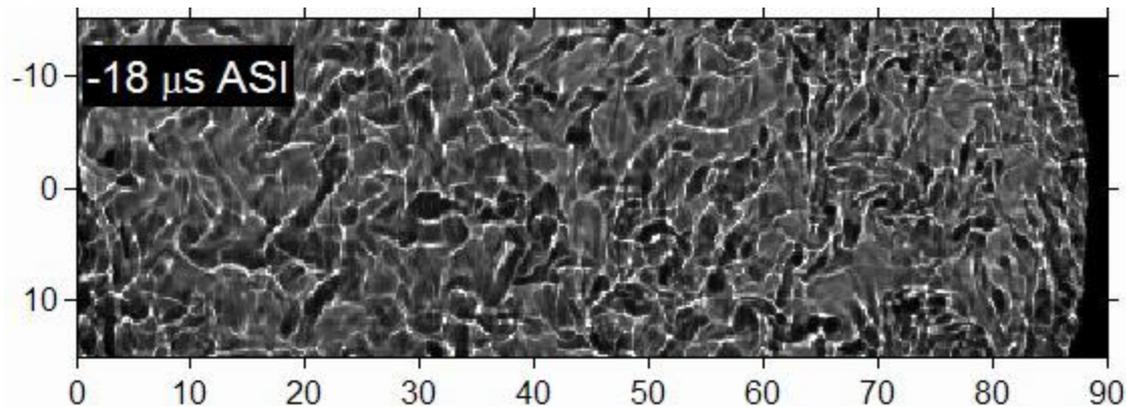


Spray Combustion Research for the Engine Combustion Network

Lyle M. Pickett*

Sandia National Laboratories

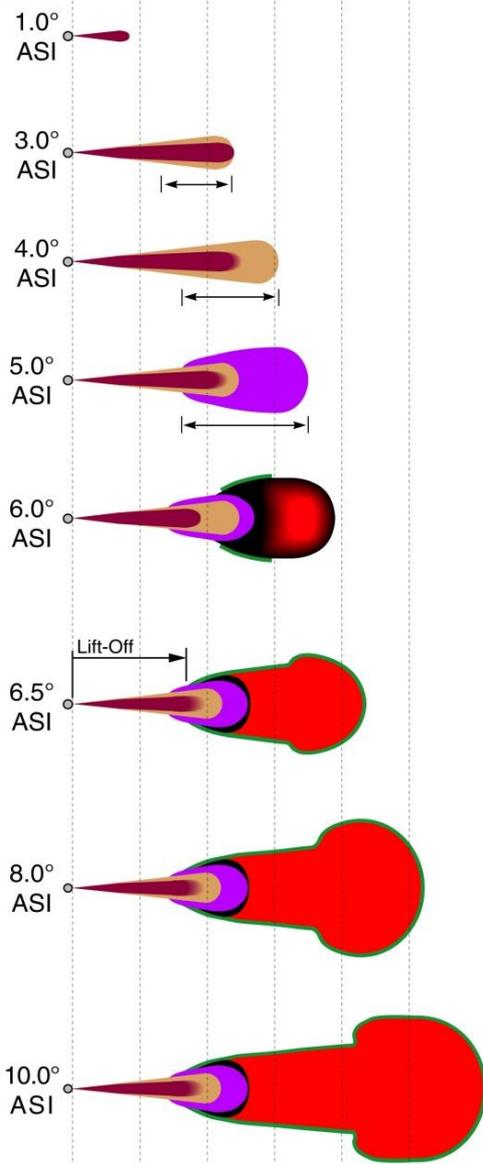
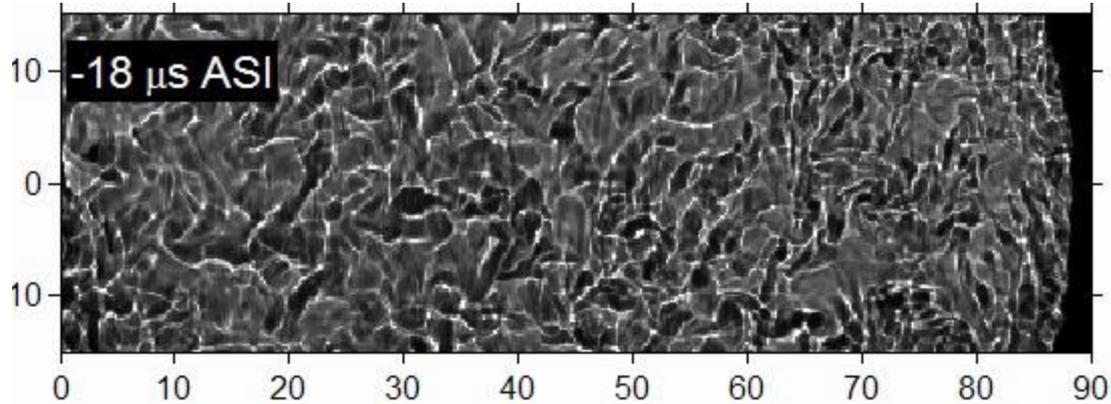


Spray "A" combustion: 60 bar, 900 K, 15% O₂

* Sponsor:
DOE Office of Vehicle
Technologies
Program Manager:
Gurpreet Singh

Current understanding of diesel combustion, summarized by a conceptual model

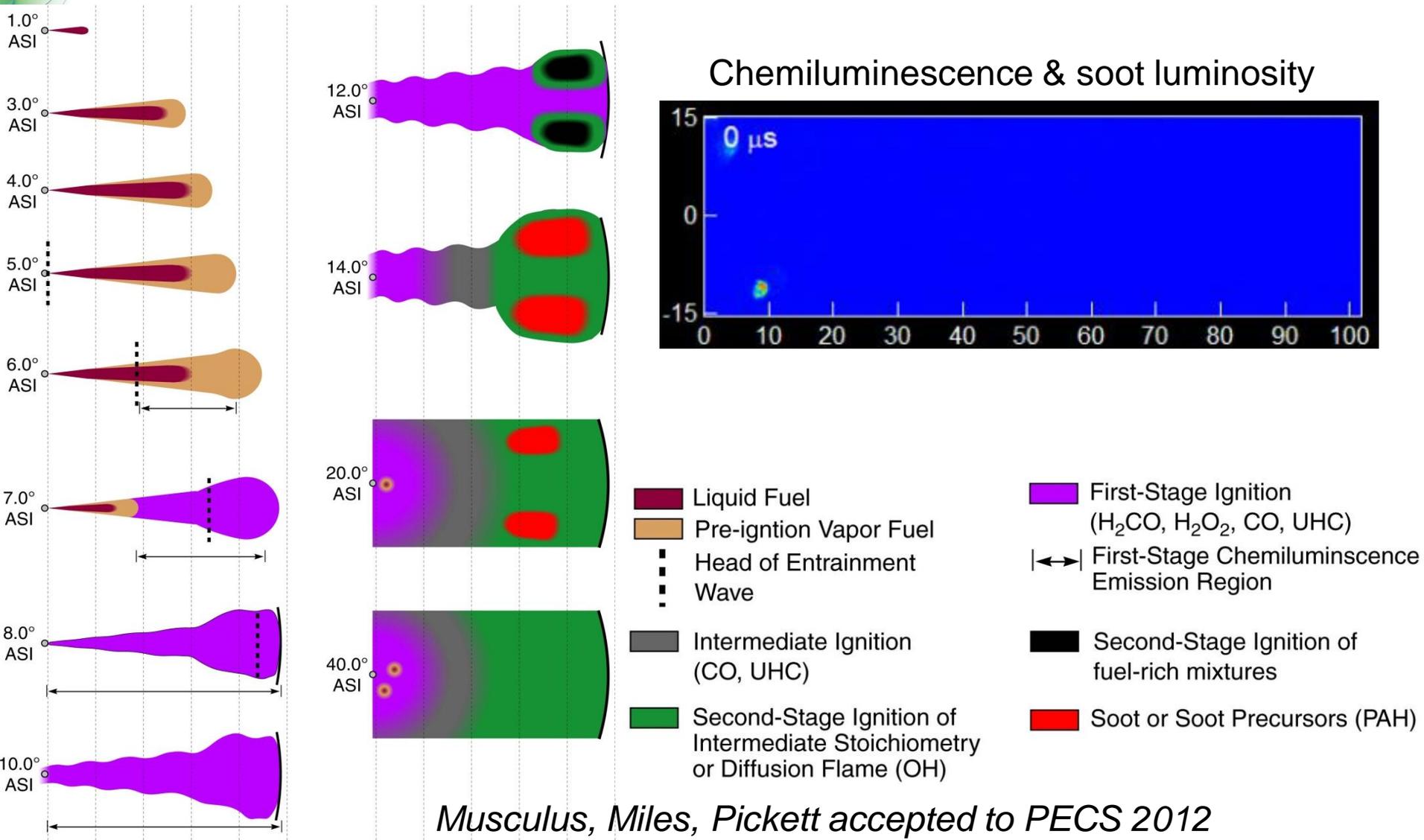
Schlieren & Mie-scatter high-speed imaging



- Liquid Fuel
- Pre-ignition Vapor Fuel
- Head of Entrainment Wave
- Intermediate Ignition (CO, UHC)
- Second-Stage Ignition of Intermediate Stoichiometry or Diffusion Flame (OH)
- First-Stage Ignition (H₂CO, H₂O₂, CO, UHC)
- Second-Stage Ignition of fuel-rich mixtures
- Soot or Soot Precursors (PAH)
- First-Stage Chemiluminescence Emission Region

based on conceptual model of John Dec, 2007

Extending this conceptual model to low-temperature diesel combustion



Musculus, Miles, Pickett accepted to PECS 2012

What DON'T we understand (even conceptually) about diesel spray combustion?

- What difficulties show up when modeling?
 - Usually, if we can't model it, we really don't understand it!
 - Knowledge is not retained until it is added to a model.
- How the conceptual model changes with operating conditions.
- Ignition location and timing.
- Lift-off stabilization.
- Jet-jet, jet-wall interactions, wall films.
- Sources of UHC and CO.
- Dense spray region.
- Why spray plume spreading angle varies.
- Structure of fuel-rich, premixed flame.
- Soot precursors and soot.
- Radiation heat transfer.

20 bar, 900 K, 15% O₂





Beyond a conceptual diesel model, what QUANTITATIVE data do we lack?

- Almost everything, at high-temperature engine conditions (>900 K).
- Liquid volume fraction and droplet size in the dense spray region and near the liquid length.
- Mixture fraction (fuel/air ratio) distribution.
- Velocity and turbulence.
- Soot volume fraction and structure distribution, particularly during transients.
- Internal injector geometry for working injectors.
- Information about internal injector cavitation and flows.
- Can we build this type of dataset?
- Can we generate predictive engine spray combustion tools/models?

Introducing the Engine Combustion Network

- Collaborative modeling/experimental data archive.
- <http://www.sandia.gov/ECN>

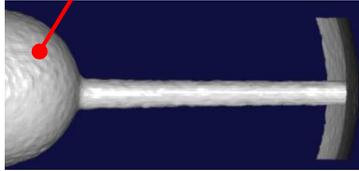
Address  <http://www.ca.sandia.gov/ecn/index.php>



<p>ECN Home</p>	<h2>Overview</h2>
<p>Experimental Data</p>	<p>The purpose of this site is to provide an open forum for international collaboration among experimental and computational researchers in engine combustion. Patterned after the Turbulent Nonpremixed Flame Workshop, the objectives of the Engine Combustion Network (ECN) are to:</p>
<p>Related Internet Sites</p>	<ol style="list-style-type: none"> 1. Establish an internet library of well-documented experiments that are appropriate for model validation and the advancement of scientific understanding of combustion at conditions specific to engines.
<p>References</p>	<ol style="list-style-type: none"> 2. Provide a framework for collaborative comparisons of measured and modeled results.
<p>Tutorial: Diesel Spray Visualization</p>	<ol style="list-style-type: none"> 3. Identify priorities for further experimental and computational research.
	<p>Maintained by the Engine Combustion Department of Sandia National Laboratories, data currently available on the website includes reacting and non-reacting sprays in a constant-volume chamber at conditions typical of diesel combustion. The website will be expanded in the future to include datasets and modeling results of scientific interest to participants in the ECN.</p>

Collaborative research at specific target conditions

Injector
90° C, 1500 bar

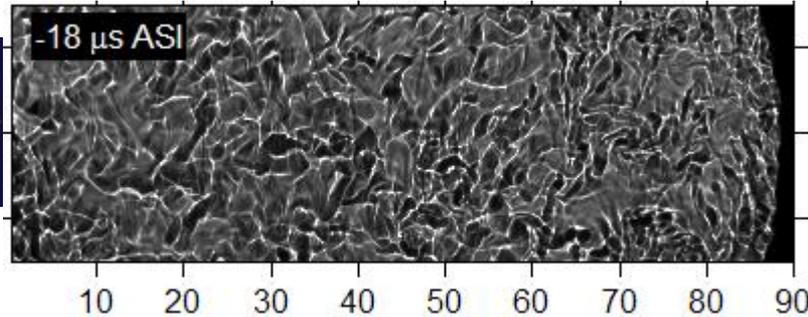


Internal nozzle geometry

Ambient

900 K, 60 bar

Spray A



Other defined targets:

- Spray H (baseline n-heptane)
- Spray B (3-hole version of Spray A).
- Gasoline DI and engine flows.

- Opportunity for the greatest exchange and deepest collaboration.
 - Understanding facilities/boundary conditions.
 - Understanding diagnostics and quantification.
 - Standardize methodologies for post-processing.
- Leverages the development of quantitative, complete datasets.
 - Unique diagnostics to build upon past understanding.
 - Moves from “qualitative” to “quantitative”.
 - Sharing results/meshes/code/methods saves time and effort.
- Pathway towards predictive spray and engine CFD.

Measurements to date at Spray A conditions

Quantity	Experiment	Contributors (Inst. and/or person)
Gas T distribution	fine-wire TC, variable diameter TC	CAT, CMT, Sandia, IFPEN, TU/e
Ambient gas minor species existence and effects	kinetics modeling	Mich. Tech. U. (Jaclyn Nesbitt Johnson)
Nozzle internal temperature	thermocouple	Sandia, CAT, IFPEN, CMT, TU/e, Aachen
Nozzle surface temperature	laser-induced phosphorescence	IFPEN (Louis-Marie Malbec, Gilles Bruneaux)
Nozzle geometry	x-ray tomography	CAT (Tim Bazyn)
Nozzle geometry	phase-contrast imaging	Argonne (Alan Kastengren, Chris Powell)
Nozzle geometry	silicone molds	CMT (Raul Payri, Julien Manin)
Nozzle exit shape	optical microscopy, SEM	Sandia (Julien Manin, Lyle Pickett)
Educated nozzle grids	Smoothing and analysis of all data	GaTech, Umass-Amherst, Sandia Argonne
Mass rate of injection	bosch tube method	CMT (Raul Payri, Julien Manin)
Rate of momentum	force piezo	CMT, Sandia, CAT
Total mass injected	gravimetric scale	CMT, Sandia, IFPEN
Nozzle Cd, Ca	momentum + mass	CMT, Sandia
Liquid penetration	Mie scatter	IFPEN, Sandia, CMT, CAT, TU/e
Liquid penetration	Diffuser back illumination	Sandia, CMT, IFPEN, TU/e
Liquid optical thickness	laser extinction	Sandia (Julien Manin, Lyle Pickett)
Liquid structure	long-distance microscopy	Sandia (Julien Manin, Lyle Pickett)
Liquid vol. fraction (300 K)	x-ray radiography extinction	Argonne (Alan Kastengren, Chris Powell)
Vapor boundary/penetration	schlieren / shadowgraphy	Sandia, IFPEN, CAT, CMT, TU/e
Fuel mixture/mass fraction	Rayleigh scattering	Sandia
Velocity (gas-phase)	PIV	IFPEN (L.-M. Malbec, G. Bruneaux, M. Meijer)
Ignition delay	high-speed chemiluminescence	Sandia, CAT, CMT, IFPEN, TU/e
Lift-off length	OH or broadband chemilum.	Sandia, IFPEN, CAT, CMT, TU/e
Transient lift-off/ignition	intensified OH chemiluminescence	Sandia, IFPEN, CAT, CMT, TU/e
Pressure rise/AHRR	high-speed pressure	Sandia, IFPEN, TU/e
Soot luminosity	high-speed luminosity imaging	Sandia, IFPEN, CAT, CMT, TU/e
Soot volume fraction	laser-induced incandescence, laser extinction	IFPEN/Duisberg-Essen (Emre Cencer)

26 types of experiments

8 different international institutions



Workshops organized with voluntary participation (for ECN2: 8 experimental, 16 modeling teams)

- Different than a conference, designed to promote active experimental and modeling exchange.
- Coordinators gather experimental and modeling results before conference to compare side by side.
- Discussed standardization, quantification of uncertainties, and best practices for model comparison.
 - Are modeling and experimental results actually talking about the same thing?
 - Are measurements delivering the type of data needed for model improvement?

ECN2, Sept 2012 in Germany

- Overall:
 - Gilles Bruneaux (IFPEN), Lyle Pickett (Sandia)
- Internal Nozzle Flow
 - Chris Powell (Argonne), David Schmidt (UMassAmherst), Marco Arienti (Sandia)
- Spray Development and Vaporization
 - Julien Manin (Sandia), Sibendu Som (Argonne), Chawki Habchi (IFPEN)
- Mixing and Velocity
 - Louis-Marie Malbec (IFPEN), Gianluca D'Errico (Pol. Milano)
- Ignition and Lift-off Length
 - Michele Bardi (CMT), Evatt Hawkes (UNSW), Christian Angelberger (IFPEN)
- Soot
 - Emre Cenker (Duisburg/IFPEN), Dan Haworth (Penn St.)
- Gasoline Sprays
 - Scott Parrish (GM)
- Engine Flows
 - Sebastian Kaiser (Duisburg-Essen)



Outline

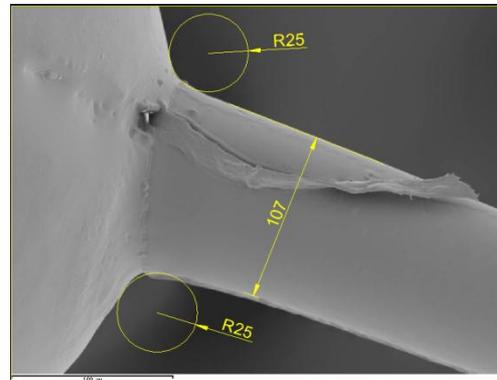
- Nozzle internal geometry and needle-valve movement
- Near-nozzle mixture fraction
- Near-nozzle visualization
- Vapor-phase mixture fraction and velocity
- Ignition delay and lift-off length

Nozzle internal geometry measurements

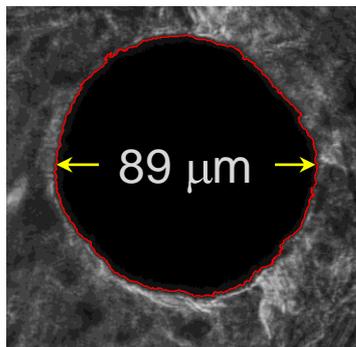
X-ray phase-contrast
(Argonne)



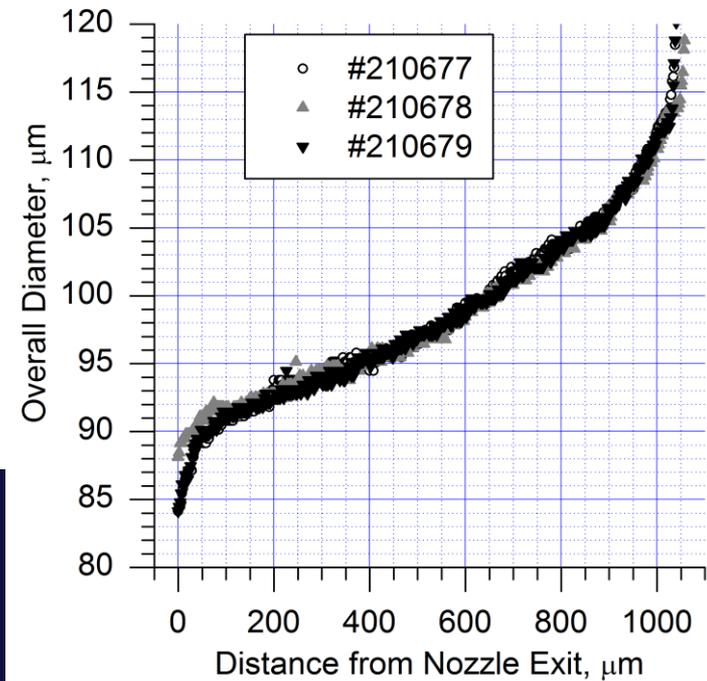
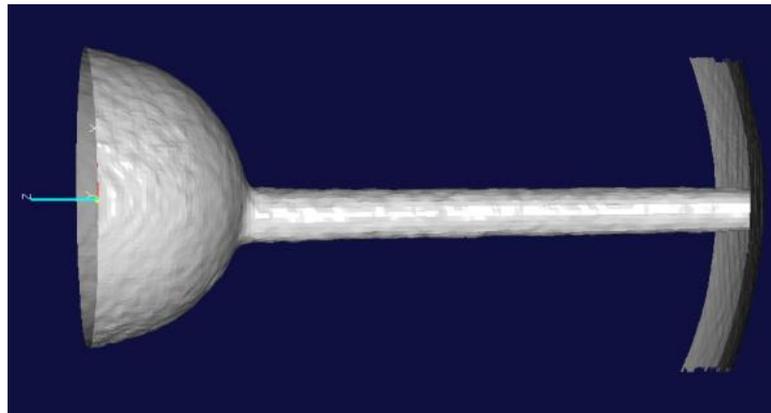
Silicone molds (CMT)



Optical
(Sandia)

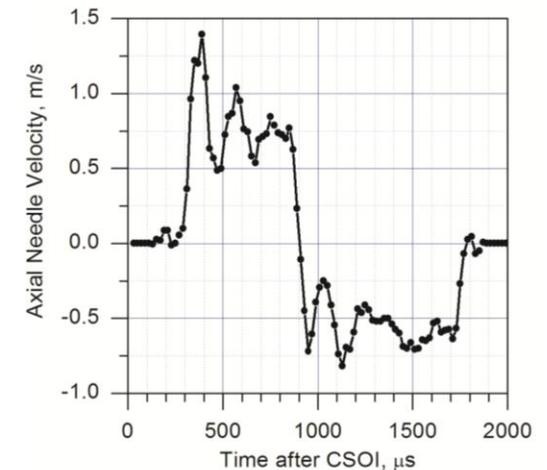
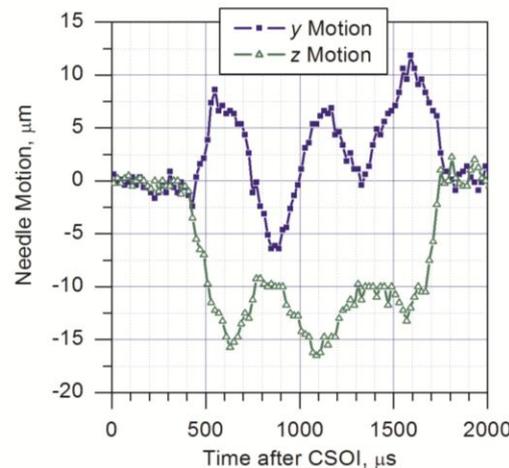
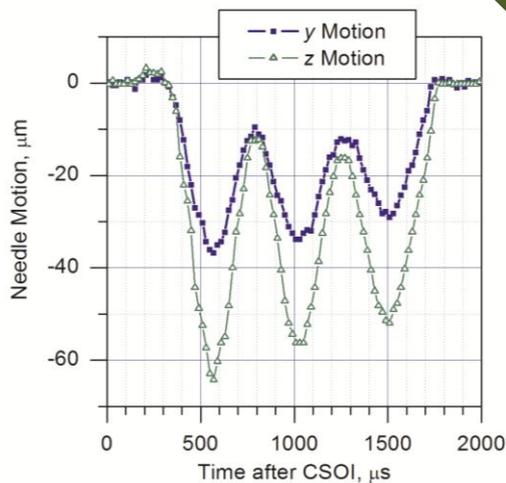
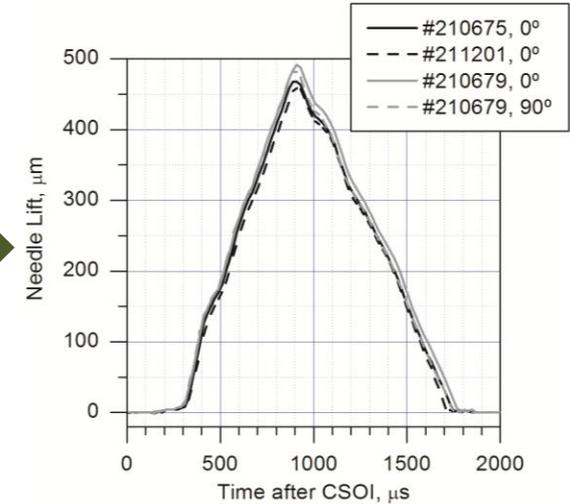
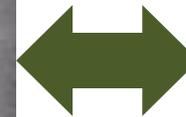
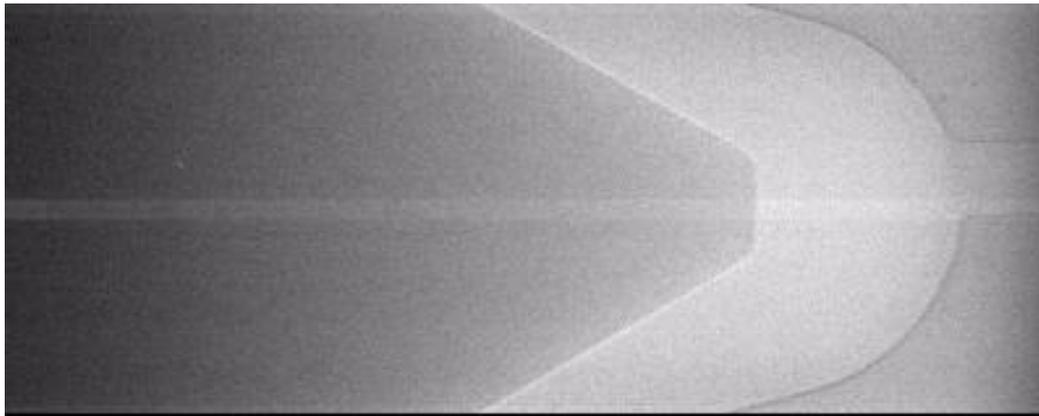


X-ray tomography
(Caterpillar)



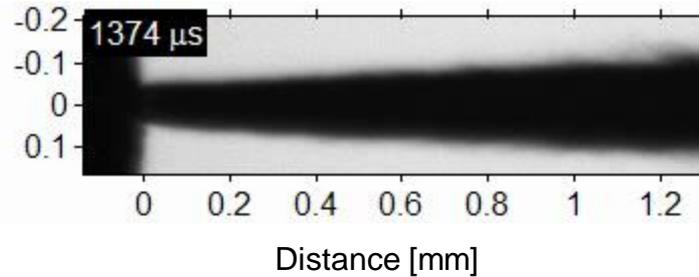
X-ray phase-contrast imaging of needle motion

Experiment by Alan Kastengren & Chris Powell, Argonne National Laboratory



Near-nozzle high-speed visualization at > 100 kfps

5 bar, 440 K (3.8 kg/m³)
n-dodecane, 150 MPa, 90°C



High-speed CMOS
150 kfps

Long-distance
microscope

Combustion vessel

Field
lens

Custom LED:
<50 ns pulse at
high frequency.

Engineered
diffuser

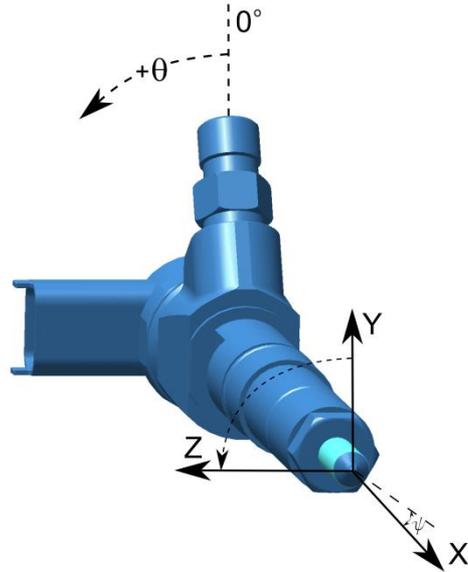
Quad-die
Blue LED
($\lambda \sim 460$ nm)

Experiments performed by
Julien Manin, *Sandia*, and
Michele Bardi, *CMT*.

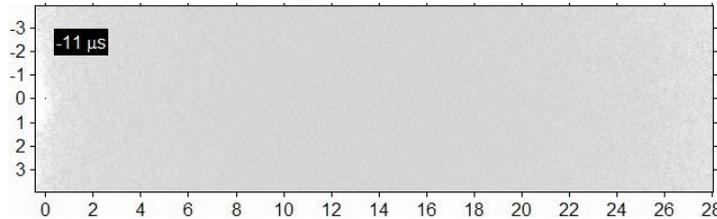
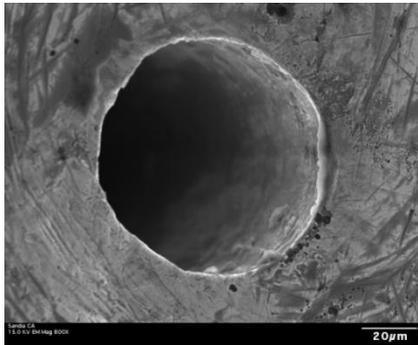
150 mm 600 mm

Fuel injector

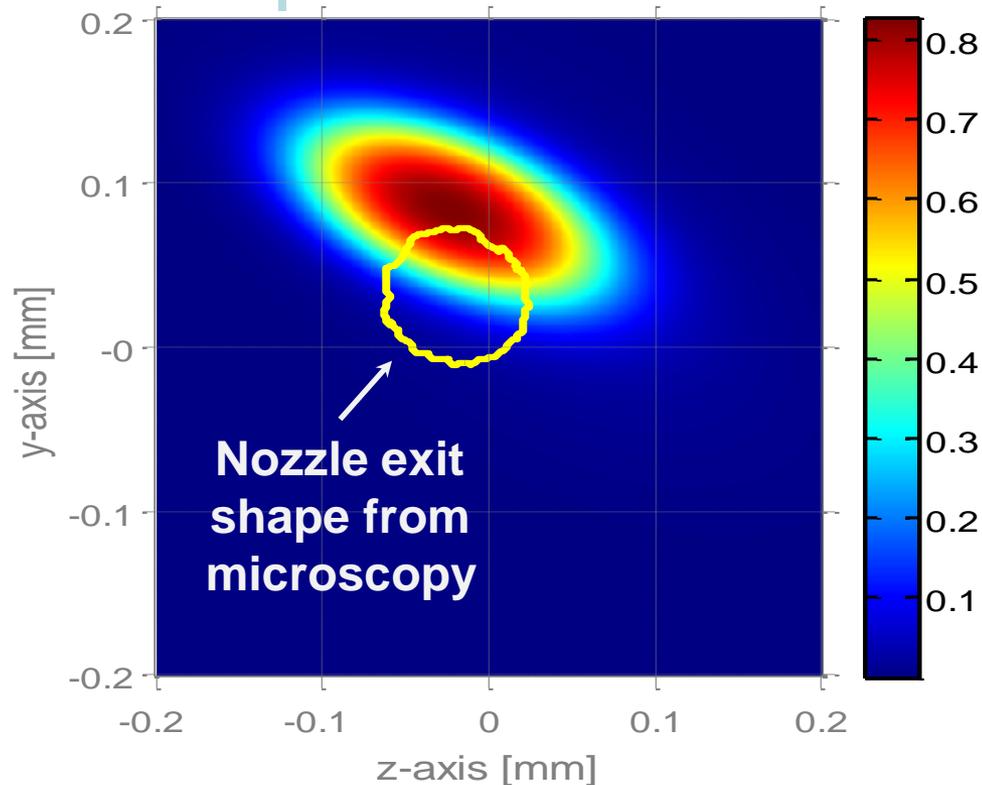
Spray asymmetry explanations



SEM of nozzle



$x = 3.2 \text{ mm}$

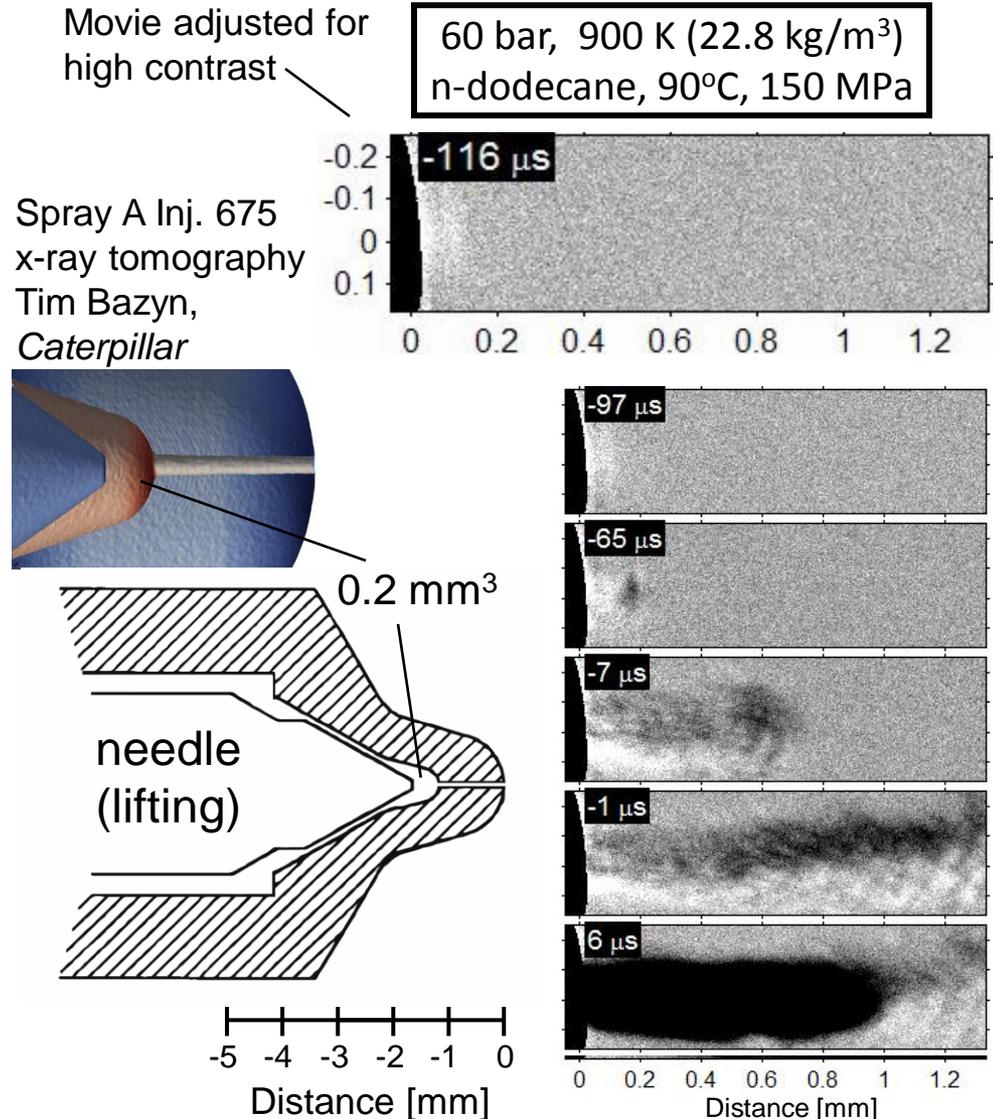


Mixture fraction derived from x-ray radiography

Argonne:
Chris Powell,
Alan
Kastengren

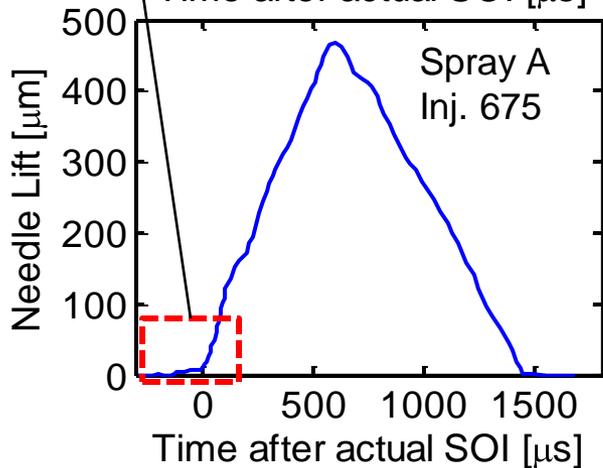
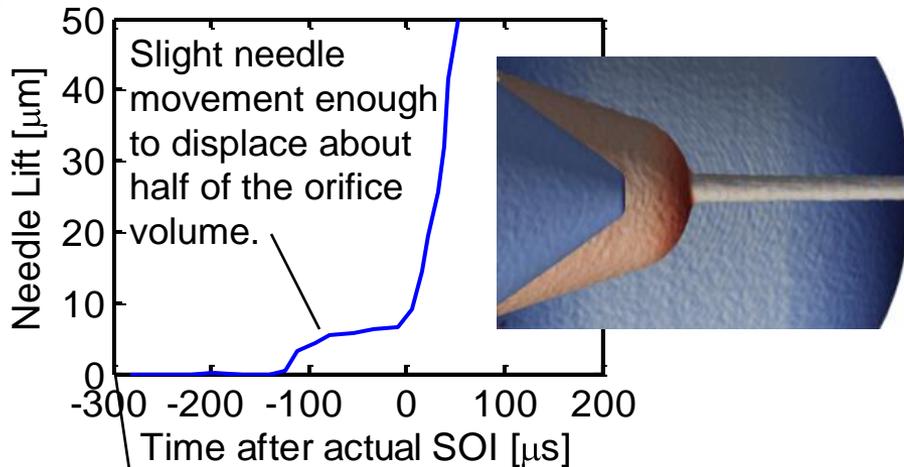
The beginning stages of injection show a vapor injection leading a liquid injection.

- What is the status of the sac volume at the start of injection?
 - Voids will be pressurized during compression cycle in an engine.
- Gases in the sac are pushed out by incoming liquid as the needle valve opens.
 - Vapor jet precedes liquid by approximately $10 \mu\text{s}$.
 - Some venting/gas exchange starts at about $-70 \mu\text{s}$.
 - Volume of the early vapor injection appears similar to that of the 1-mm long orifice.
 - Will affect initial rate of injection and penetration.
 - > Typical targets for experimental/modeling comparison.



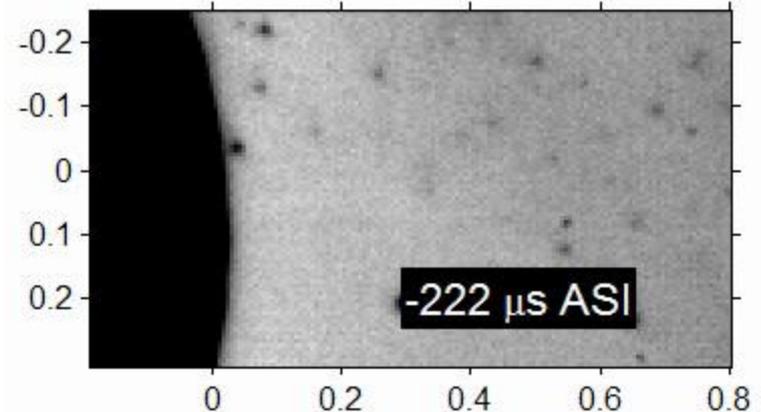
Leading vapor injection also shown recently by Crua et al. [SAE 2010-01-2247]

Needle movement actually pulls gas into the sac/orifice during first opening.



Multiple injection situation:
earlier injections have left
droplets inside the chamber.

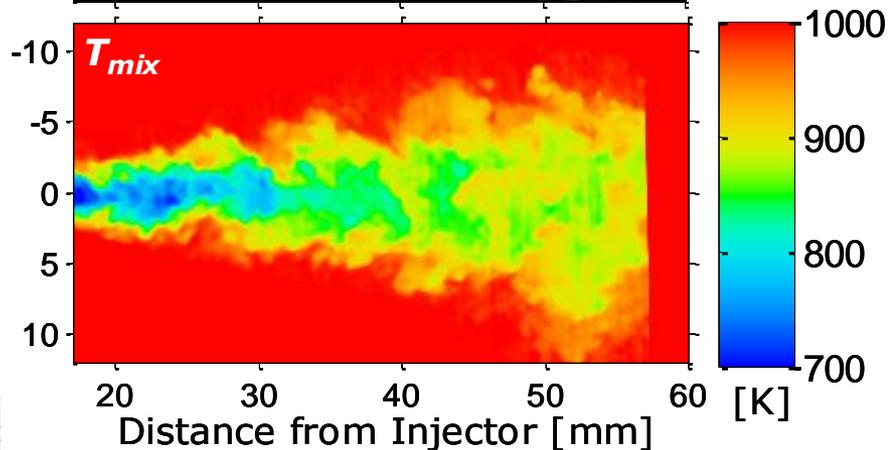
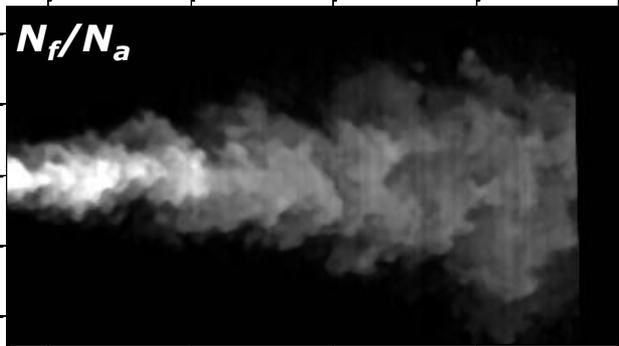
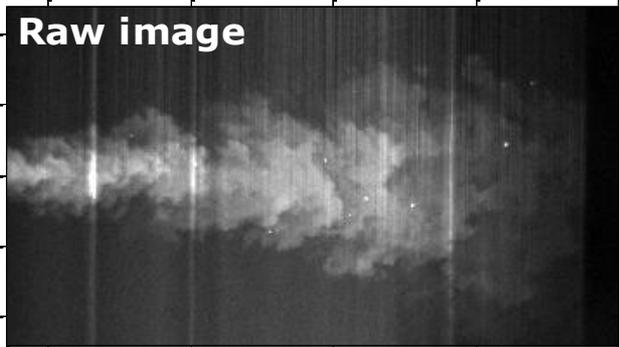
440 K, 29 bar



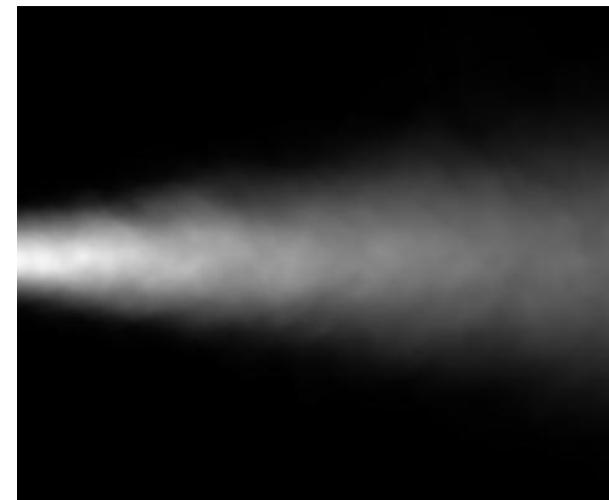
- Early needle movement momentarily creates a vacuum to pull droplet (and ambient gases) into the injector.
- Gas transfer into the sac could draw soot particles or other debris into the sac or orifice.

Rayleigh scattering performed to quantify mixing, rather than relying on vapor boundary.

- Measurement provides
 - Fuel mixture fraction (mass fraction)
 - Mixture temperature
- Performed at Sandia
 - see SAE 2011-01-0686.



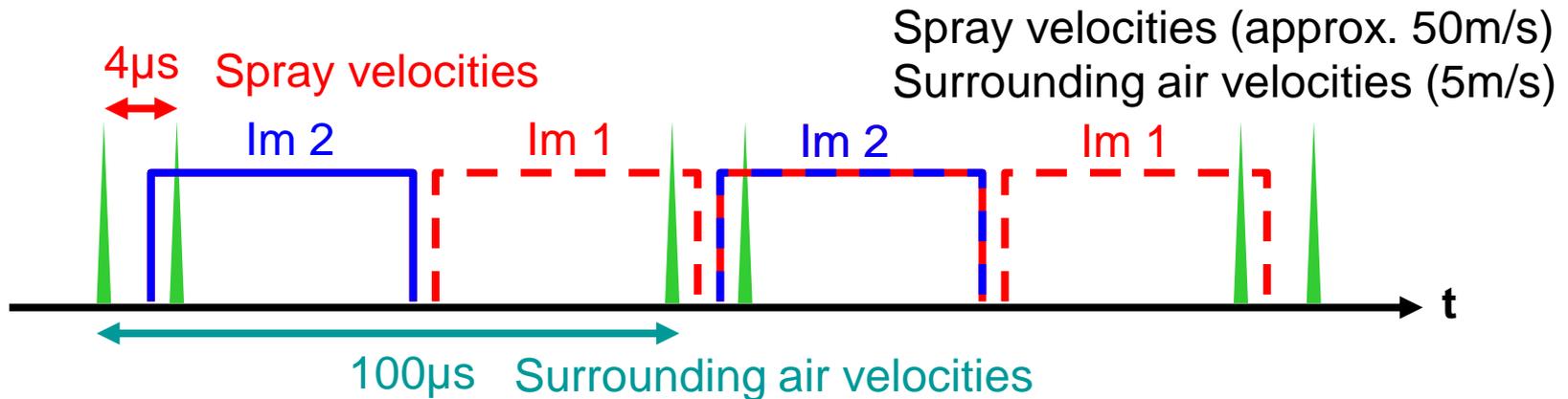
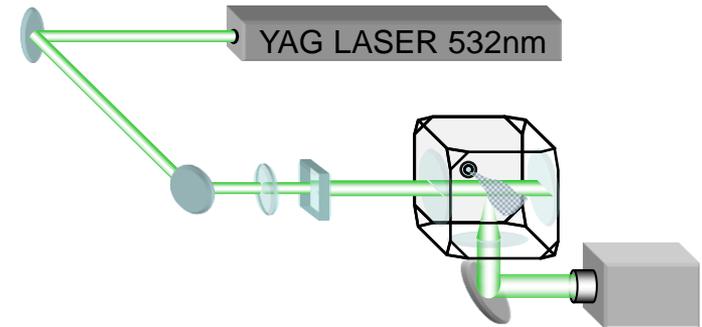
Mean mixture fraction



PIV measurements at IFPEN

Louis-Marie Malbec, Gilles Bruneaux

- ❖ High speed time-resolved PIV (10000 Hz)
 - ❖ Camera Photron SA1
 - ❖ YAG Laser 532nm (2 mJ per pulse)
 - ❖ Seeding particle: zirconium oxide, $<5\mu\text{m}$

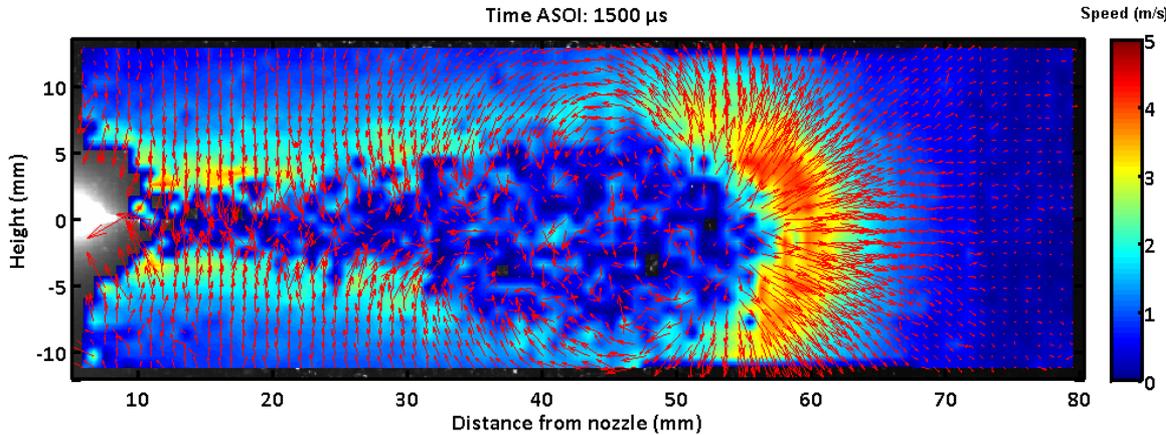


⇒ On a single injection event, 2 ranges of velocities can be resolved

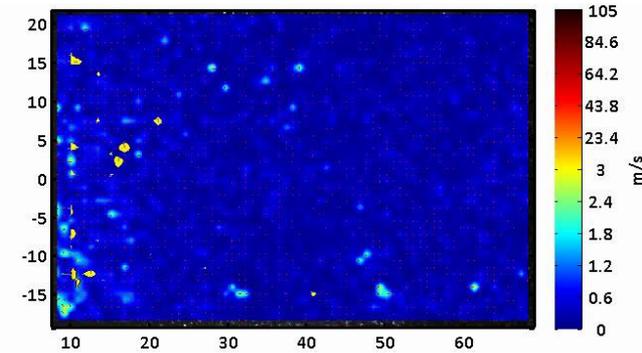
Velocity measurements performed downstream of the liquid region

Jet velocity

Time ASOI: 1500 μ s

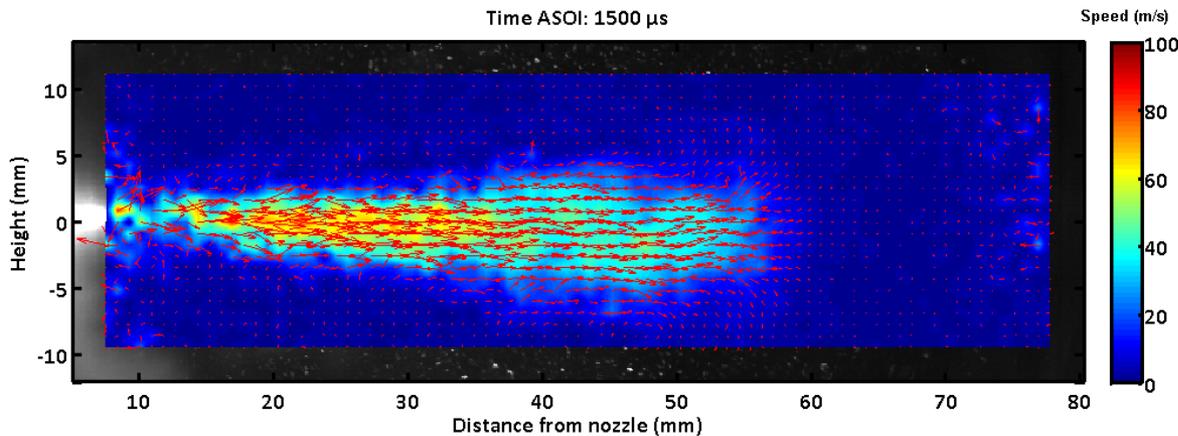


Velocity data "joined"

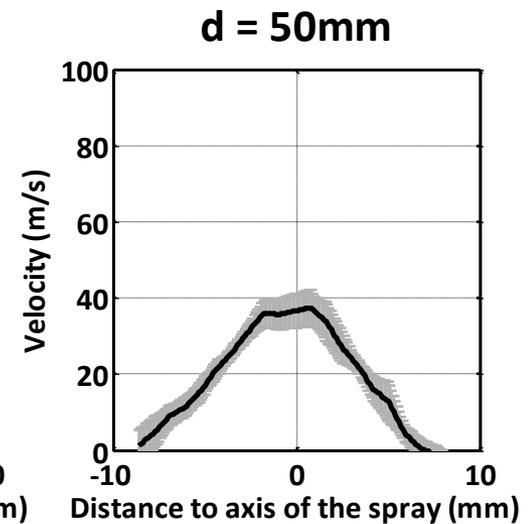
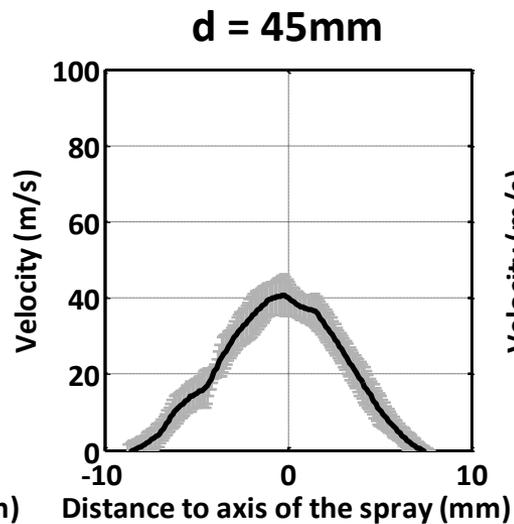
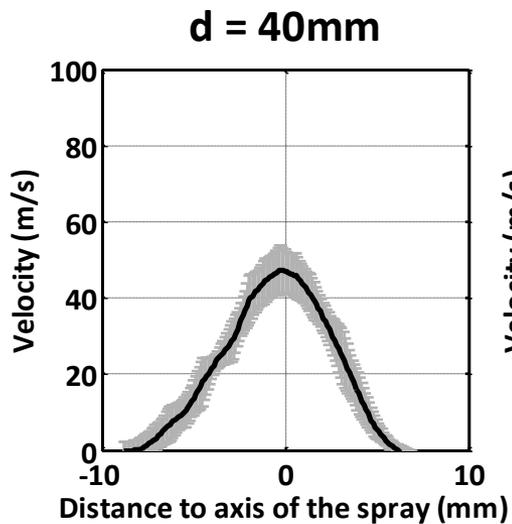
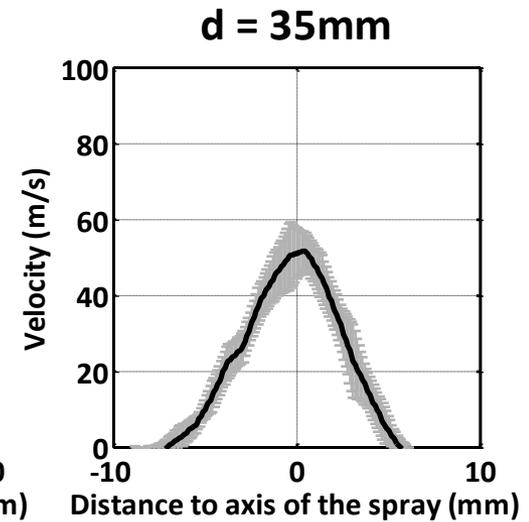
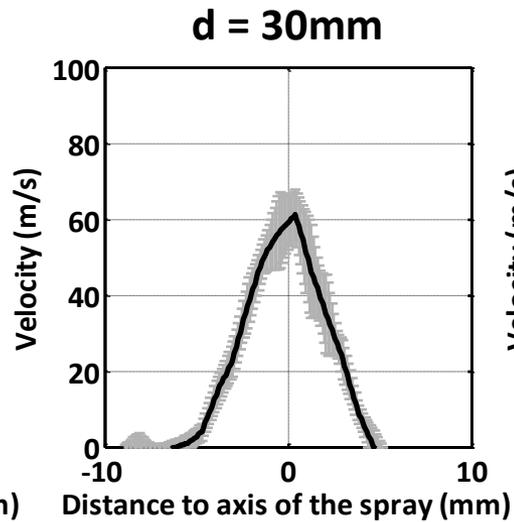
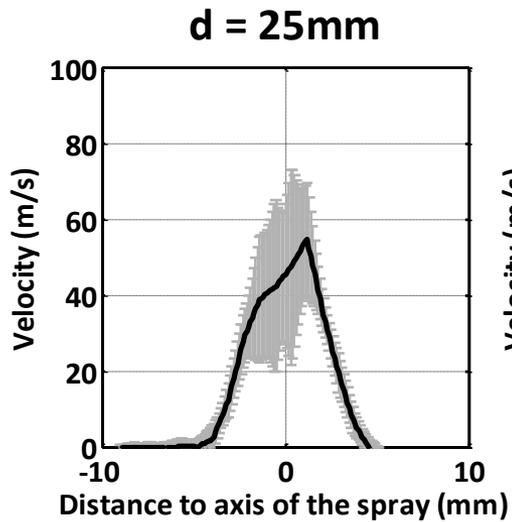
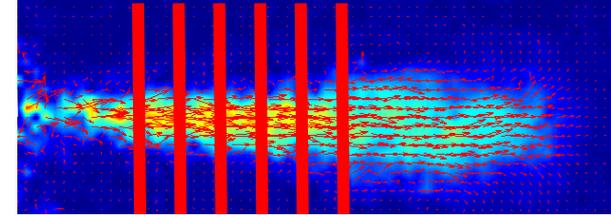


Surrounding air velocity

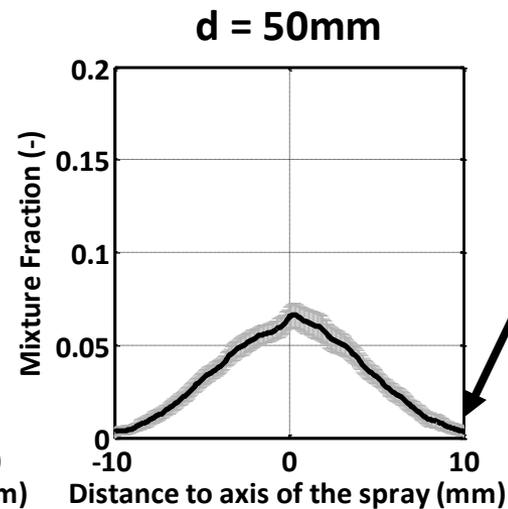
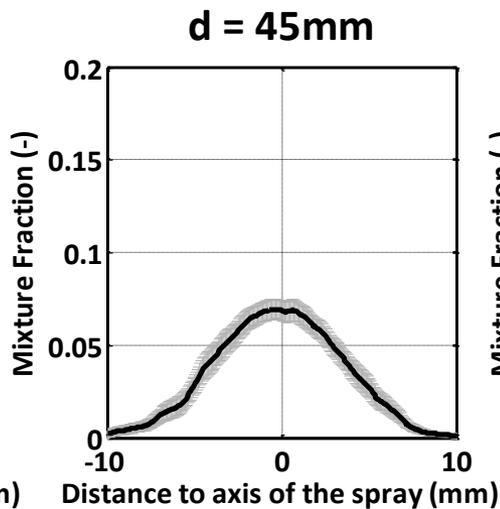
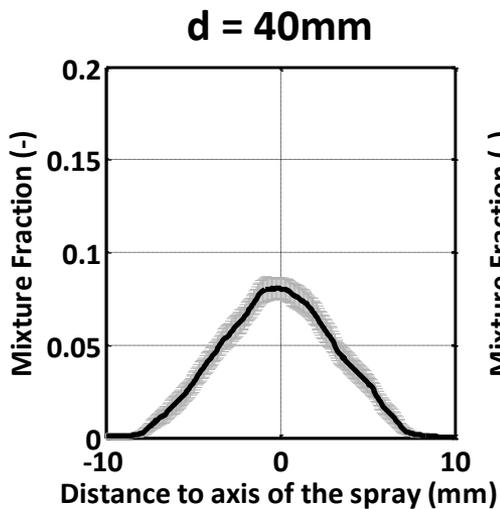
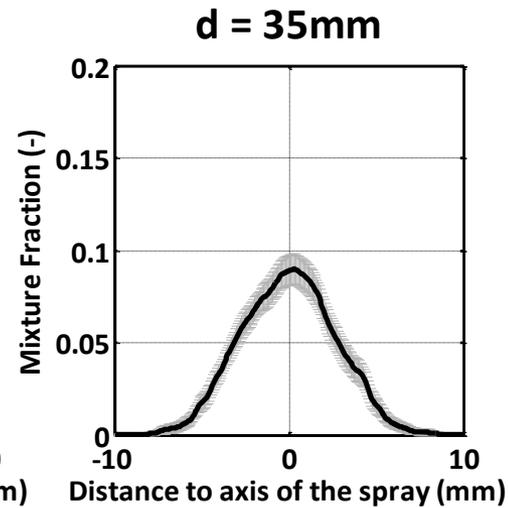
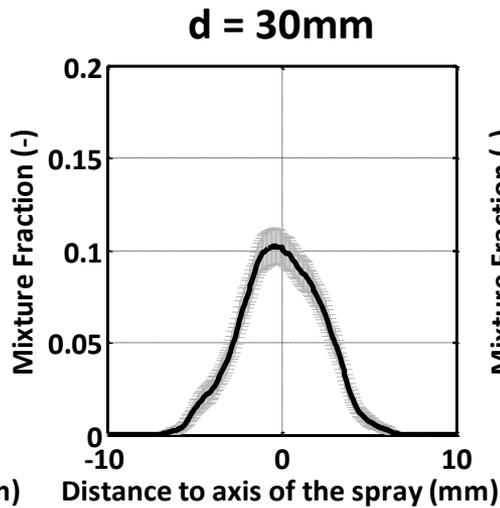
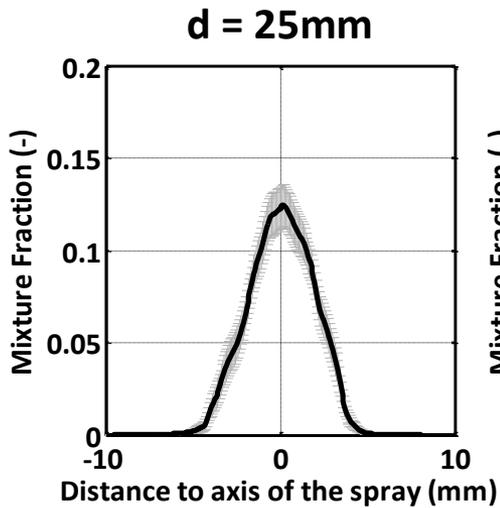
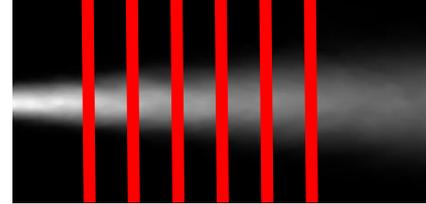
Time ASOI: 1500 μ s



Radial profiles of axial velocity in steady-state



Mixing and velocity fields are self-consistent.



schlieren
border



Modeling contribution examples

	ANL	Chalmers	CMT	PolIMI	UNSW	ERC	GA-Tech
Code	CONVERGE	OpenFOAM	OpenFOAM	OpenFOAM+LibICE	Fluent	OpenFOAM	KIVA-3V
Turbulence Model	RANS: RNG k- ϵ	RANS: k- ϵ	RANS: std k- ϵ with $C_{1\epsilon}=1.6$	RANS: k- ϵ	RANS: k- ϵ	RANS: RNG k- ϵ	RANS: k- ϵ
Spray Model:							
Injection	blob	blob		Huh	group	blob	blob
Atomization&Breakup	KH-RT with breakup length	VS2	Eulerian Sigma-Y	Huh-Gosman+Wave	No	KH-RT	KH-RT
Collision	O'Rourke Dynamic	none		none	No	none	O'Rourke Dynamic
Drag	Dynamic	VS2		Sphere	High-Mach	Dynamic	Dynamic
Evaporation	Frossling	VS2	State rel. from Locally Homog. flow	Frossling	Frossling	Frossling	Frossling
Heat Transfer	Ranz-Marshall	VS2		Ranz-Marshall	Ranz-Marshall	Ranz-Marshall	Ranz-Marshall
Dispersion	Stochastic	Stochastic		Stocastic	Stochastic DRW	Stochastic	Stochastic
Grid:							
dimensionality	3-D	3-D	2D axsiymetric	3-D	2D axisymm.	3-D	2D axisymm.
x	0.25 mm	0.25mm	0.009 mm	0.5 mm	0.84 mm	1 mm	0.5 mm
y	0.25 mm	0.25mm	0.009 mm	0.5 mm	0.29 mm	1 mm	0.5 mm
z	0.25 mm	0.5mm		0.5 mm		1 mm	
time-step	Min: 5e-7	1e-6 s	Min: 1e-8 s	5e-7 s	4e-6 second	Cou < 0.1 (DT_ini= 5e-7 s)	0.000487 s

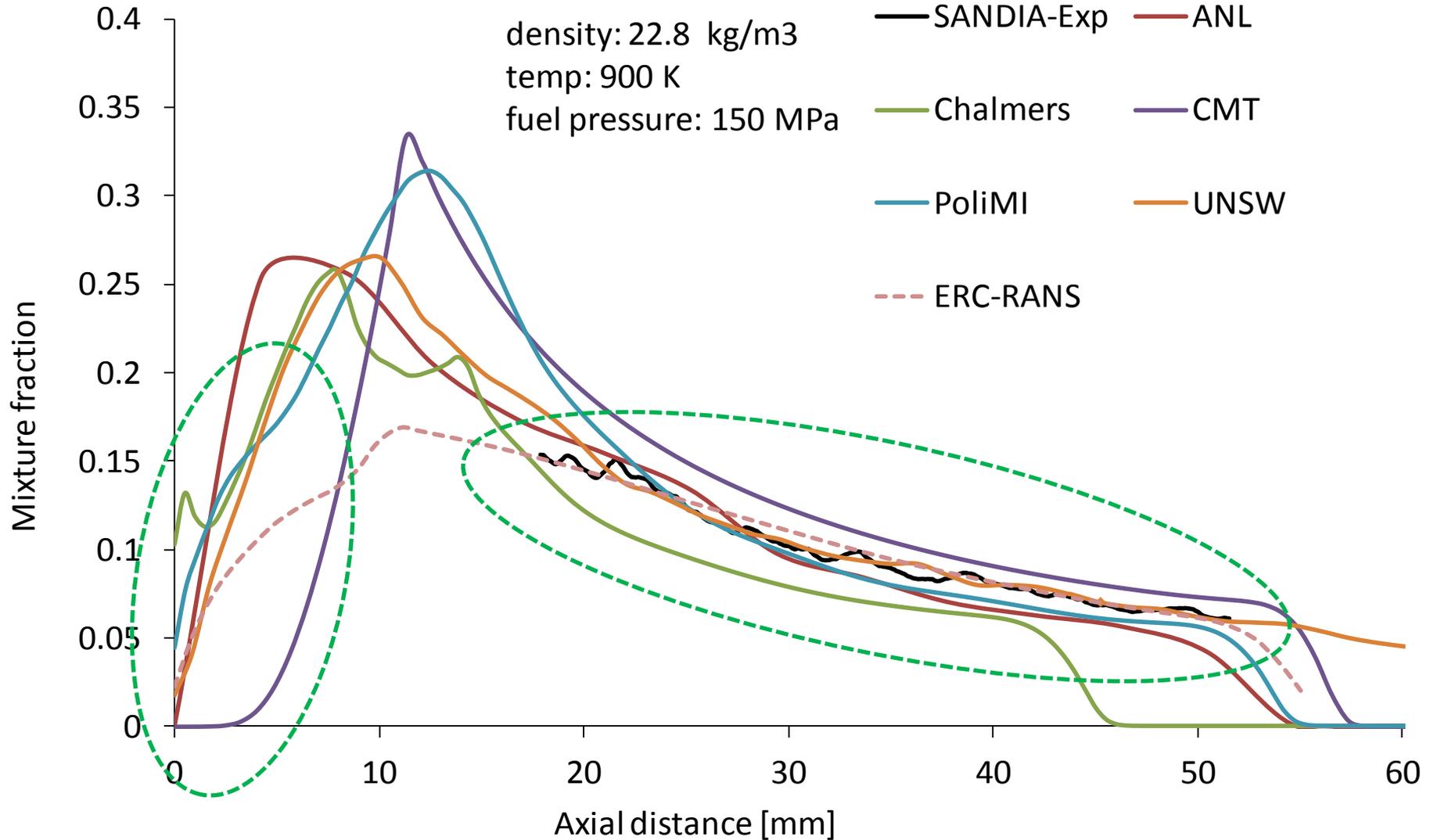
Models show variance in near-nozzle region, self-similarity downstream of liquid length

Axial profile - Vapor mixture fraction Z

density: 22.8 kg/m³

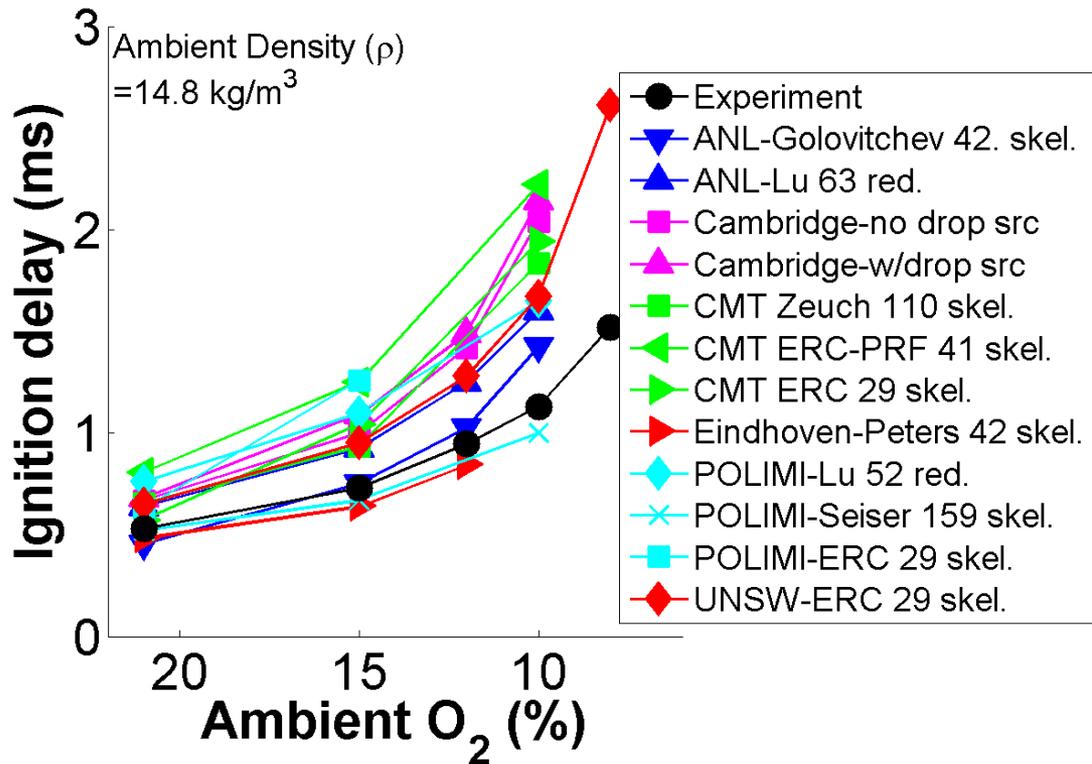
temp: 900 K

fuel pressure: 150 MPa



Evolution of model predictions between ECN1 and ECN2

n-heptane “Spray H”

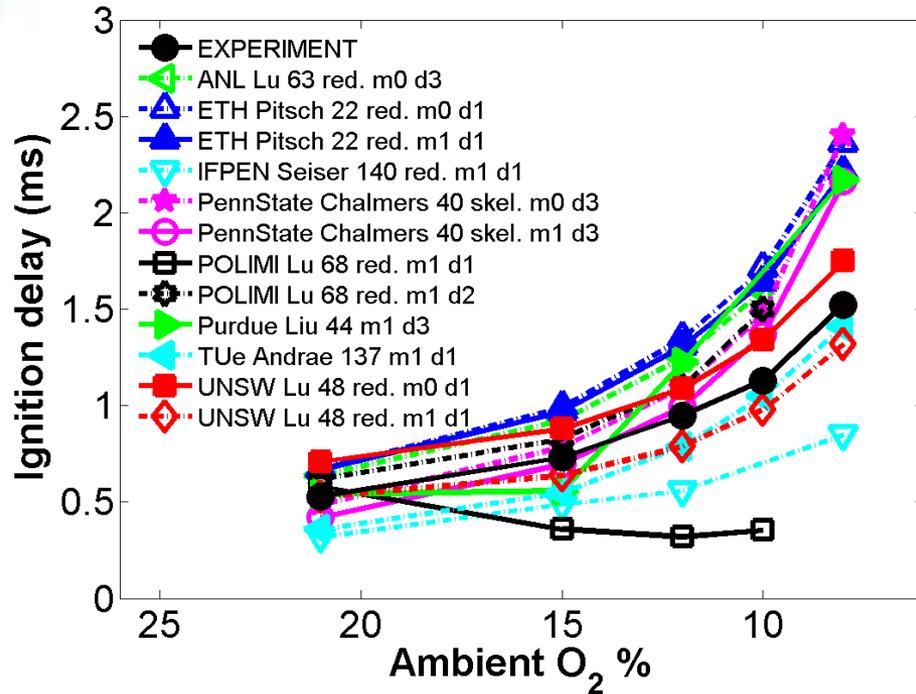


- At ECN1:
- Submissions did not necessarily have consistent definitions.
- No group successfully predicted ignition for “Spray A” using developed n-dodecane chemistry.

Ignition delay at ECN2

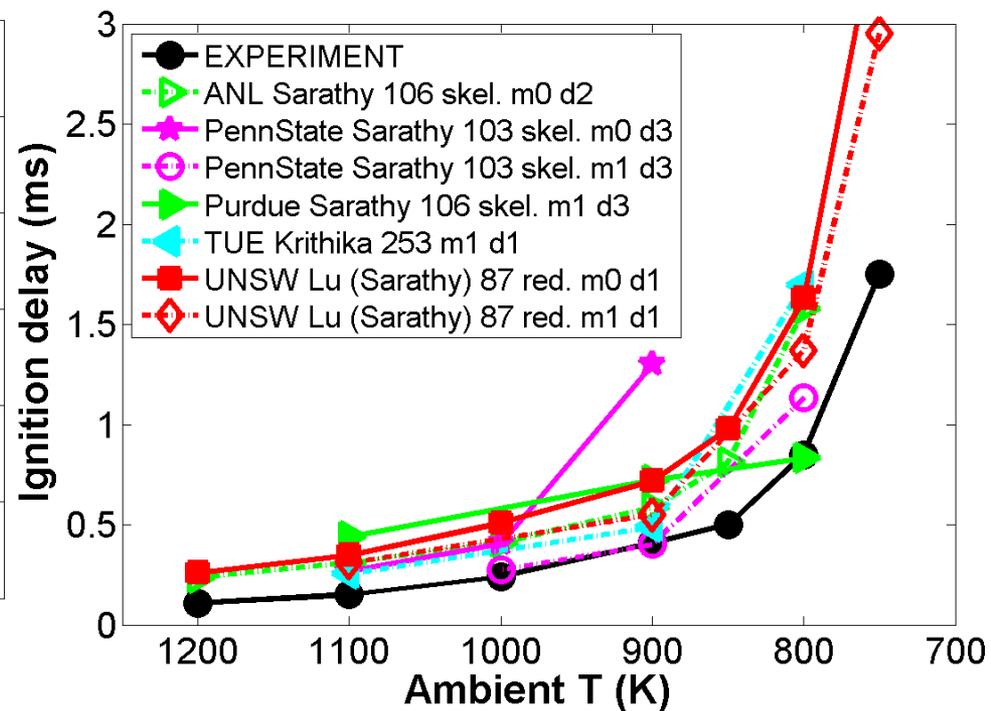
Spray H

C_7H_{16} , 1000 K, 14.8 kg/m^3 , 150 Mpa



Spray A

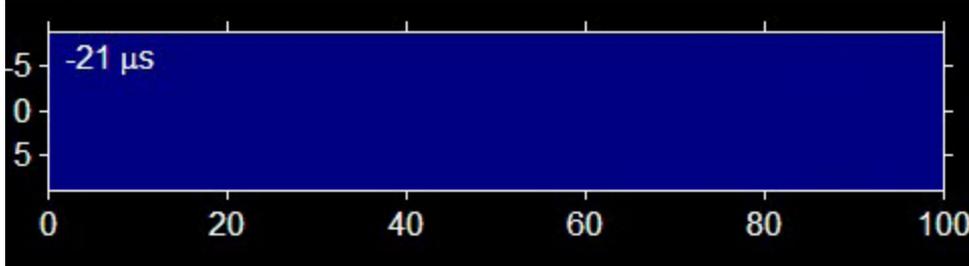
$C_{12}H_{26}$, 15% O_2 , 22.8 kg/m^3 , 150 Mpa



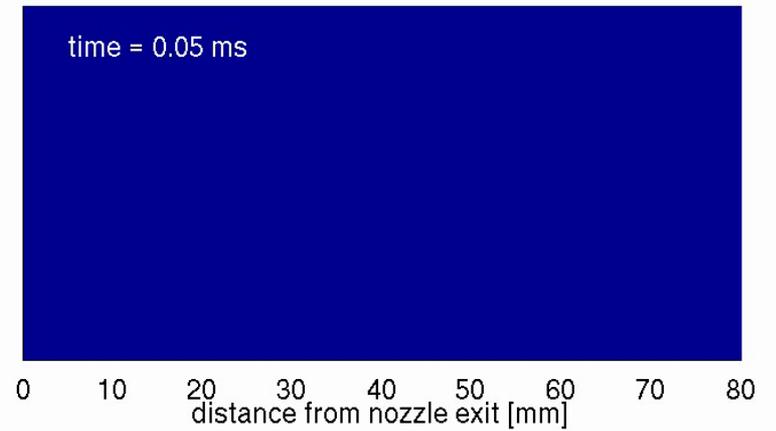
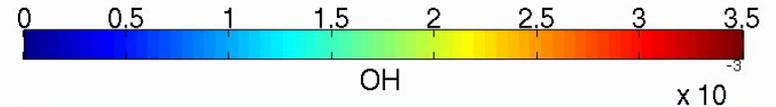
Observation of model predictions compared to experimental imaging.

Baseline n-heptane conditions

Experimental OH chemiluminescence Sandia



Eindhoven (LES)

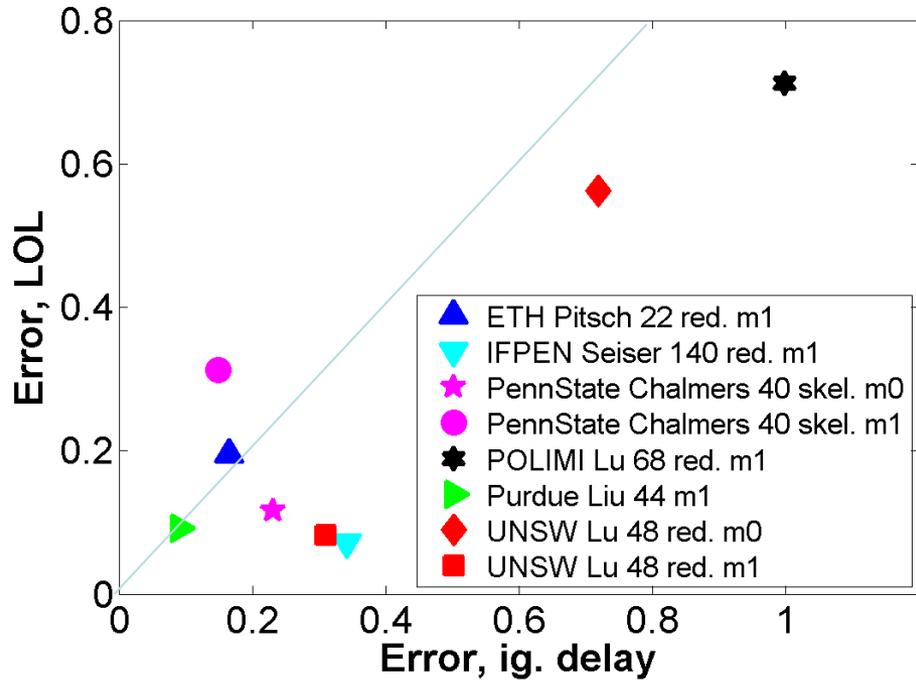


→
ANL

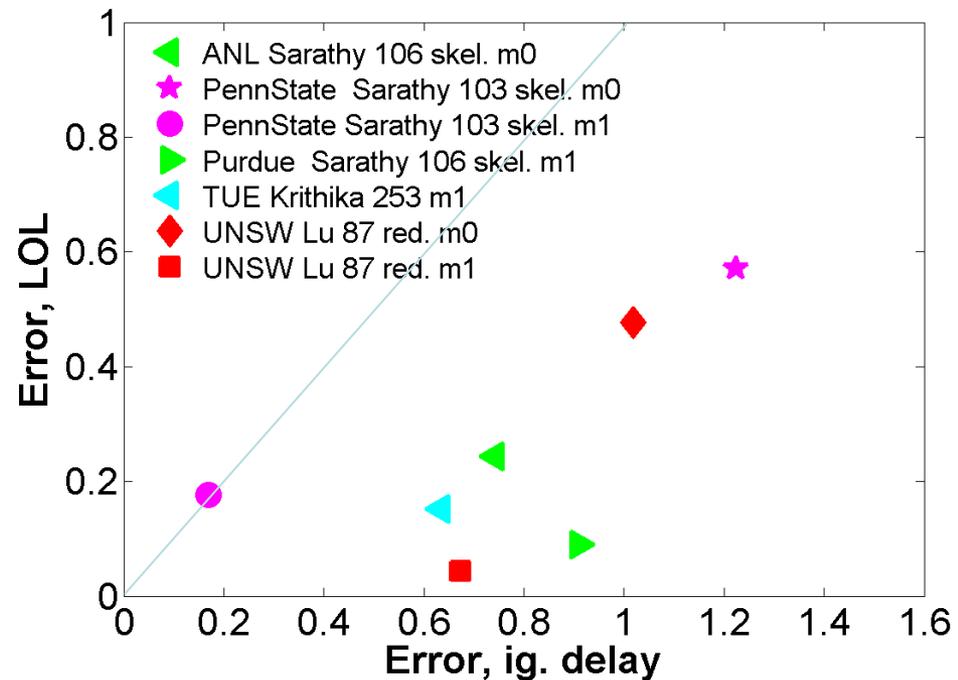
←
UNSW



C7H16, 21% O₂, 14.8 kg/m³, 150 Mpa



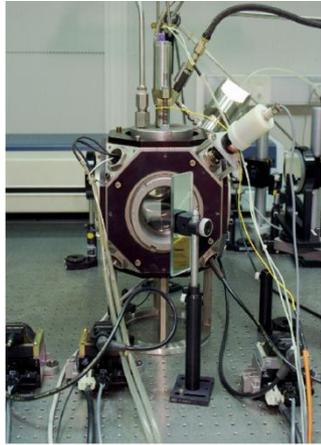
C12H26, 15% O₂, 22.8 kg/m³, 150 Mpa



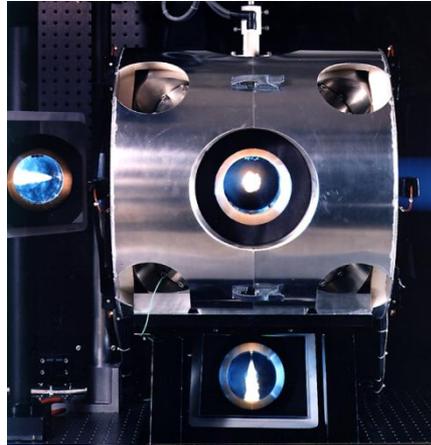
- Currently more difficult to capture ignition than lift-off, particularly for Spray A.
- Spray H generally better than Spray A.
- But 40% error will have major impact on combustion.

Ignition and lift-off length measurements are consistent for different types of HP-HT facilities.

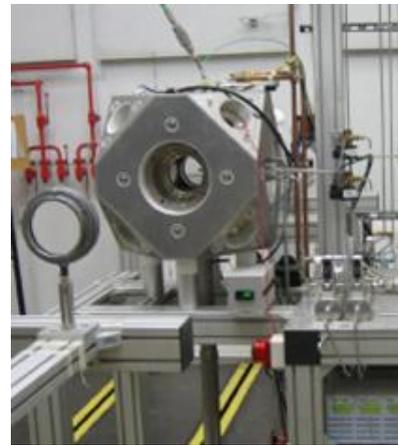
IFPEN



SNL



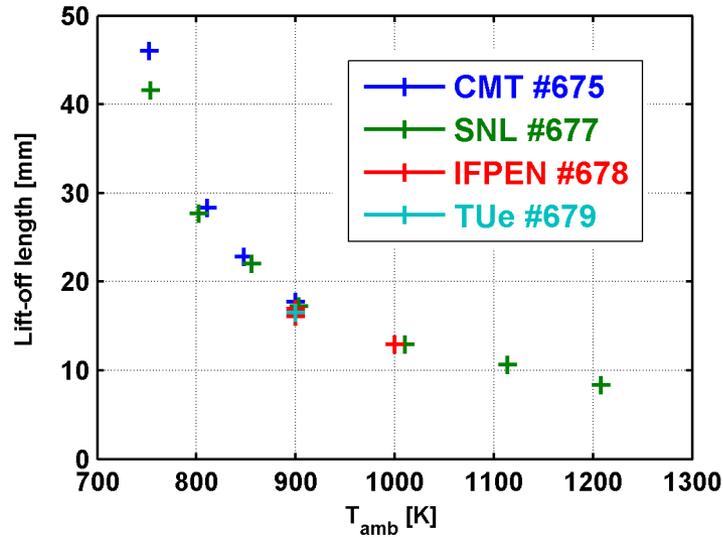
TU/e



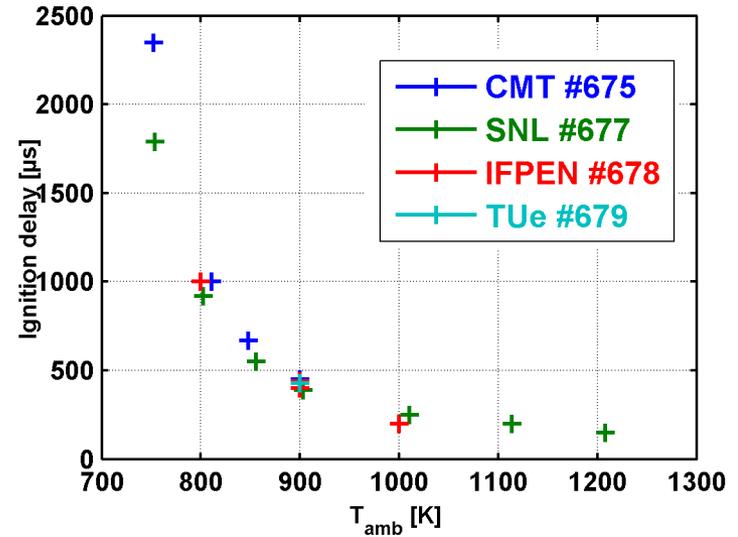
CMT



Lift-off length $\rho = 22.8 \text{ kg/m}^3$, $P_{\text{rail}} = 150 \text{ MPa}$



Ignition Delay $\rho = 22.8 \text{ kg/m}^3$, $P_{\text{rail}} = 150 \text{ MPa}$





Summary

- Our current understanding of diesel combustion is summarized in conceptual model form.
 - But there are many holes in the conceptual model, and quantification is needed.
- New “Spray A” initiative started for the Engine Combustion Network.
 - Filling the need for an advanced (quantitative) experimental dataset.
 - Provides a pathway towards more predictive spray combustion, more efficient optimized engines.
 - ECN workshops held. Data is available online.
- Results demonstrate reasonable similarity between institutions.
 - Opportunity to leverage experimental effort.
- CFD model improvement may proceed in a more quantitative way.



Questions