SAND2018-4887C

Spray Combustion Cross-Cut Engine Research

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Sandia National Laboratories

FY 2018 DOE Vehicle Technologies Program Annual Merit Review
Project ACS005, 2:00 PM, Tue. 19 June 2018

Sponsor: **DOE Vehicle Technologies Program**
Program Managers: **Gurpreet Singh and Michael Weismiller**

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Overview

Timeline

- Project provides fundamental research that supports DOE/ industry advanced engine development projects.

- Project directions and continuation are evaluated annually.

Budget

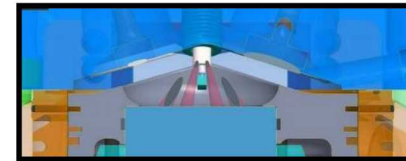- Project funded by DOE/VT: FY17 - $845K
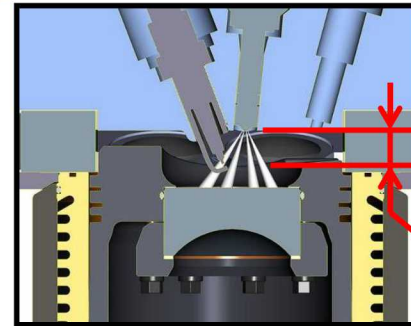
Barriers

- Engine efficiency and emissions

- Understanding direct-injection sprays

- CFD model improvement for engine design/optimization
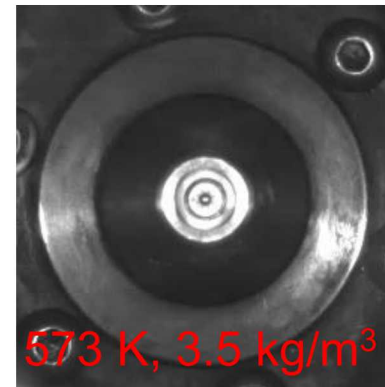
Partners

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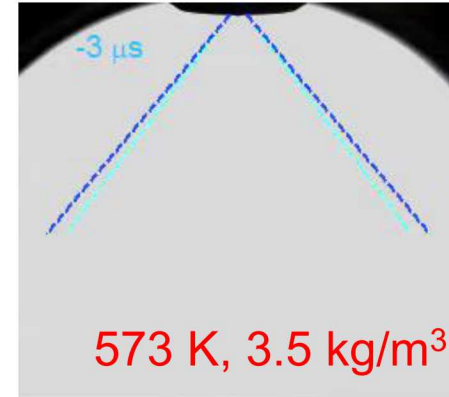
- **Barriers for high-efficiency gasoline**
  - Particulate emissions
  - Engine knock
  - Slow burn rate or partial burn
  - Heat release control when using compression ignition
  - Lack of predictive CFD tools
- **Barriers for high-efficiency diesel**
  - Particulate emissions
  - Heat release rate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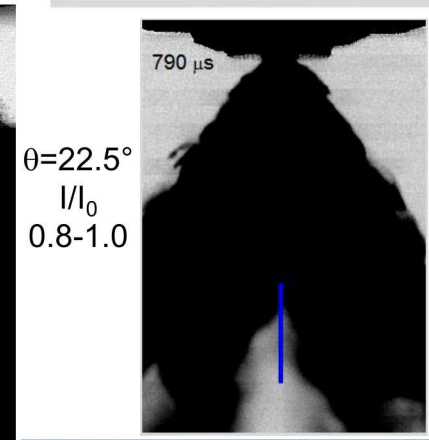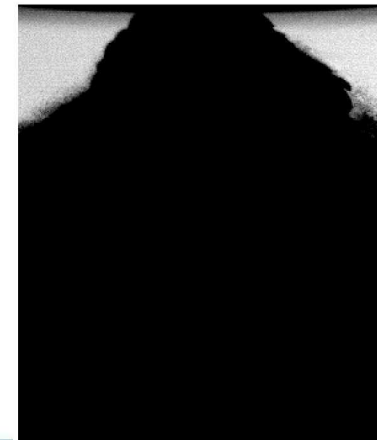 - Lack of predictive CFD, particularly for short and multiple injections

8-hole, gasoline
80° total angle
~15mm

-3 µs

573 K, 3.5 kg/m^3

573 K, 3.5 kg/m^3

High-speed microscopy at nozzle exit

790 µs

θ=22.5°
I/I_0
0.8-1.0

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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
  - Negative consequences of spray collapse must be understood, alleviated
  - Mixing measurements in sprays challenging due to liquid droplets amid vapor—robust diagnostic needed
- Pursue discoveries relating spray and mixing to combustion emissions
  - How/why does soot form from films/drops in stoichiometric GDI operation?
- Support development of diesel surrogate fuels
  - Generate target spray, combustion, and soot data for validation of surrogate fuels

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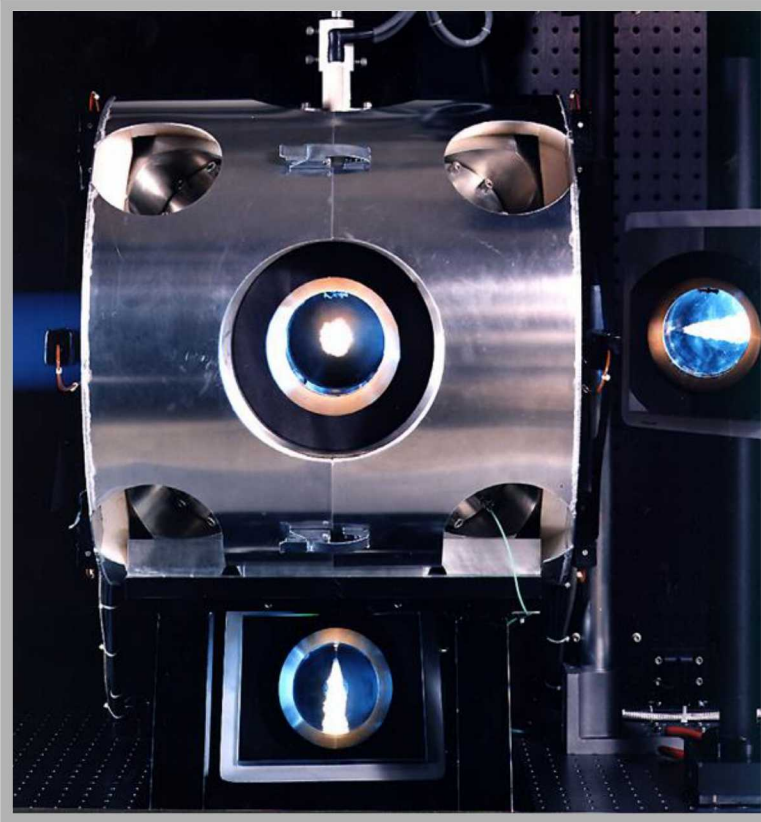
- Well-defined ambient conditions:
  - 300 to 1300 K
  - up to 350 bar
  - 0-21% O_2 (EGR)
- Injector
  - single- or multi-hole injectors
  - diesel or gasoline (cross-cut)
- Full optical access
  - 100 mm on a side
- Boundary condition control needed for CFD model development and validation
  - Better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

Responses to previous year reviewer comments

- How are priorities chosen for experiments at engine relevant spray conditions for development of predictive computational tools.
  - We focus on conditions agreed upon within the ECN because they draw international collaboration and provide long-term impact.
- The reviewer said that progress has been satisfactory, but output can be increased. This reviewer wondered about work that was proposed last year to probe particulate formation at the tip of gasoline injectors; it was not reported on this year.
  - High-throughput vessel will increase productivity significantly (300-500x)!
  - Major effort devoted to GDI soot in FY2018.
- The reviewer wondered what the fate of the spray bomb is, and asked if the new facility makes the spray bomb obsolete, or will you continue to do work in that chamber.
  - Spray bomb (constant volume premixed combustion chamber) capabilities extend those available in new facility enabling unique experiments that will continue.
- The reviewer asked if the project PI is planning to leverage the particulate formation for GDI systems from the project ACS001 regarding multiple injections.
  - Yes, collaboration with respect to diagnostics and mixing characteristics is planned.
- The reviewer suggested that the investigation of particulate formation in GDCI engines be given very high priority, especially with regard to soot from large droplets produced when the pintel closes at the end of injection.
  - We agree, and have devoted major attention to this work in FY18 and plan additional work in FY19.
- The reviewer also recommended a further study of the collapsing behavior of gasoline multi-hole sprays. Other variables that are of great interest to the industry are the back pressure, the conicity of the nozzle, the pitch diameter of the circle where the holes are located, and the number of holes.
  - With the development of the high-throughput spray chamber, we will have the ability to study injector variables previously not possible due to time constraints.

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Collaborative research through the Engine Combustion Network accelerates CFD model development
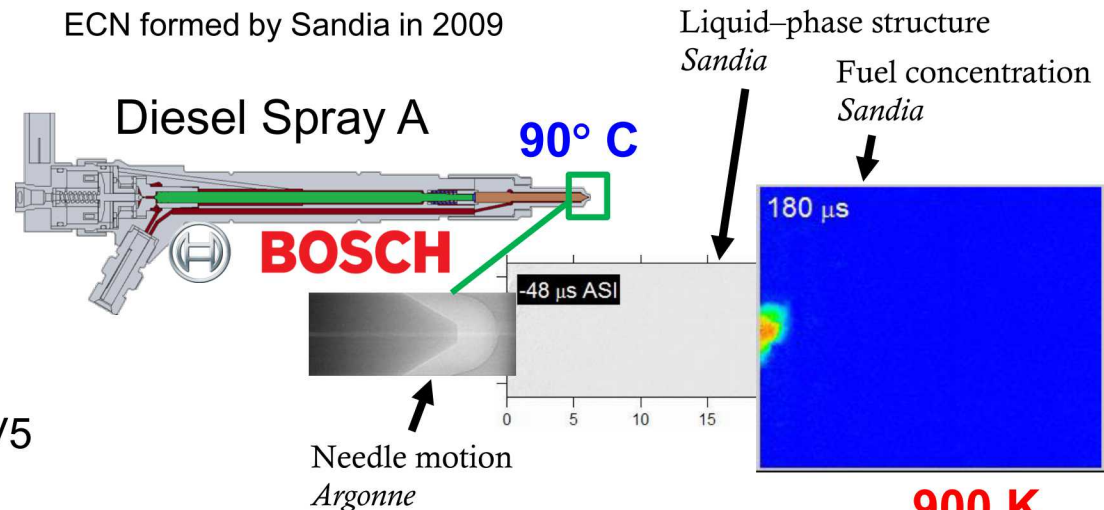
Approach

- 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, multi-hole HDEV5

- Results submitted to online archive with fields (like geometry and uncertainty) specifically tailored for CFD simulations
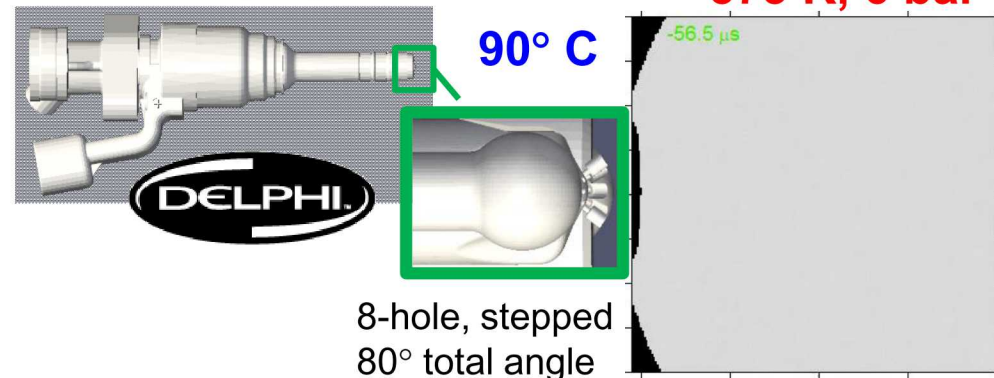
Impact

- 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

Liquid–phase structure
Sandia

Fuel concentration
Sandia

Diesel Spray A

90° C

BOSCH

180 µs

-48 µs ASI

0   5   10   15

Needle motion
Argonne

**900 K
60 bar**

>70 measurements/diagnostics contributed from >15 institutions

Gasoline Spray G

573 K, 6 bar

90° C

-56.5 µs

DELPHI

8-hole, stepped
80° total angle

Approach - Milestones

✓ **Apr 2017**

Investigate spray and combustion behavior of AVL-18a diesel surrogates relative to a commercial diesel fuel

✓ **Jun 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 (proof-of-concept)

✓ **Aug 2017**

Develop high-speed imaging extinction diagnostic for spray mixture quantification

✓ **Sept 2017**

Determine minimum 355-nm pulse energy required to detect formaldehyde PLIF with a non-intensified CMOS camera in preparation for pulse-burst laser experiments

✓ **Oct 2017**

Santoro burner extinction measurements at multiple wavelengths for soot refractive index study

✓ **Nov 2017**

Analyze high-speed planar mixing measurements for mixture quantification at ignition

✓ **Jan 2018**

GDI multi-injection spray PIV

✓ **Feb 2018**

Expand soot extinction imaging diagnostic to wall impinging jets and wall films

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Transient spray mixture fraction measured (non-reacting) in vaporized region

- Apply custom pulse-burst laser
- Jet mixing characterized by large structures shed to the side and re-entrained
  - Larger residence time in hot mixtures
- Obvious target for high-fidelity LES studies
  - verify accurate mixing field as a preliminary step towards predicting ignition/combustion
  - quantify variance, intermittency, scalar gradients

Parameter	Quantity
Frequency	100 kHz
Burst duration	5 ms
Pulse width	4 – 8 ns
Wavelength	532 nm
Pulse energy	15 mJ
Polarization	Horizontal

Julien Manin et al., Sandia, 2017

150 kHz schlieren imaging

67 µs
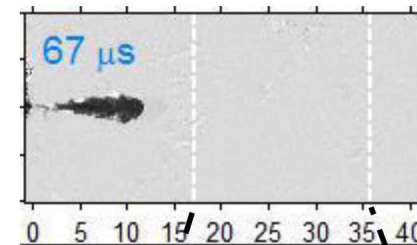
Axial distance [mm]

Ambient Gas
900 K
60 bar
15% O_2

Region of interest for ignition and lift-off stabilization

Fuel mixture fraction

Planar Rayleigh

Equiv. Ratio (15% O_2)

180 µs

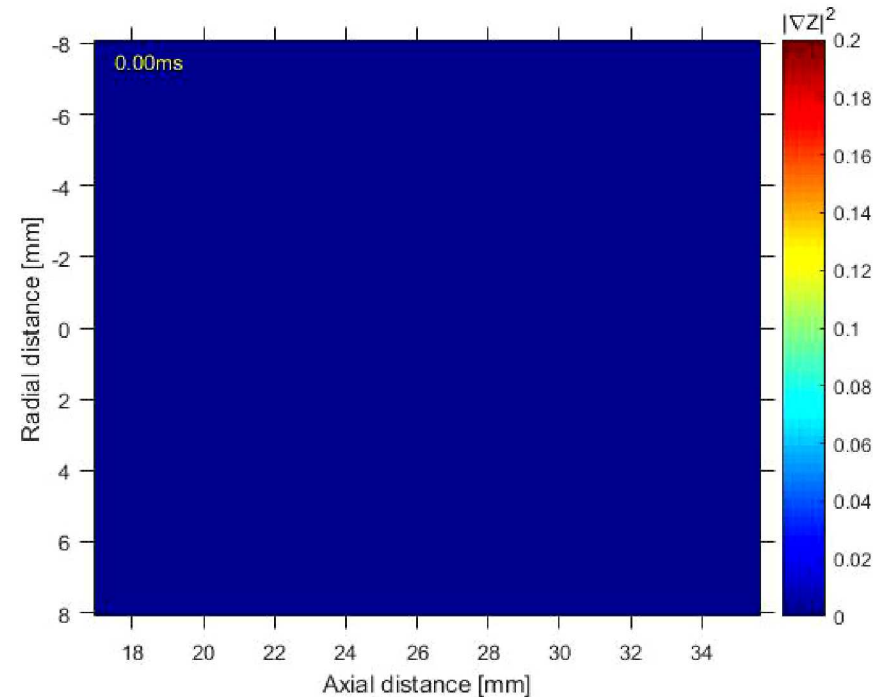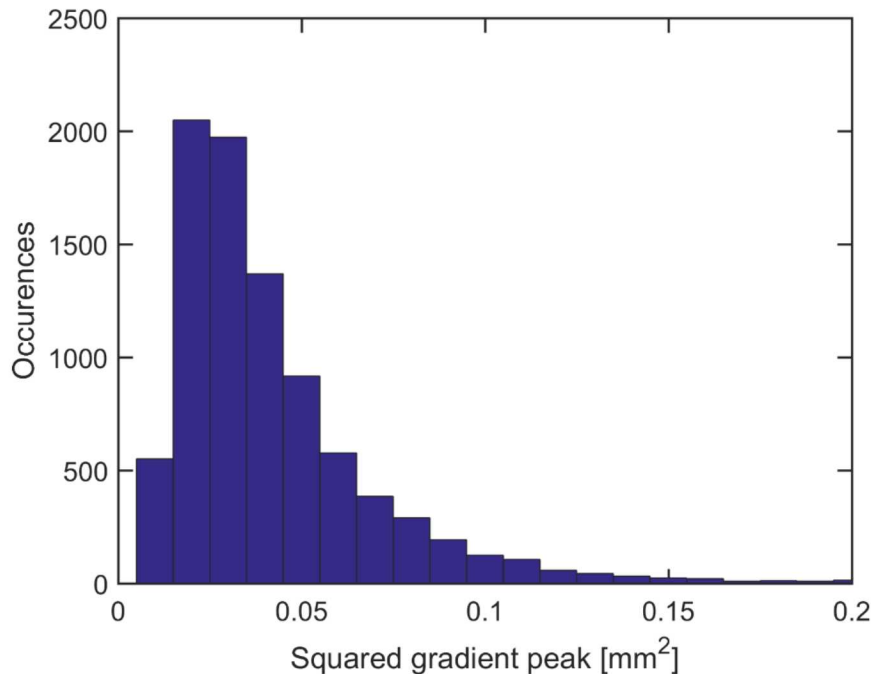Ambient Gas
900 K
60 bar
0% O_2

High-repetition rate laser/imaging system yields time-resolved mixing gradients

- The squared gradients of the mixing fields can be computed to estimate scalar dissipation rates

$$\chi = 2D. |\nabla Z|^2$$

- Broad distribution of dissipative structures over the visualized region

  - Maximum squared gradients on the order of 0.2 mm^2

  - Mean of squared gradients distribution slightly above 0.04 mm^2

Rayleigh scattering limitations

Planar Rayleigh Scattering

Cold vapor fuel beam steering
Mitigation: Develop wavelet-based algorithm to correct for local, pixel-by-pixel laser intensity variations, from shot to shot.

Window and vessel "flare"
Mitigation: Use "recessed" laser-access windows and internal baffles. Make internal surfaces flat and black using special cured paint. Move shiny spark electrodes to different position. Measure background flare often to detect changes with time.

Liquid scatter
Mitigation: Choose illumination region downstream of the liquid-phase penetration length

Window thermal boundary layer beam steering
Mitigation: Use reference ambient as built-in laser intensity correction.

Ambient gas particles (original)
Mitigation: Filter delivery gases with 3 nm filter. Use slow discharge through intake valves. Limit heavy-oil condensates.

Ambient gas particles (preburn combustion sources)
Mitigation: Special covers for seals and window glue lines. "Bake-in" heating with many combustion events for pain/internal surface.

Fuel particles
Mitigation: Install special high-pressure syringe pump with few moving parts. Extensive flushing of lines and injectors. Selection of "pure" fuels. Filtering and centrifuging.

Window laser damage
Mitigation: Use high-grade optics, AR coated if possible, and kept very clean.
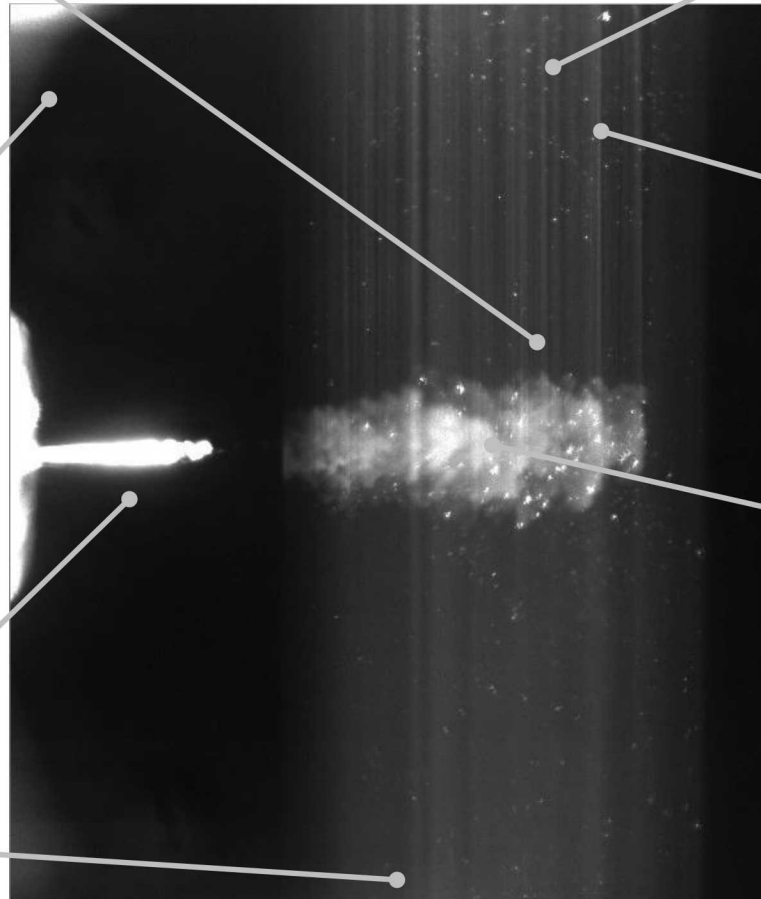
Develop extinction imaging diagnostic for quantitative mixing measurement

- Need method resilient to:
  - presence of fuel droplets amid fuel vapor
  - beam steering
  - particulate contaminants

- Extinction diagnostics have proven ability to overcome these challenges
  - However, previous efforts required UV sources and noisy intensified cameras
- Sandia developed extinction imaging diagnostic robust under conditions with high beam steering
  - Uses visible CMOS sensor
- Need for a "visible" spectrum absorption tracer
  - C70 fullerene "buckyballs"
  - Characterized by strong absorption in the visible spectrum
  - C70 fullerene highly soluble in toluene
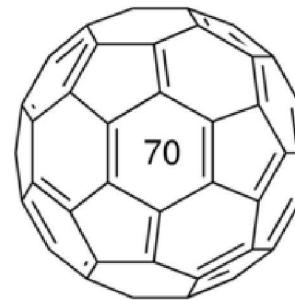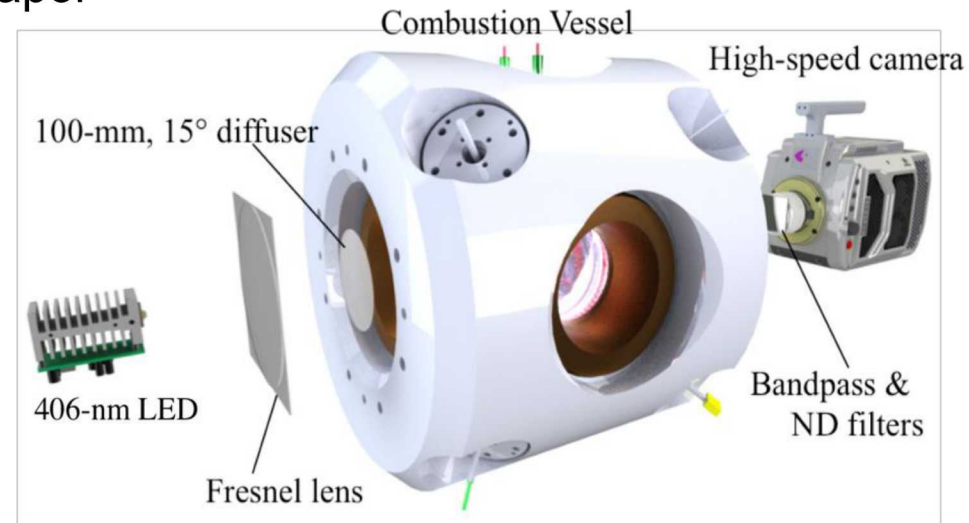
# Extinction based mixture fraction measurements using C70 fullerene

- Line-of-sight diagnostic provides direct measure of total fuel mass
- Symmetry in time- and ensemble-averaged images permit tomographic inversion returning quasi-steady mixture fraction distribution along center plane
- Sufficient statistics or simultaneous orthogonal perspectives will permit quantification of transients
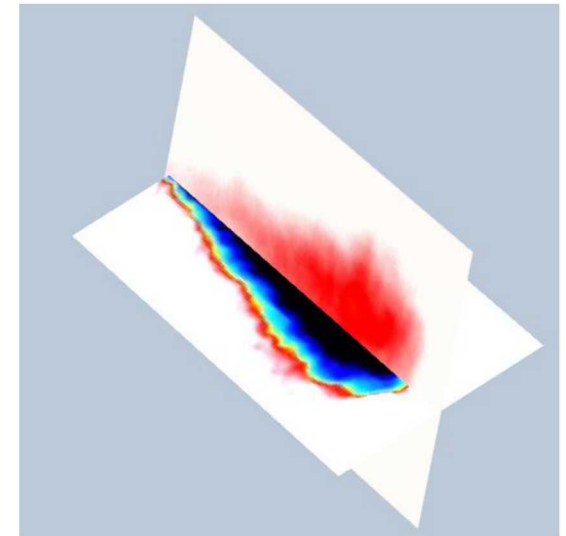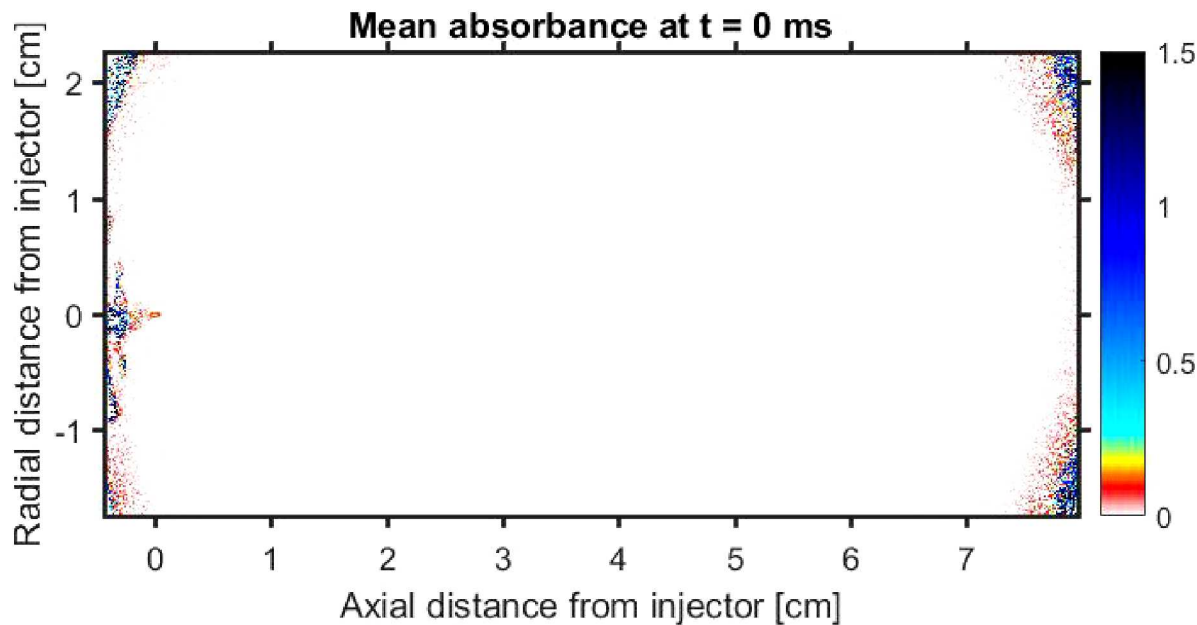
What are the mechanisms of soot formation in stoichiometric GDI operation?

- Use constant volume vessel to mimic stoichiometric GDI engine
  - Create fuel film
  - Premixed flame propagates past film, consumes available oxygen
  - Investigate fate of fuel film and interrogate soot formation process

0.0 ms after spark command

OH*
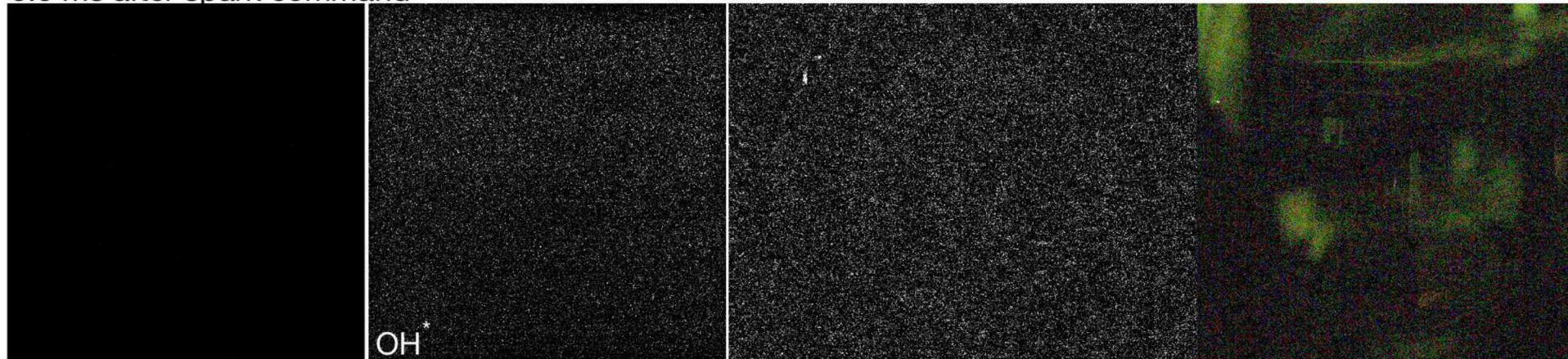
What are the mechanisms of soot formation in stoichiometric GDI operation?

- Does liquid film on piston surface combust as a pool fire (i.e., diffusion flame)?

  — OR

- Are there fuel-rich ($\varphi > 2$) pockets created in the vicinity of the film as it vaporizes?

  — OR

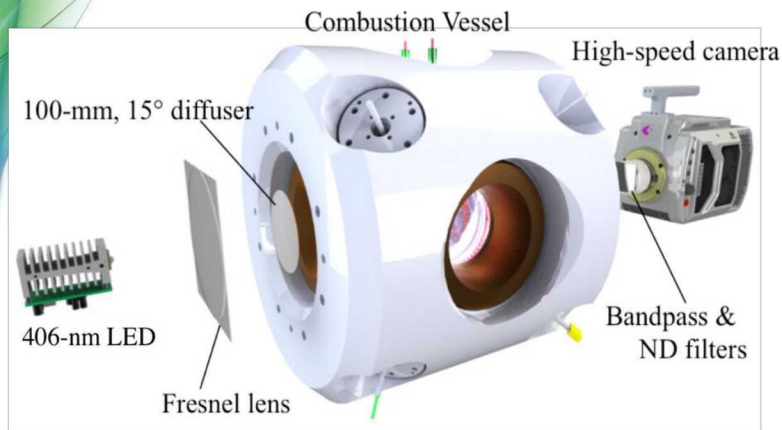- Is oxygen mostly consumed during premixed burn leaving fuel film to pyrolyze?

194.5 ms after spark
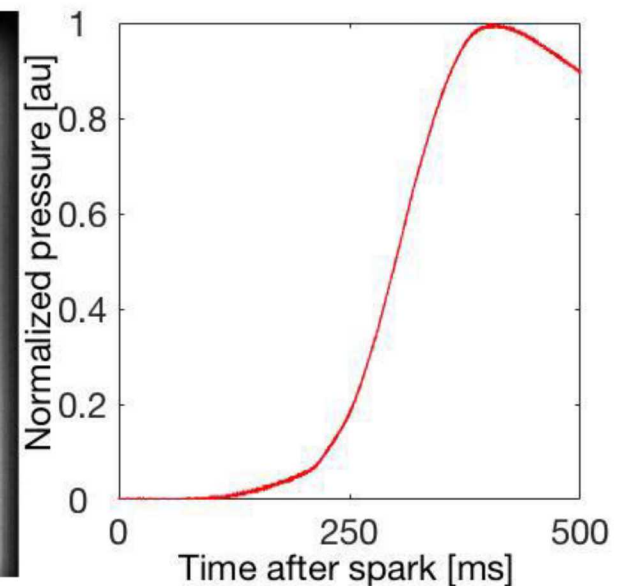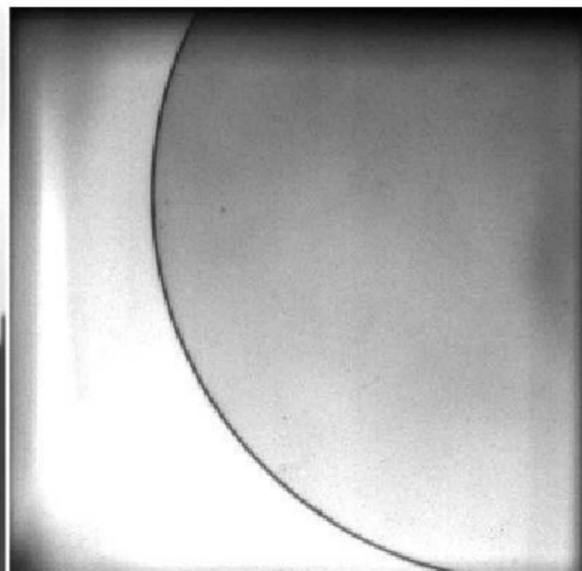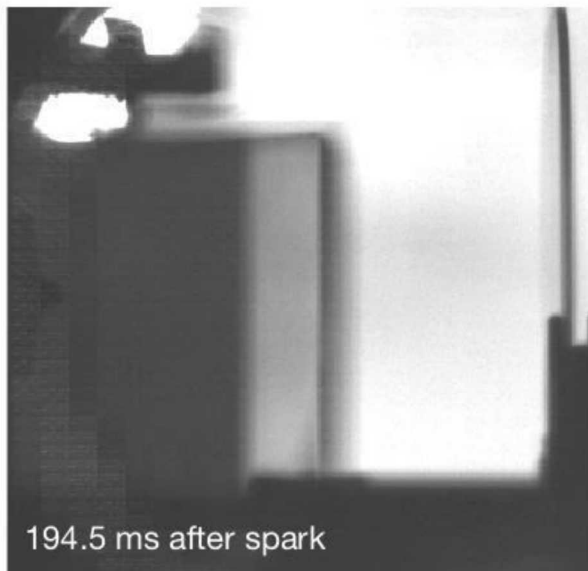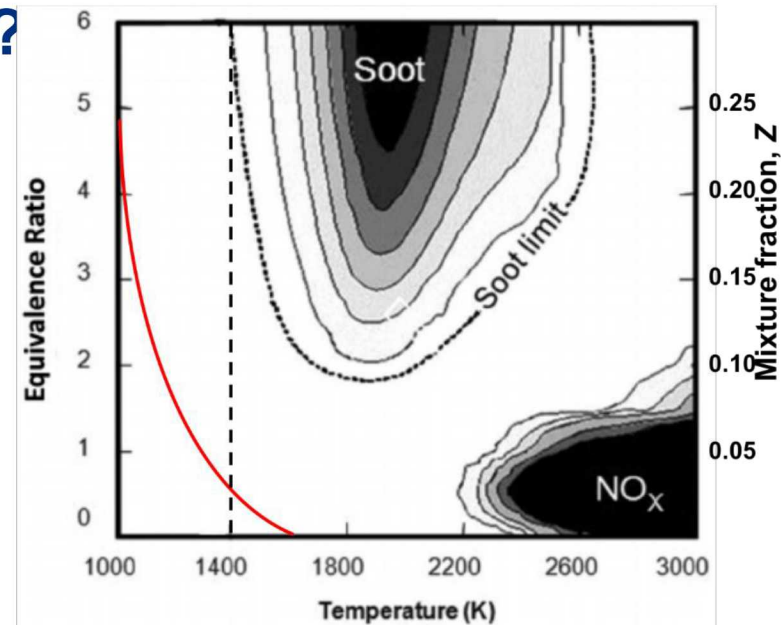
Soot formation in pyrolyzing sprays—even at low *Z?*

Diffused back-illumination extinction imaging yields time-resolved total soot mass

$$f_v L = -\ln\left(\frac{I}{I_0}\right) \cdot \frac{\lambda}{k_e}$$
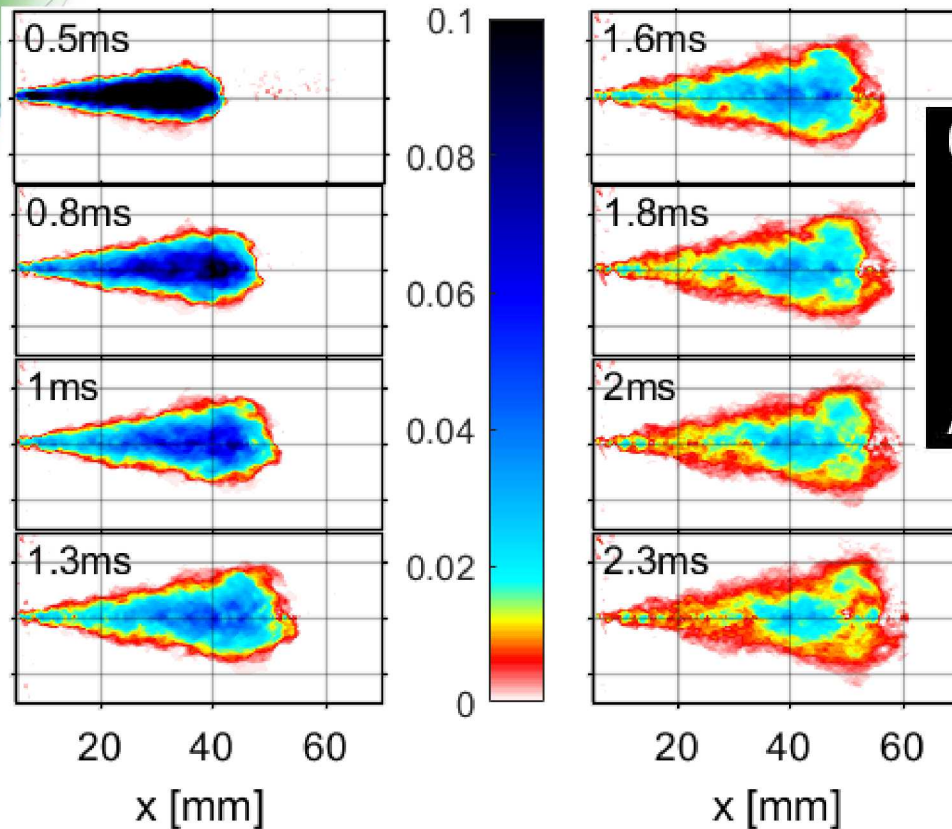
$$m_{soot} = \iint \rho_{soot} \cdot f_v L \cdot dA = -\iint \rho_{soot} \cdot \frac{\lambda}{k_e} \cdot \ln\left(\frac{I}{I_0}\right) \cdot dA$$

- ~200 µs injection
- 0% oxygen, 1600 K ambient
- Rapid mixing with ambient inert gases
- Sooting "limit" temperature of 1450K identified by exploring a range of temperatures and pressures
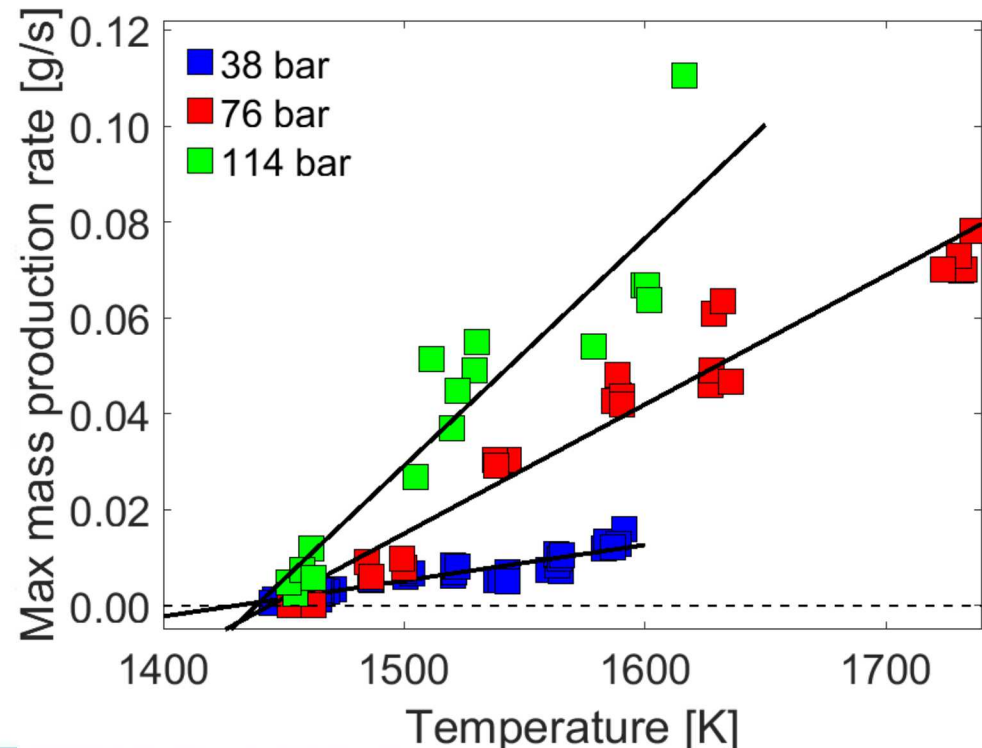
Soot formation in pyrolyzing sprays—even at low *Z!*
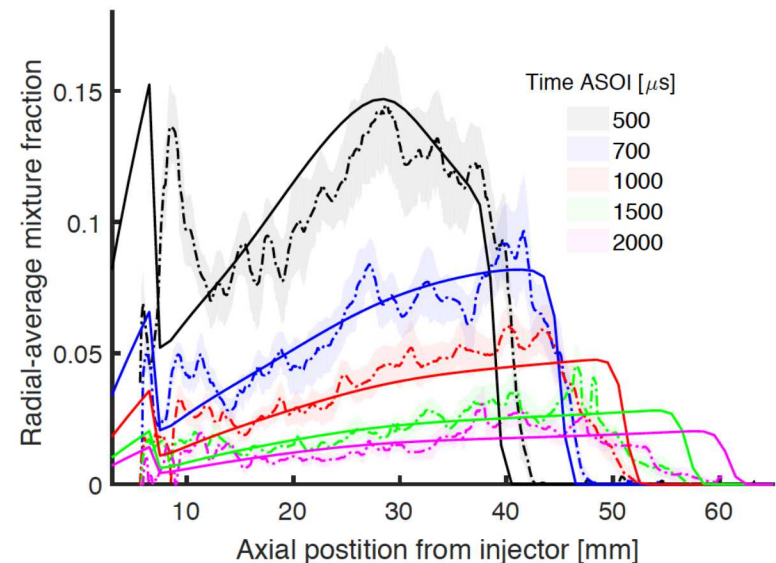

Pyrolyzing spray at 1600 K
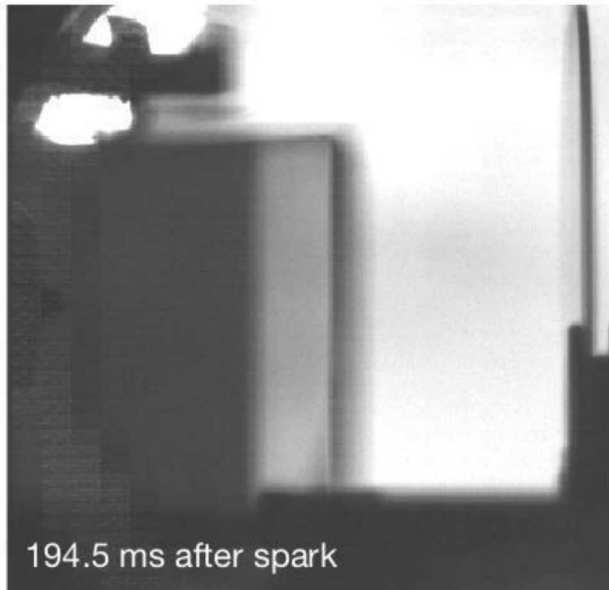

0.00 ms ASOI

KL

- Liquid injection observed, rapid vaporization
- Soot "onset" observed near 2 ms ASOI
- Highest *Z* measured at 2 ms ASOI in a ~350 μs injection is ~0.04.
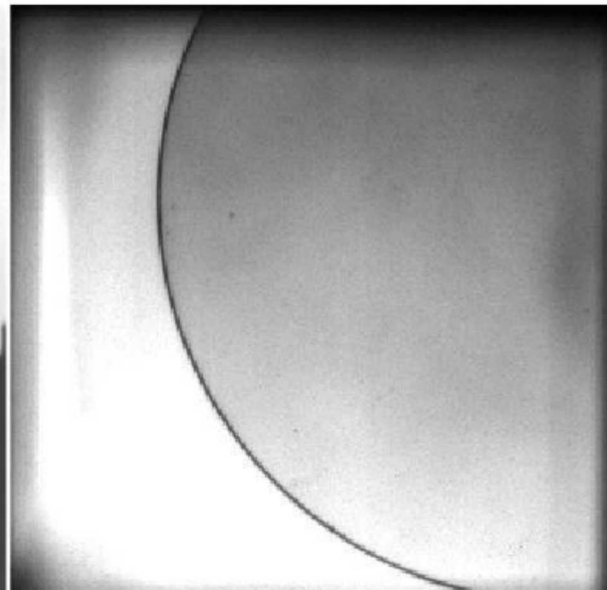- Radial avg. *Z* this late is relatively uniform and < 0.02

Soot formation in stoichiometric GDI operation due to wall impingement – pyrolysis pathway!
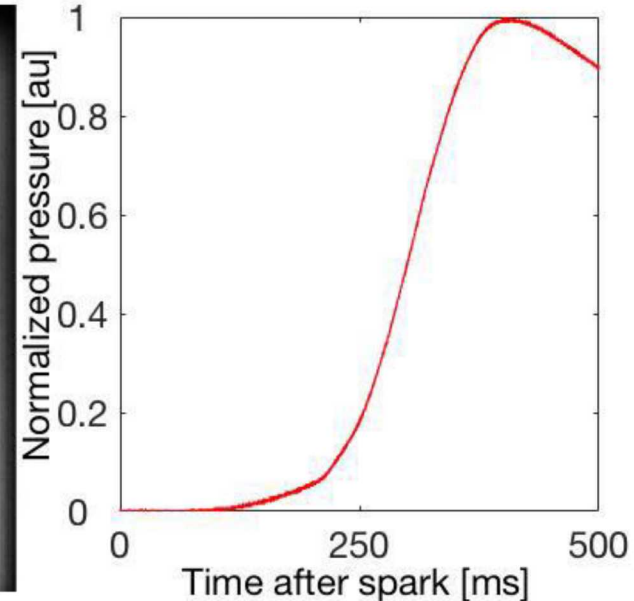
Extinction Imaging: side view   Extinction Imaging: head-on view   Normalized vessel pressure

194.5 ms after spark

- First demonstration of extinction imaging for wall impinging spray
- Beam steering along wall indicates preburn flame passes over fuel film without igniting film and/or generating soot – products calculated to be ~1750K
- Soot forms several milliseconds after flame passes over film, time required to heat and vaporize fuel film to the soot limit temperature
- Soot ejected away from wall as it forms, convective forces at play may be critical
- A detailed look at CFD results for soot in GDI is warranted!

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How do multiple injections influence spray collapse and can they be used to reduce wall impingement?

- Plumes diverge inward from drill angle during late stages of single injection event – potentially enhancing wall wetting
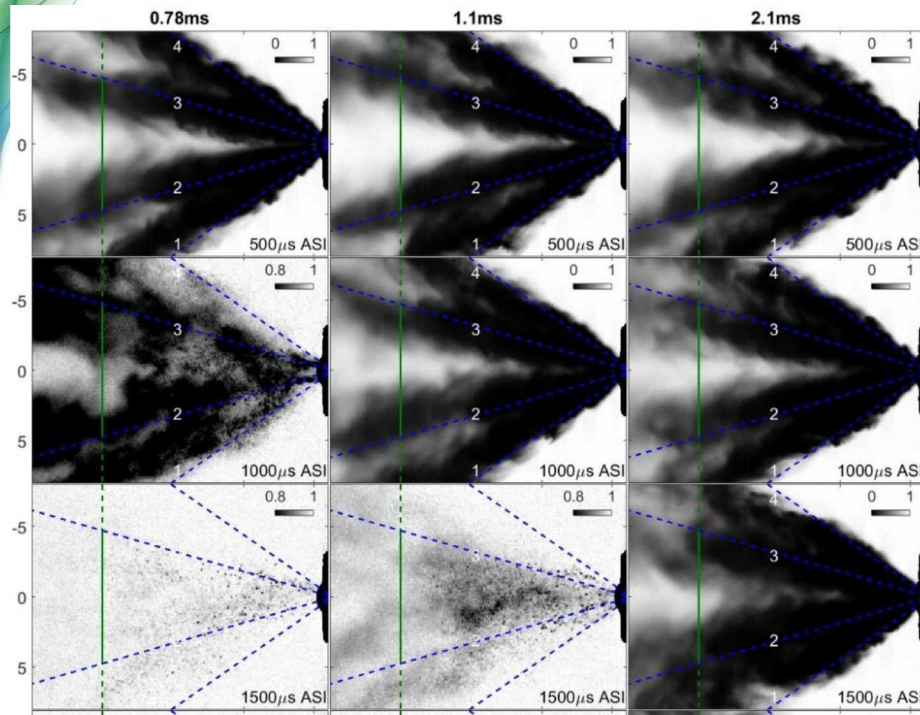
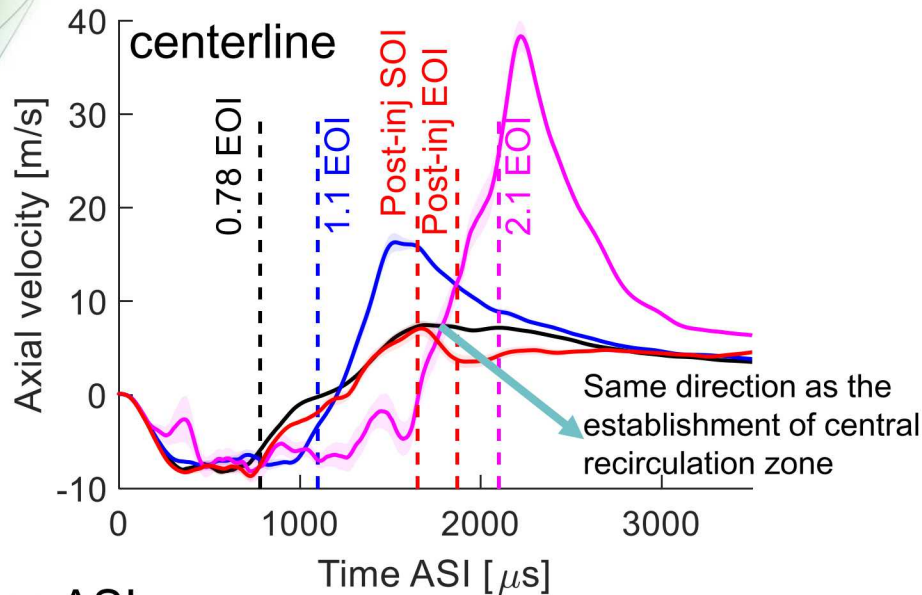- Second injection "resets" plume angle to injector drill angle – may help to inhibit wall wetting by reducing penetration
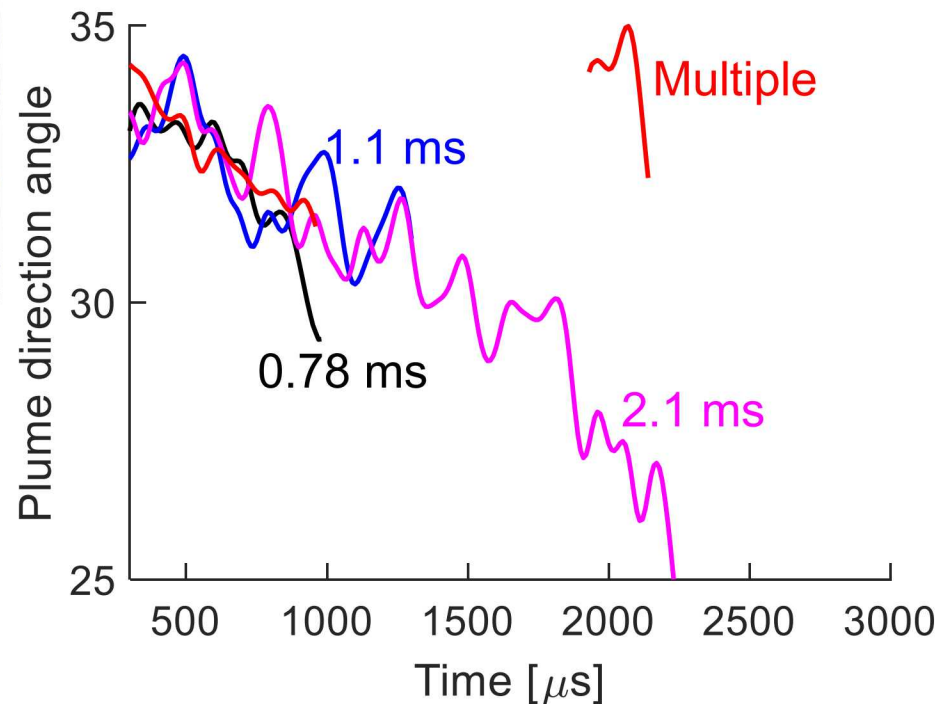
Centerline velocity driven lower by second injection

centerline

Axial velocity [m/s]

0.78 EOI
1.1 EOI
Post-inj SOI
Post-inj EOI
2.1 EOI

Same direction as the establishment of central recirculation zone

Time ASI [μs]

- **Resistance to spray collapse demonstrated by using multiple injections**
- **Conclusion: velocity and mixing analysis both indicate more effective mixing with second injection**

time ASI

0.8ms   1.1ms   multiple injection

EOI

Velocity [m/s]

axial velocity time evolution at z = 15 mm

radial position [mm]

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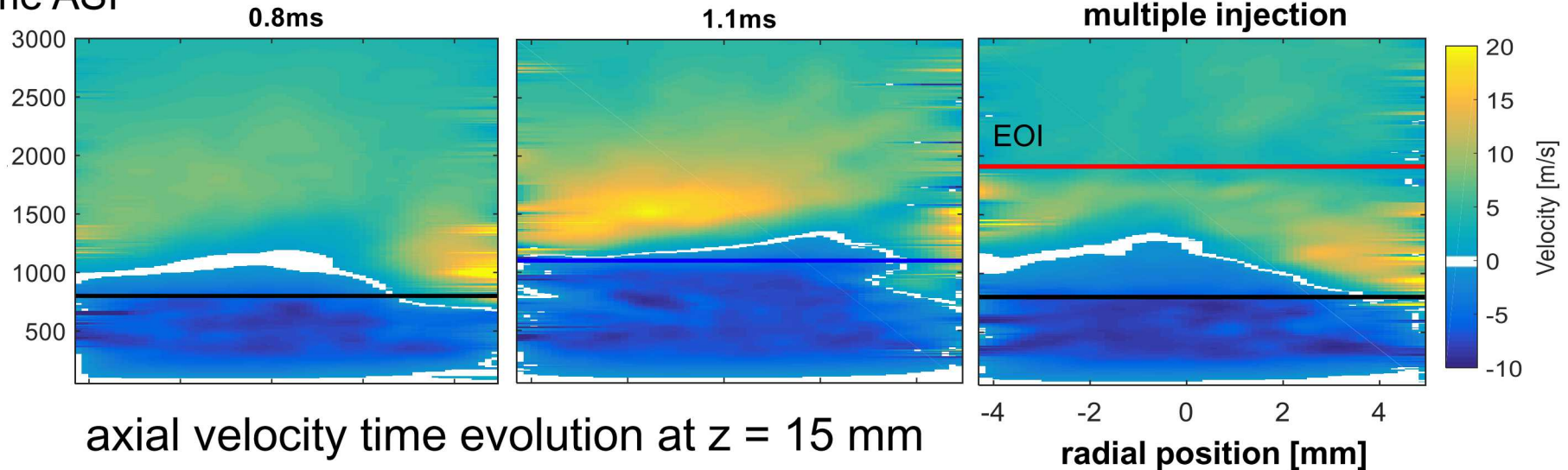
Future work

- Gasoline direct-injection activities (FY19)
  - Extend soot extinction imaging of soot in films for quantitative measurements
  - Quantify soot in spark/laser ignited gasoline sprays
  - Explore effectiveness of multiple injections to limit liquid penetration for reduced soot from wall wetting but also to understand bulk gas and droplet mixing
  - Further development of extinction imaging diagnostic for mixture fraction

- Diesel research activities (FY19)
  - Investigate transient internal flows (including cavitation) using transparent nozzles
  - Interrogate the (miscible) structure of fuel droplets under supercritical reacting conditions (relevance to soot from injector dribble)
  - Perform high-speed planar imaging of mixing and ignition (custom 100 kHz pulse burst laser) over wider range of conditions
- Begin experiments in new high-throughput laboratory (funded via Co-Optima) to improve efficiency of this research
  - Investigate GDI flash-boiling conditions
  - Model validation datasets will have lower uncertainty
  - New opportunities for gas sampling with offline mass spectrometry
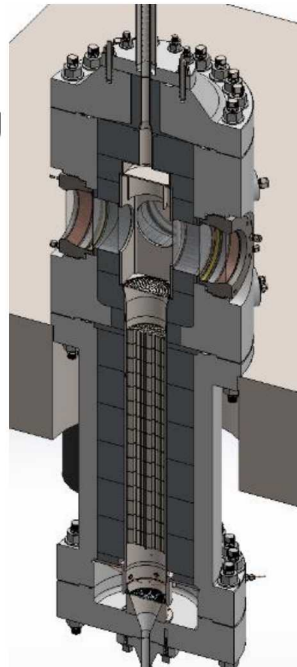
Presentation Summary

- 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
- FY18 approach yields increased understanding of key phenomena
  - Quantitative, high-speed mixing measurements provide critical target data for model improvement and first-ever spray mixing statistics
  - Novel combustion vessel operation reveals new insights on soot formation pathway in stoichiometric GDI operation
  - Advanced spray diagnostics (PIV in GDI sprays) demonstrate utility of multiple injections to inhibit spray collapse by "resetting" plume angle
- 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

First comprehensive spray study of AVFL-18a diesel surrogates demonstrates promise for combustion and soot characteristics
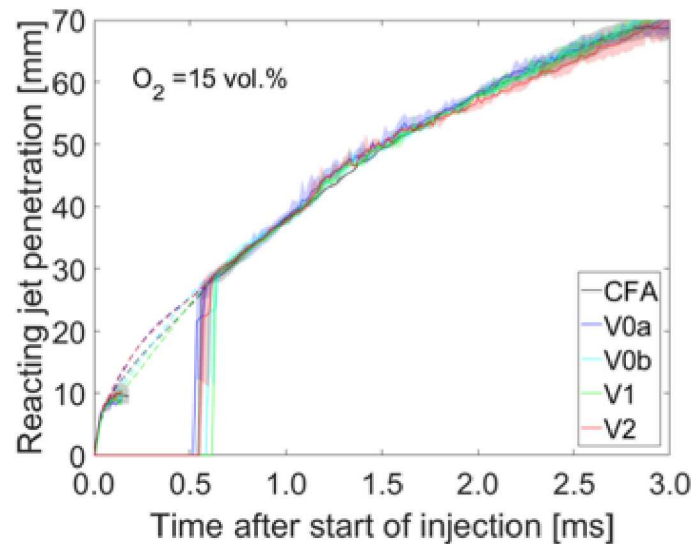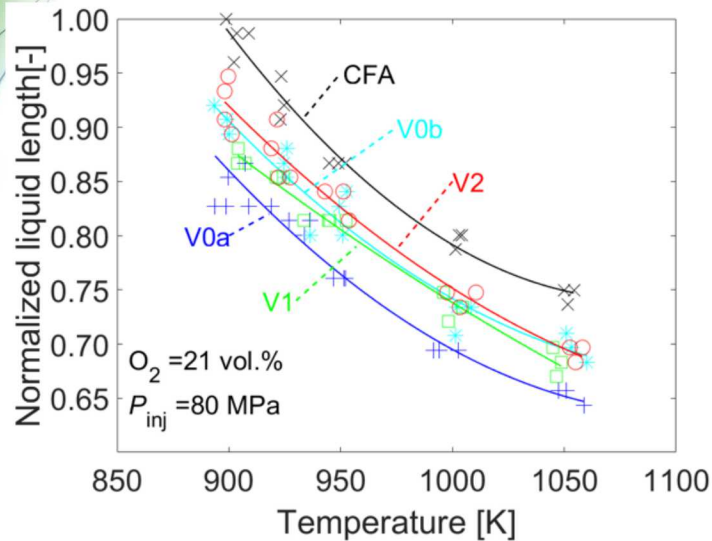

- Four AVFL-18a surrogate fuels (4,5,8,9 component) compared with diesel certification fuel (CFA)
- Large experimental matrix:
  - 5 ambient temperatures, 2 injection pressures (80,150 MPa), 2 oxygen concentrations (15%,21%)
- Liquid length, vapor penetration, ignition delay and lift-off length, and soot mass
- Sandia Combustion Vessel, 22.8 kg/m^3

- Differences in liquid length can be explained by fuel properties—90% distillation temperatures and heats of vaporization
  - CFA > V2≈V0b≥V1>V0a
- In spite of fuel physical property differences, vapor penetration is consistent as it is controlled by momentum (which is conserved)
  - $V_f \propto \sqrt{2\Delta P/\rho_f}$ (velocity)
  - $\dot{M} = \rho_f V_f^2 A \propto 2\Delta PA$ (momentum flux)

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First comprehensive spray study of AVFL-18a diesel surrogates demonstrates promise for combustion and soot characteristics
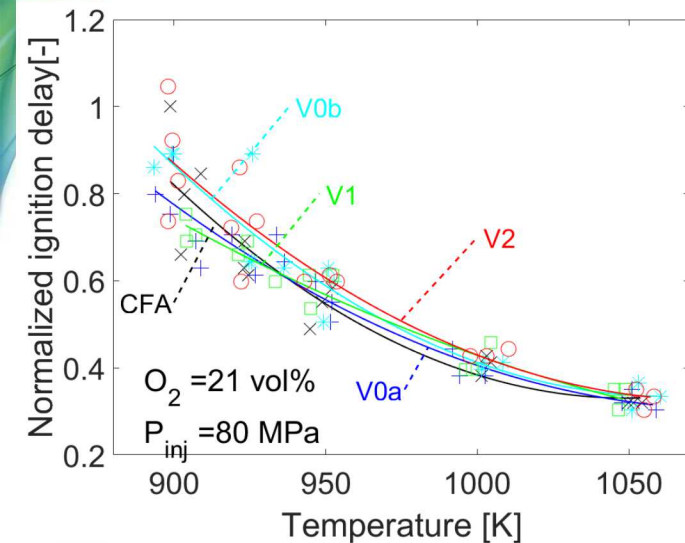

- Scatter plots of individual data points highlight consistency among data for ignition delay and lift-off length (not shown)—shot-to-shot variability remains a topic of interest
- Surrogates show slight trend toward longer ignition delays relative to CFA (not predicted by DCN)
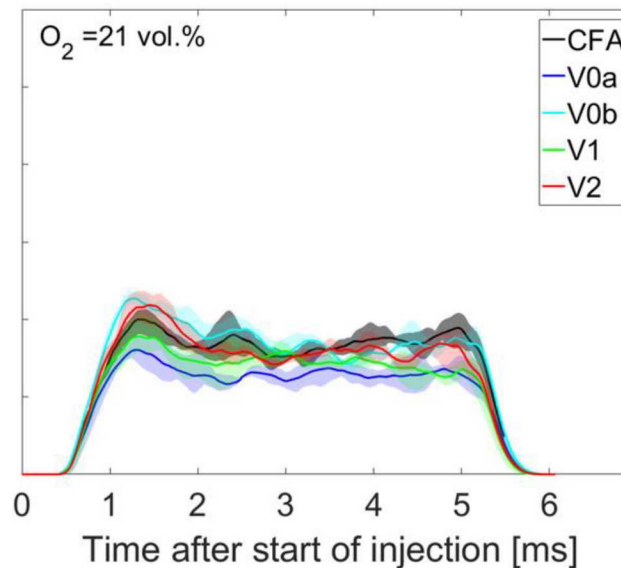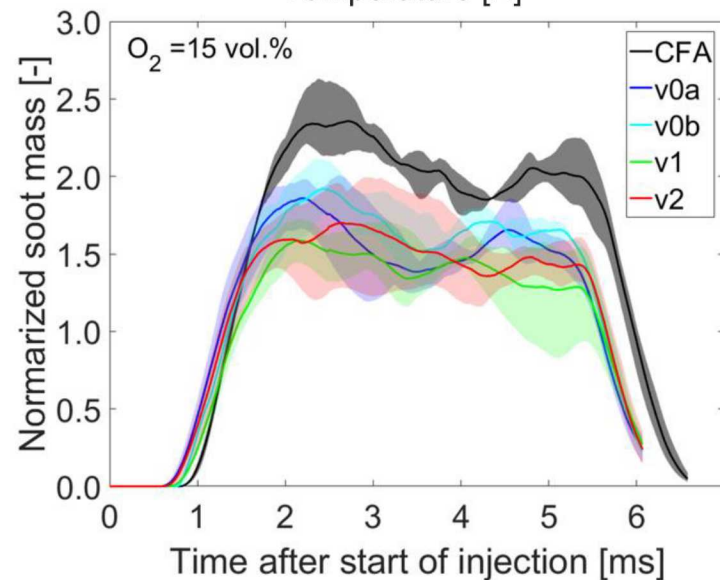
Unique high-speed velocity diagnostic applied

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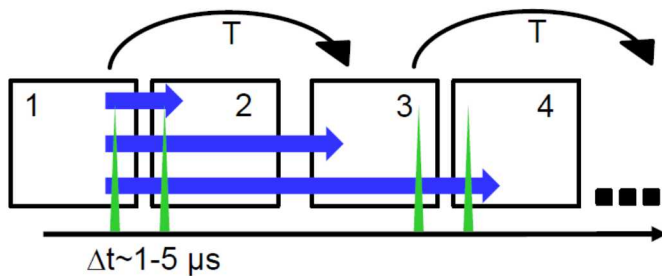
- Applied PIV
  - 1 μm zirconia seed in gas phase
  - 200 kHz imaging on high-speed CMOS camera
  - Liquid-phase avoided by probing between plumes and moving downstream

Spray G
fuel: iso-octane, 200 bar
gas: 573 K, 6 bar

Axial distance from injector [mm]

Plumes 2&3 Plumes 1&4   Plumes 8&5 Plumes 7&6
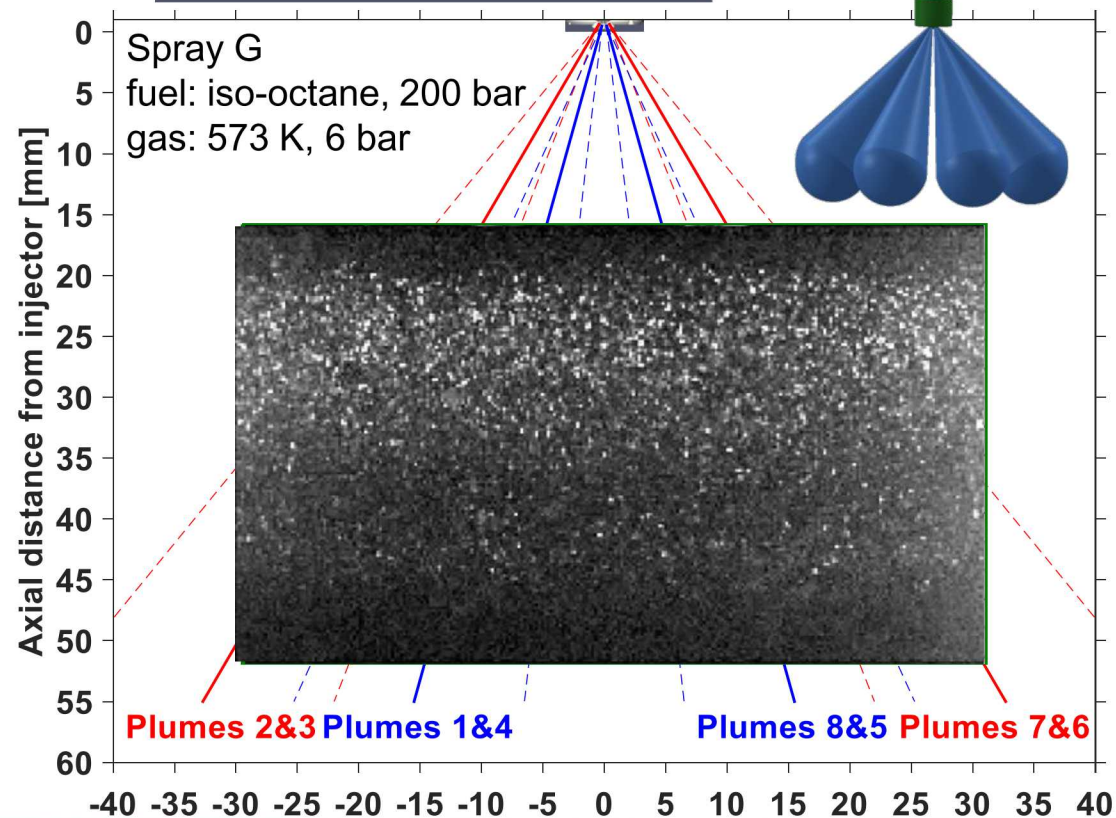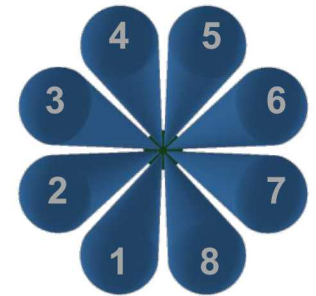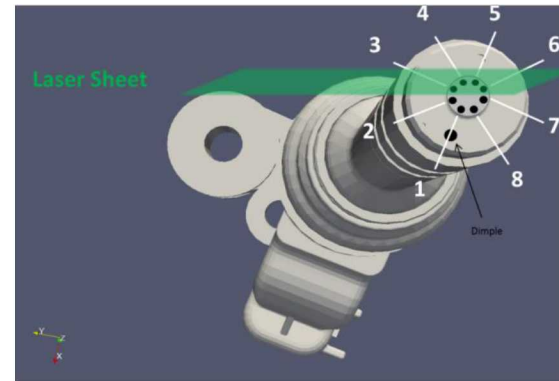
Close collaboration and pathway to better CFD tools

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
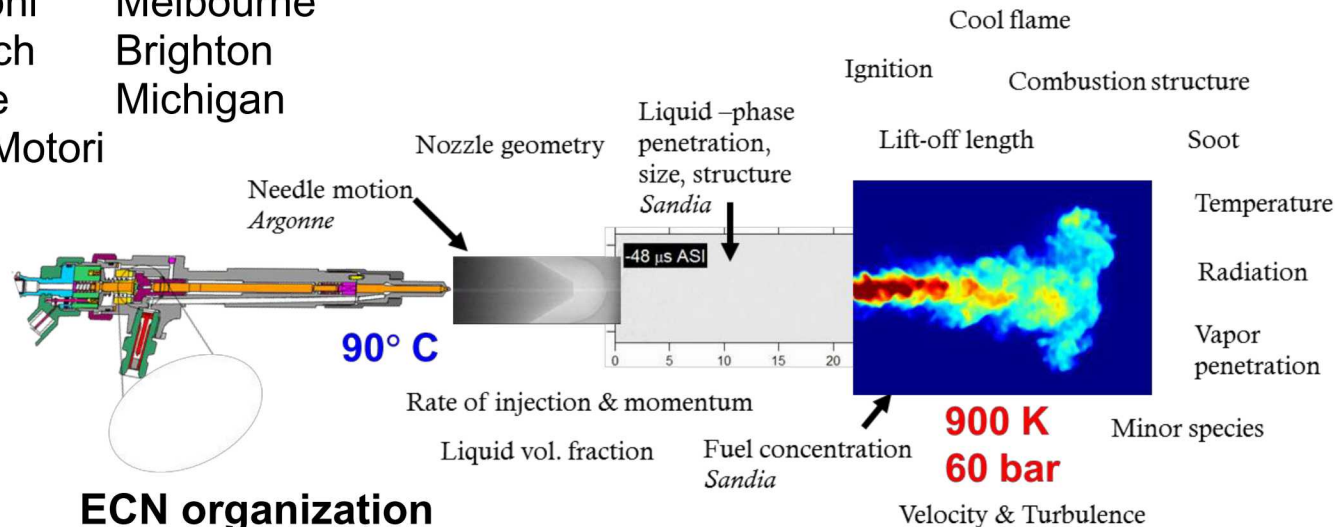Eulerian-Eulerian
Eulerian-Lagrangian
Dense fluid
many spray and
combustion variants…

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…

Most industry use ECN data to test their CFD practices

Nozzle geometry

Needle motion *Argonne*

90° C

Liquid –phase penetration, size, structure *Sandia*

-48 μs ASI

0 5 10 15 20

Rate of injection & momentum

Liquid vol. fraction

Fuel concentration *Sandia*

Cool flame

Ignition

Lift-off length

Combustion structure

Soot

Temperature

Radiation

Vapor penetration

900 K 60 bar

Minor species

Velocity & Turbulence

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

Reviewer-only Slides

Reviewer Slides: Recent Publications

"Measuring the soot onset temperature in high-pressure n-dodecane spray pyrolysis," Scott A. Skeen and Koji Yasutomi, Combustion and Flame 188:483-487, 2018.

"Inter-plume aerodynamics for gasoline spray collapse" Panos Sphicas, Lyle M. Pickett, Scott A. Skeen, and Jonathan H. Frank. International Journal of Engine Research:1468087417740306, 2017.

"Internal and near nozzle measurements of Engine Combustion Network "Spray G" gasoline direct injectors," Daniel J. Duke, Alan L. Kastengren, Katarzyna E. Matusik, Andrew B. Swantek, Christopher F. Powell, Raul Payri, Daniel Vaquerizo, Lama Itani, Gilles Bruneaux, Ronald O. Grover, Scott Parrish, Lee Markle, David Schmidt, Julien Manin, Scott A. Skeen, and Lyle M. Pickett. Experimental Thermal and Fluid Science 88:608-621, 2017.

"Ducted fuel injection: A new approach for lowering soot emissions from direct-injection engines," Charles J. Mueller, Christopher W. Nilsen, Daniel J. Ruth, Ryan K. Gehmlich, Lyle M. Pickett, and Scott A. Skeen. Applied Energy 204:206-220, 2017.

"On the transcritical mixing of fuels at diesel engine conditions," Cyril Crua, Julien Manin, and Lyle M. Pickett, Fuel 208:535-548, 2017.

"Diffuse back-illumination setup for high temporally resolved extinction imaging," Fredrik R. Westlye, Keith Penney, Anders Ivarsson, Lyle M. Pickett, Julien Manin, and Scott A. Skeen, Appl.Opt. 56 (17):5028-5038, 2017.

"Transcritical mixing of sprays for multi-component fuel mixtures," Julien Manin, Cyril Crua, Lyle M. Pickett, ILASS-Europe, 2017.

COMBUSTION RESEARCH FACILITY

Sandia National Laboratories