Spray Combustion Cross-Cut Engine Research

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Sandia National Laboratories

FY 2017 DOE Vehicle Technologies Office Annual Merit Review
Project ACS005, 11:30 AM, Wed. 7 June 2017

Sponsor: DOE Vehicle Technologies Office
Program Managers: Gurpreet Singh and Leo Breton

This presentation does not contain any proprietary, confidential, or otherwise restricted information.

Overview

Timeline

- Project provides fundamental research that supports DOE/ industry advanced engine development projects.
- Project directions and continuation are evaluated annually.

Budget

- Project funded by DOE/VTO: FY17 - $950K

Barriers

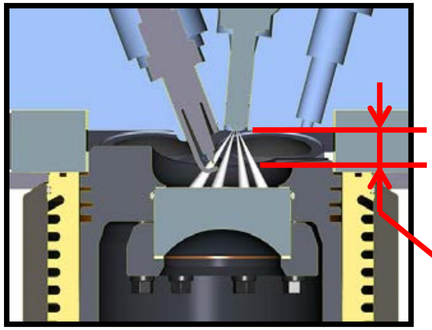
- Engine efficiency and emissions
- Understanding direct-injection sprays
- CFD model improvement for engine design/optimization

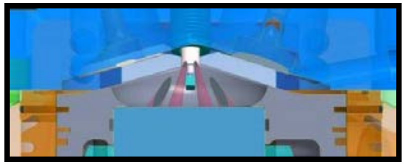
Partners

- 15 Industry partners in MOU: Advanced Engine Combustion
- Engine Combustion Network
  - >20 experimental + >20 modeling
  - >100 participants attend ECN5
- Project lead: Sandia
  - Lyle Pickett (PI), Scott Skeen

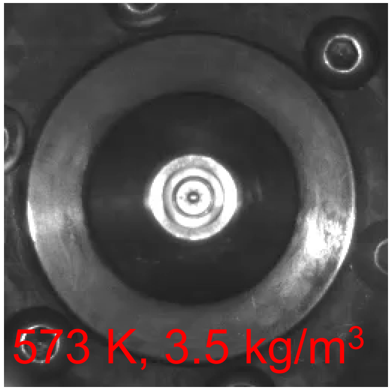
Engine efficiency gains require fuel (DI spray) delivery optimization

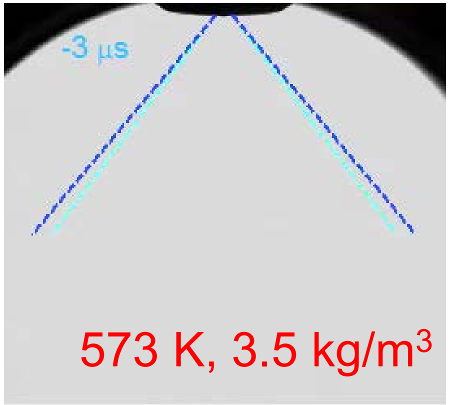
- Barriers for high-efficiency gasoline
  - Particulate emissions
  - Engine knock
  - Slow burn rate or partial burn
  - Heat release control when using compression ignition
  - Lack of predictive CFD tools
- Barriers for high-efficiency diesel
  - Particulate emissions
  - Heat release rate and phasing
  - Lack of predictive CFD, particularly for short and multiple injections



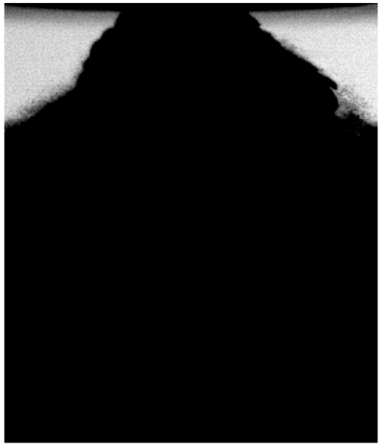


8-hole, gasoline
80° total angle

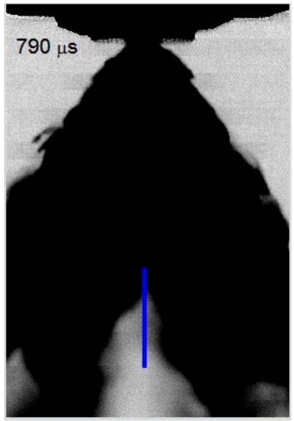




High-speed microscopy at nozzle exit



θ=22.5°
I/I_0
0.8-1.0

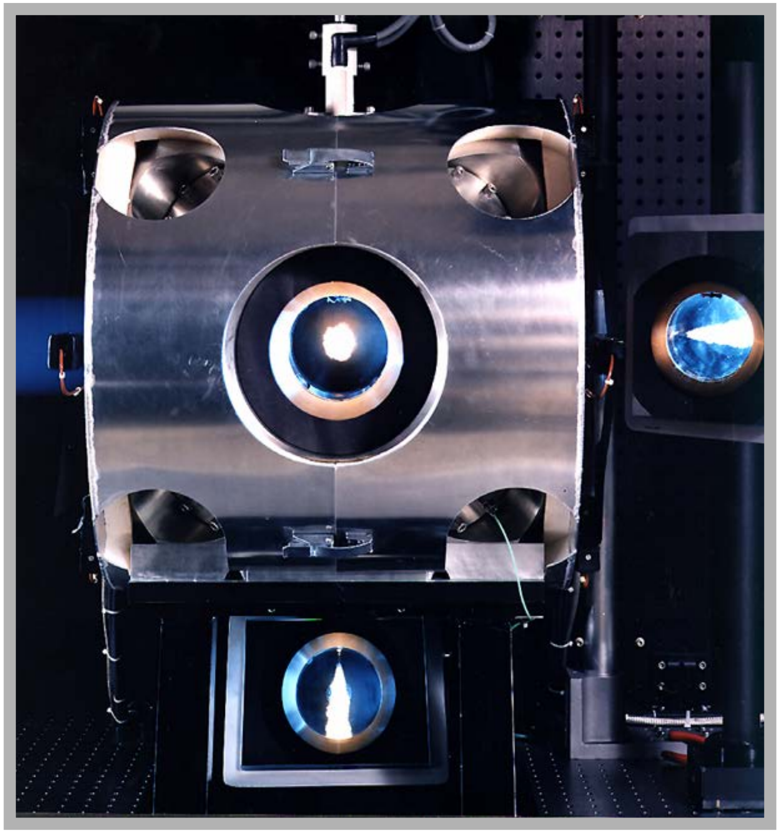


Project Objectives – Relevance

Major objective: experimentation at engine-relevant spray conditions, allowing development of predictive computational tools used by industry

- Provide fundamental understanding to make transient gasoline and diesel spray mixing and velocity predictive
  - Predictive combustion must be preceded by predictive mixing—still a weak link
  - Plume-plume interactions and aerodynamics leading to spray collapse
  - Focus on targets for with significant CFD activity as part of the Engine Combustion Network
- Provide a link between spray mixing and combustion
  - Characterize vaporization, ignition, soot formation processes
  - Models are deficient in these areas with serious consequences on emissions and efficiency
  - Guide model development and evaluation using quantitative, CFD-validation datasets

Experimental approach utilizes well-controlled conditions in constant-volume chamber



- Well-defined ambient conditions:
  - 300 to 1300 K
  - up to 350 bar
  - 0-21% O_2 (EGR)
- Injector
  - single- or multi-hole injectors
  - diesel or gasoline (cross-cut)
- Full optical access
  - 100 mm on a side
- Boundary condition control needed for CFD model development and validation
  - Better control than an engine
  - Easier to grid

Project does not include a funded CFD activity

Responses to previous year reviewer comments

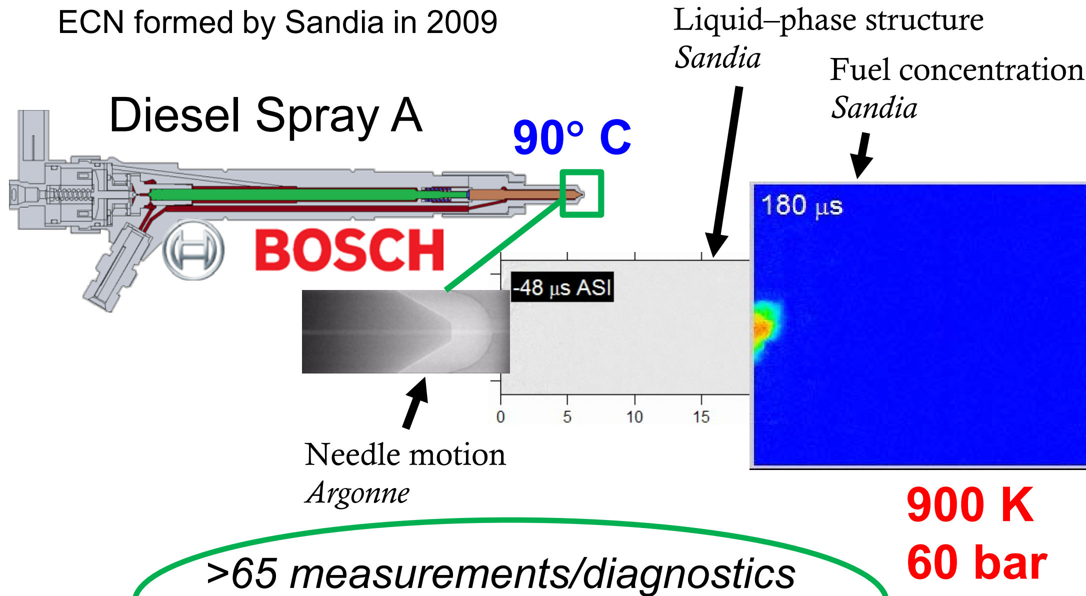
- How do your experiments actually affect CFD modeling tools:
  - "Better demonstration of how CVC data are used in CFD development"
  - "How diagnostic capabilities to quantify velocity are being used in CFD"
  - "How the spray data are being used in the CFD modeling should be demonstrated"
  - "Better specificity of precisely what data will be developed that the codes will predict should be provided"
- Clarify your collaboration in the Engine Combustion Network:
  - "Many CFD collaborators are listed in the ECN but how is the "very tight coordination executed"?
  - "Precise roles of the ECN collaborators were not evident"
  - "Are ECN participants free to define their own niche, and if not, how are they being steered in ways that will create a synergistic whole?"
- General:
  - "Consider developing a diagnostics consortium across the national laboratories"
  - "What is being done in the area of flash-boiling sprays"?

Collaborative research through the Engine Combustion Network accelerates CFD model development

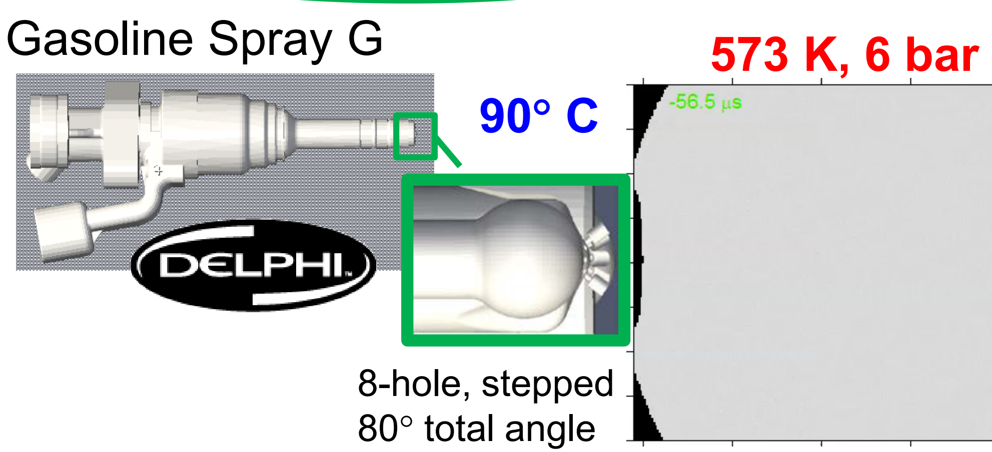
Approach
- Develop diesel and gasoline target conditions with emphasis on CFD modeling shortcomings
- Comprehensive experimental and modeling contributions
- Diesel Spray A, B, C, D
- Gasoline Spray G
- Results submitted to online archive with fields (like geometry and uncertainty) specifically tailored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

Impact
- Established in 2009, there are already 1400 citations of the ECN data archive
- ALL US 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



ECN Workshop Activities

- Most recent workshop: ECN5 held Apr 2017 at Wayne St. Univ. (Thank you to local host Marcis Jansons)
- Sandia contributes experimental data to all topics
- Topic organizers establish guidelines a year in advance of in-person workshop
- Organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review
- Sandia PIs have deep, specific engagement in CFD efforts
- Monthly web meetings are held to provide individual institutions the opportunity to present their ECN work

organizer role	**ECN5 Topics**
	Internal flow diesel
	Near-nozzle diesel
	Evaporative diesel
	Reactions and ignition
	Diesel combustion
Skeen	Soot
	Multi-hole diesel
	Internal flow gasoline
Pickett	Evaporative gasoline

Snippet from Spray G "evaporative gasoline" guidelines

Lagrangian or Eulerian simulations data request::
- Priority for Spray G, G2, G6, G4 conditions
- Provide liquid/vapor axial penetration with respect to time

☐ Liquid (liquid volume fraction = 0.1%)
☐ Vapor axial penetration (fuel mixture fraction = 0.01)

At 0.1-2ms (or max) in 0.1 ms steps, provide at axial positions z=2,15,10 mm.

☐ 3 component gas and liquid velocities
☐ Total liquid and vapor fuel mixture fraction (mass of liquid fuel and vapor fuel/mass of all mixture)
☐ mass liquid fuel / volume (not liquid density)
☐ total mixture density (fuel and all other gases / volume)
☐ Sauter mean diameter droplet size

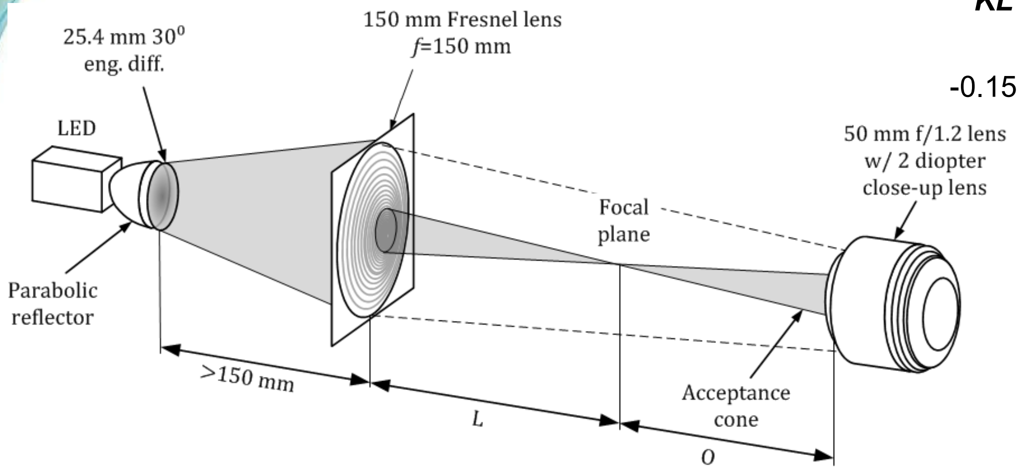
- At 0.1-2ms (or max) in 0.1 ms steps provide at the side view "primary" and "secondary" cut planes (0-40 mm or domain max). ....

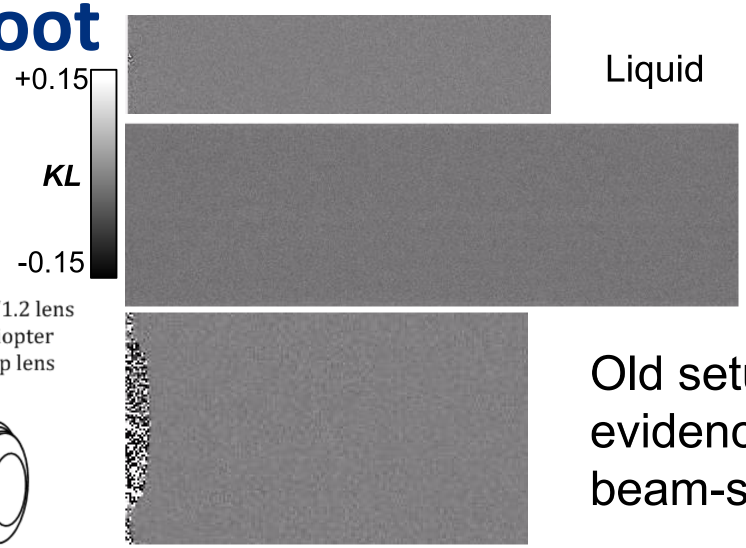
Approach - Milestones

- ✓ **Jul 2016**
  Using high-speed and formaldehyde imaging, analyze the effects of cool flame on high-temperature ignition
- ✓ **Aug 2016**
  Investigate effect of fuel type and blend on liquid structure at “supercritical” conditions
- ✓ **Sept 2016**
  Apply extinction imaging to define plume centers and their interaction in multiple-injection gasoline direct injection scenarios
- ✓ **Nov 2016**
  Research visit to continuous-flow chambers at GM & Caterpillar to obtain statistically resolved quantities of soot extinction, ignition, and lift-off length for CFD comparison
- ✓ **Dec 2016**
  Analyze high-speed planar mixing measurements for mixture at ignition
- ✓ **Mar 2017**
  Conduct ECN5, performing analysis of the state-of-the art experiment and CFD with respect to gasoline spray modeling and diesel (ignition & lift-off length) soot formation
- ● **May 2017**
  Apply filtered-Rayleigh scattering for Spray G (multi-hole gasoline) vapor concentration
- ● **Jul 2017**
  Use long-distance microscopy and high-speed imaging to investigate soot formation due to poorly atomized droplets and fuel films remaining on GDI injectors

Optimization and standardization of DBI setup for liquid and soot

DBI: Diffused Back Illumination





Liquid

(Sandia Spray A)

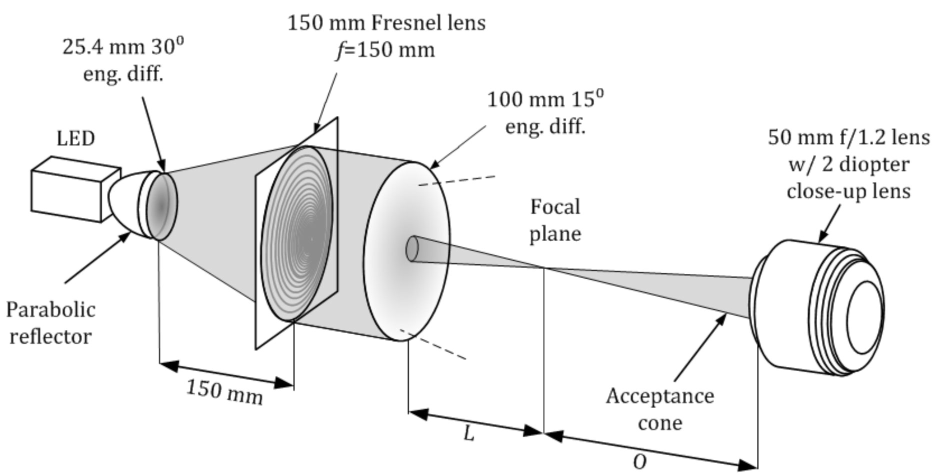
Soot

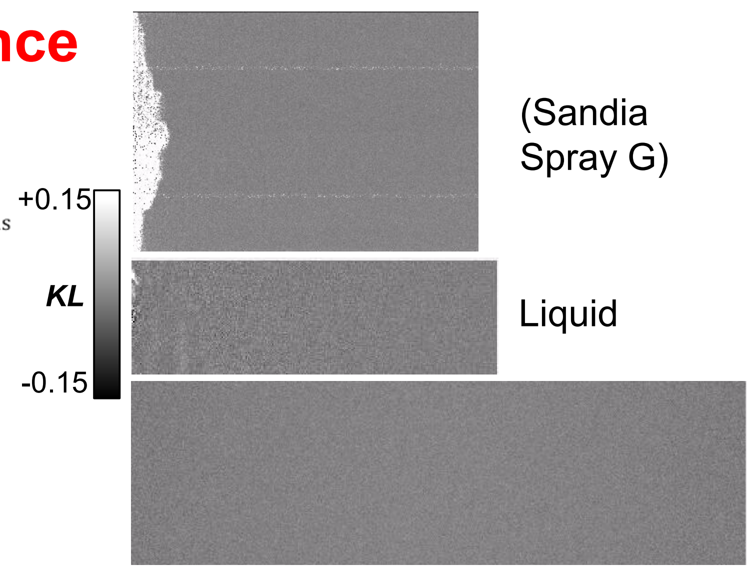
Old setup shows evidence of beam-steering

(Sandia Spray G)

Liquid

New DBI setup performance





(Sandia Spray G)

Liquid

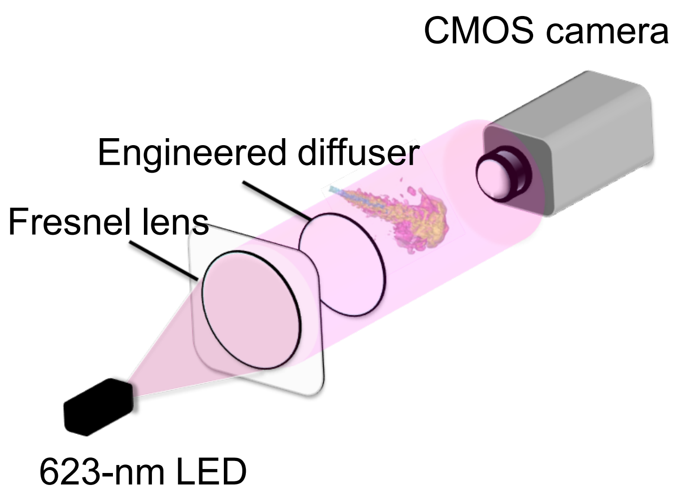
(Sandia Spray A)

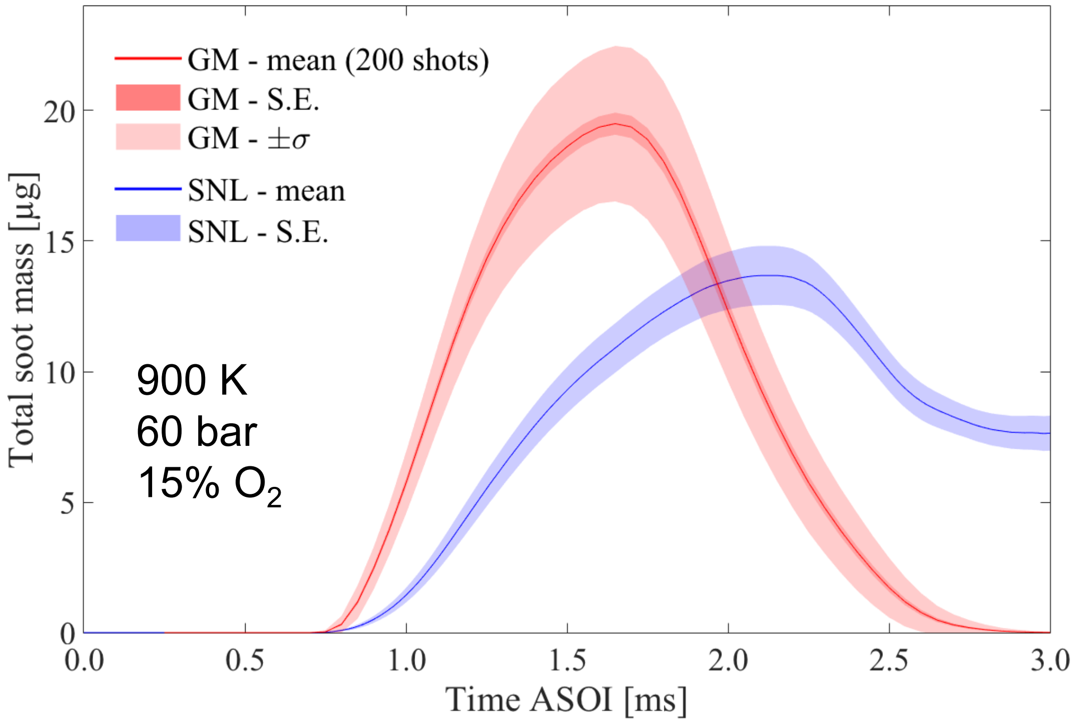
Soot

Collaborative efforts with industry provide insight into EGR effects and shot-to-shot variability

Total Soot Mass

- 200 consecutive Spray A injections performed at GM research with Sandia-developed extinction imaging diagnostic (Spray C & D studied at Caterpillar)
- GM constant pressure vessel ambient contains O_2/N_2, whereas SNL pre-burn vessel contains H_2O and CO_2 from pre-burn products
- GM results show earlier onset of soot formation and higher peak soot in spray head relative to SNL data in spite of consistent ignition delay and lift-off length

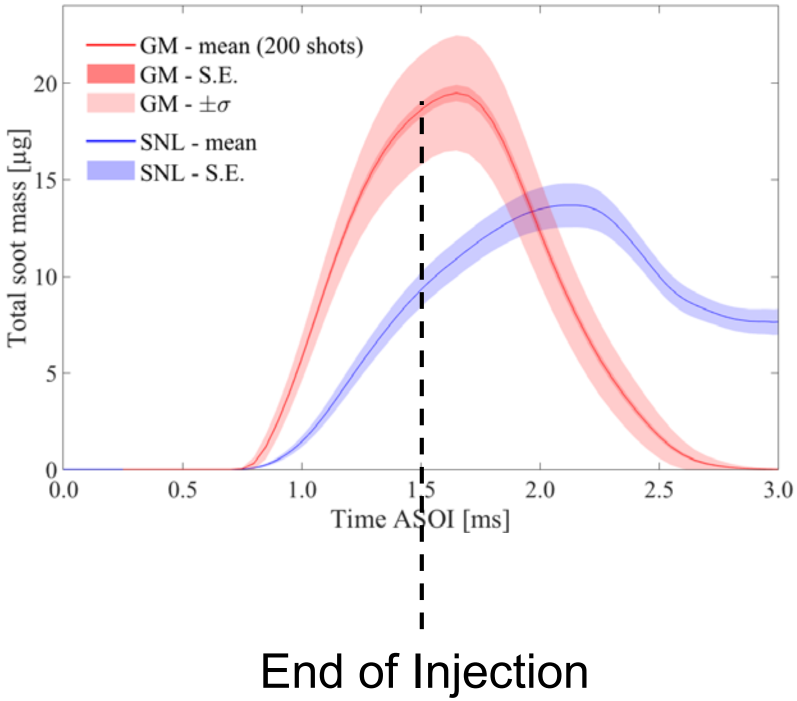




Shot-to-shot variability in total soot mass increases significantly before end of injection

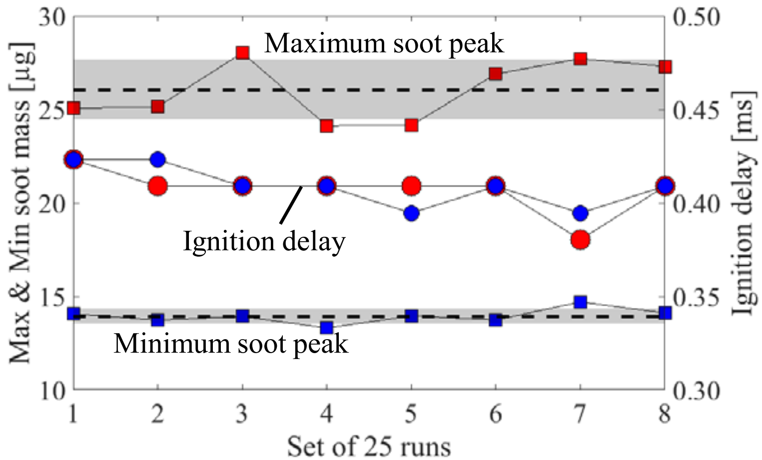
Shot-to-shot variability

- Standard Error (S.E.) with 200 consecutive injections ranges from <1% to approximately 5% of the mean transient soot mass during injection
- Standard deviation begins to increase well before end-of-injection (EOI) with the largest variability observed near (EOI)

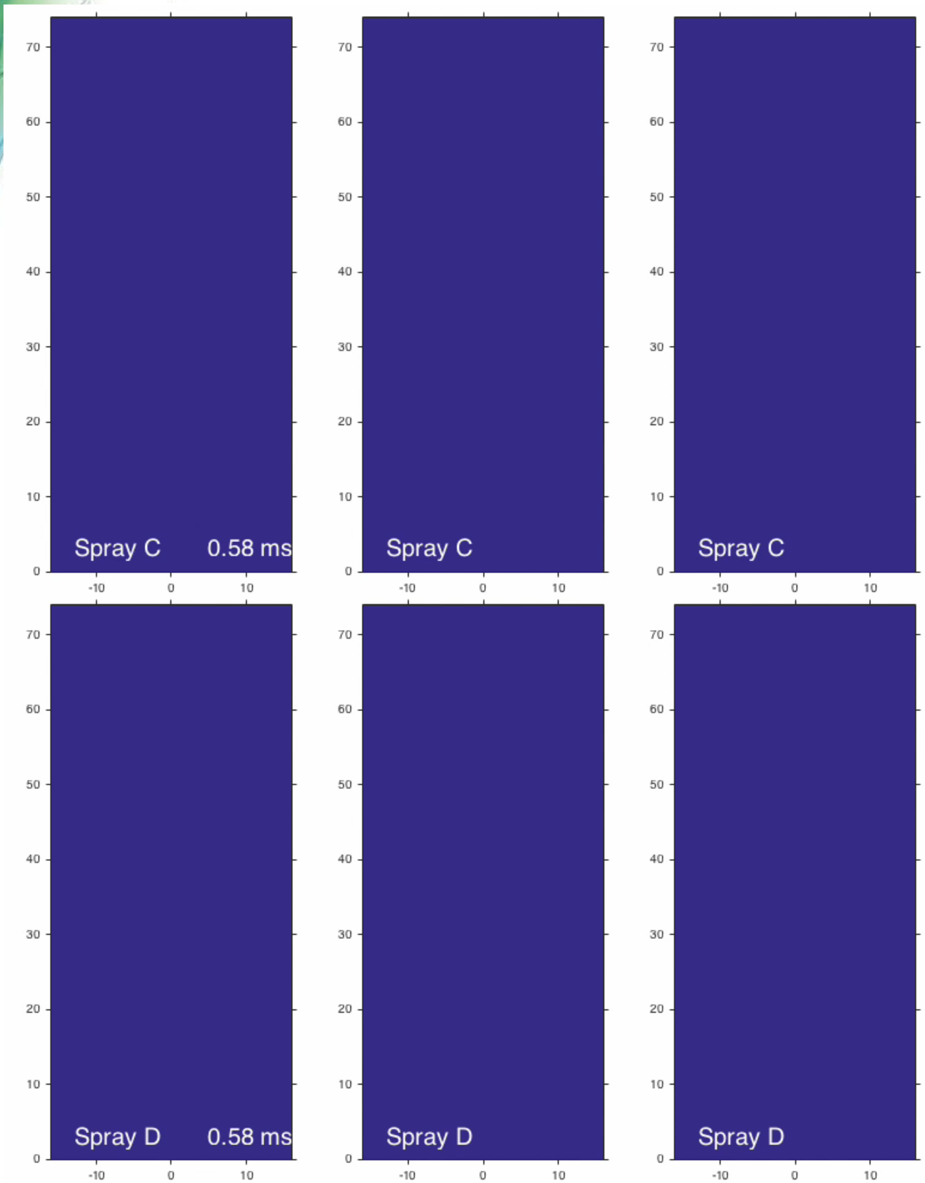


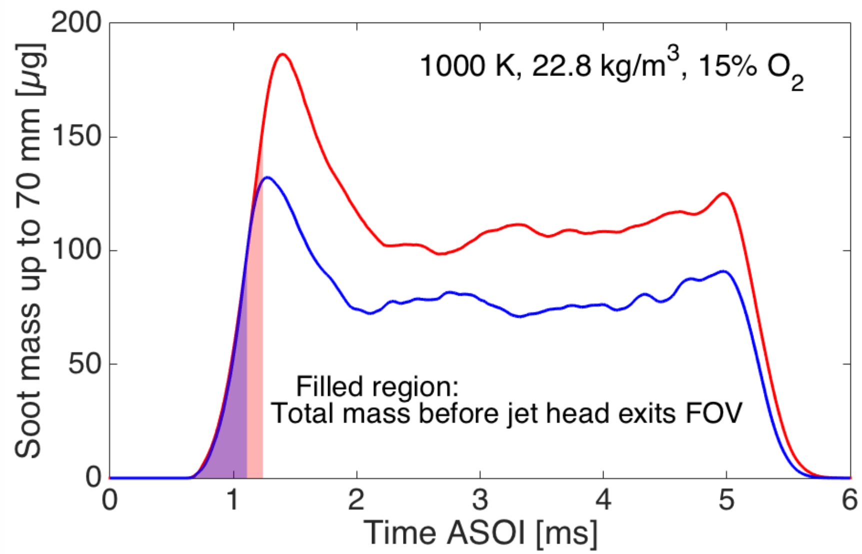
Ignition delay

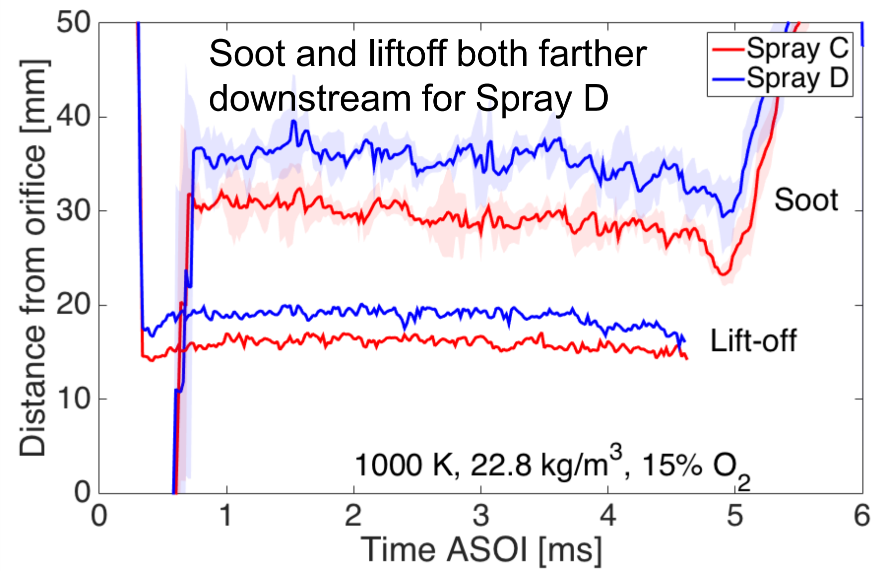
- No correlation between ID for runs with largest soot differences



Soot mass much greater for heavy-duty injectors – Spray C and D > 120 µg, partial sample; Spray A ~50 µg, near-full sample

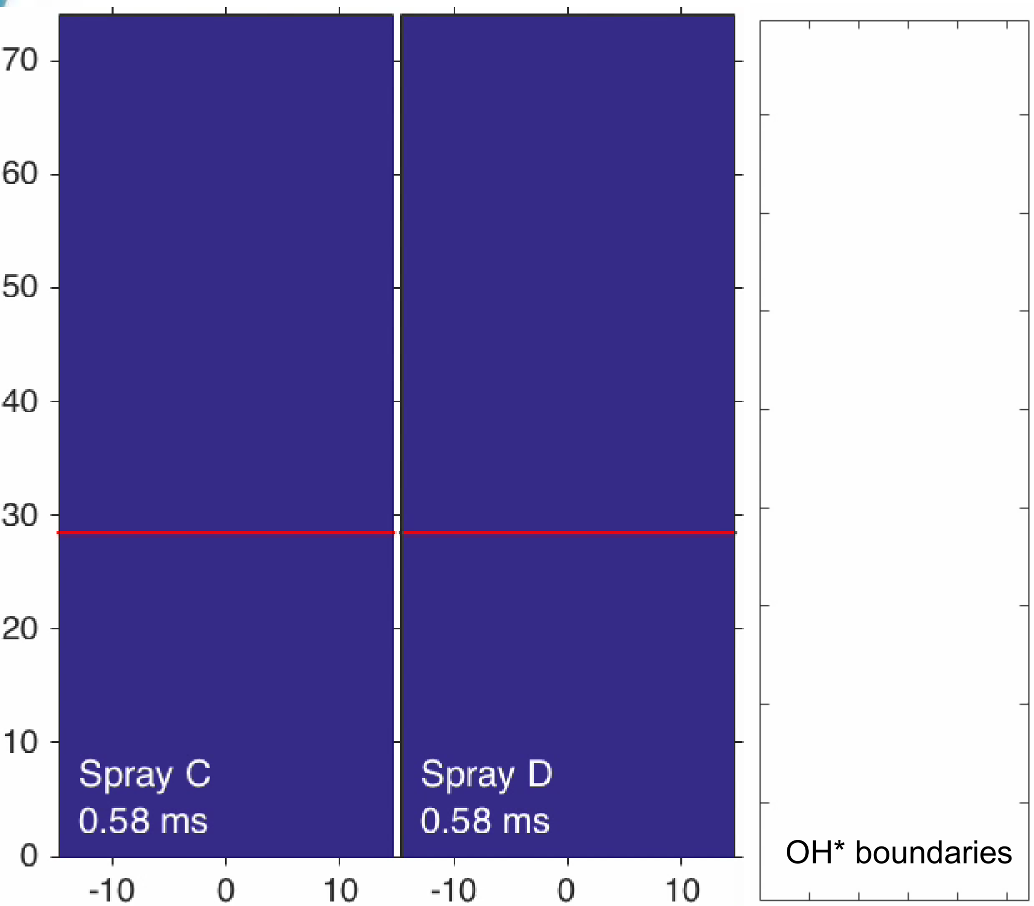




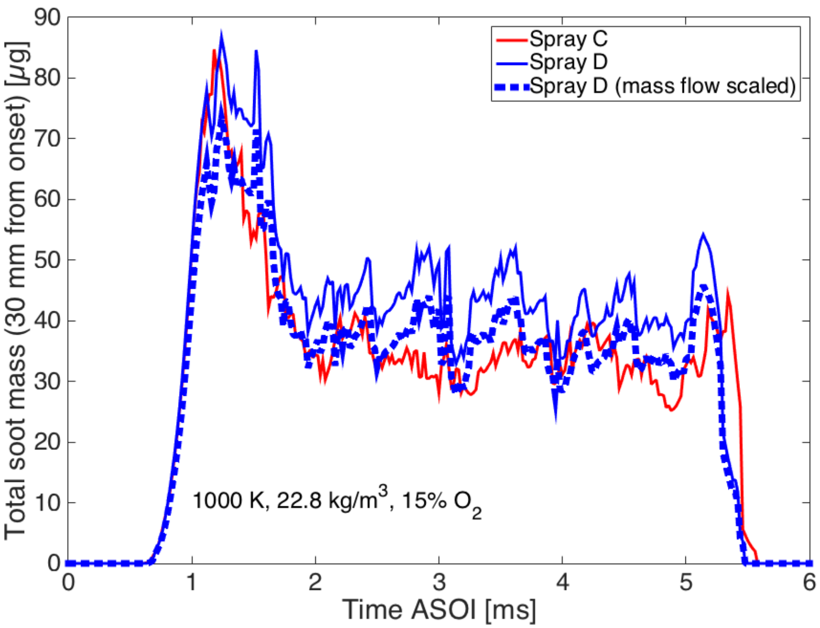


Comparison of soot mass within consistent spatial bounds shows similar soot for cavitating or non-cavitating injectors

Cavitating - Spray C - red
Smooth KS - Spray D - blue



- Determine axial location where optical thickness, *KL*, first exceeds 0.005 (99.5% transmission).
- Extend 30-mm downstream from this position and integrate total soot only within these bounds



- BUT, spatial location of flame is much different! This changes jet-jet interaction, penetration, wall interaction.

Example of ECN organizer role (Lyle Pickett)
Contributors to "Lagrangian Spray G" session at ECN5

Experiment

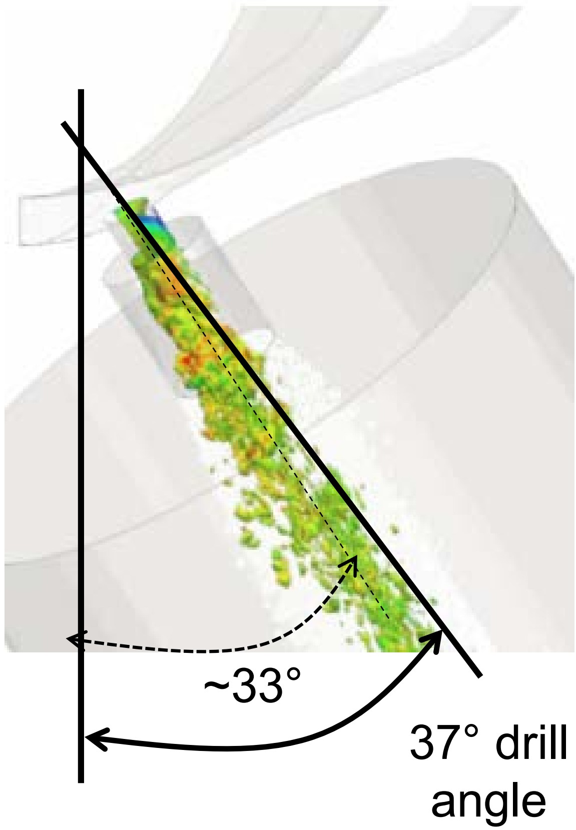
- Argonne National Laboratory
  - Radiography/tomography measurements: Daniel Duke, Chris Powell, Katie Matusik, Alan Kastengren
- General Motors R&D
  - Rate of injection &
  - Droplet velocity/sizing: Scott Parrish
- Delphi
  - Patternation: Lee Markle
- Sandia National Laboratories
  - High-speed PIV gas-phase velocity: Panos Sphicas (visiting from Imperial College), Scott Skeen, Lyle Pickett, Jonathan Frank
  - Liquid and vapor penetration
  - Liquid extinction imaging

Modeling

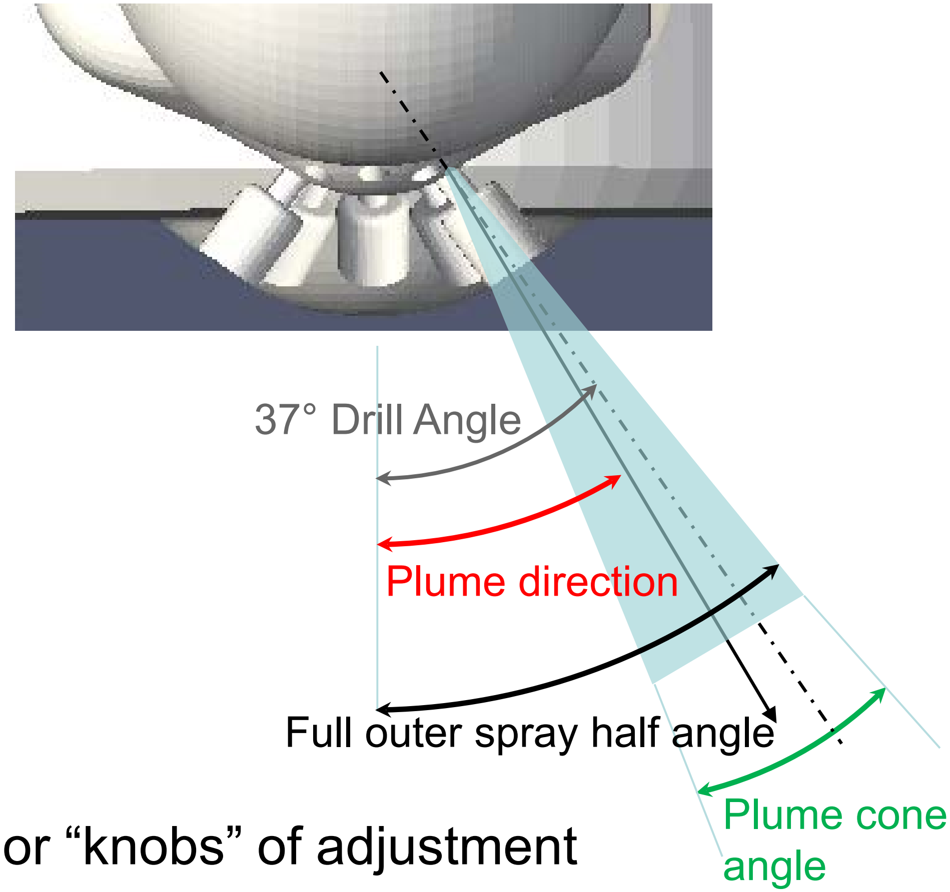
- Argonne National Lab. (ANL)
  - LES & RANS simulation, CONVERGE: Kaushik Saha, Sibendu Som
- Politecnico di Milano (PoliMi)
  - RANS simulation, Open-FOAM: Tommaso Lucchini, David Sinoir, Davide Paredi, Gianluca d'Errico
- KAUST-Hong G. Im, F. E. Hernandez Perez
  Wisconsin - Chris Rutland, Hongjiang Li
  AramCo - Jihad A. Badra, Jaeheon Sim
  - LES simulation, Open-FOAM
- ETH-Zurich
  - LES simulation, CD-adapco: Lucas Zeugin, Yuri Wright

Modeling Spray G via Lagrangian particle tracking is complex/difficult

VOF simulation of internal flow



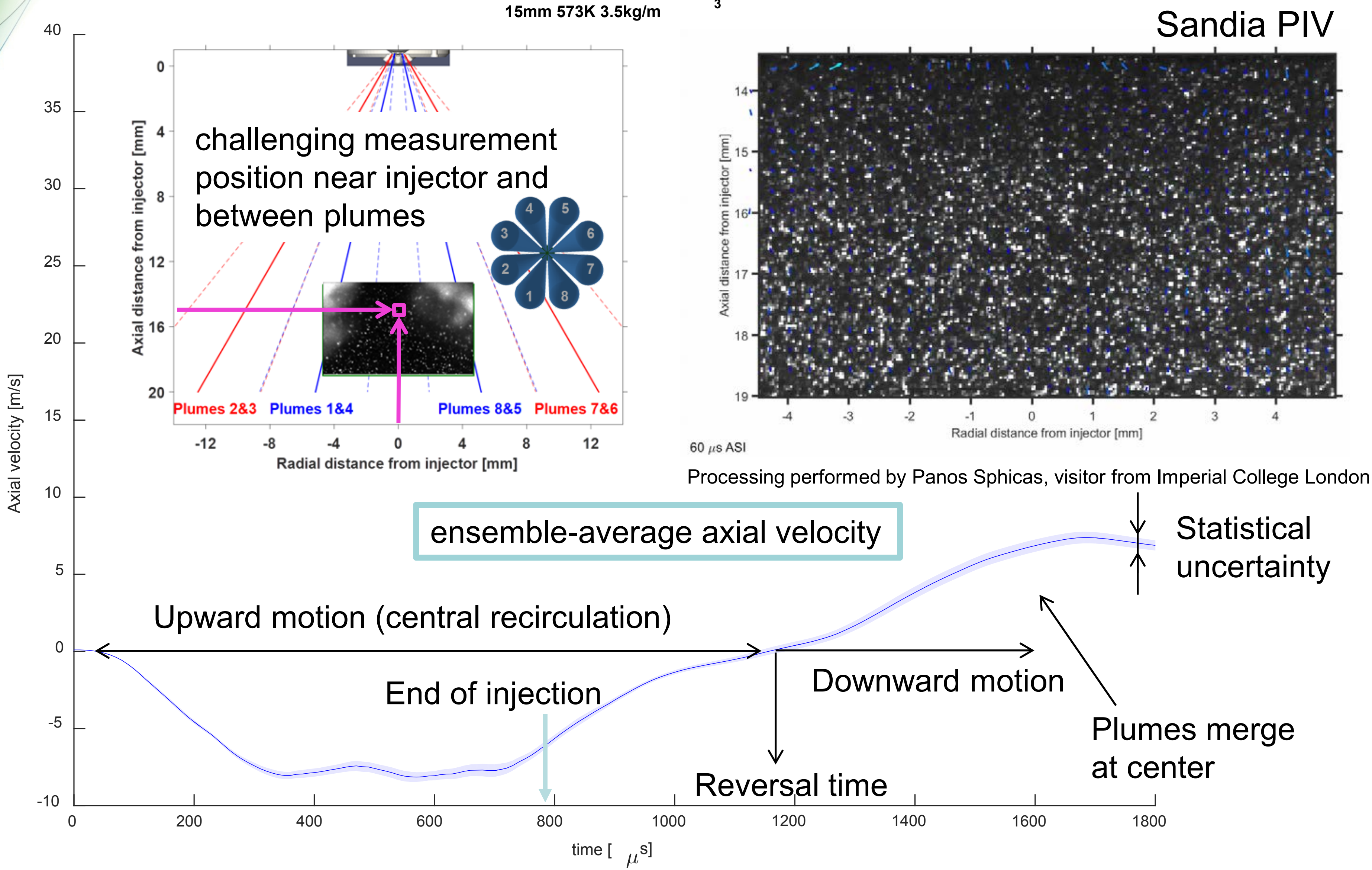
ECN4: courtesy Bizhan Befrui, Delphi



- Major "knobs" of adjustment
  - "Plume direction" angle relative to injector
  - Individual plume "cone angle"

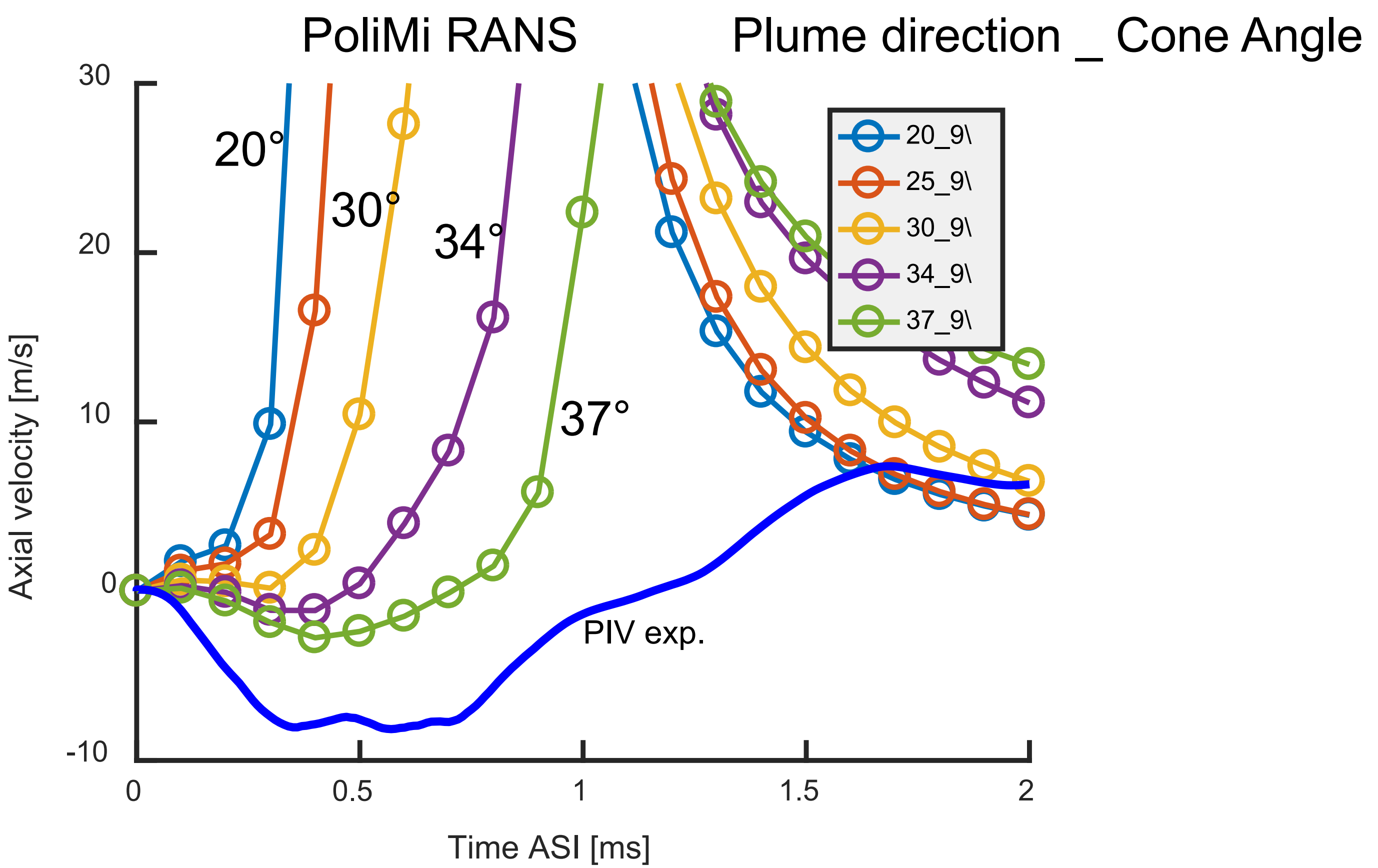
Will one simulation consistently "best match" all experimental data?
Which experimental data is the most useful for model tuning?

Gas velocity data between plumes is available for the first time as a metric to evaluate CFD



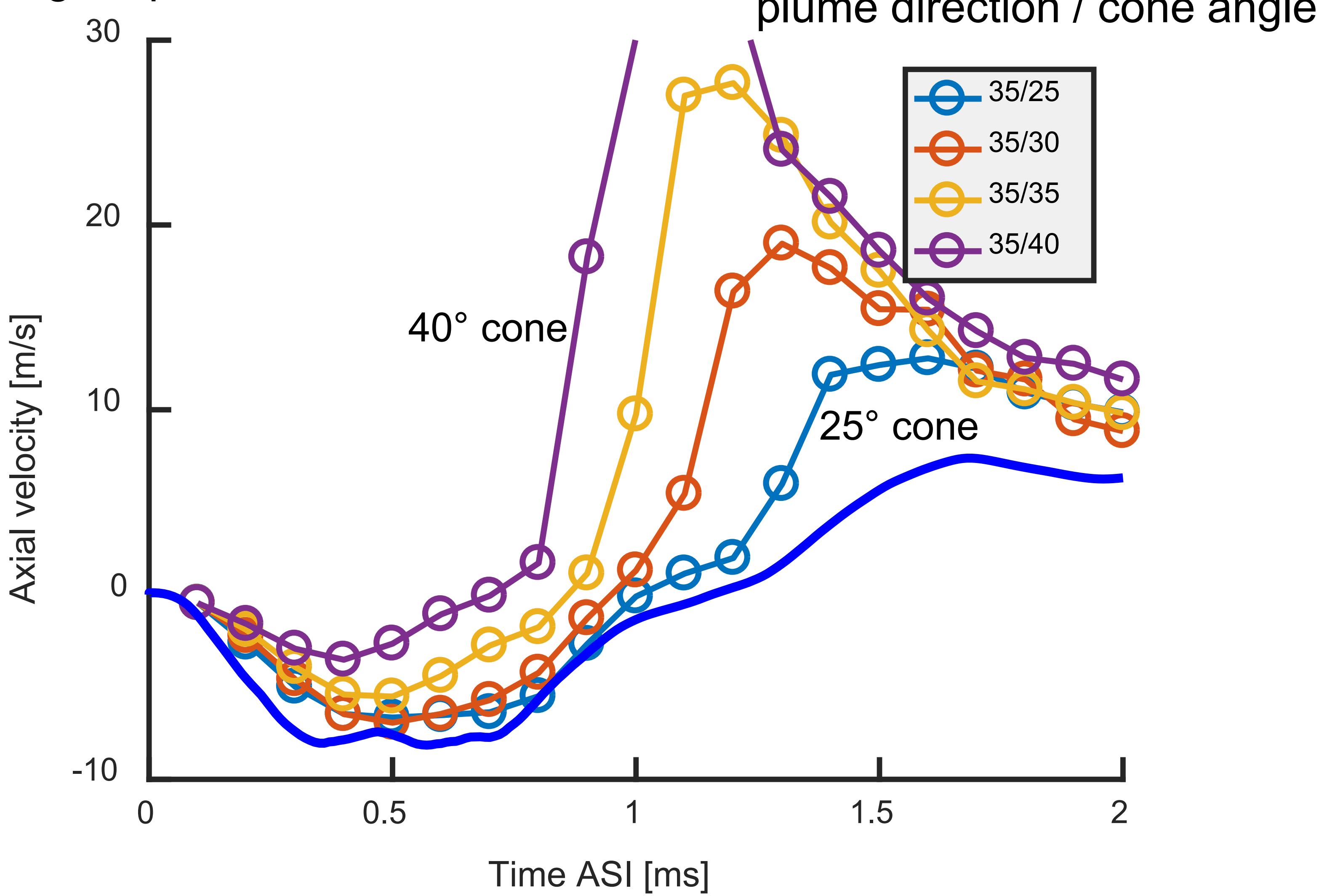
Compare simulations against experiments at the centerline, z = 15 mm location

- Central recirculation zone increases with higher plume direction, but does not meet level of experiment

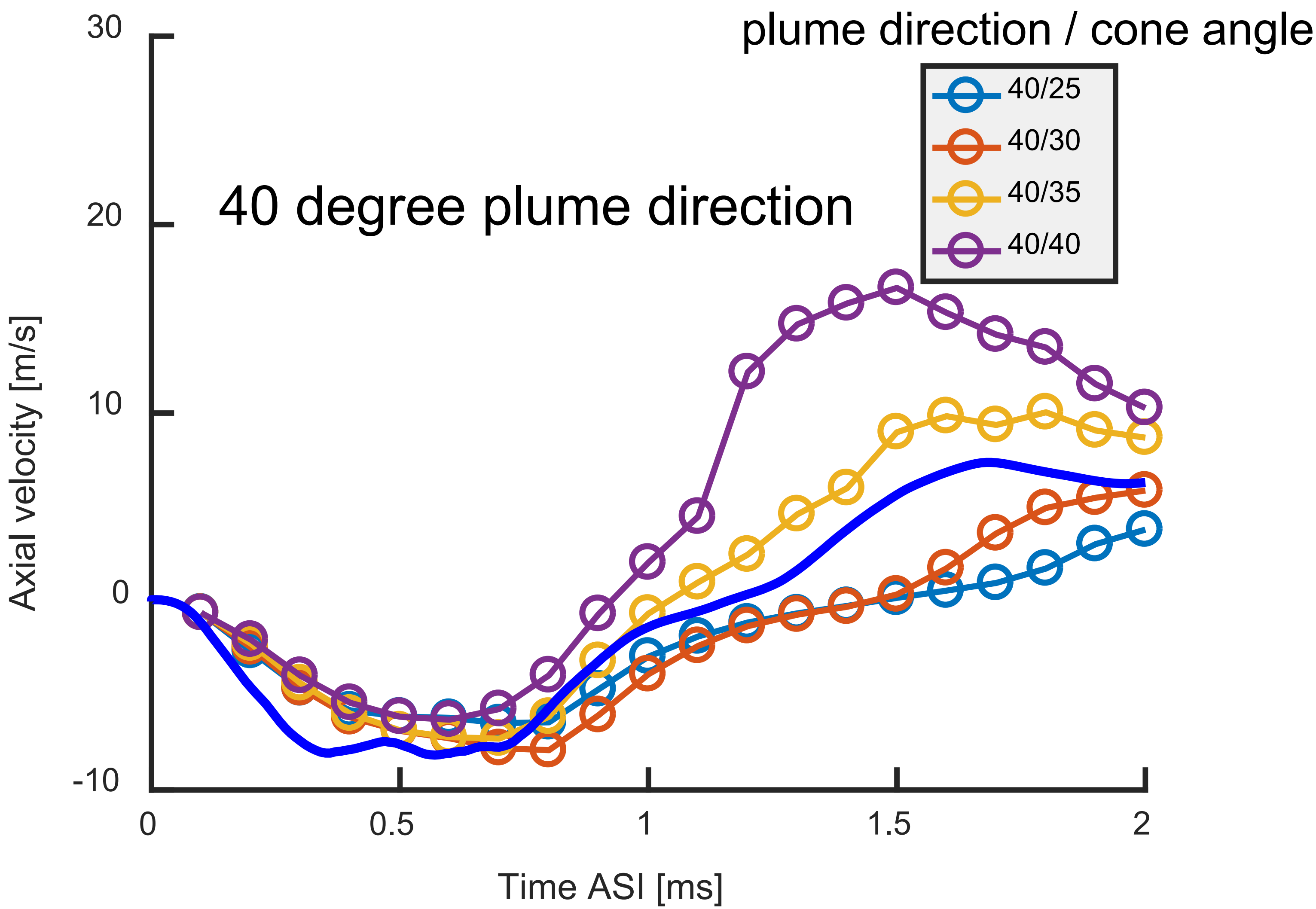


KAUST-WI-ARAMCO (KWA) LES picks up central recirculation zone and merge of jets at end of injection

35 degree plume direction

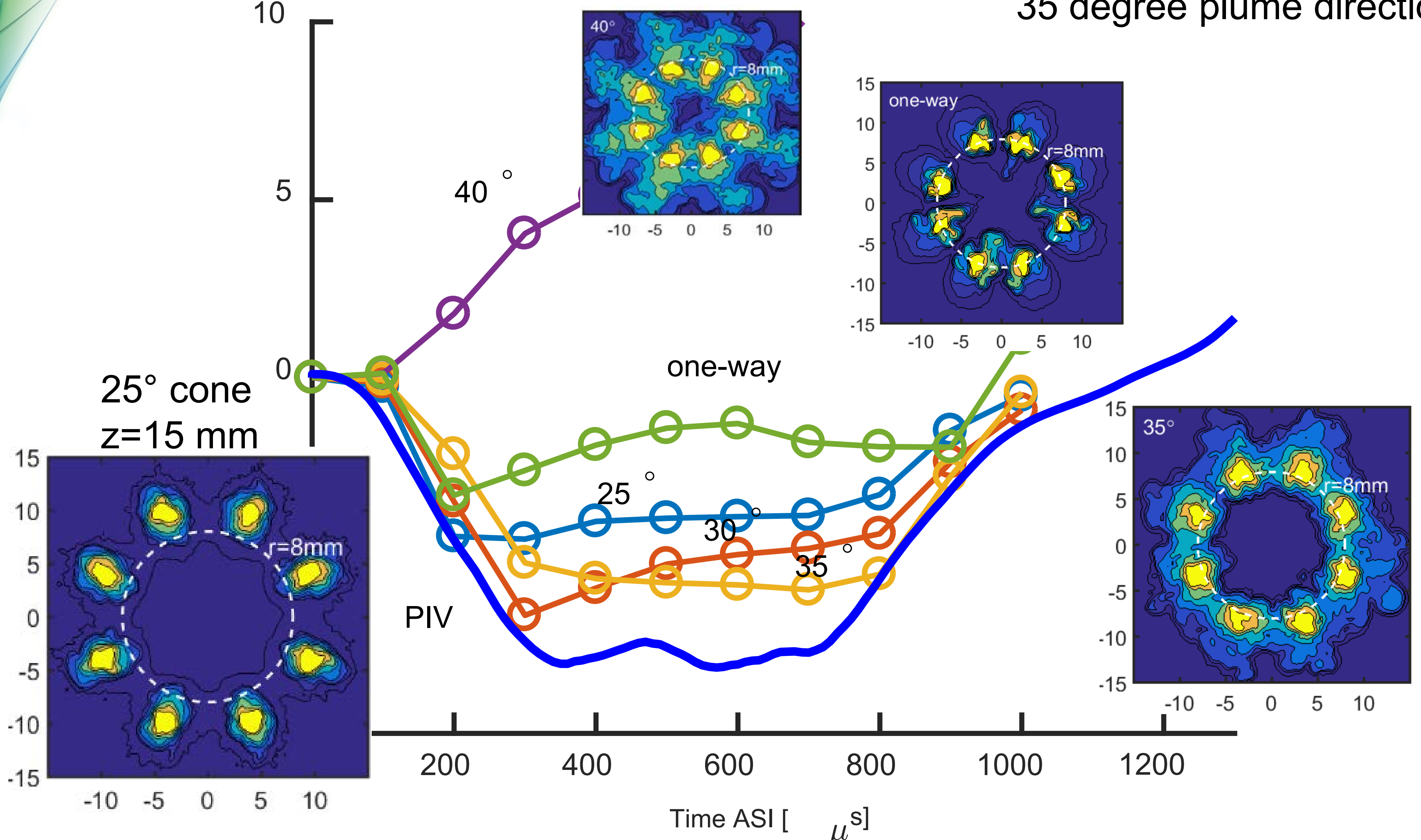


KWA LES: Larger plume direction increases recirculation velocity



Argonne LES: experiences a toggling/collapse with increased plume cone angle

35 degree plume direction

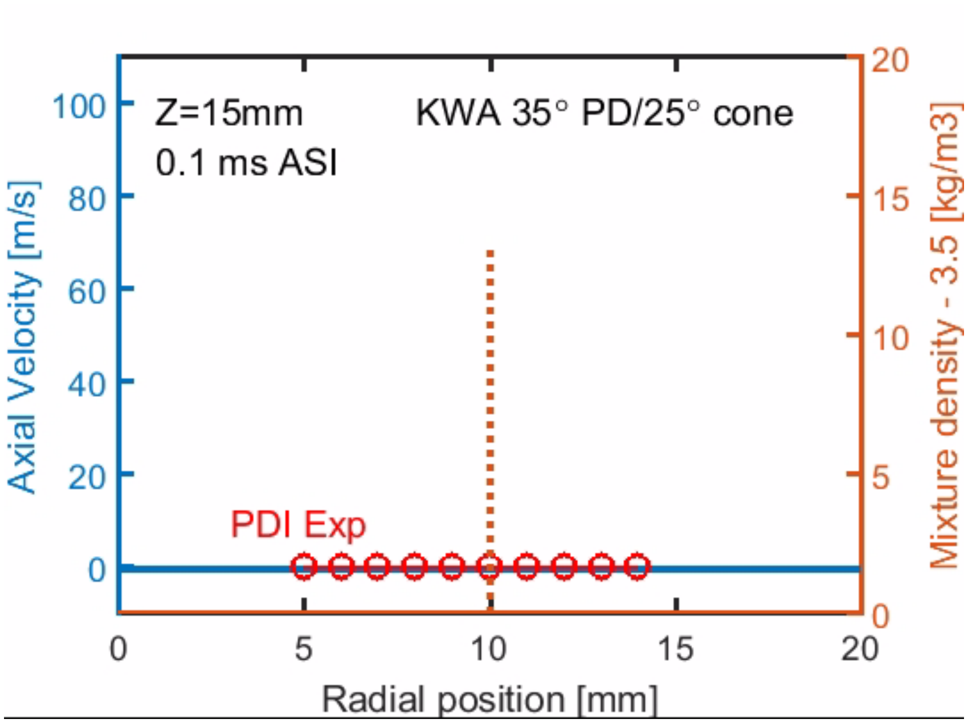


Mixture density at 600 μs ASI

See Sandia/Argonne/PoliMi publication: SAE 2017-01-0837

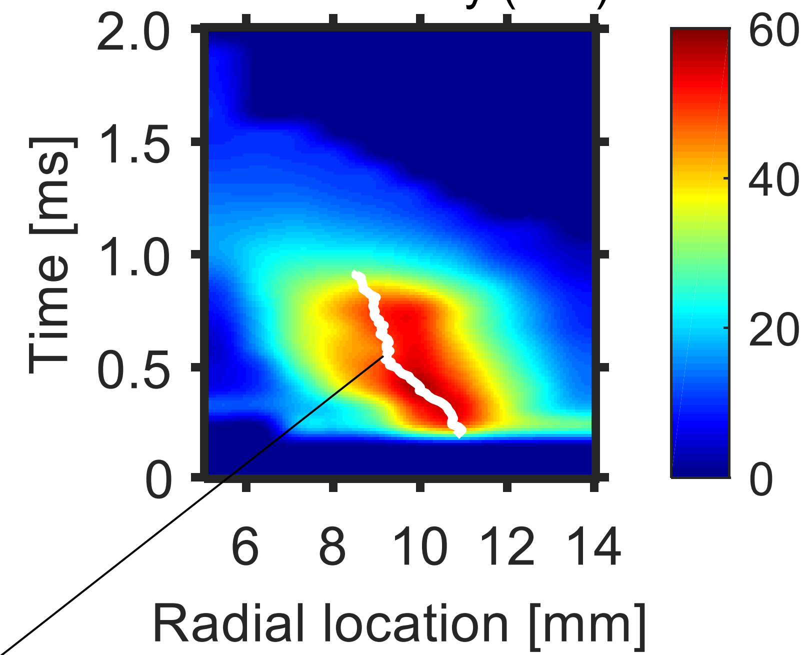
Profiles of velocity, density, mixture fraction used to identify plume center

- Nice agreement with measured liquid velocity
- Plume center moves towards injector axis during injection
- Plume center measured with DBI extinction imaging also consistent



Average of all 8 plumes, and average of 5 LES realizations

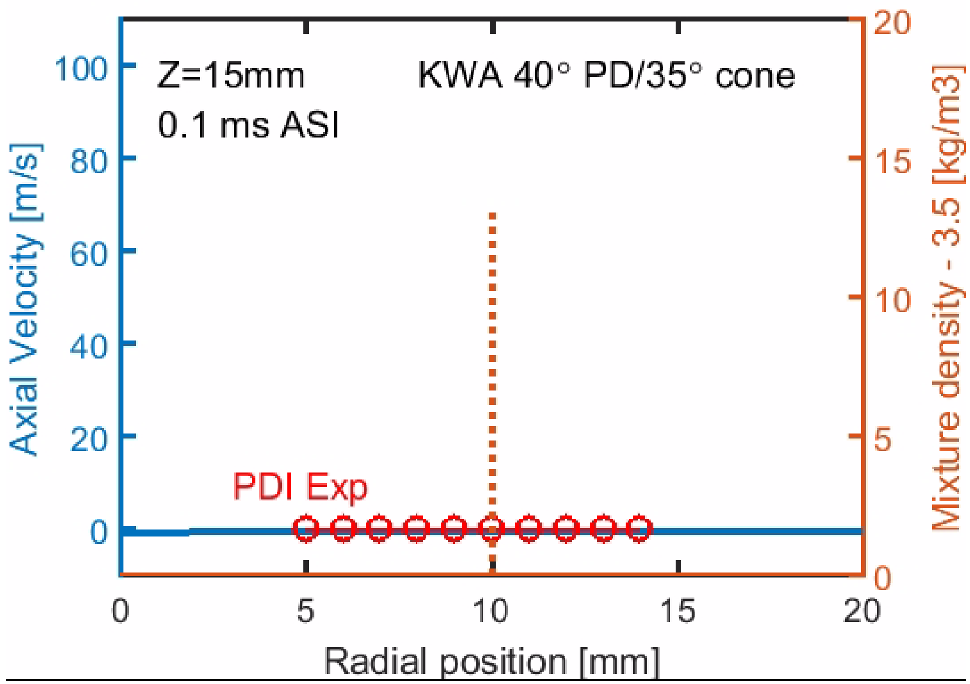
Measured liquid velocity magnitude by phase-Doppler interferometry (GM)



Plume center from Sandia extinction imaging

Larger plume direction is unrealistic

- Some combinations of plume direction angle and cone angle provided decent fits to centerline gas velocity or penetration, but this practice cannot be justified when considering measured plume center

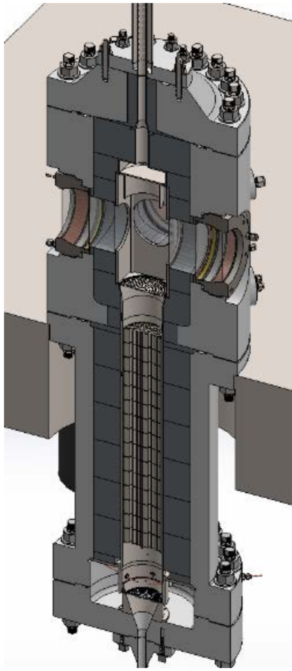


ECN5 Spray G Lagrangian model observations

- Advisable to tune plume cone angle over plume direction
- A single cone-angle/plume direction simulation does consistently provide "best match" against detailed gas and liquid data
- LES models inherently show better capacity to track central recirc. zone
- Dispersion of plume appears to have little correlation with input cone angle
  - RANS very dispersive, requiring small cone-angle inputs
  - LES implementation not consistent with different platforms
- Other concerns identified:
  - Large differences in velocity slip between liquid and gas
  - Lack of correct trends with increased temperature (vaporization)
  - Do not predict large SMD at the end of injection

Future work

- Comprehensive investigation of particulate formation for gasoline direct-injection systems
  - Investigate the fate of soot from large droplets expelled at EOI
  - Use multiple injections, to limit liquid penetration and wall wetting but also to understand bulk gas and droplet mixing
- Diesel research activities (FY18)
  - Investigate the (miscible) structure of fuel sprays with fuel blends and realistic diesel fuel, including the use of cavitating fuel injectors
  - Perform high-speed planar imaging of ignition and mixing (using custom 100 kHz pulse burst laser
  - Quantify ignition and sooting characteristics of diesel certification fuel and proposed surrogates
- Expanding to a new high-throughput laboratory (funded via Co-Optima) will improve the efficiency of this research
  - Available during FY18
  - Achieves flash-boiling conditions
  - Heated chamber allows 300x speedup
  - Model validation datasets will have lower uncertainty

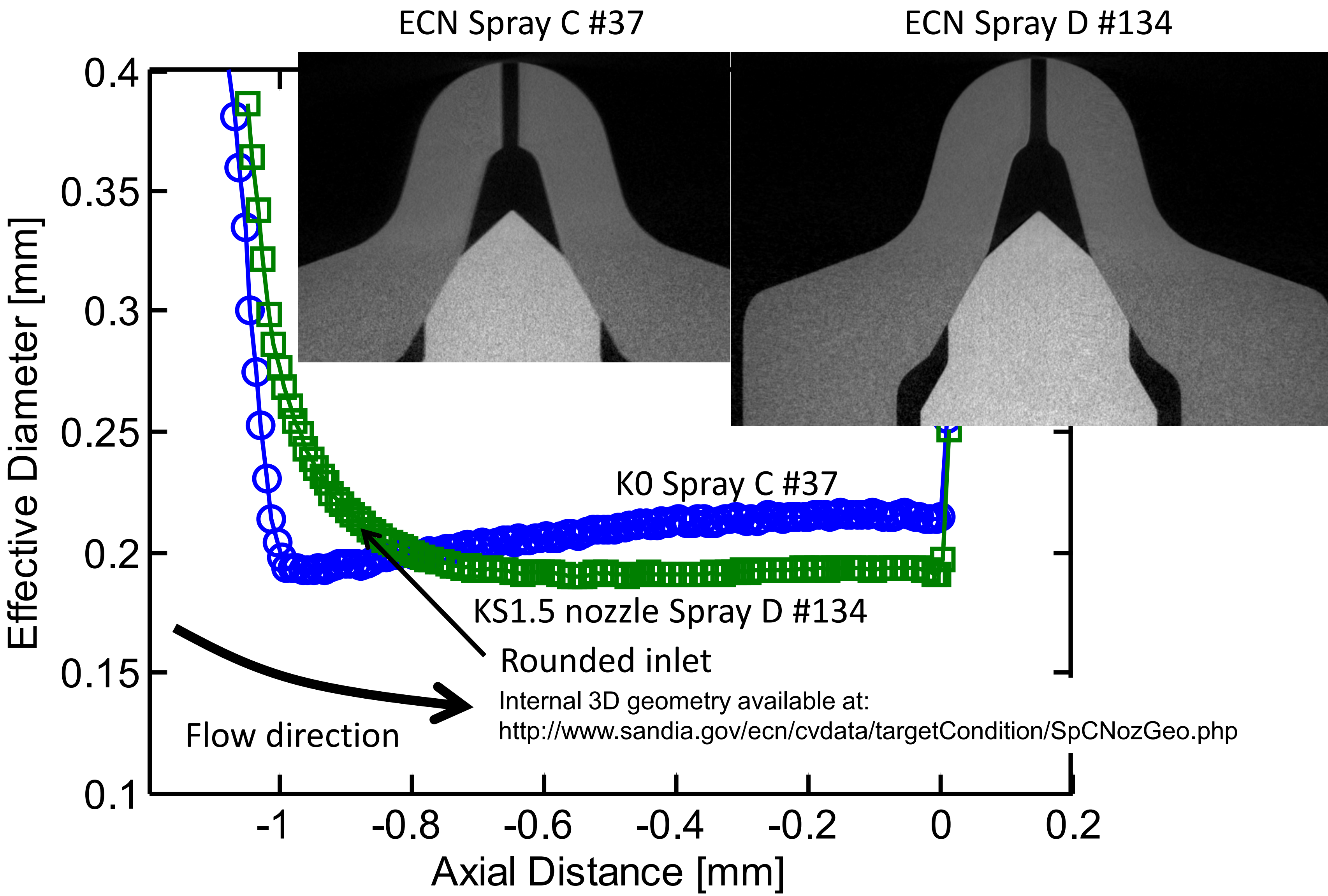


Presentation Summary

- Project is relevant to the development of high-efficiency, low-emission engines, which all use direct-injection sprays
  - Observations in controlled environment lead to improved understanding/models for engine development
  - We address specific challenges facing current injection systems as well as future concepts
- FY17 approach addresses deficiencies in spray combustion modeling
  - Unique, quantitative soot datasets available, coupled to in-depth knowledge of ignition/combustion behavior.
  - Advanced gasoline direct-injection experiments show consistency, and highlight needs for future CFD development
- Collaboration through the ECN used as a tool to accelerate research and provide a pathway for improved CFD tools used by industry
- Future plans will continue research in gasoline and diesel sprays using unique tools and facilities

Technical Backup Slides

Nozzle inlet shape effect on spray development and combustion investigated



Internal 3D geometry available at:
http://www.sandia.gov/ecn/cvdata/targetCondition/SpCNozGeo.php

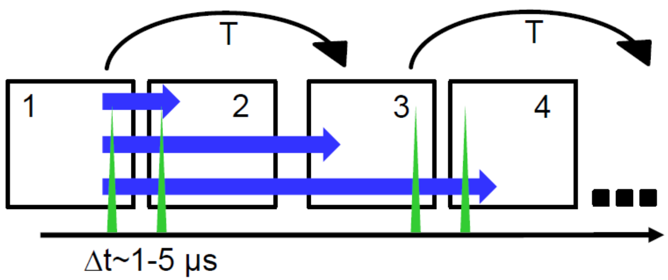
Comparison of C and D nozzle flow rates

- Specification called for larger cylindrical (K0) nozzle diameter for Spray C to account for smaller flow coefficients and match flow rate of Spray D
  - But actual minimum diameter was only slightly larger
- Mass and momentum flow rate measurements (provided by CMT, Valencia, Spain) confirm lower flow rates, lower flow coefficients
  - Effective nozzle diameter is smaller for Spray C compared to Spray D
  - This issue addressed during analysis of results

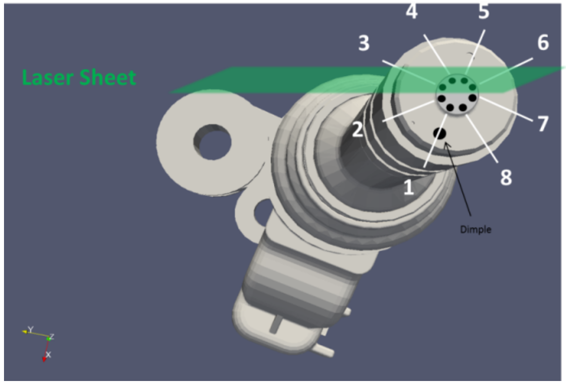
	(Spray D)	(Spray C)
Serial number	209134D	210037C
[μm] (specified)	186	200
(measured)	186	187
[μm] (measured)	193	188
[μm] (measured)	186	208
K-factor [-] (specified)	1.5	0
K-factor [-] (measured)	0.55	-2.3
Nozzle shaping/hyroerosion	to C_d = 0.86	5%
[g/s] (150 – 6 MPa)	11.96	10.12
[N] (150 – 6 MPa)	7.13	5.83
[-] Discharge coefficient. , where and	0.97	0.81
Area-contraction coefficient Ca = *Ca > 1 is not physical but is most likely reflective of experimental uncertainties to derive its value	1.03*	0.89

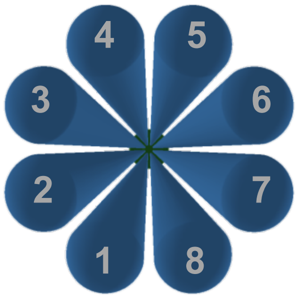
Unique high-speed velocity diagnostic applied

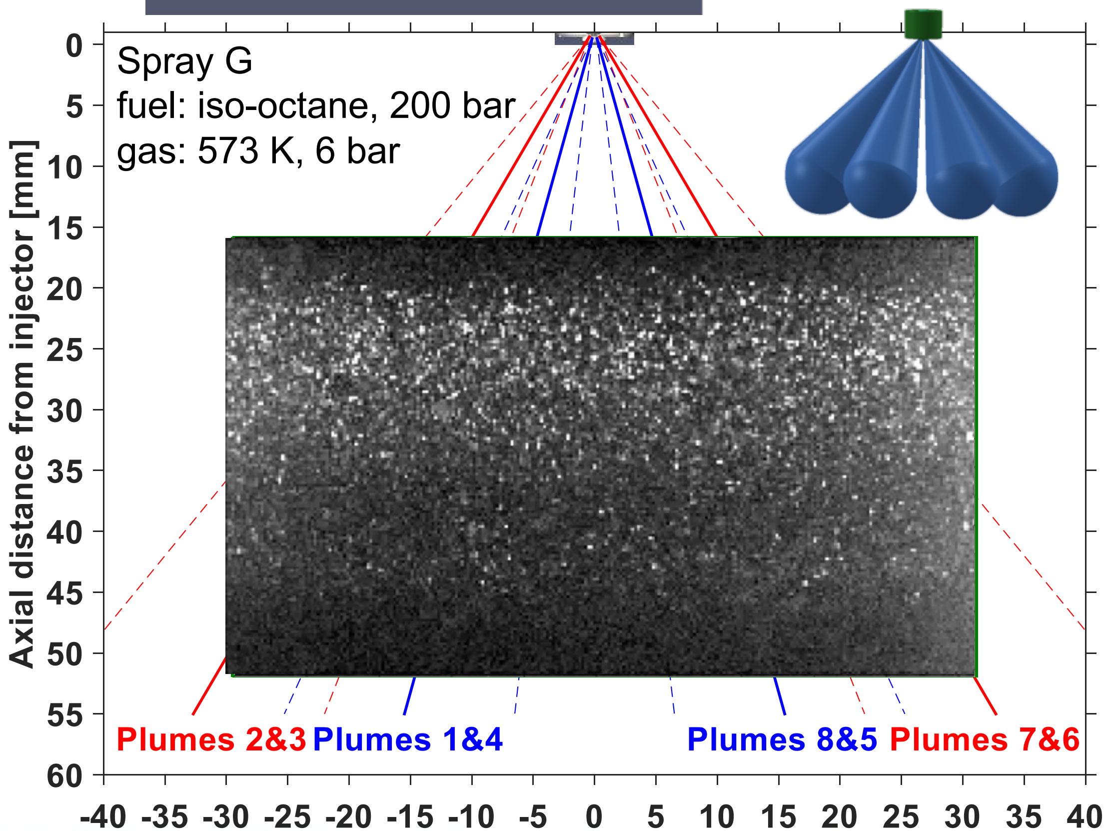
- Custom pulse-burst laser system developed
  - 100 kHz pulse pairs
  - 500 pulse pairs (5 ms burst)
  - 15 mJ/pulse at 532 nm
  - Funded by internal Sandia project (PI J. Frank)



- Applied PIV
  - 1 µm zirconia seed in gas phase
  - 200 kHz imaging on high-speed CMOS camera
  - Liquid-phase avoided by probing between plumes and moving downstream



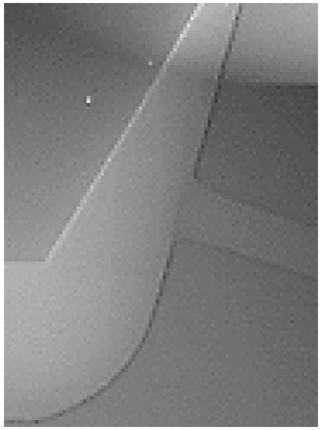


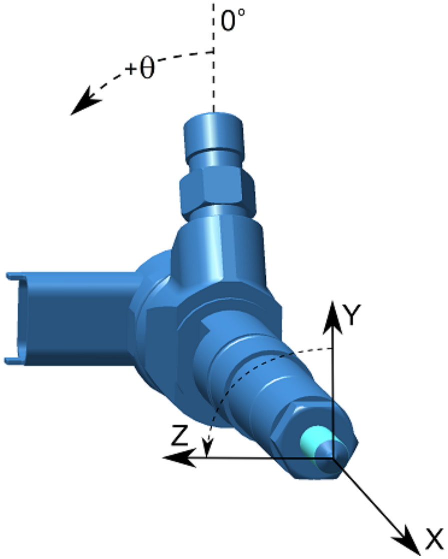


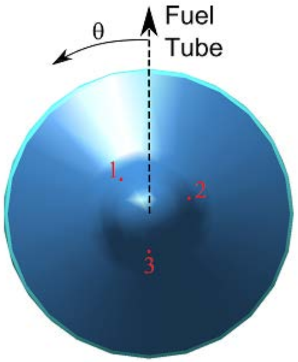
ECN Spray B nozzle

- Has the same size and KS specification as Spray A, but with a shorter length
- Side hole with ψ = 72.5° (145° full included angle)
- Plume 3, opposite the fuel tube, is the plume of interest

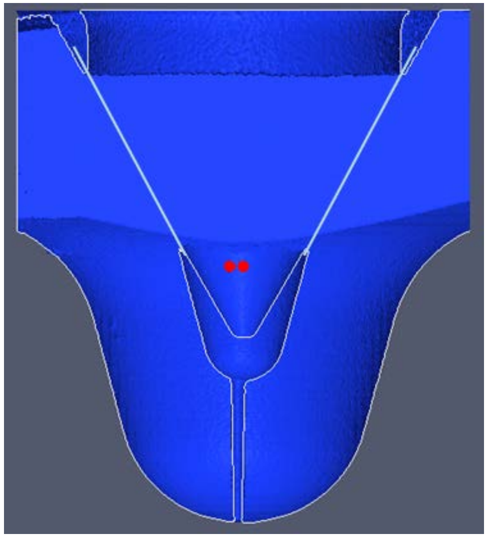
Spray B

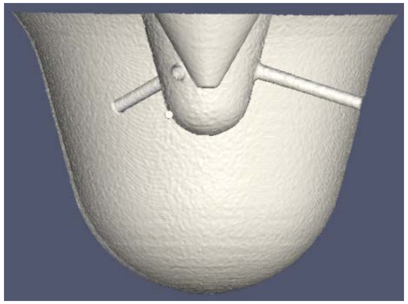






Spray A





Close collaboration and pathway to better CFD tools

Experiment

Sandia	Mich. Tech.
Argonne	Meiji
IFPEN	Infineum
CMT	Chalmers
CAT	KAIST
GM	Aachen
Delphi	Melbourne
Bosch	Brighton
TU/e	Michigan
Ist. Motori	

CFD codes used

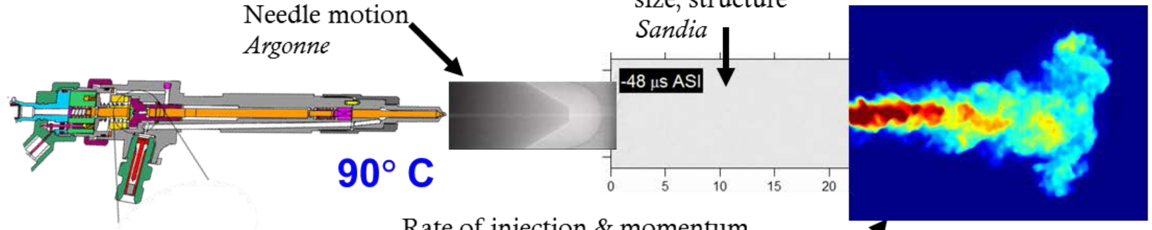
CONVERGE
Star CD
Open FOAM
KIVA
ANSYS Fluent & CFX
FORTE
RAPTOR
other research codes…

CFD approaches

RANS
LES
High-fidelity LES
Eulerian-Eulerian
Eulerian-Lagrangian
Dense fluid
many spray and combustion variants…

Modeling submissions

Sandia
Argonne
IFPEN
CMT
PoliMi
UMass
UNSW
Penn St.
TU/e
UW-Madison
Purdue
ETH-Zurich
Aalto
Aachen
DTU
Cambridge
Georgia Tech
Chalmers
GM…



ECN organization

- Monthly web meetings
- Workshop organizers gather experimental and modeling data, perform analysis, understand differences, provide expert review
- Very tight coordination because of target conditions

Most industry use ECN data to test their CFD practices

Simulation contributions for ECN5

	Polimi RANS	Argonne RANS	Argonne LES	KAUST-Aramco-UW LES	ETH-Zurich LES
Domain Dimensions	169 x 248 mm	108 x 108 mm	108 x 108 mm	100 x 60 x 60mm	100 x 100 x 100mm
Base Cell Size	4 mm	1 mm	1 mm	1 mm	2 mm
Min Cell Size	1 mm	0.125 mm	0.125 mm	0.5 mm	0.125 mm
Nozzle tip included	No	No, Yes for one-way	No, Yes for one-way	Yes	Yes
Radial position of droplet parcel	0.5 mm	0.79 mm	0.79 mm	0.79 mm	0.79 mm
Adaptive or Static Refinement	Adaptive	Both	Both	Both	Static
Cell Type	Cartesian & oriented	Cartesian cut-cell	Cartesian cut-cell	Cartesian	Cartesian
Total/Maximum Cell Count	115,000	14 million	14 million @ 1ms; 20 million @ 2ms	2.2 million	3.5 million
Number of spray parcels	20k per plume	400k per plume	200k per plume	200k per plume	500K per plume
CPU cost	1 realization 3 processors 40 minutes for 2 ms **2 CPU hrs for 2 ms**	?	5 realizations 36 processors 10 hours for 1 ms **3600 CPU hrs for 2 ms**	5 realizations 32 processors 10 hours for 2 ms **1800 CPU hrs for 2 ms**	1 realization 96 processors 5 hours for 2 ms **480 CPU hrs for 2 ms**

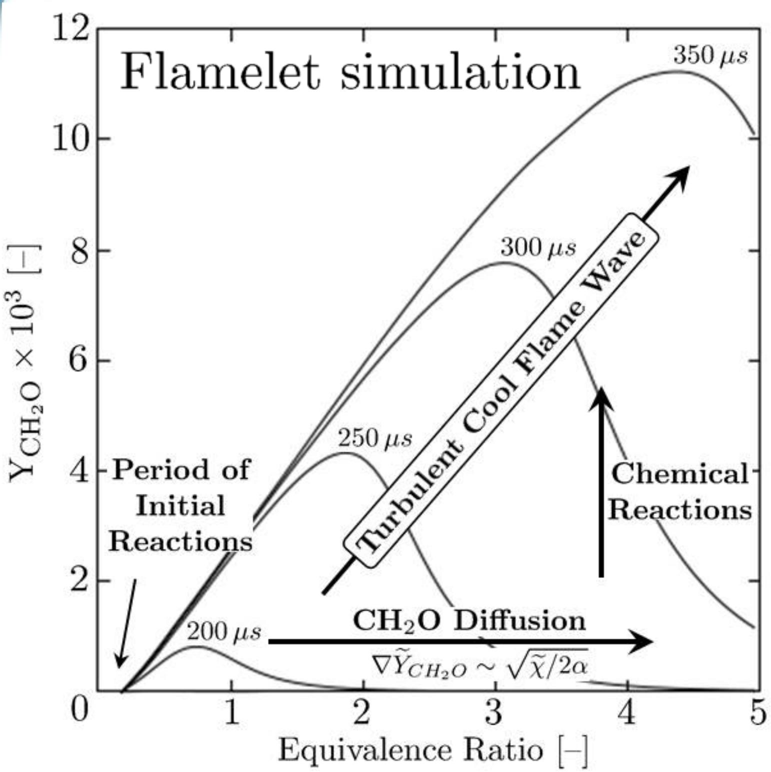
- Can less-expensive simulations be used to define bc's used later for more expensive simulations?

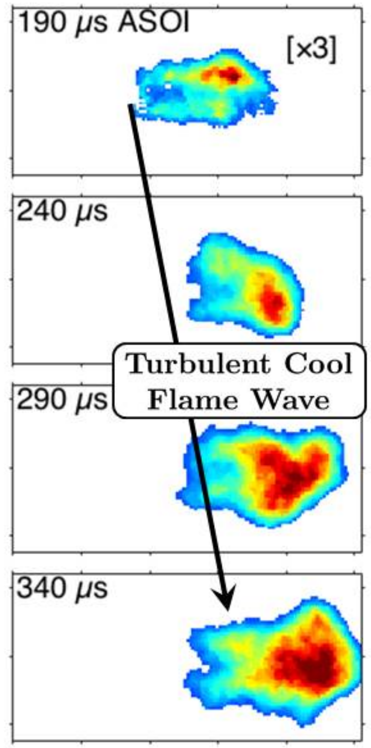
Summary of models and setup

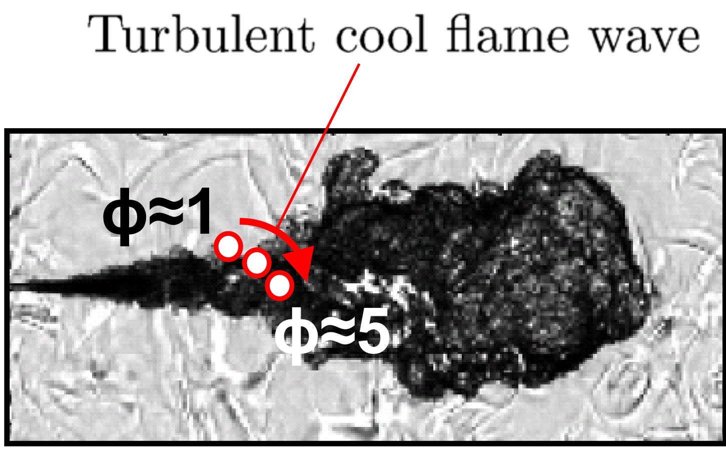
	Polimi RANS	Argonne RANS	Argonne LES	KAUST-UW-Aramco LES	ETH-Zurich LES
CFD Code	OpenFOAM + Lib-ICE	CONVERGE	CONVERGE	OpenFOAM	Star-CD
Turbulence Model	Standard k-ε	Standard k-ε	LES – dynamic structure	LES dynamic structure with spray source/sink	LES – sub-grid k model
Injection Model	Lagrangian/Huh	Lagrangian/Blob	Lagrangian/Blob	Lagrangian/Blob	Lagrangian/Blob
Primary Break-up Model	Huh-Gosman	Kelvin-Helmholtz (KH)	Kelvin-Helmholtz (KH)	KH (Cb = 1.0, B1= 35)	Kelvin-Helmholtz (KH)
Secondary Break-up	Kelvin Helmholtz (KH) + Rayleigh Taylor (RT)	Rayleigh-Taylor (RT)	Rayleigh-Taylor (RT)	KH/RT competing	Rayleigh-Taylor (RT)
Vaporization	Spalding Number-based (mass-based)		Frössling	Frössling	Spalding Number-based (mass-based)
Heat Transfer	Ranz-Marshall		O'Rourke	Ranz-Marshall	Ranz-Marshall
Collision	None		NTC	None	O'Rourke
Droplet Drag	Dynamic without spherical correction		Dynamic	Dynamic without spherical correction	Standard
Initial gas turbulence	u' = 1 m/s; Li = 2 mm		TKE=1.0; EPS=100.0	TKE=7.9e-3 (35° PD) TKE = 1.6e-4(40° PD)	TKE=7.9e-3
Plume direction	34°, 37°		35°	35°, 40°	33°
Plume cone angle	Calculated from Huh-Gosman as 9°	25°- 40°, "one-way"	25°- 40°, "one-way"	25°, 30°, 35°, 40°	17°

Ignition mechanism in high-pressure sprays
see Dahms, Paczko, Skeen, Pickett. ProCI 36(2), 2017

→ Turbulence generates *steep* gradients and, hence, strong diffusion fluxes







Note: Pei & Gong (both using 3D LES, homogenous reactor) and Krisman (2D DNS) show cool flame accelerating rich ignition. But they must use limited chemistry or TCI assumptions. Our analysis uses full detailed chemistry and makes no sub-grid scale TCI assumptions.

Conclusion:

a) Species & temperature diffusion into neighbored mixture triggers 1^{st}-stage ignition

b) Continuous reactions & diffusion leads to cool flame wave propagation

New insights into the role of turbulence chemistry interactions (TCI) on diesel ignition

First-principles analysis of turbulent ignition

- High-turbulence, high-pressure, complex kinetics, large domains and time span
  - Revisiting Peters' derivation for burning flamelets (1984, 2000) and resolving all time and diffusion length scales & chemical pathways via LLNL kinetics

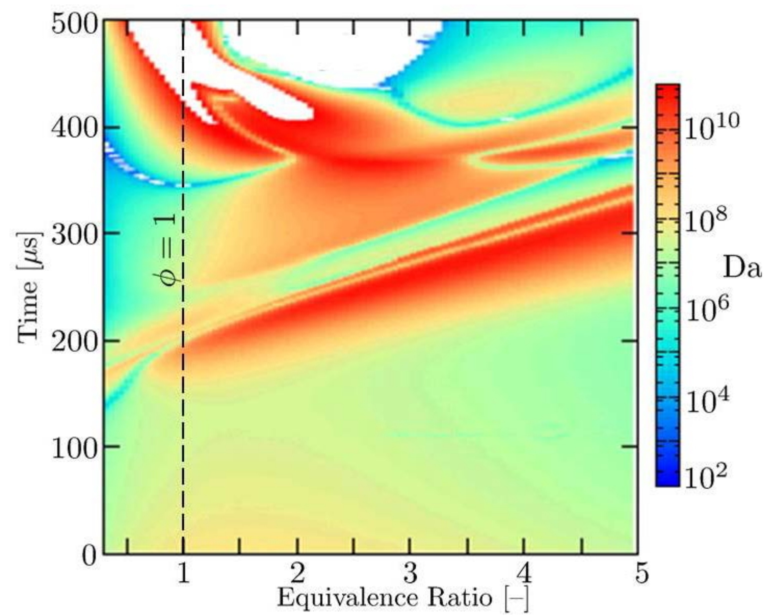
3D reactive Navier-Stokes eqs. → Two-scale asymptotic → **1D flamelet eqs. in equivalence ratio**

True solution (!) of Navier-Stokes eqs. while asymptotic is valid → Da=t_D/t_c>>1

- Chemical time scales from CEMA (Law *et al.*, *JFM*, 2010)
- Diffusion time scales (≠χ!) derived from individual species profiles

$$t_{D,i}^{-1} = \frac{1}{Y_{i,0}^2}\frac{\chi}{2}\left(\frac{\partial^2 Y_i}{\partial Z^2}\right)^2$$

- Complete LLNL kinetics for n-dodecane (2755 species; 11,173 reactions)
- ***Asymptotic holds during entire ignition event!***

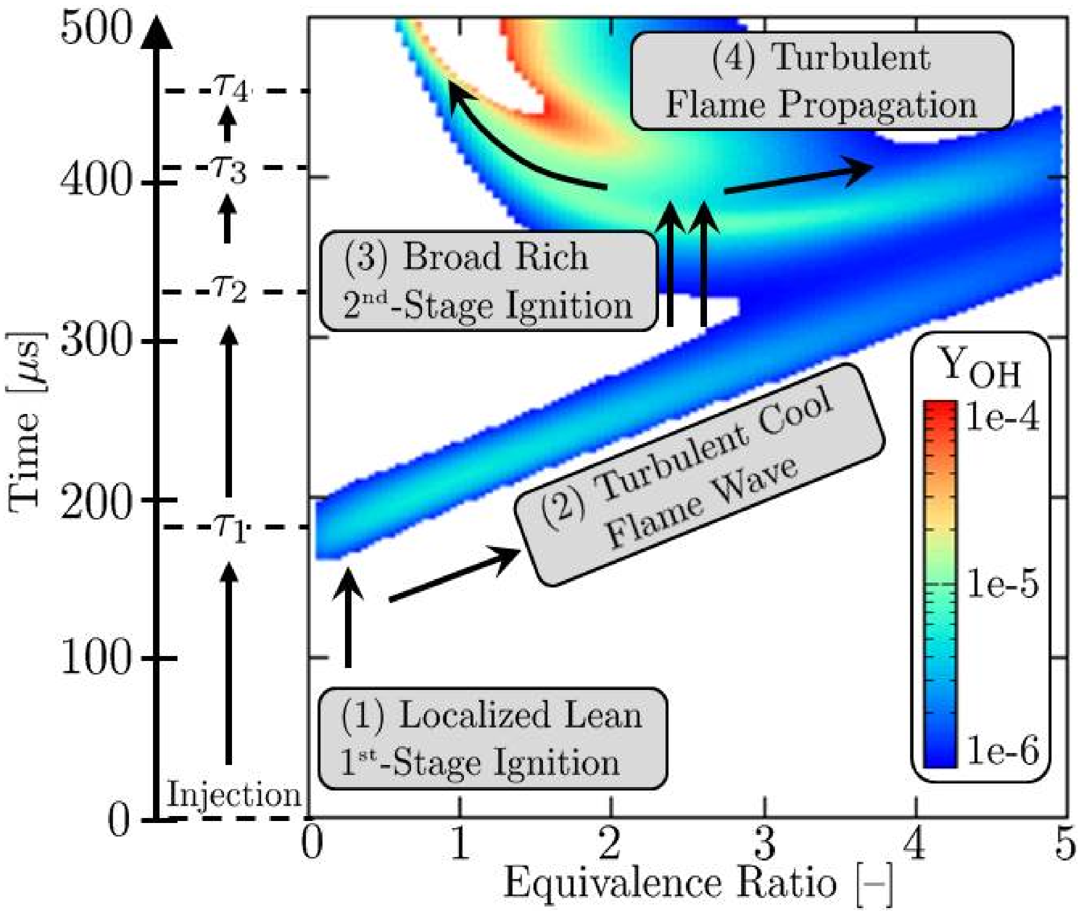


Characteristic time scales in high-pressure spray flame ignition

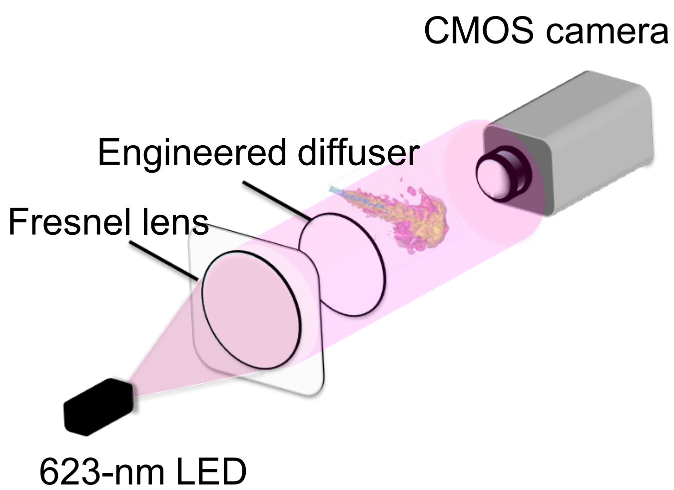
1. t_1 (~190 μs):
   Initial period of chemical activity with first ignition in hot lean mixture
2. t_2 (~200 μs):
   Turbulent cool flame wave leads to cool-flame ignition of entire mixture
3. t_3 (~50 μs):
   Localized hot ignition in rich mixture where delay between 1st and 2nd stage of ignition is minimal
4. t_4 (~30 μs):
   Auto-igniting flame front propagation

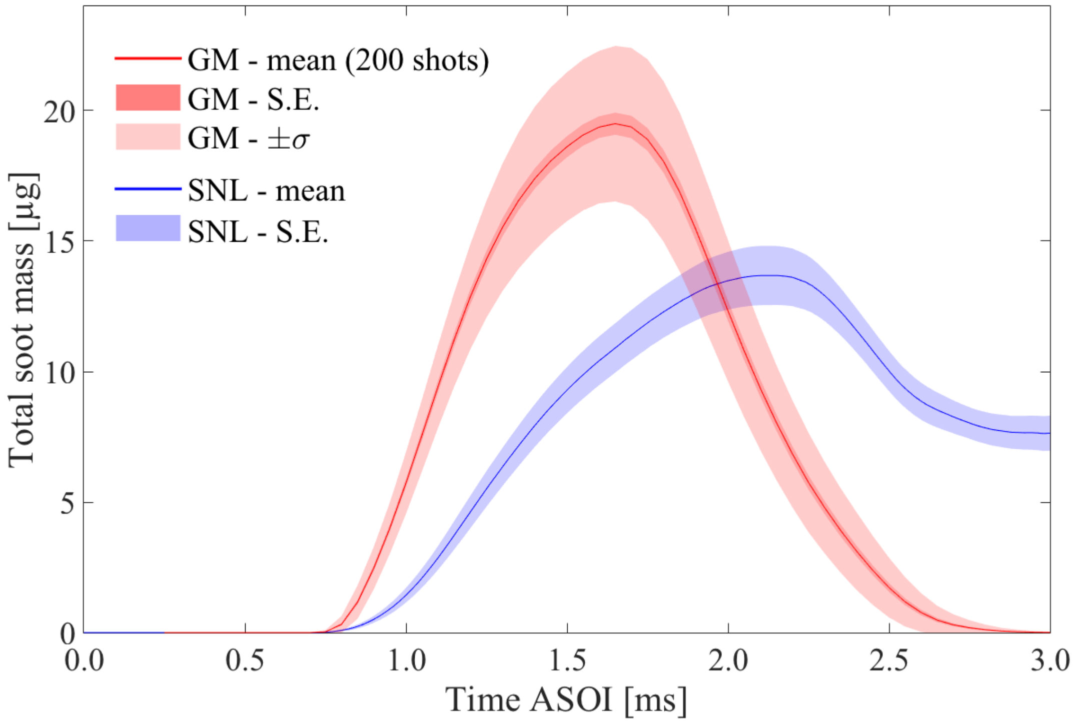
- Changes in p, T, χ, etc. modify t_1-t_4 time scales

➢ **Characteristic sequence of phenomena remains largely unaffected over wide range of conditions**



Collaborative efforts with industry provide insight into EGR effects and shot-to-shot variability





Collaborative efforts with industry provide insight into EGR effects and shot-to-shot variability

Total Soot Mass

- 200 consecutive Spray C/D injections performed at Caterpillar research with Sandia-developed high-speed extinction imaging diagnostic
- CAT constant pressure vessel ambient contains O_2/N_2, whereas SNL pre-burn vessel contains H_2O and CO_2 from pre-burn products
- CAT results show earlier onset of soot formation, but SNL data has higher peak soot in spray head even though ID and LOL are consistent.