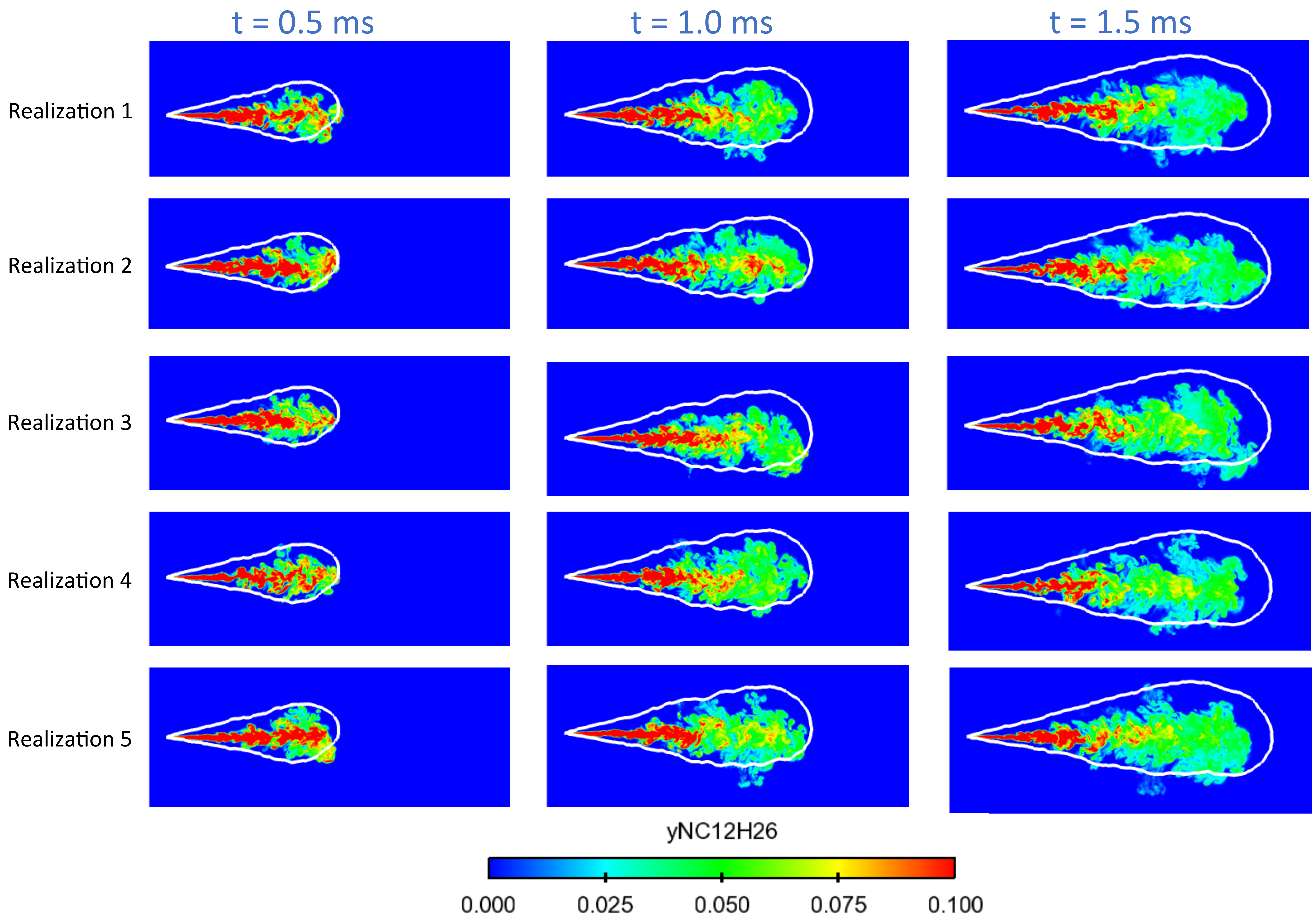
- Similarities in penetration curves suggest that a single realization is enough when looking at global parameters such as penetration

Spray A, 0.0625 mm

What About Multiple Realizations?

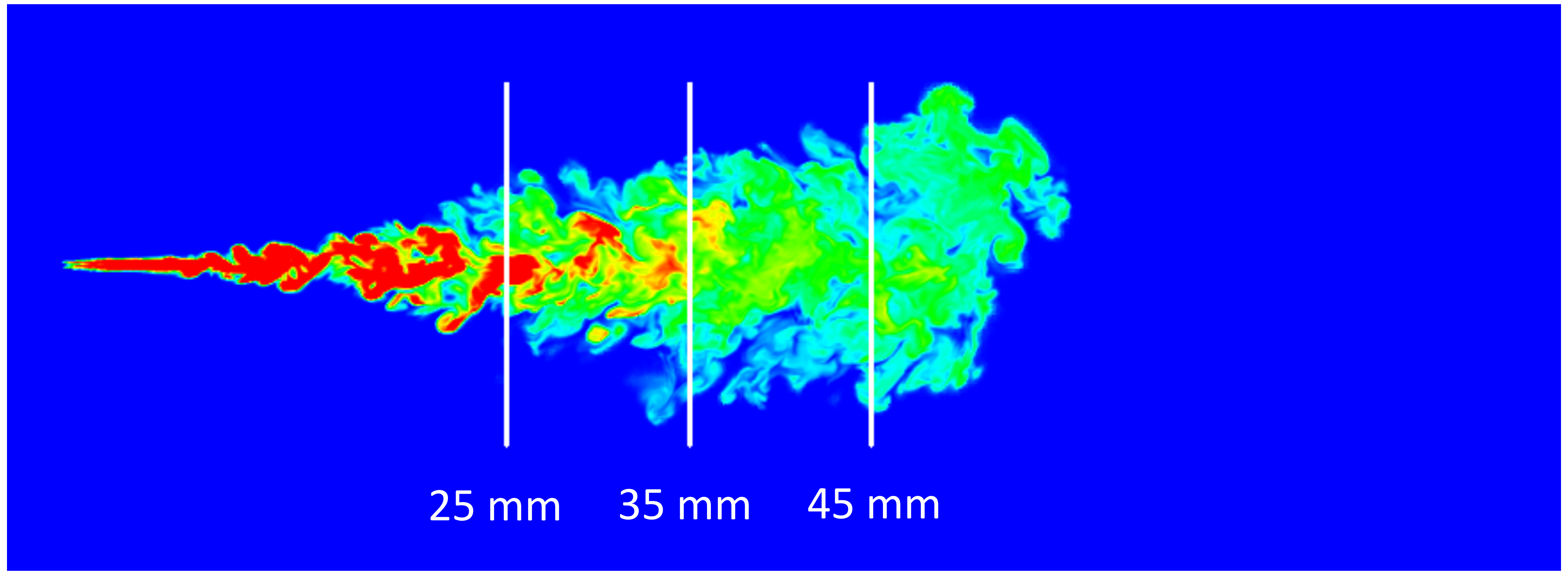
Base mesh size	1.0 mm
Fixed nozzle embedding	0.0625 mm
Velocity AMR	0.0625 mm
Maximum cell count specified	20 million
Maximum cell count at 1.5 ms	18 million

- All LES realizations do a reasonable job matching both penetration and extent of vapor in the radial direction

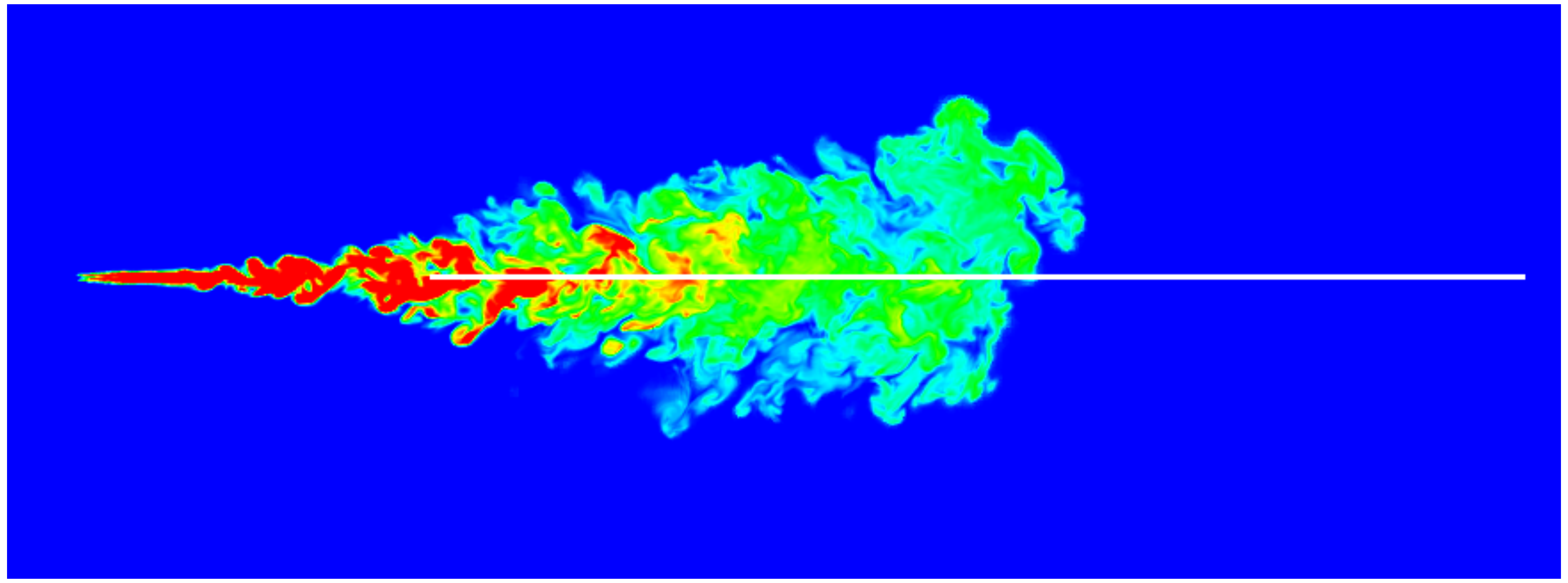


Spray A

Examining Local Quantities



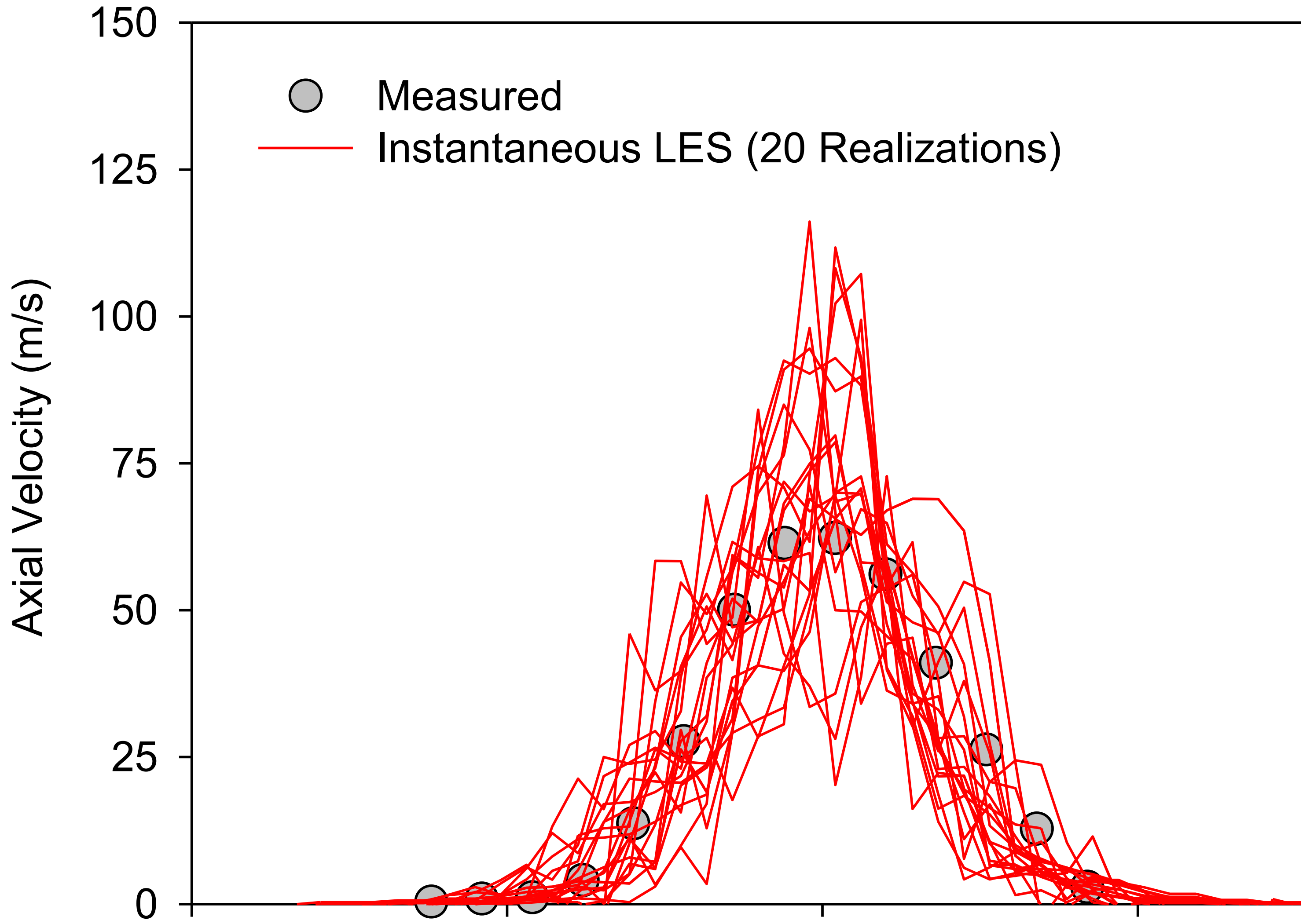
- Transverse profiles at three locations

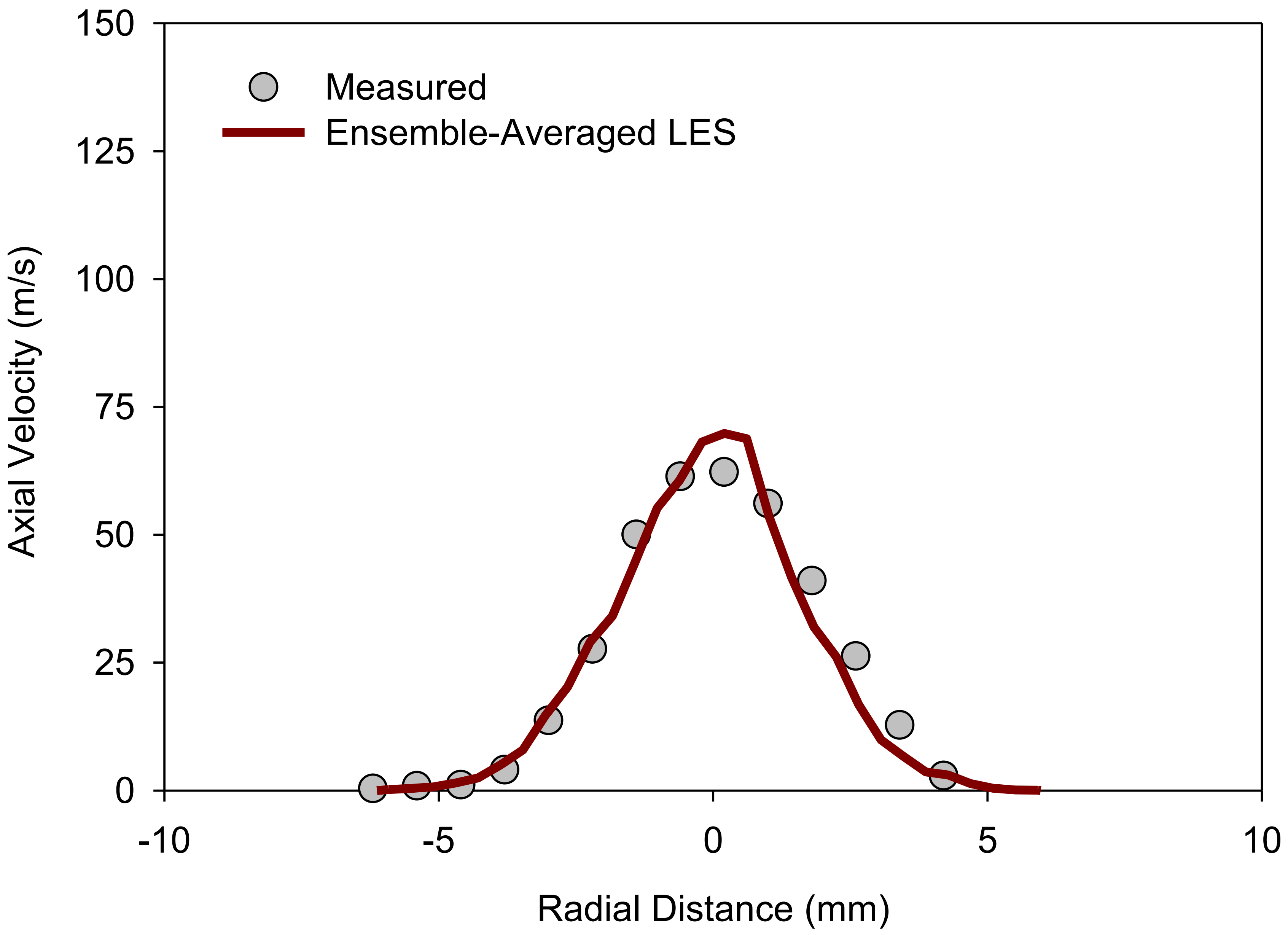


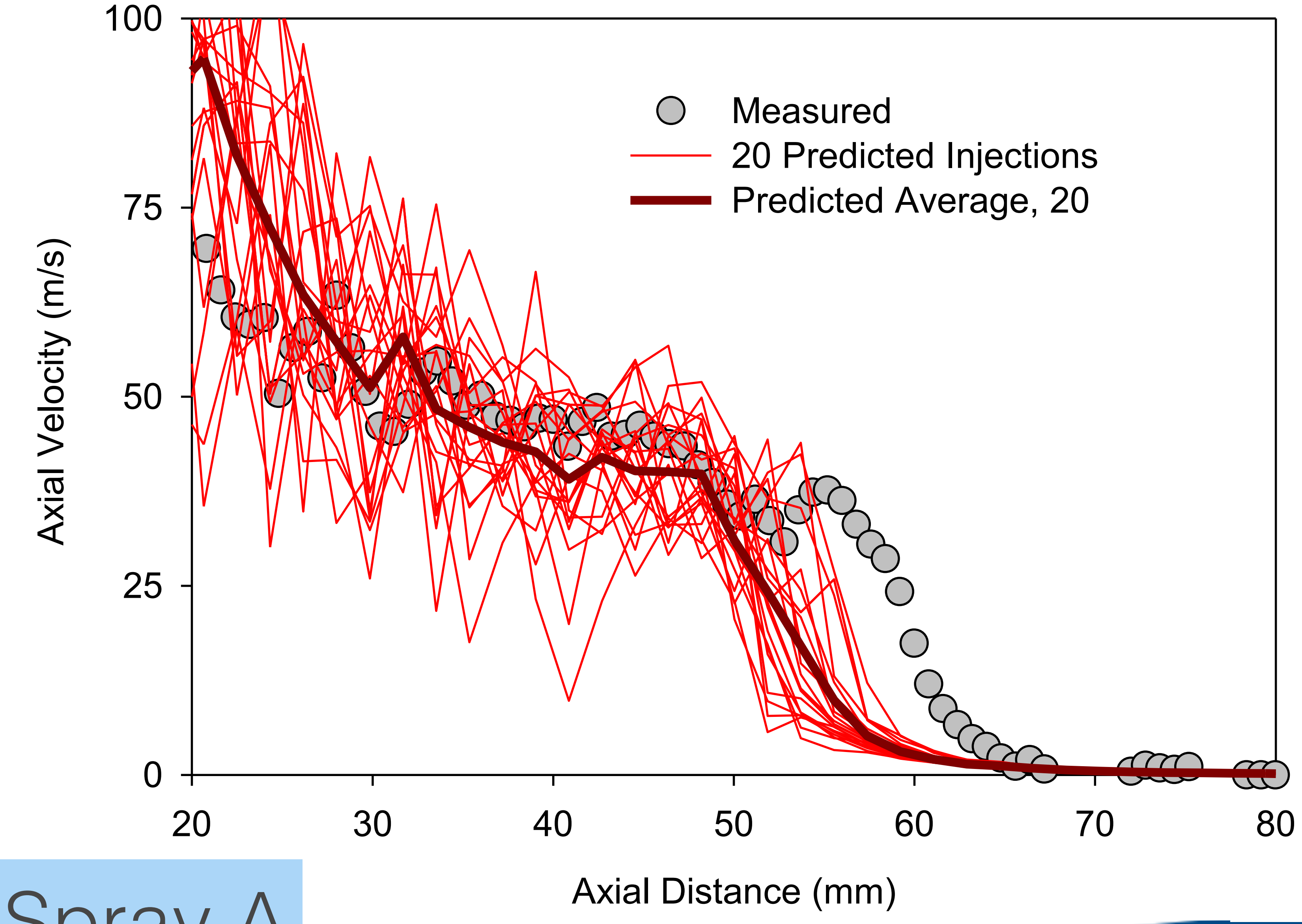
- Centerline profiles between 20 and 80 mm

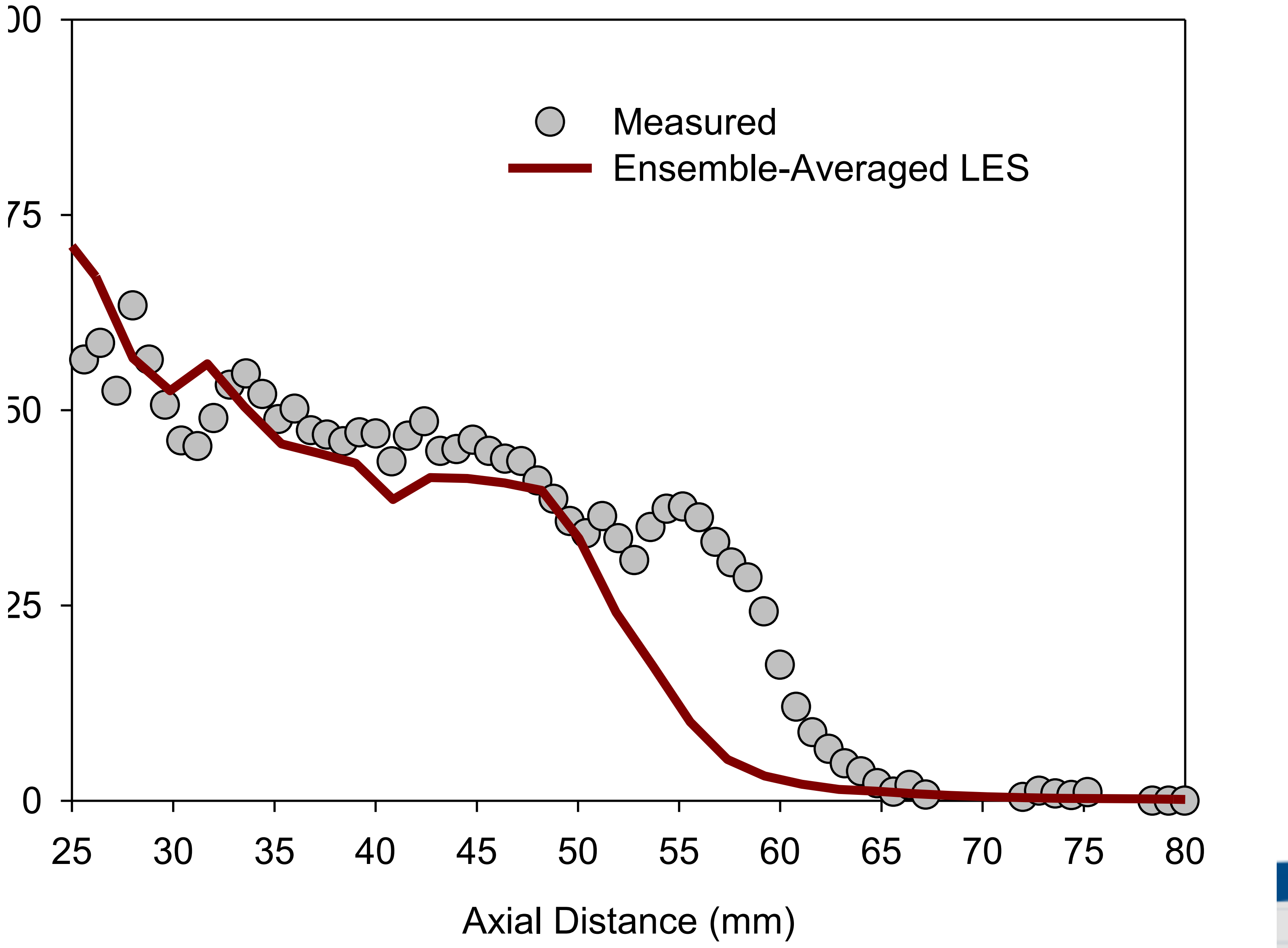
Local Quantities - Velocity

- Transverse velocity at 25 mm









- Centerline velocity

Spray A

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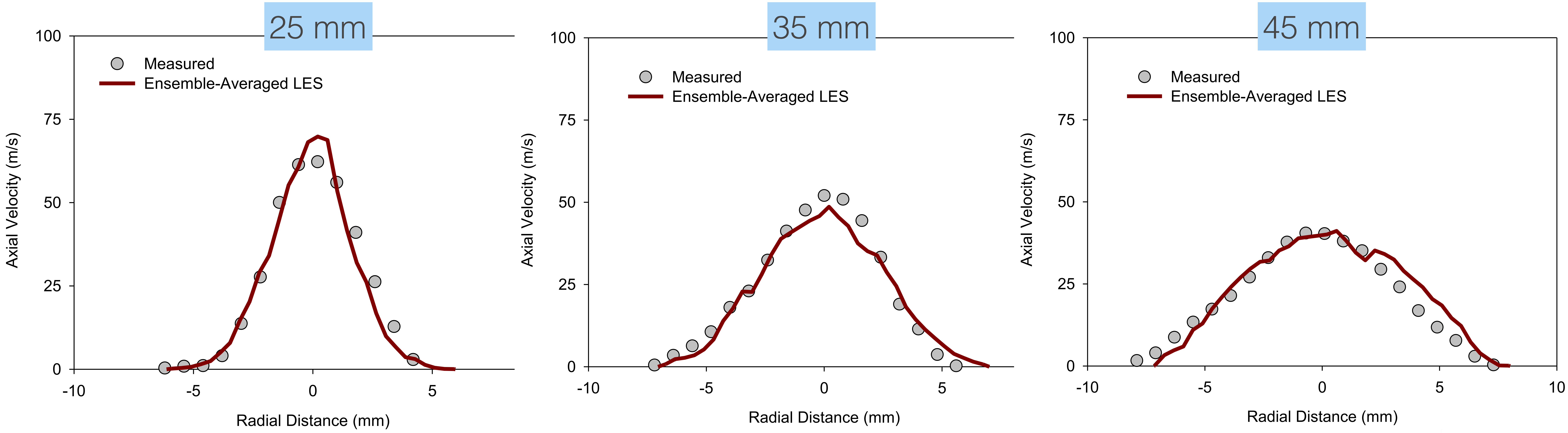
Local Quantities - Velocity



Spray A

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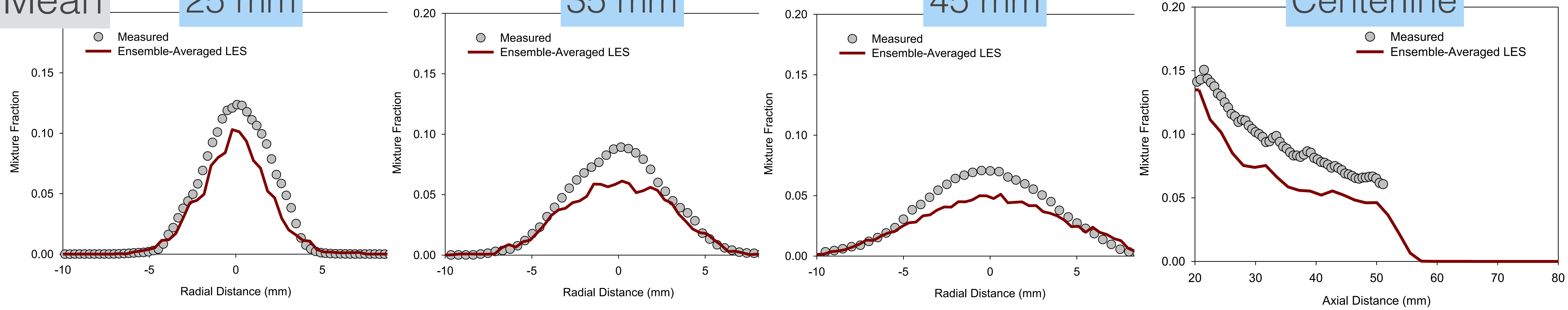
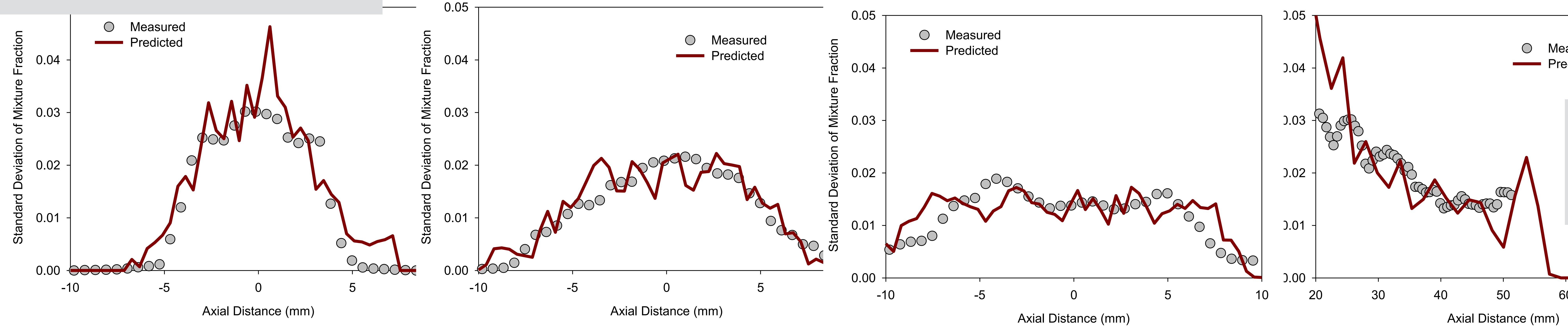
Local Quantities - Mixture Fraction

Mean



Standard Deviation

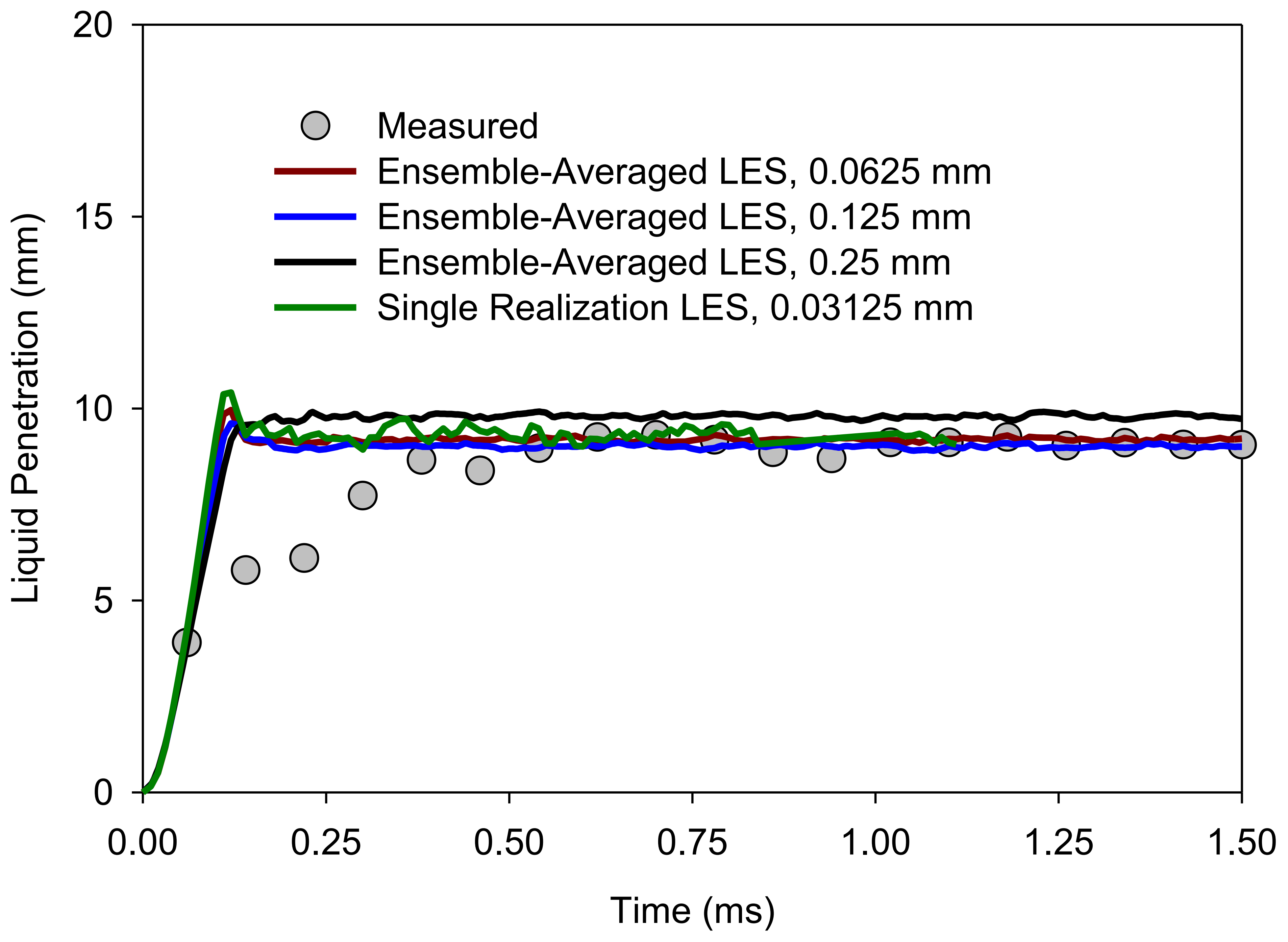


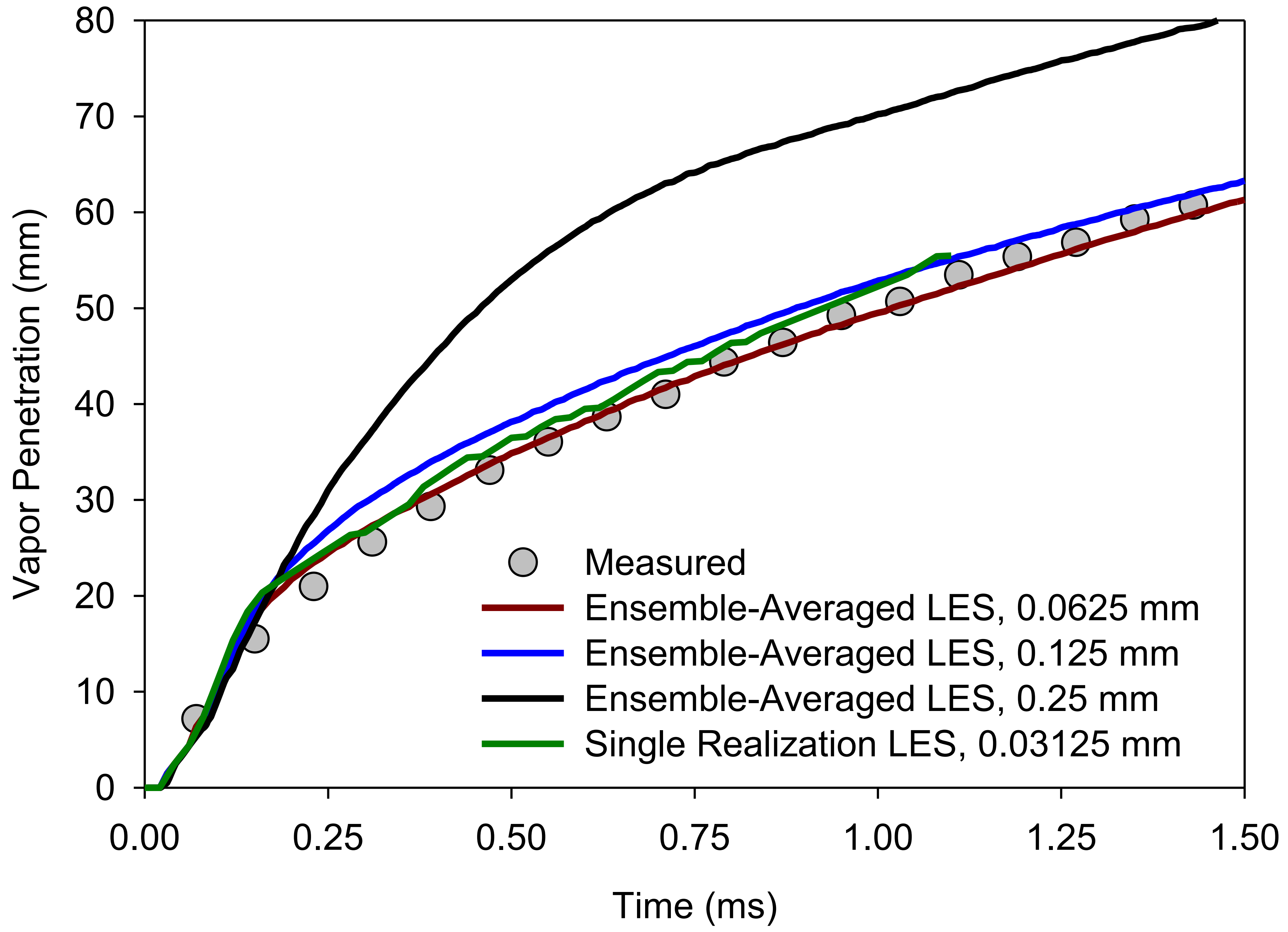
$$s = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}\left(x_i - \bar{x}\right)^2}$$

- Spread in mixing over the range of predicted realizations is similar to what is seen experimentally

Spray A

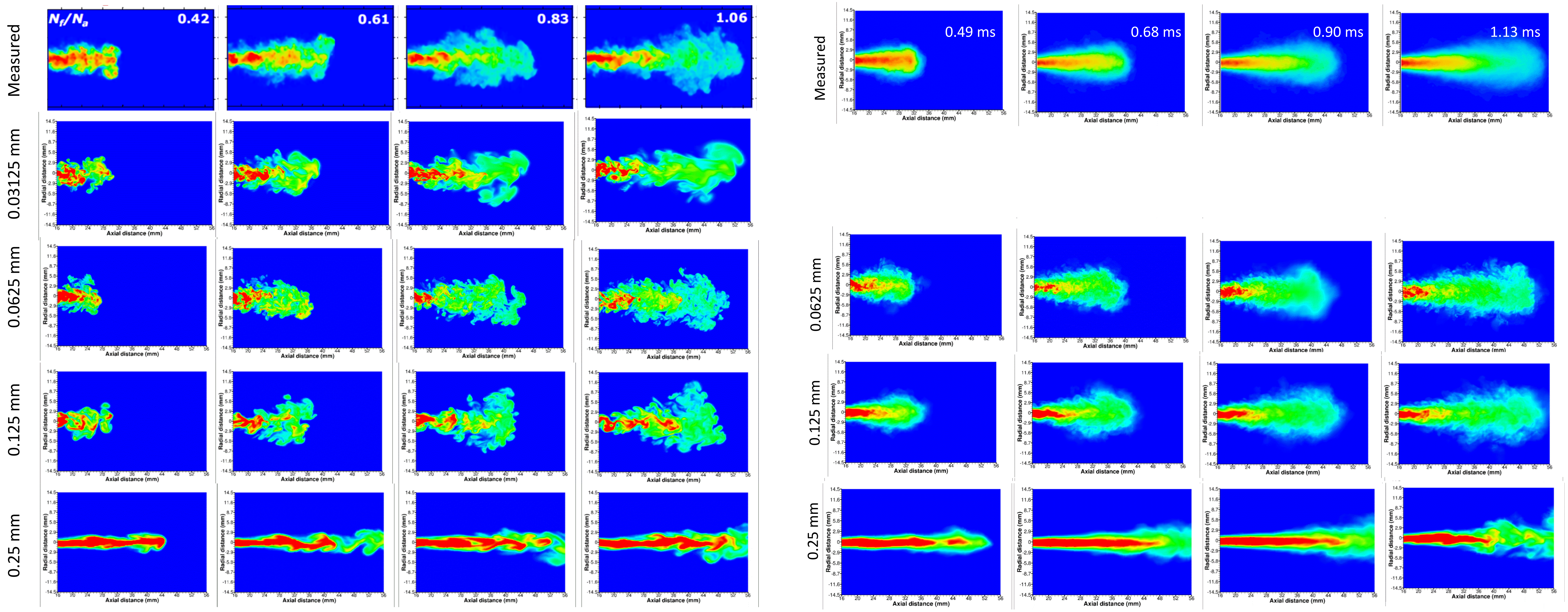
LES of Spray H





Case	0.25 mm	0.125 mm	0.0625 mm	0.03125 mm
Base mesh size	1.0 mm	1.0 mm	1.0 mm	1.0 mm
Fixed nozzle embedding	0.25 mm	0.125 mm	0.0625 mm	0.03125 mm
Velocity AMR	0.25 mm	0.125 mm	0.0625 mm	0.03125 mm
Number of realizations	28	28	28	1
Maximum cell count at 1.0 ms	1.3 million	3.1 million	15.8 million	20 million (maximum)
Number of parcels injected	50,000	200,000	800,000	3,200,000

LES of Spray H - Instantaneous & Mean Mixture Fraction



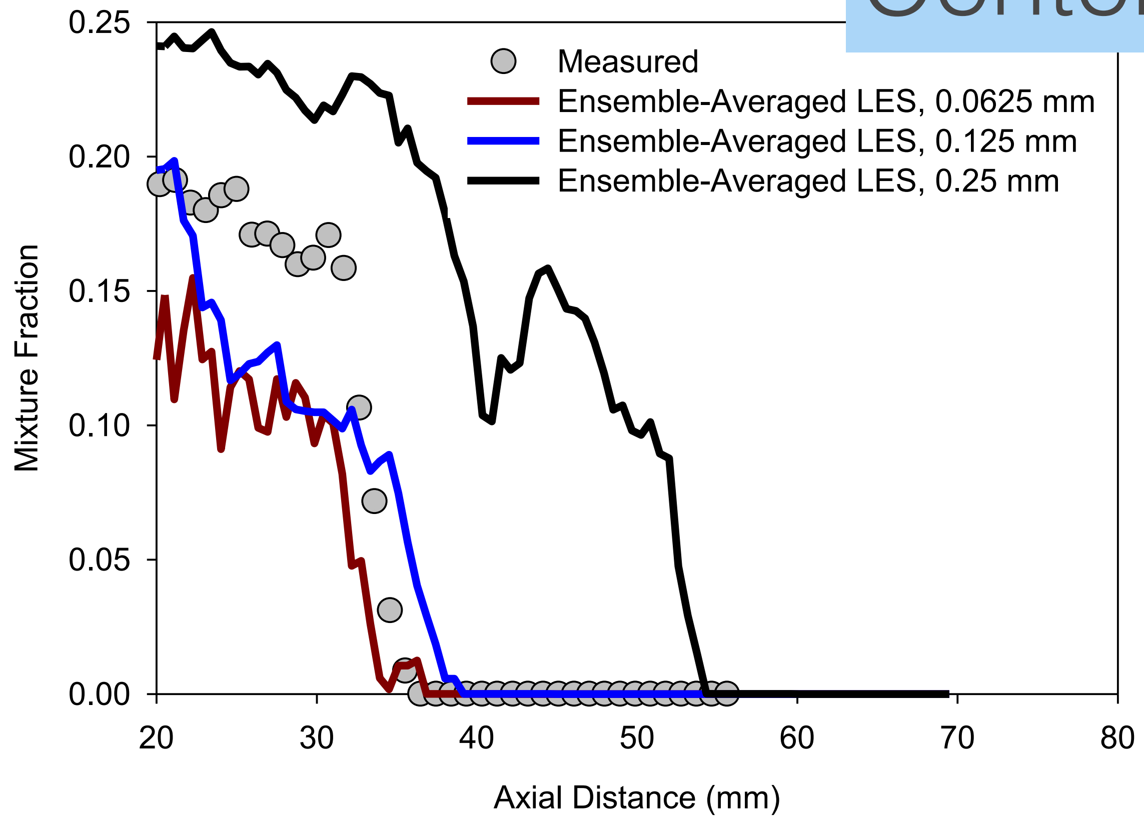
Instantaneous

Mean

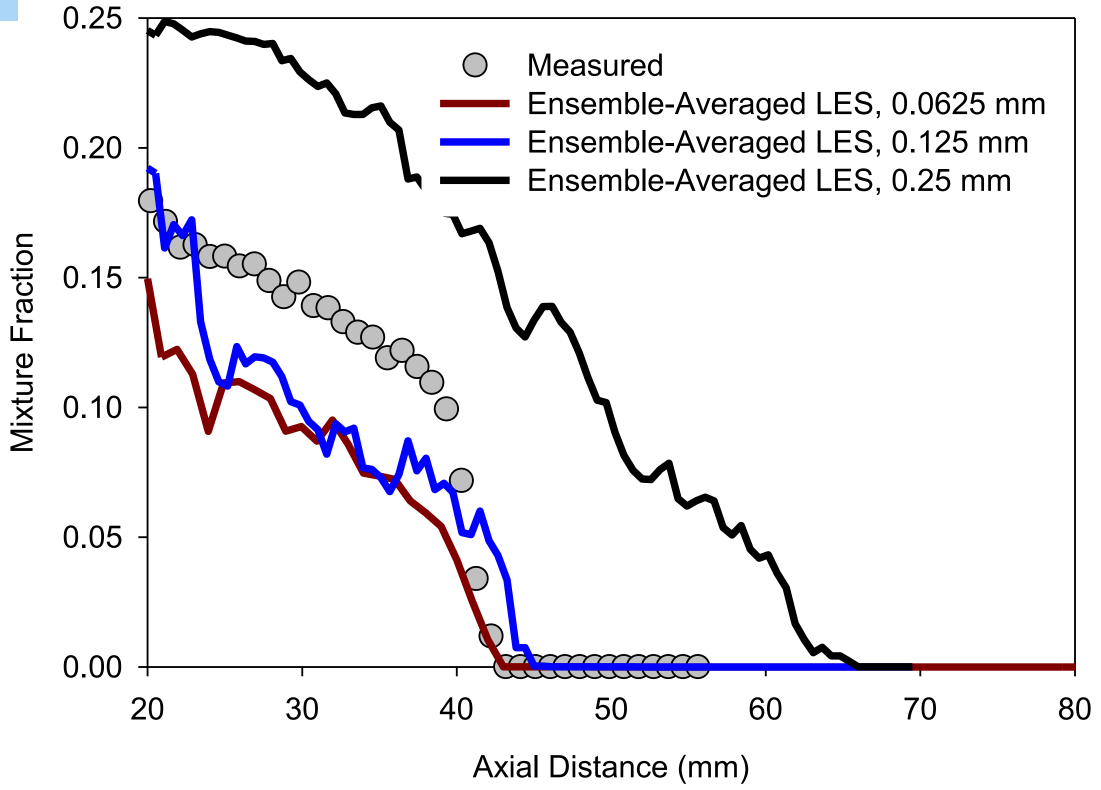
Spray H

LES of Spray H - Mixture Fraction

Centerline

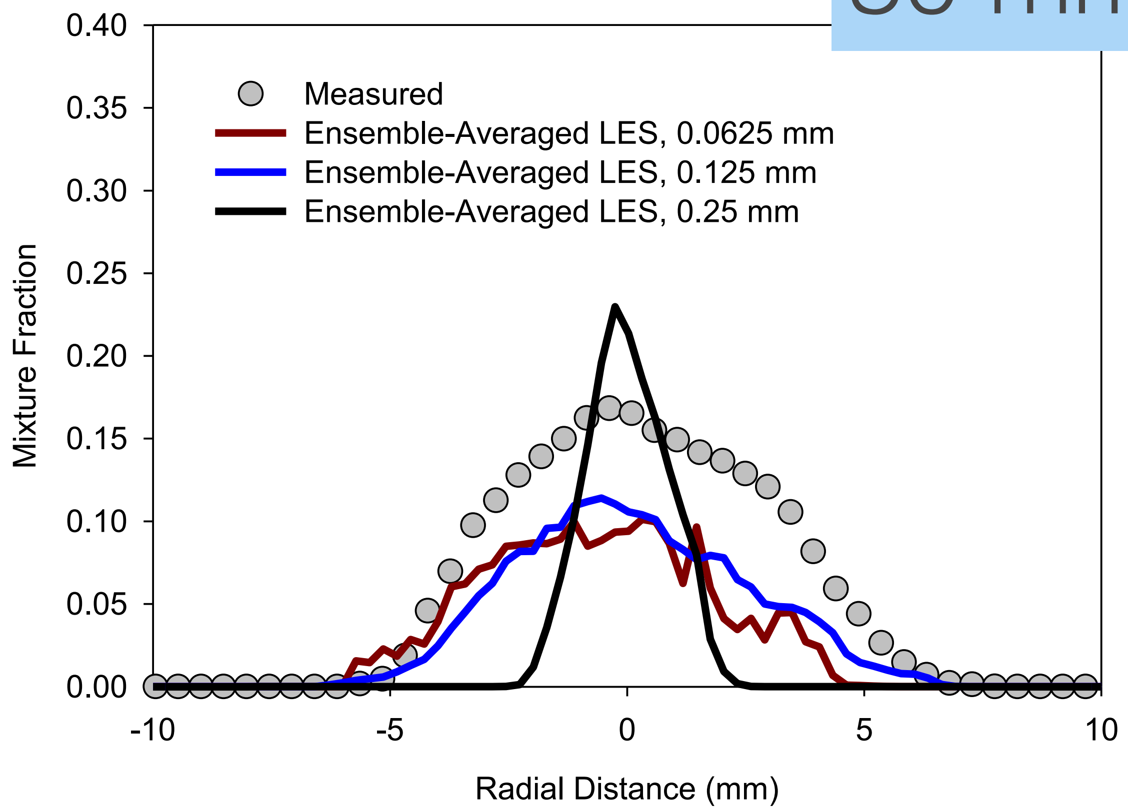


0.49 ms

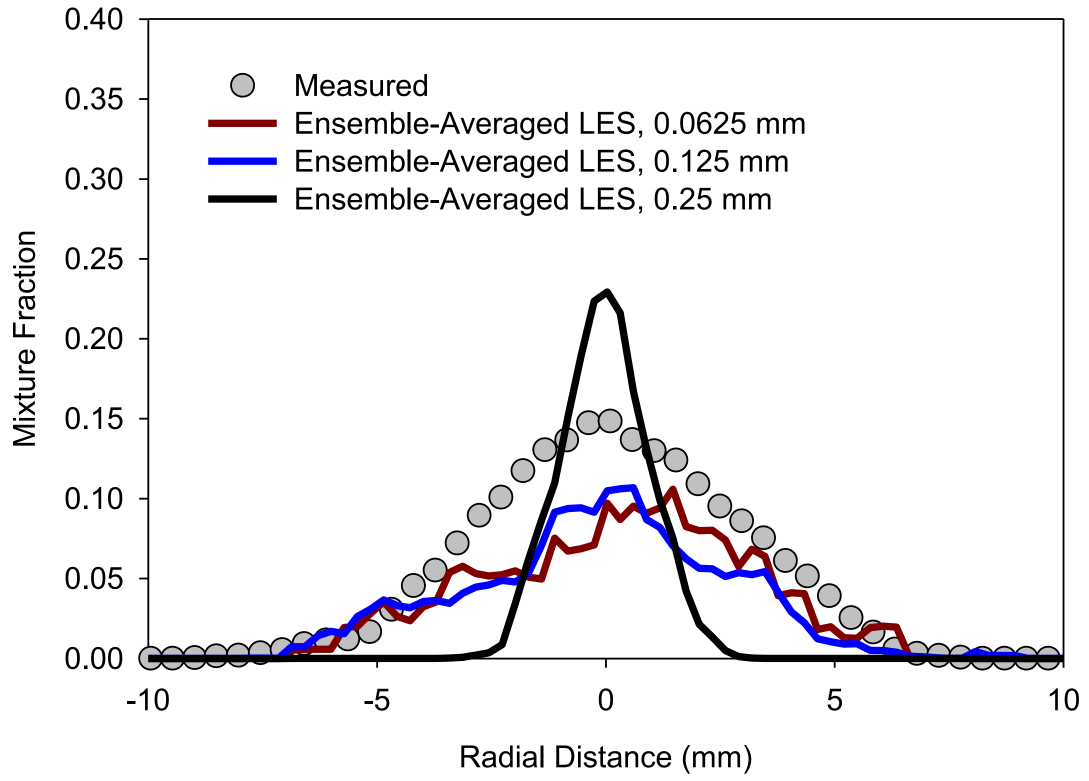


0.68 ms

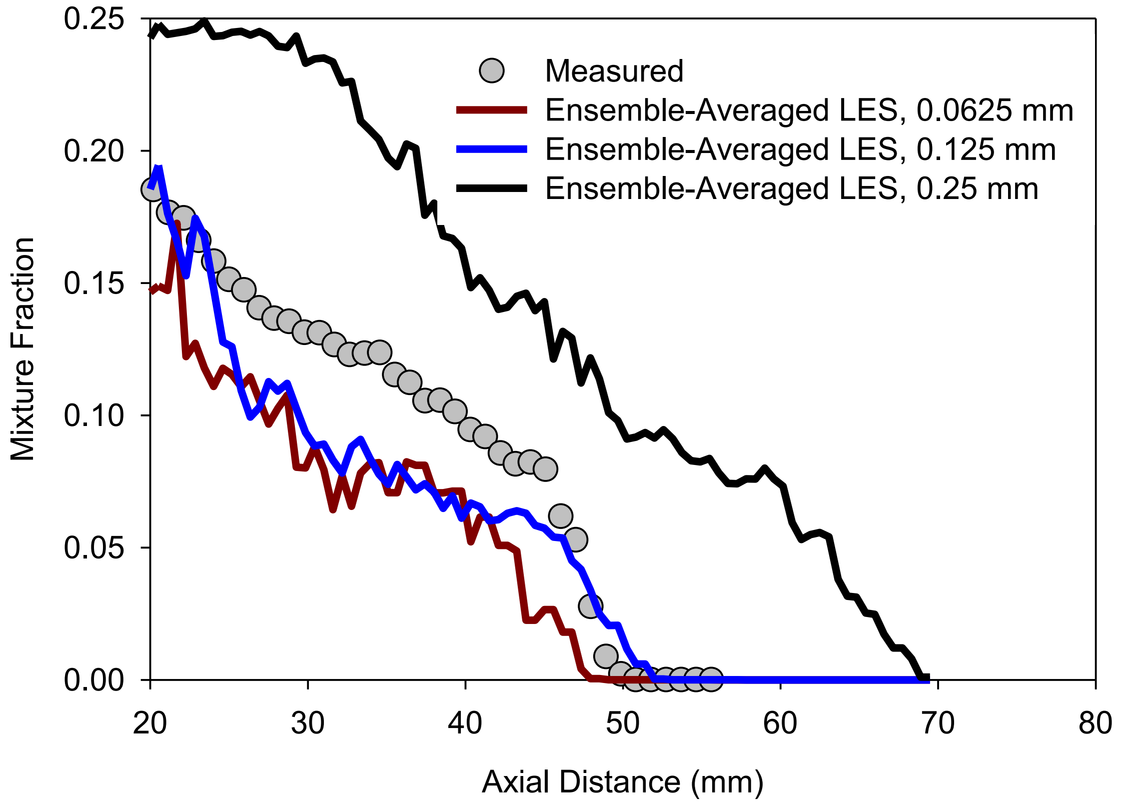
30 mm



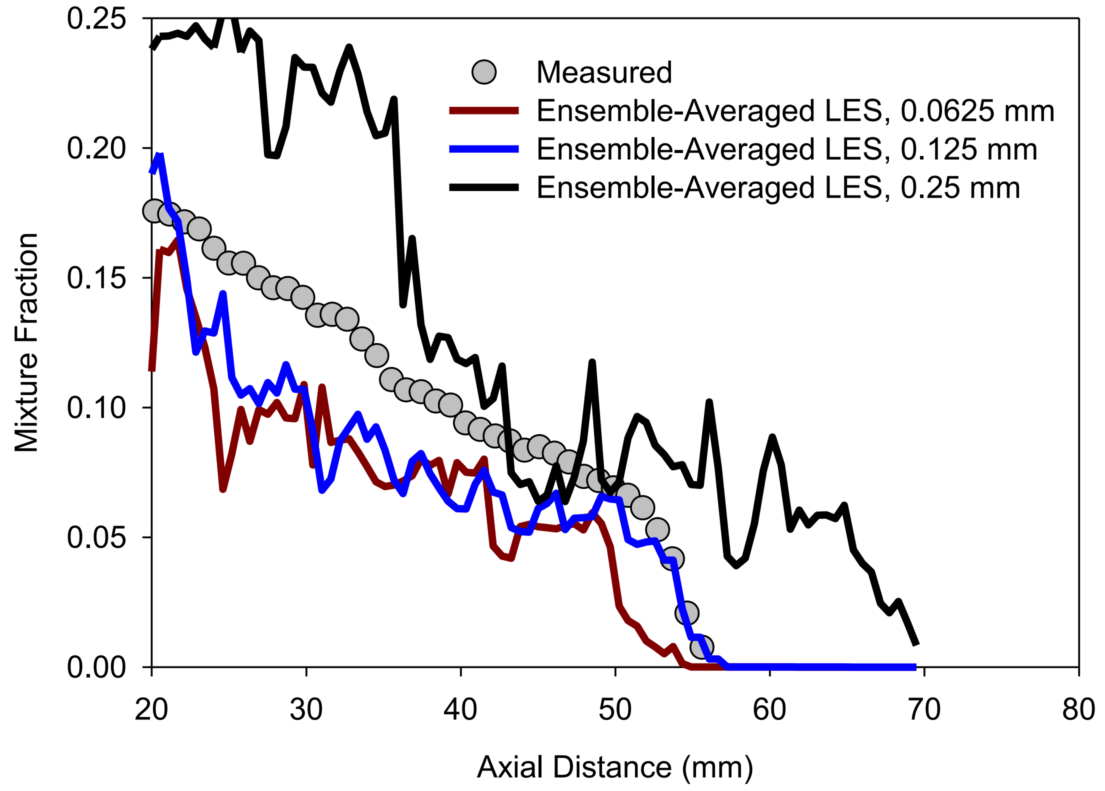
0.49 ms



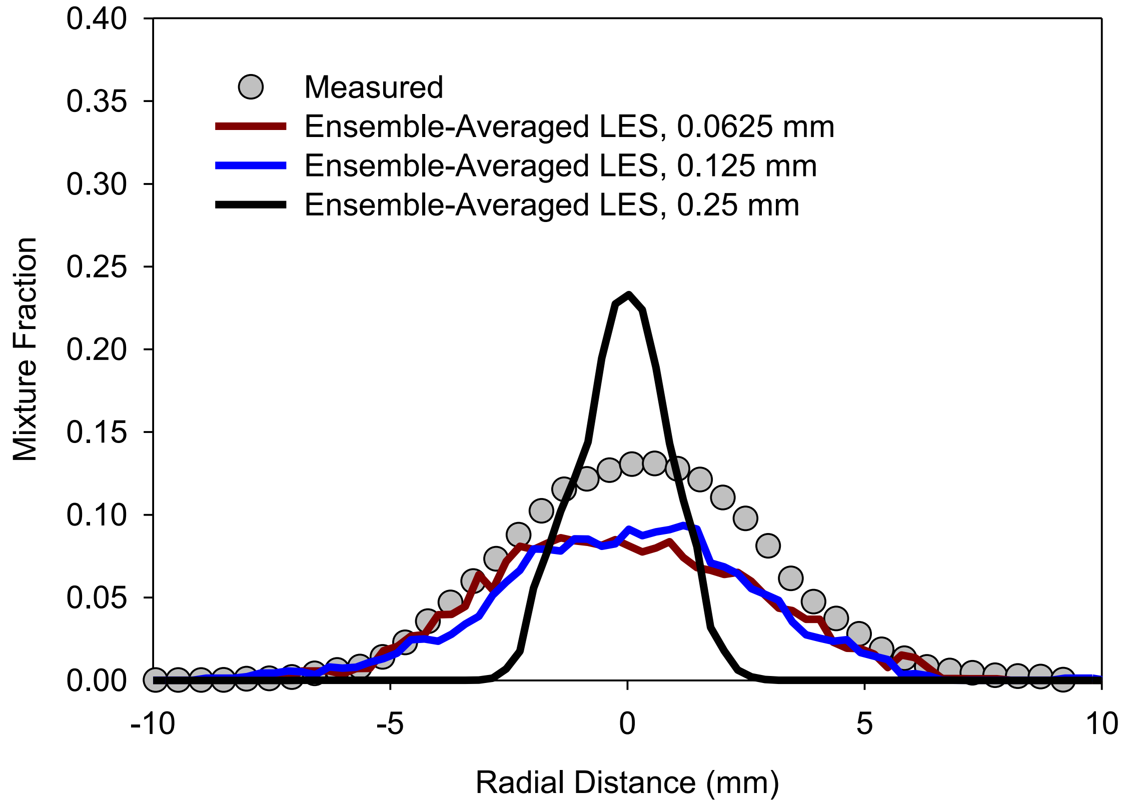
0.68 ms



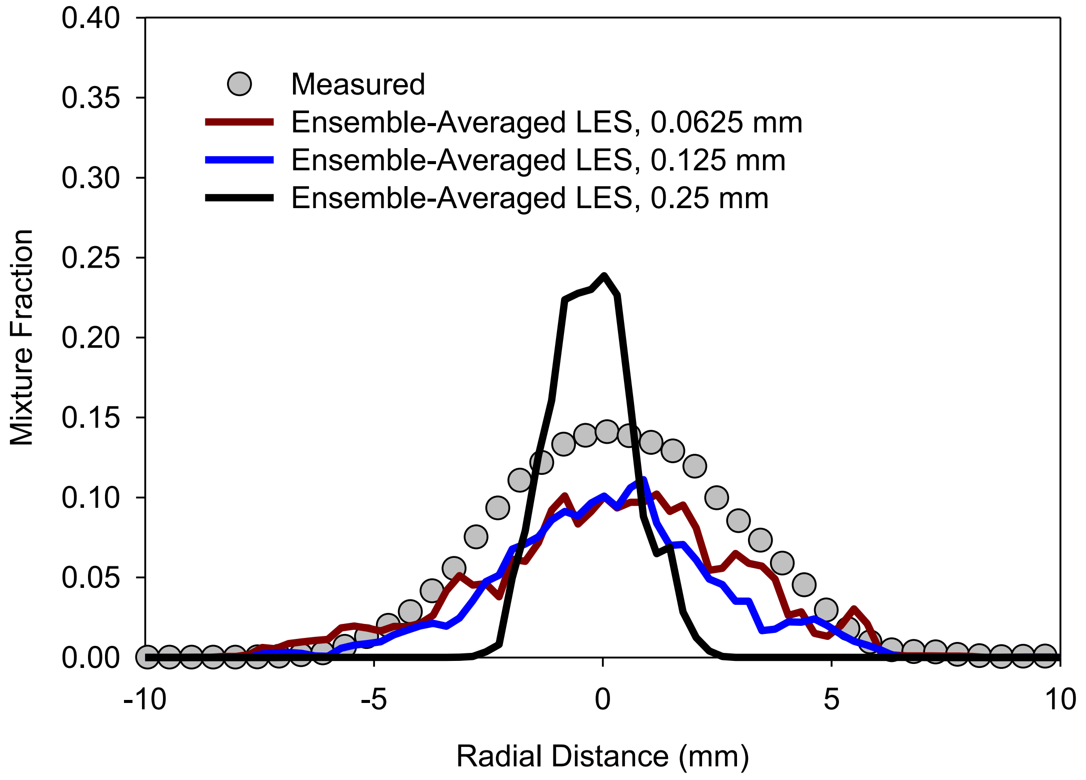
0.90 ms



1.13 ms



0.90 ms



1.13 ms

Spray H

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LES of Spray A - Reacting

Mesh resolution study at 900 K ambient temperature condition.

*Pei et al., accepted to *Combust Flame*, 2015

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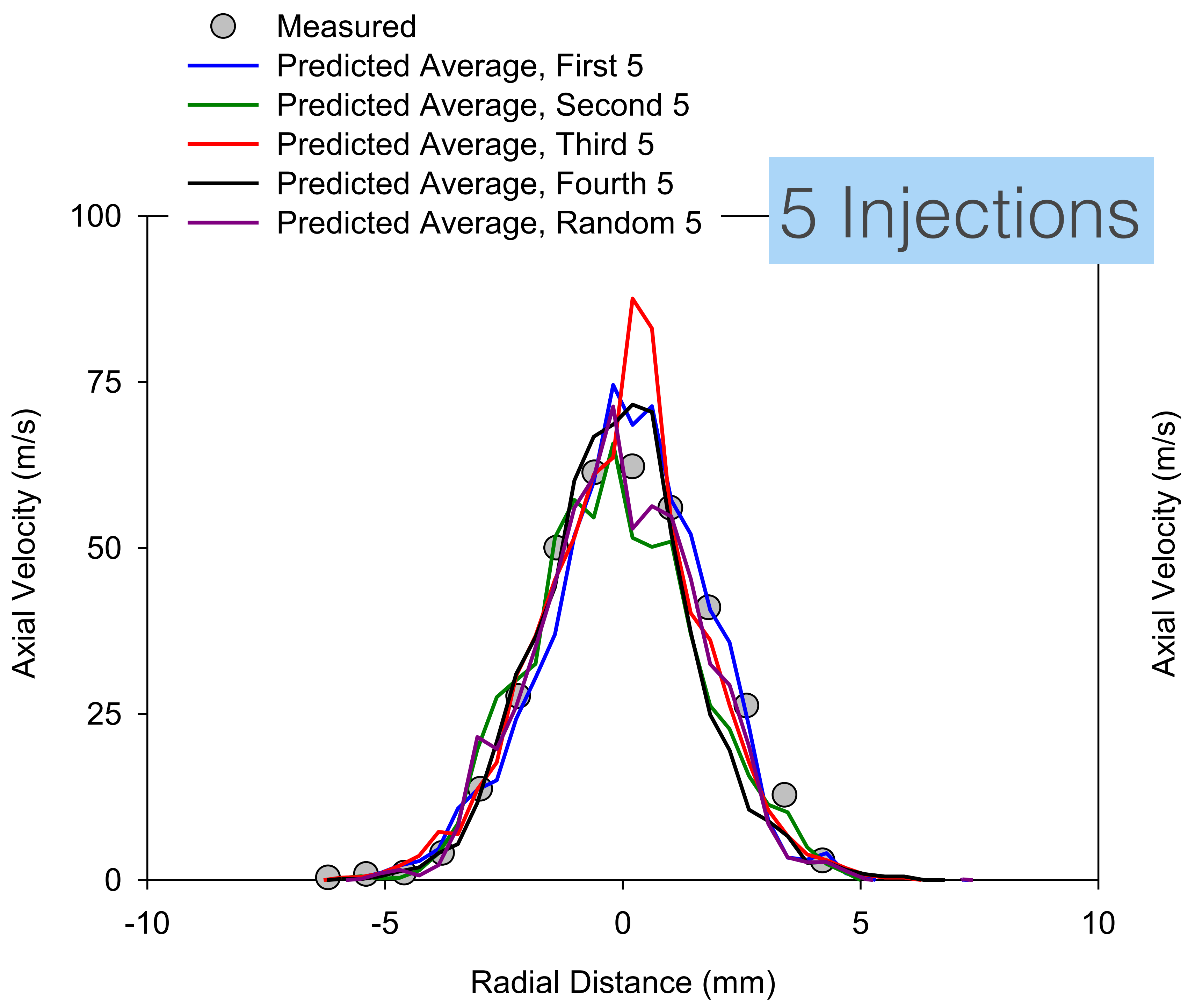
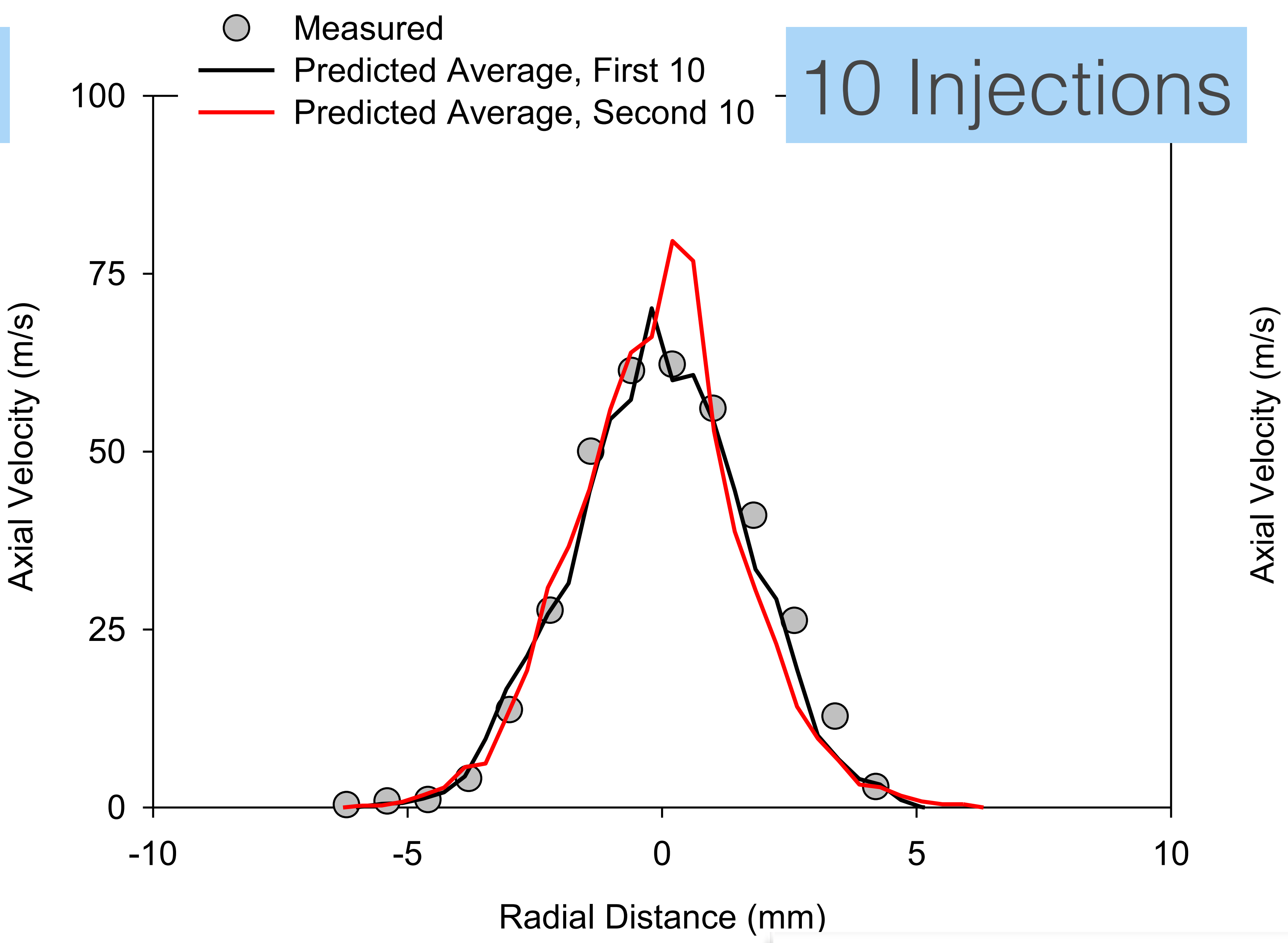
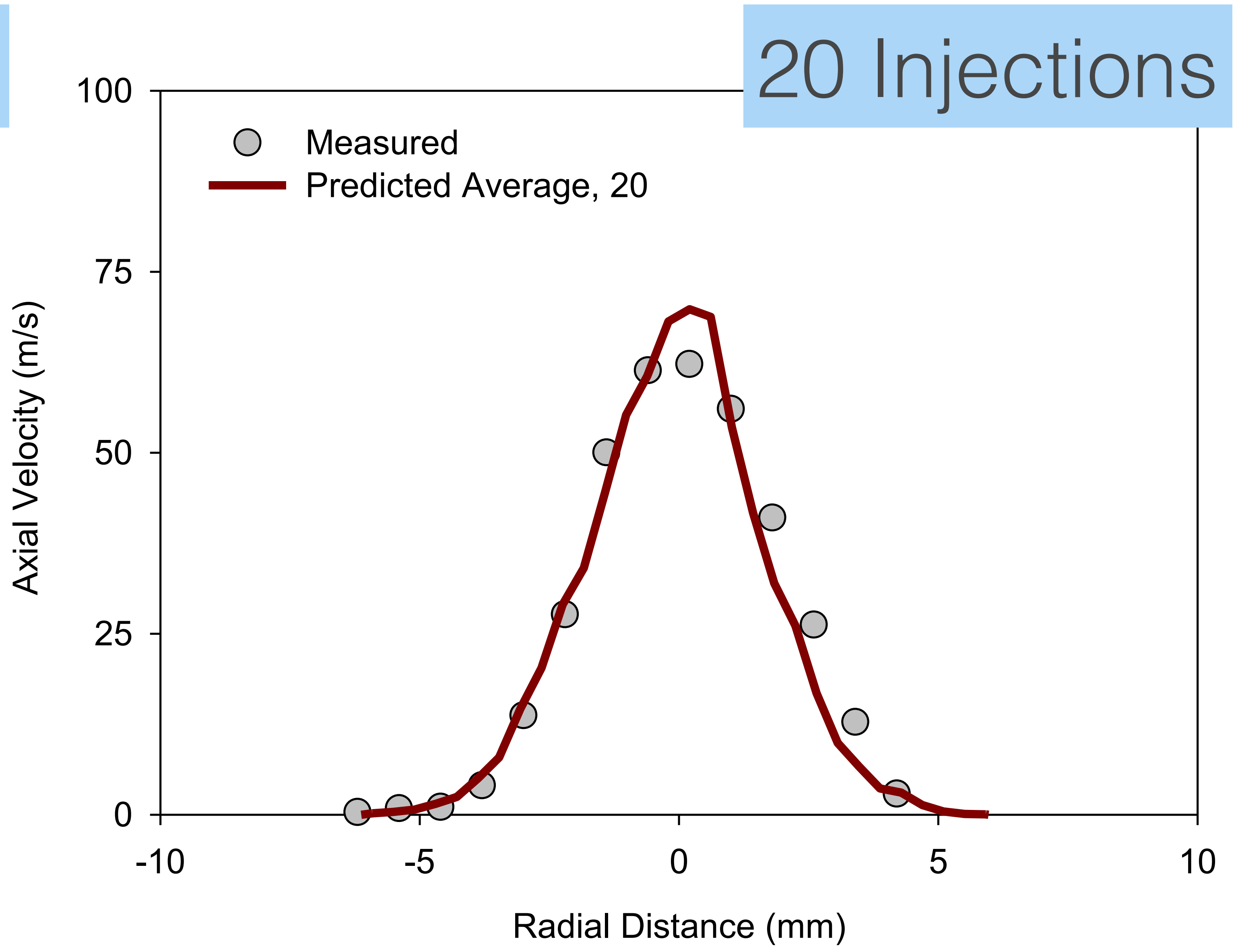
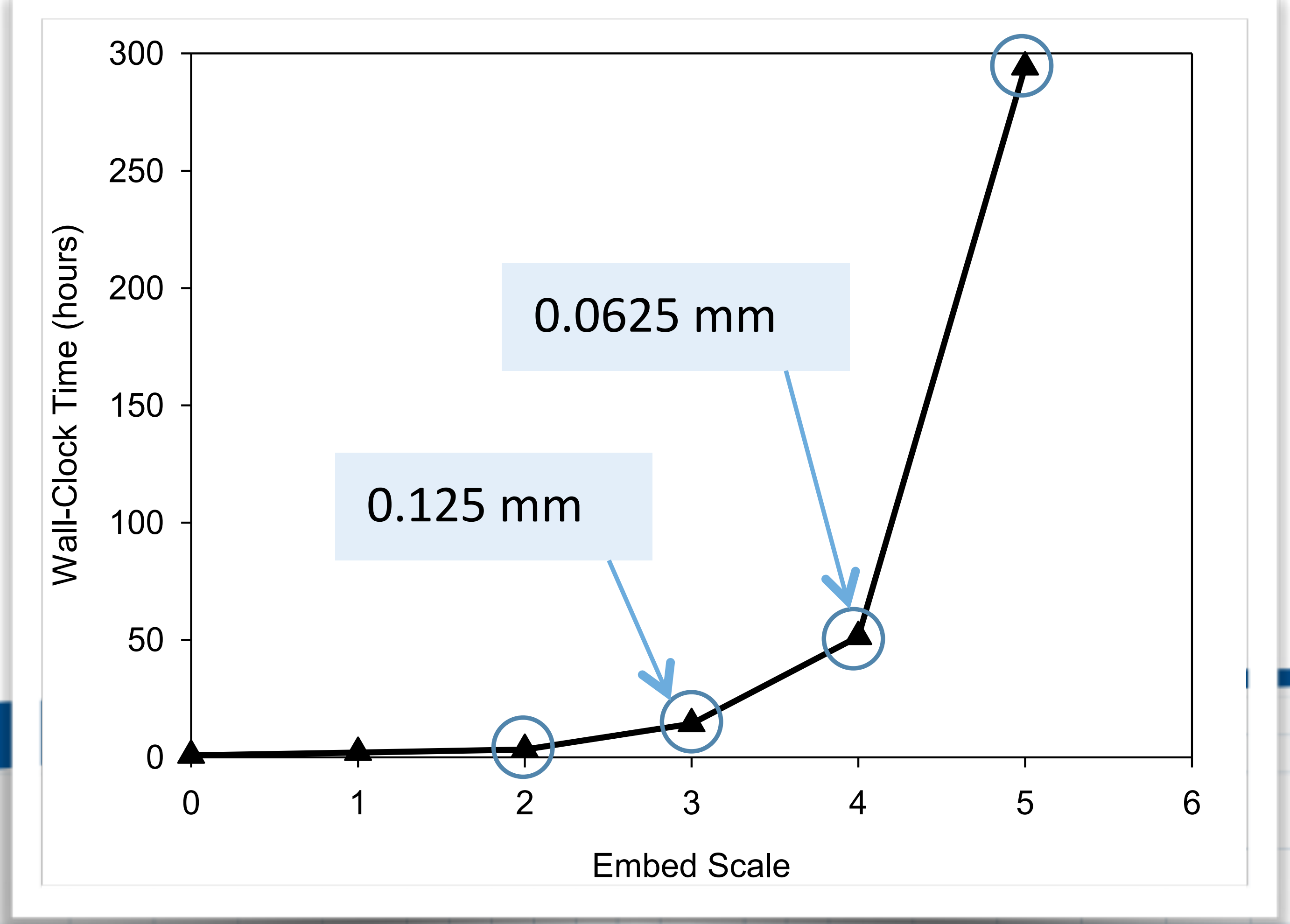
How Many Realizations are Needed?







- 1200 hours (50 days wall time) to run 20 sequential realizations on 64 cores!

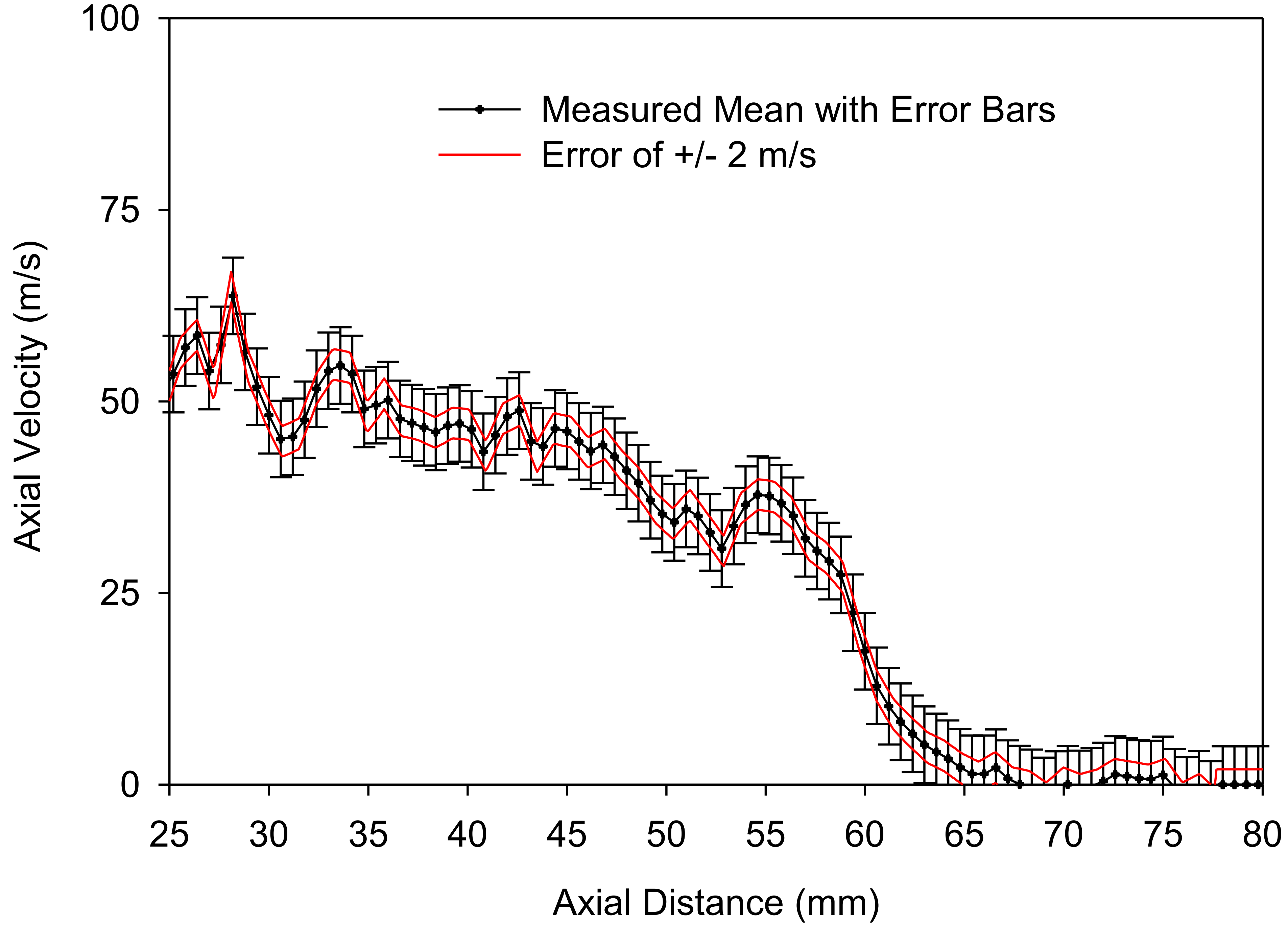


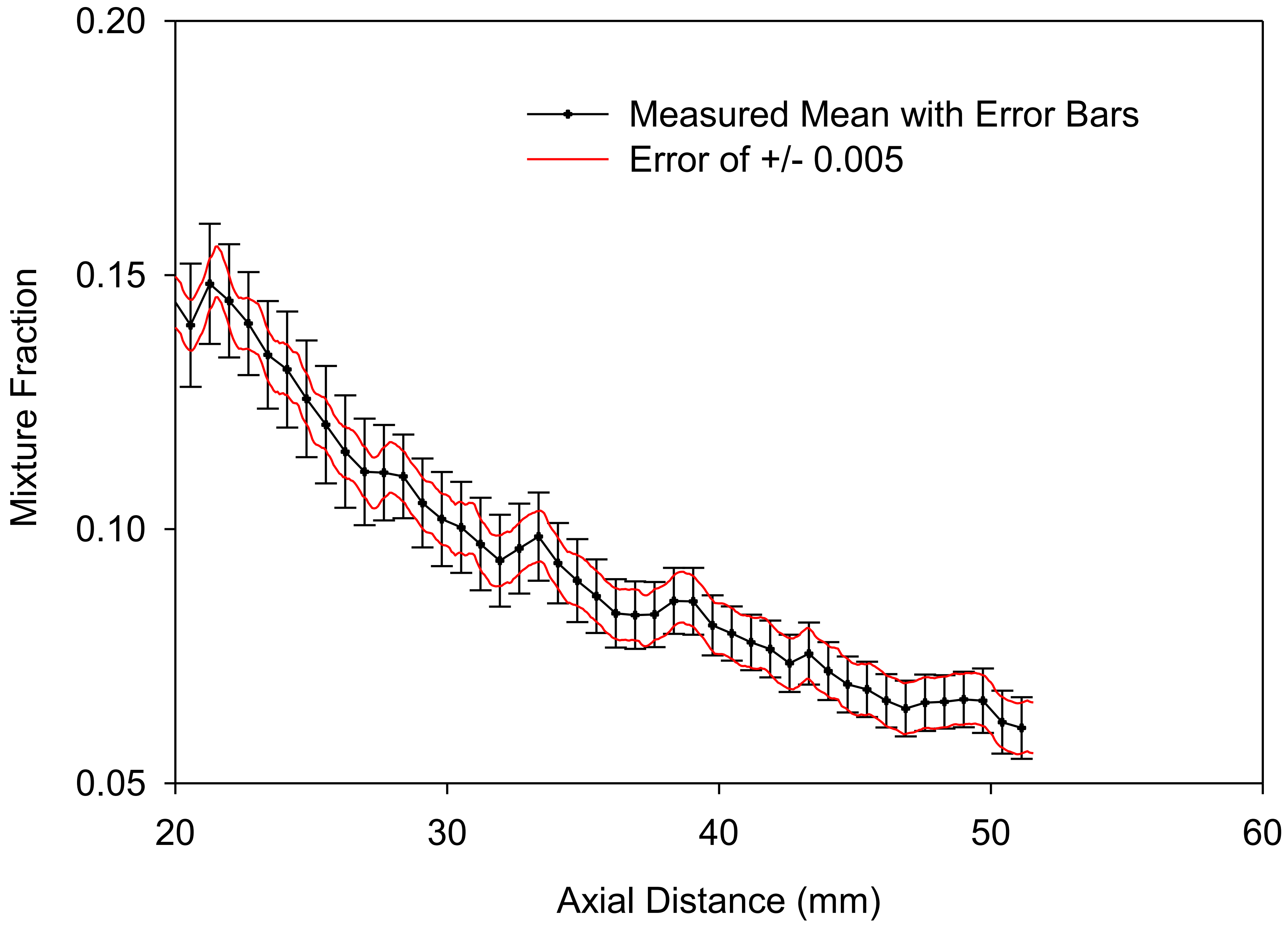
Spray A

How Many Realizations are Needed?

tol (m/s)	Cycles to exceed 90%	Cycles to exceed 95%
0.5	19	19
1.0	14	15
2.0	8	9
5.0	2	3

tol	Cycles to exceed 90%	Cycles to exceed 95%
0.001	19	19
0.002	15	15
0.005	6	7
0.010	2	3





Spray A

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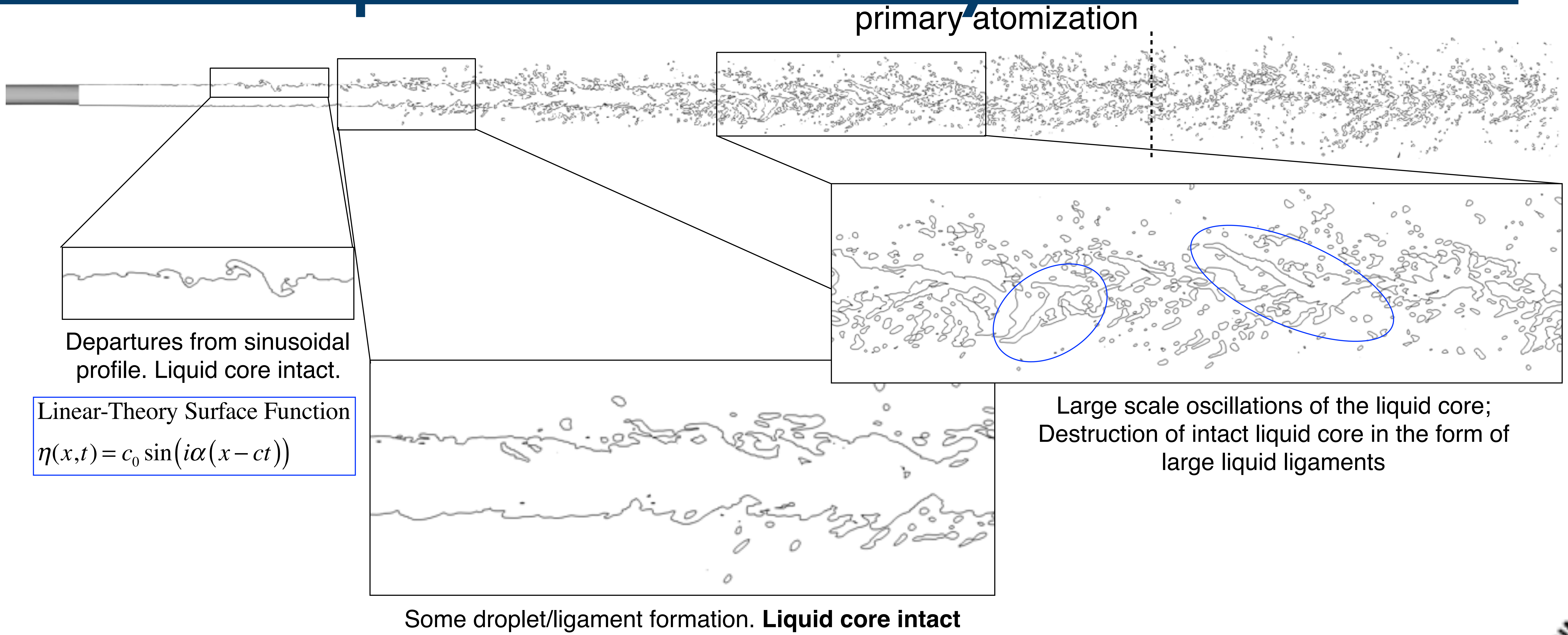
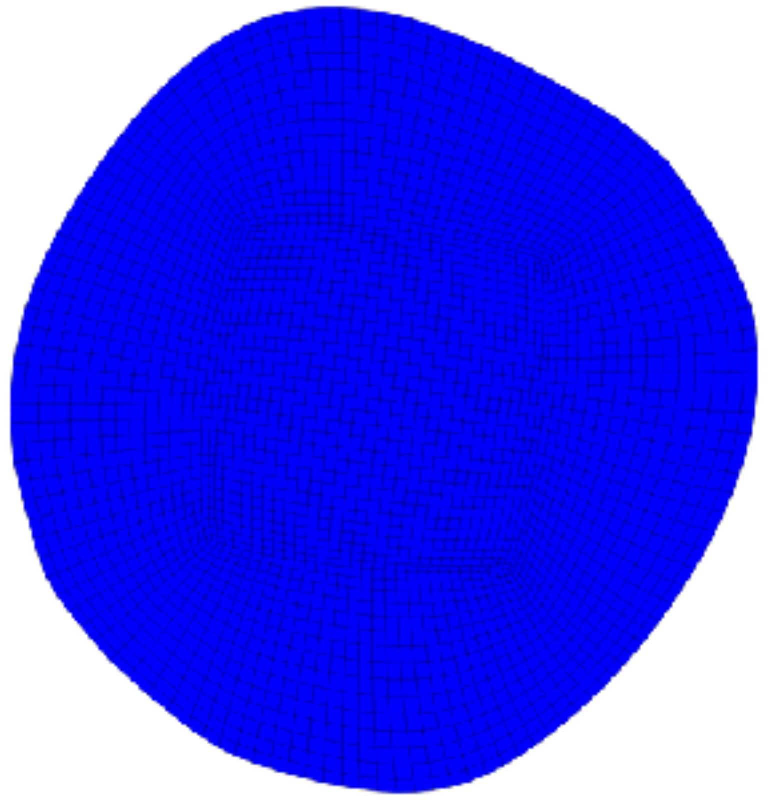
Model Assumptions - Primary Atomization



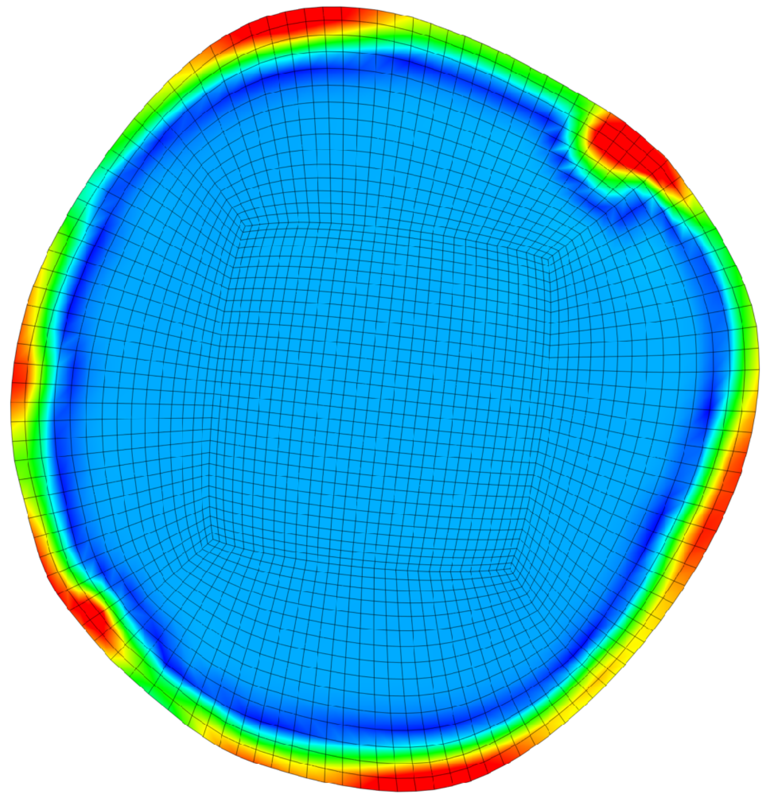
- Non-sinusoidal surface (departure from surface profile adopted in OS solution) very close to the nozzle
- Primary atomization happens downstream in the form of large scale oscillations of the liquid core

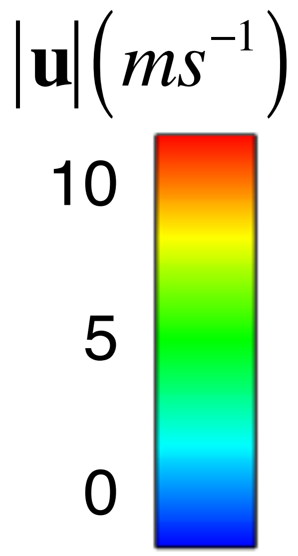
Model Assumptions - Nozzle Flow

EXTERNAL ONLY



INTERNAL + EXTERNAL



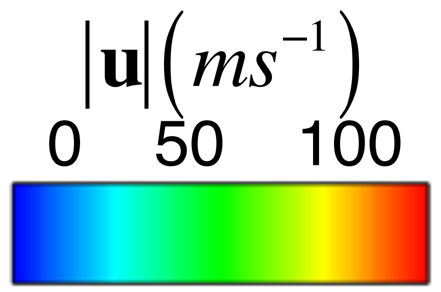


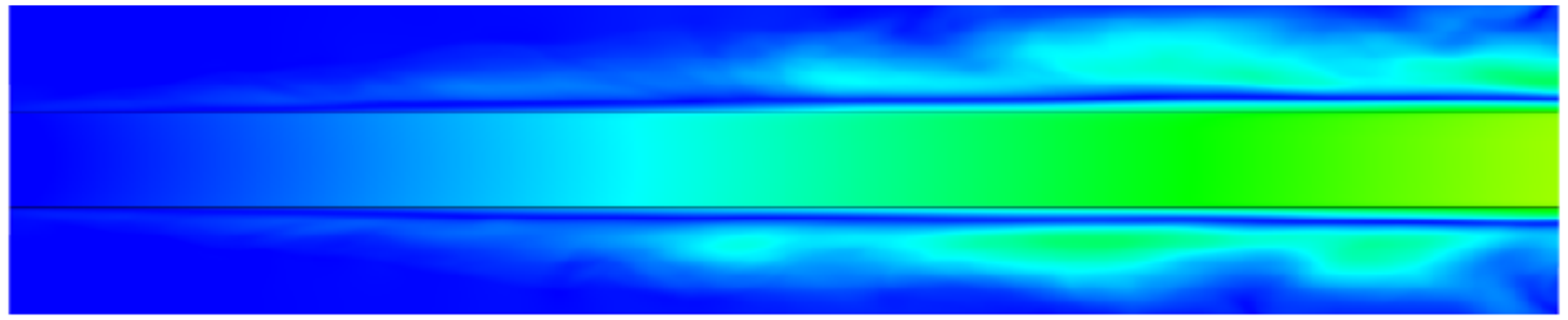
$\mathbf{U} = U_x\mathbf{e}_x + 0\mathbf{e}_y + 0\mathbf{e}_z$

$\mathbf{u} = \mathbf{0}$

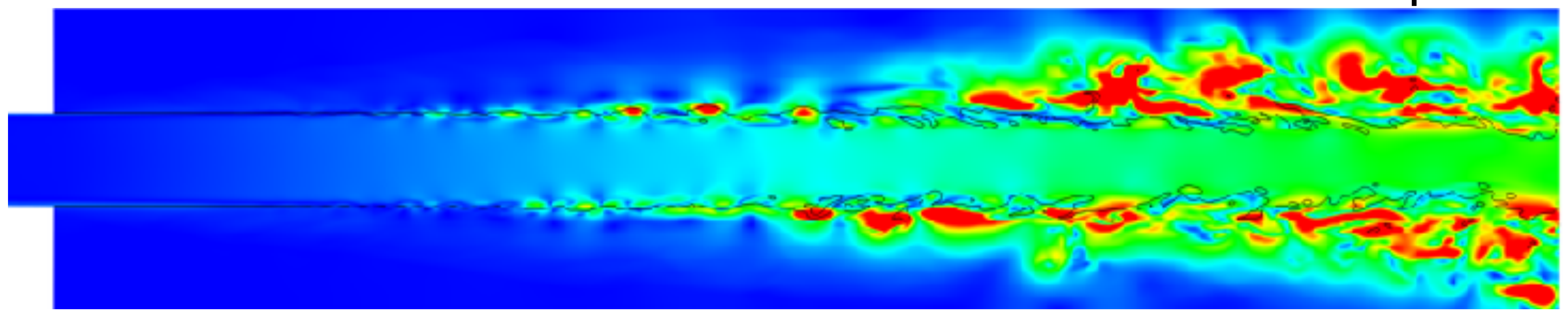
$\mathbf{U}$ from simulation

$\mathbf{u}$ from simulation





avg(Δx)=2μm
t=25μs



- Negligible initial disturbances - naturally unstable modes will dominate flow
- Flow remains smooth in initial region

- Nozzle generated disturbances - naturally unstable modes may not dominate
- Very quick and violent departure from linearity

What's Next?

- Improved scalability for multi-realization LES on more cores
- Incorporate non-linear effects into the atomization models
- Dynamic coupling of nozzle flows and the downstream spray
- Transition criteria and drop initialization for ELE models
  - ★ Allows for two-way coupling
- Flash boiling
  - ★ Especially for GDI sprays
  - ★ Effect on atomization
- Wallfilm!
  - ★ Impingement outcomes
  - ★ Film boiling

THANK YOU!

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