ACE001: Heavy-Duty Low-Temperature and Diesel Combustion & Heavy-Duty Combustion Modeling

Mark P. B. Musculus
Combustion Research Facility
Sandia National Laboratories

FY 2016 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D/Combustion Research
8:00 – 8:30 AM, Wednesday, June 8, 2016

Sponsor: U.S. Dept. of Energy, Office of Vehicle Technologies
Program Managers: Leo Breton, Gurpreet Singh

ACE001

Overview: Heavy-duty combustion project

Timeline

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

Barriers

From 2013 US DRIVE Adv. Comb. & Emission Tech. Team Roadmap:

- Inadequate understanding of LTC control technologies, esp. for mixed-mode
- LTC aftertreatment integration
- Impact of future fuels on LTC

Budget

- Project funded by DOE/VTP:
  FY14-SNL/UW: $735k/99k
  FY15-SNL/UW: $720k/99k

Partners

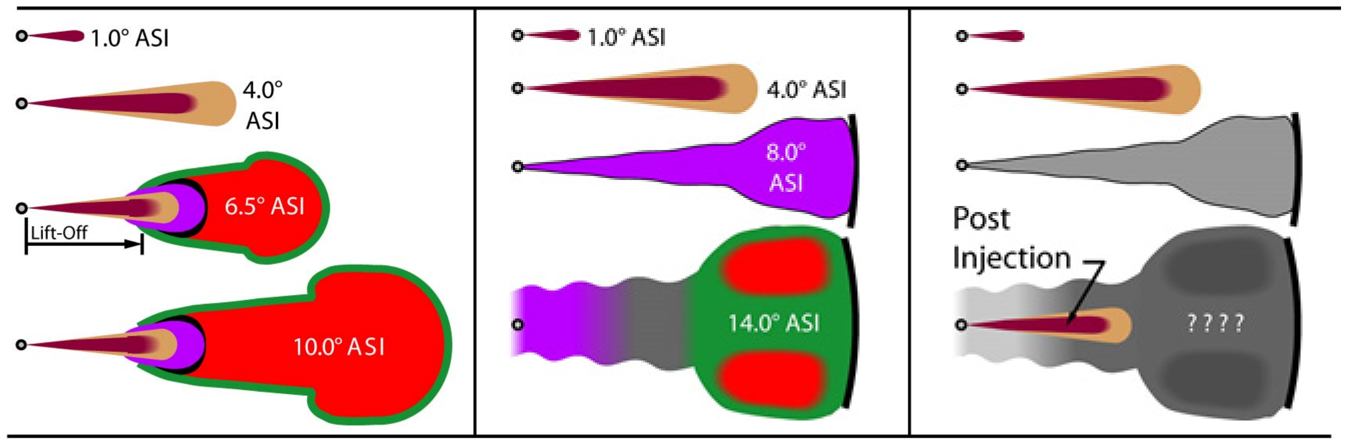
- U. of Wisconsin, Cummins, Delphi, Convergent Science, Wayne State U., Lund, IFPEN
- 15 AEC MOU industry partners
- Project lead: Sandia (Musculus)

Relevance/Objectives: HD in-cylinder combustion

Long-Term Objective

Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines

1997: **Conventional Diesel** (Single Injection) | 2012: **LTC Diesel** (Single Injection) | 2013+: **Multiple Injection** (Conventional & LTC)



- Liquid Fuel
- Pre-ignition Vapor Fuel
- First-Stage Ignition (H_2CO, H_2O_2, CO, UHC)
- Intermediate Ignition (CO, UHC)
- Second-Stage Ignition of Intermediate Stoichiometry or Diffusion Flame (OH)
- Second-Stage Ignition of fuel-rich mixtures
- Soot or Soot Precursors (PAH)

Milestones/Objectives: H-D In-Cylinder Combustion

Long-Term Objective

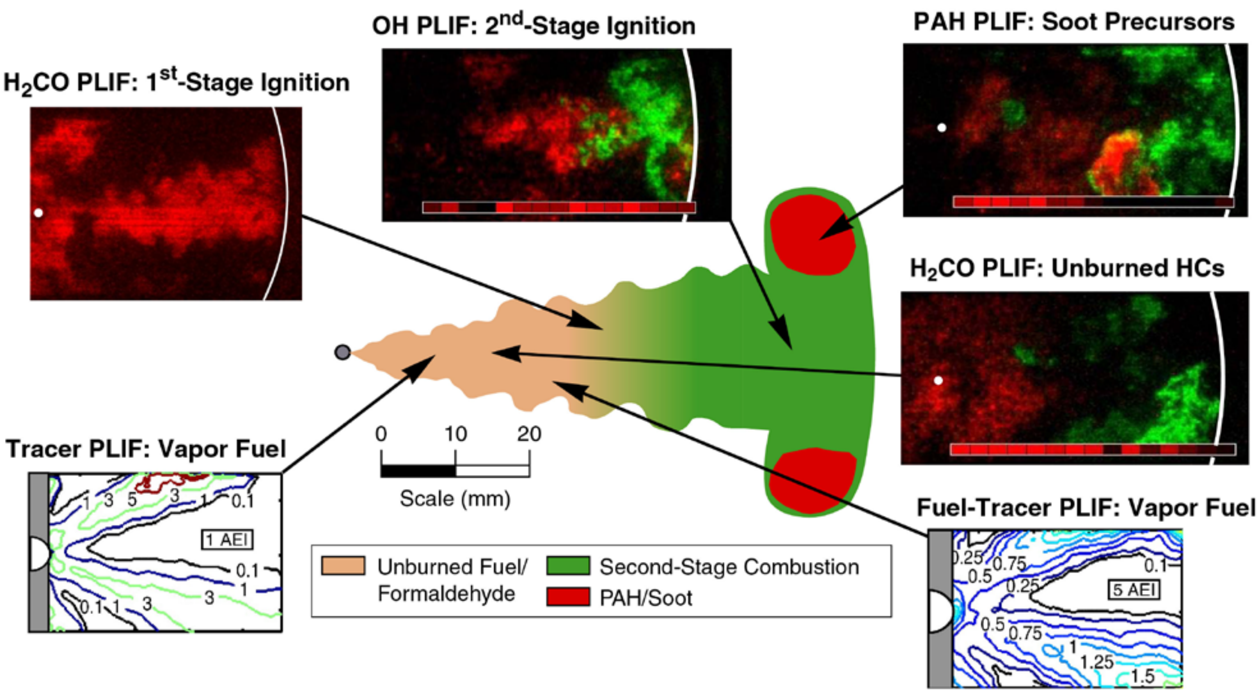
Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines

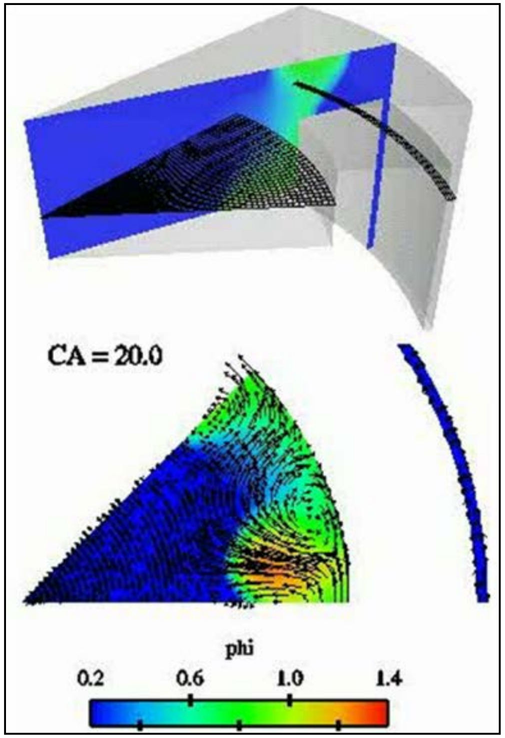
Current Milestones/Objectives:

1. SNL – Provide Spray B in-cylinder engine data and uncertainty estimates for ECN
2. SNL – End-of-injection mixing effects on ignition
3. SNL – In-cylinder surface heat transfer diagnostic
4. UW & SNL – Use computer-model simulation/analysis tools to complement experimental data

Approach/Strategy: Optical imaging and CFD modeling of in-cylinder chemical/physical processes

- Combine planar laser-imaging diagnostics in an optical heavy-duty engine with multi-dimensional computer modeling (KIVA) to understand LTC combustion
- Transfer fundamental understanding to industry through working group meetings, individual correspondence, and publications





Collaborations

- All work has been conducted under the Advanced Engine Combustion Working Group in cooperation with industrial partners
  – Cummins, Caterpillar, DDC, Mack Trucks, John Deere, GE, International, Ford, GM, Daimler-Chrysler, ExxonMobil, ConocoPhillips, Shell, Chevron, BP, SNL, LANL, LLNL, ANL, ORNL, U. Wisconsin
- New research findings are presented at biannual meetings
- Tasks and work priorities are established in close cooperation with industrial partners
  – Both general directions and specific issues
- Industrial/University partnerships support laboratory activities
  – FY2016: Wayne State University – IR diagnostic development
  – FY2016: DOE/NSF proposal on soot/precursor modeling with UW//Convergent Science
  – FY2016: Collaborations/visits with IFPEN and Lund University

Responses to Previous Year Reviewers' Comments

Comment: ***"Focusing on fewer topics might provide greater leadership and progress in these areas ... with four areas worked on, there would be concern that each got less time than it deserved for the value of each area individually ...* more significant progress could be made with more focused study of fewer topics*"***

Response: This year's project directions are more focused, with less dilution over multiple efforts.

Comment: *"Soot formation and oxidation work is very exciting, and is a perfect example of the value of optical engine work since these results would be unobtainable anywhere else"*

Response: We are in the process of developing new diagnostics to extend soot formation and oxidation work, which will be presented at the FY17 review and in other meetings/publications.

Comment: *"Thermal imaging for vapor penetration is very interesting and would like to see more development and validation of the technique to understand it better"*

Response: We have plans to better understand IR imaging for fuel vapor, and we're also exploring other diagnostic opportunities like soot luminosity imaging and CO absorption.

Comment: *"It would be great to expand on the idea of tailoring the mixing and scalar gradient distribution. [and] how that can be physically controlled with some injector or combustion bowl design changes"*

Response: The scalar gradient distribution question is difficult to explore in the high-pressure in-cylinder engine environment, but we have made progress, as detailed in this year's report. We'll continue to work in this area, and we have hardware in place for investigating a production bowl shape as well.

Comment: *"The plans to continue building the conceptual model of multiple injection processes and determining how combustion design affects heat transfer and efficiency, should continue the very good progress that has been made"*

Response: This is a multi-year effort that we will continue to follow.

Technical Accomplishments & Progress

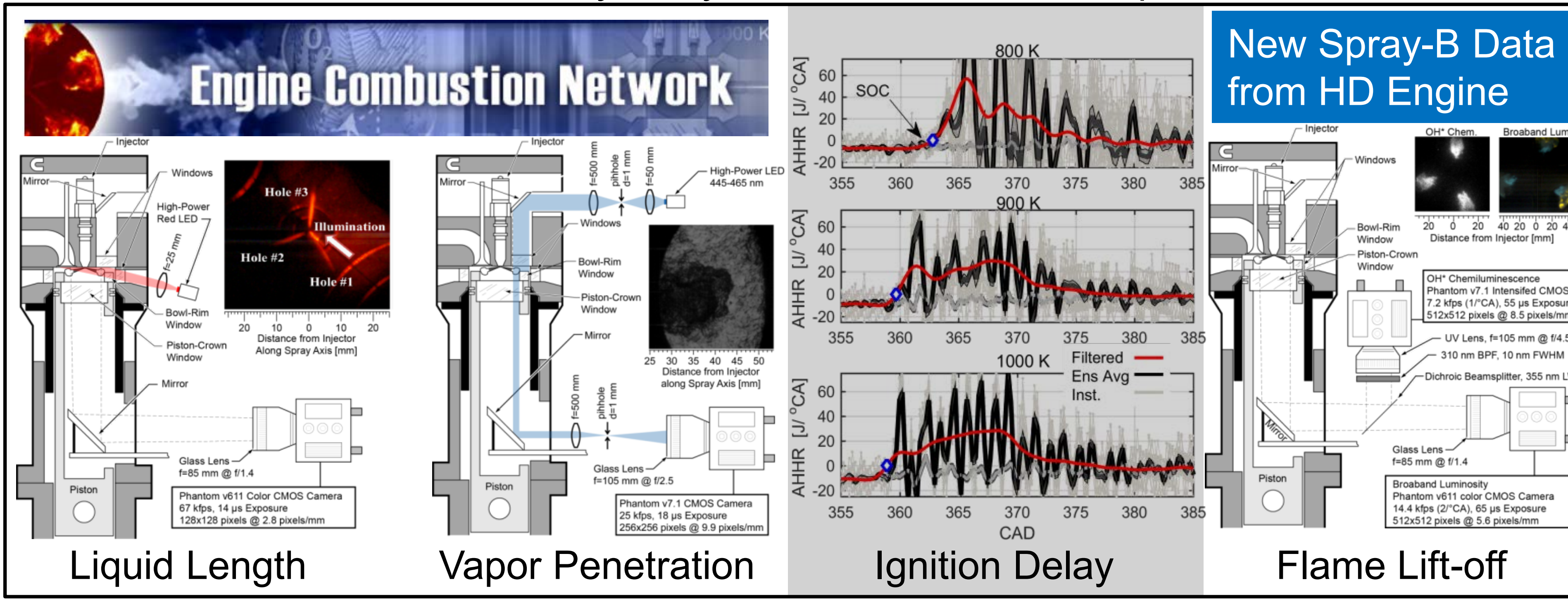
- Accomplishments for each of the four current milestones / objectives below are described in the following four sections

Current Milestones/Objectives:

1. **SNL – Provide Spray B in-cylinder engine data and uncertainty estimates for ECN**
2. **SNL – End-of-injection mixing effects on ignition**
3. **SNL – In-cylinder surface heat transfer diagnostic**
4. **UW & SNL – Use computer-model simulation/analysis tools to complement experimental data**

① ECN is collaboration & model validation resource for const. vol. vessels, now adding engine data

- The Engine Combustion Network (ECN) is a forum and database for collaboration on engine combustion
  - Initial ECN data: single-hole, constant-volume combustion vessels
  - FY15 AMR: added first vapor penetration data for multi-hole injectors and engines using new IR vapor-penetration diagnostic
- FY16: Provide full dataset with multiple spray/combustion diagnostics, *with detailed uncertainty analysis*, to aid model development



ECN's "Spray B" is closer to production injectors than the early ECN-standard, single-hole Spray A

Engine

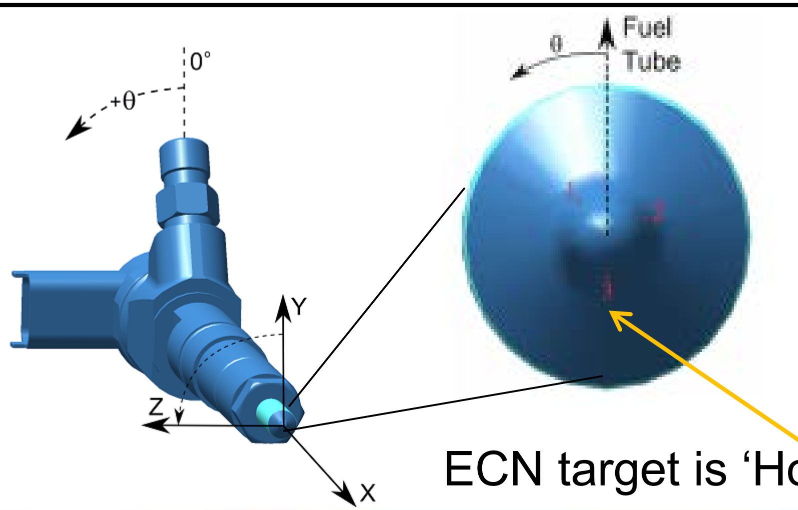
Intake valves	2
Exhaust valves	1 [a]
Swirl ratio	0.5
Bore × Stroke	139.7 × 152.4 mm
Bowl width × depth	97.8 × 15.5 mm
Displacement	2.34 L
Compression ratio	11.22:1 [b]
Connecting rod length	304.8 mm

[a] One exhaust valve has been replaced by an optical periscope.
[b] TDC conditions typical of 16:1 compression ratio are met by boosting and heating the intake stream.

Spray B

Common rail fuel injector	Bosch solenoid-activated, generation 2.4
Nominal nozzle outlet diameter	90 μm
Nozzle k-factor	1.5
Nozzle shaping	Smoothed by hydro-erosion
Mini-sac volume	0.2 mm^3
Discharge coefficient at 10MPa pressure drop	0.86
Number of holes	3
Holes #1,2,3 angular position	36.4, -62.3, 180°
Holes #1,2,3 exit diameter	90.9, 91.7, 90.9 μm
Hole pattern included angle	145°

- Spray A has single axial hole, Spray B has three holes
- Spray B internal turning flow more characteristic of diesel injectors
- Widely spaced holes give minimal spray interactions external to injector and facilitate optical diagnostics

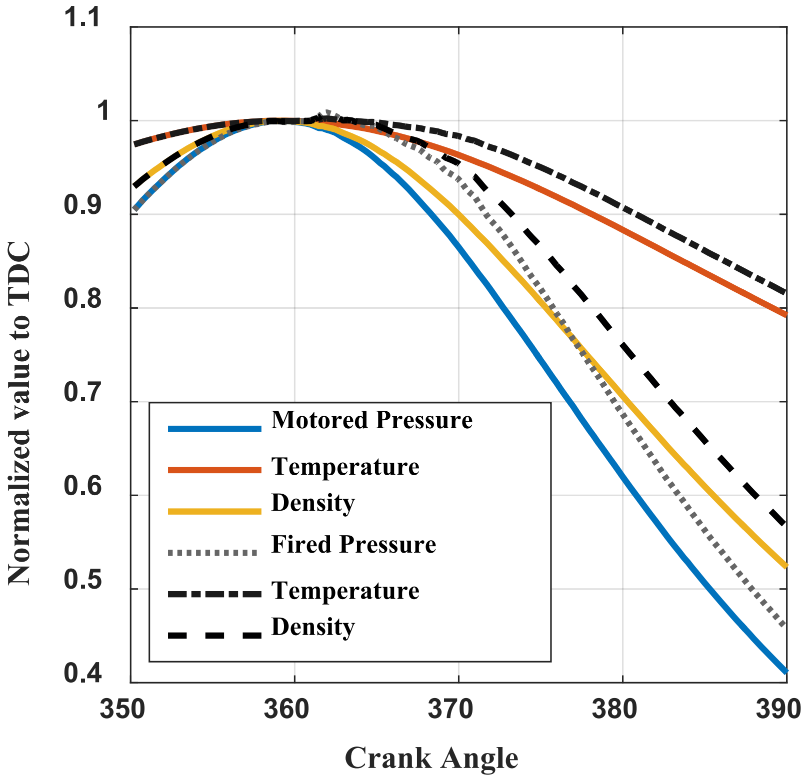


ECN target is 'Hole 3'

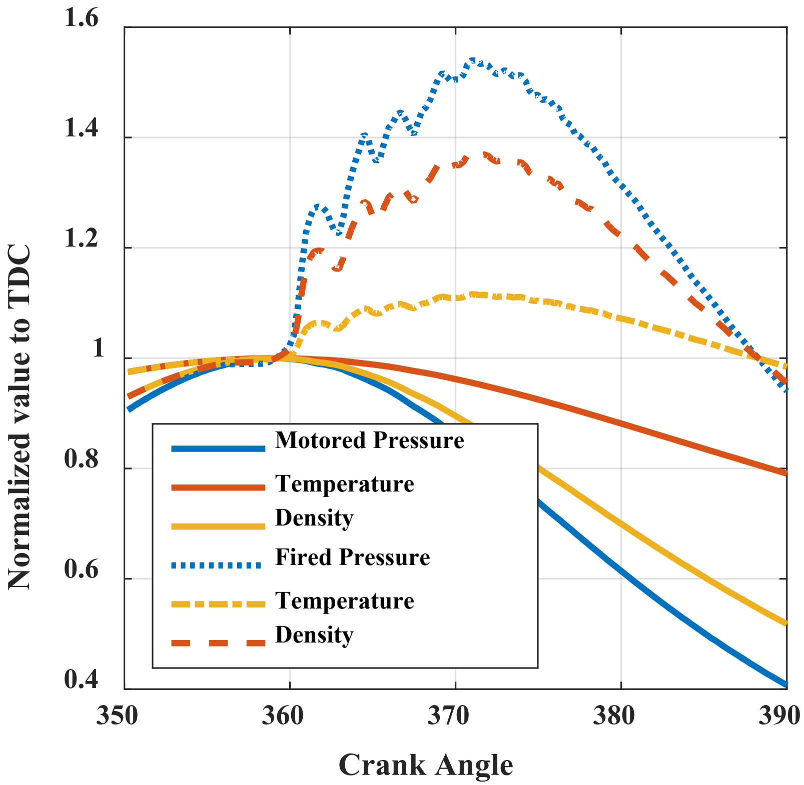
① ECN Spray B with 3x90-micron holes yields small combustion pressure rise in heavy-duty engine

- Thermodynamic conditions are nearly constant with combustion, similar to constant-volume vessels
- Standard multi-hole injectors yield large pressure rise, complicating comparisons between engines and const.-vol. vessels

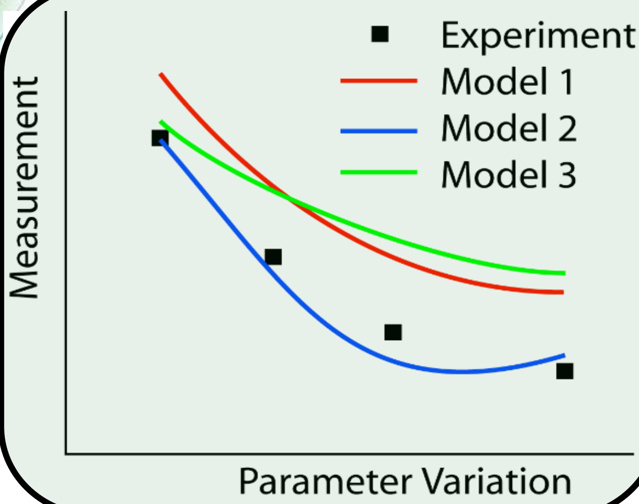
Three-hole Spray B



Seven-hole HD injector

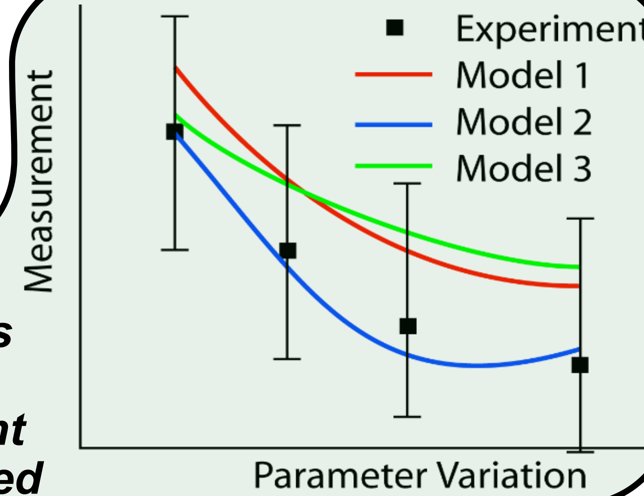


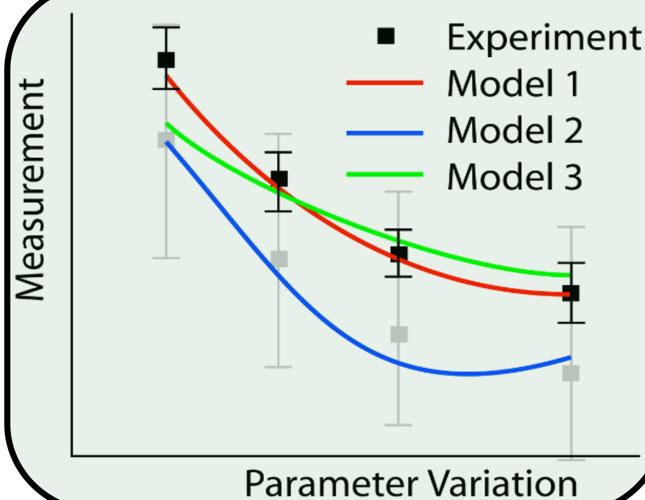
Spray B data include detailed uncertainty analysis: essential for justifying/directing modeling efforts



Without uncertainty analysis, Model 2 seems to perform best of the three.

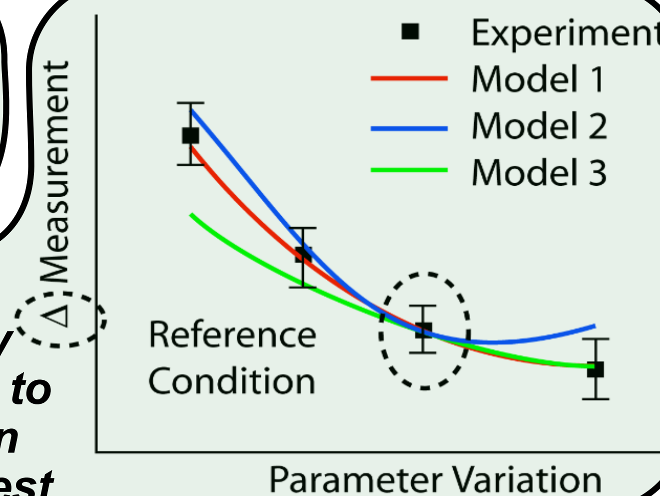
With uncertainty analysis, all models may be equivalent: further development of models unjustified





Option #1: Get better data with lower uncertainty – Model 1 is now best

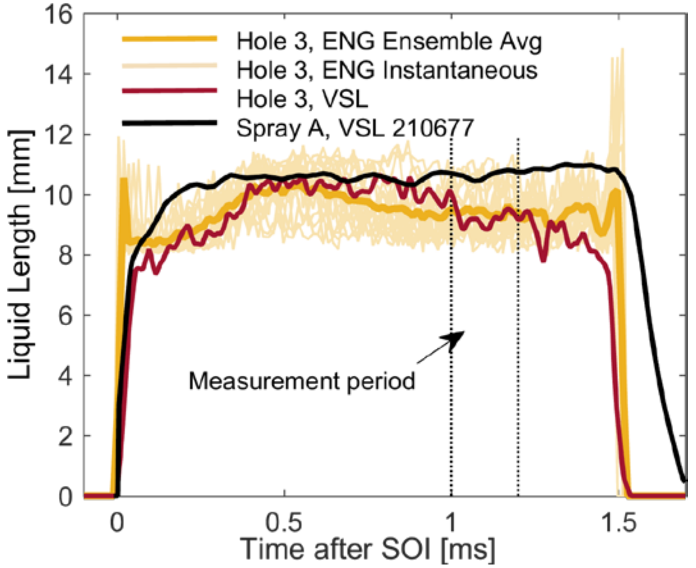
Option #2: remove bias uncertainty by using data relative to reference condition – Model 1 is still best

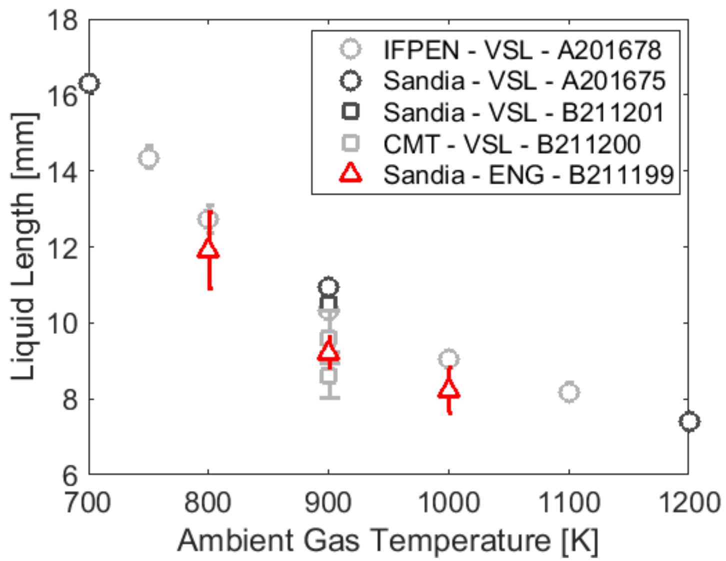


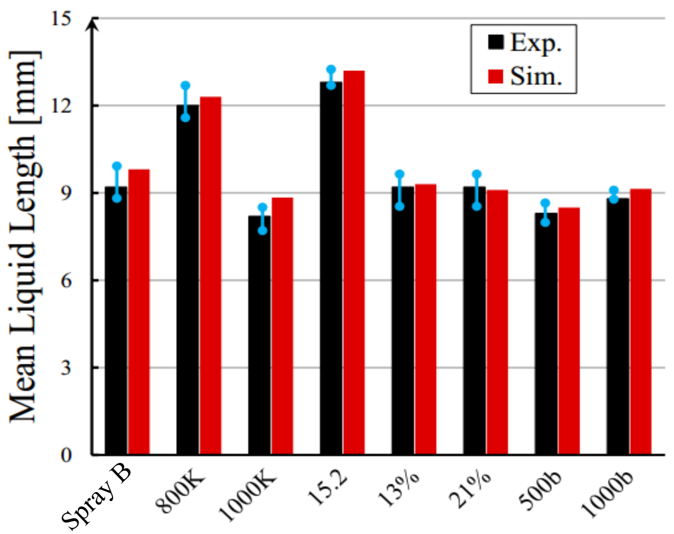
Uncertainty analysis details in back-up slides & SAE 2016-01-0743

Spray B LL shorter, more variable more than Spray A; similar to vessels within uncertainty

- Spray B shows more variation in the liquid length (LL) during injection, both in constant-volume vessels (VSL) and in the engine (ENG)
- During the relatively steady period, 1.0-1.2 ms after start of injection (SOI), VSL and ENG Spray B LL are similar & shorter than Spray A
- RANS LL simulations (Polytechnic University of Milan collaboration) show good agreement within exp. uncertainty (SAE 2016-01-0577)

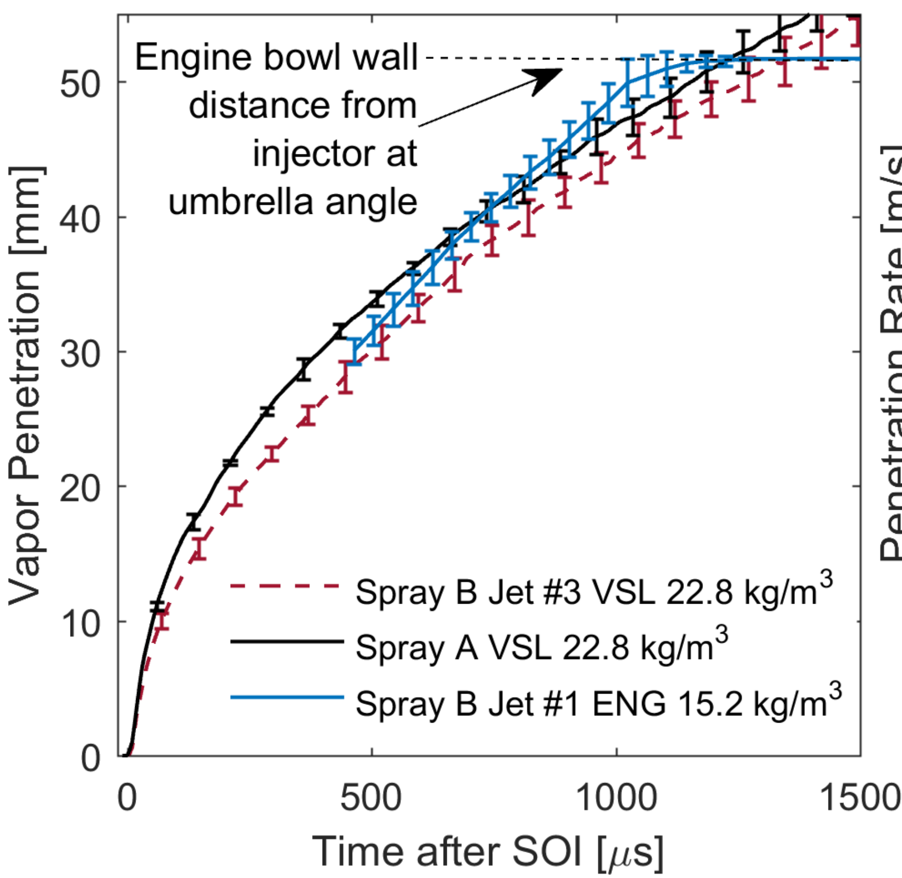


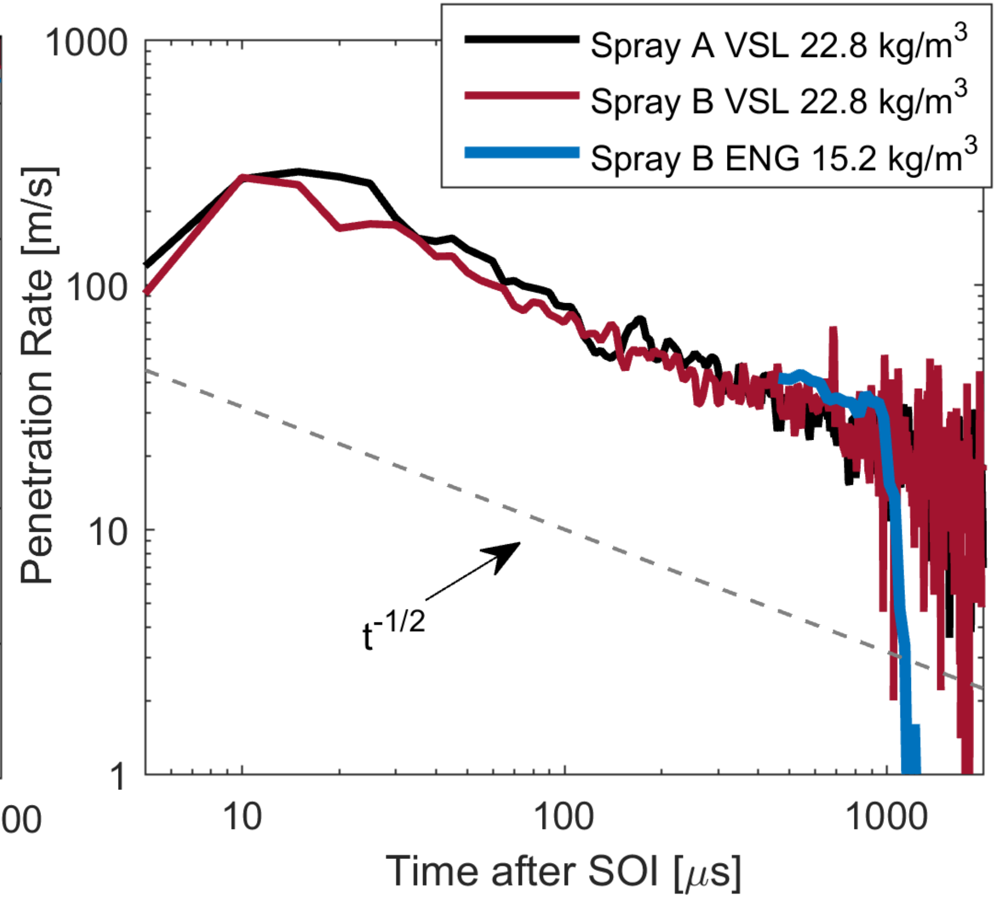




① Initial engine vapor-jet penetration is slower than expected, slows at wall, similar $t^{-1/2}$ dependence

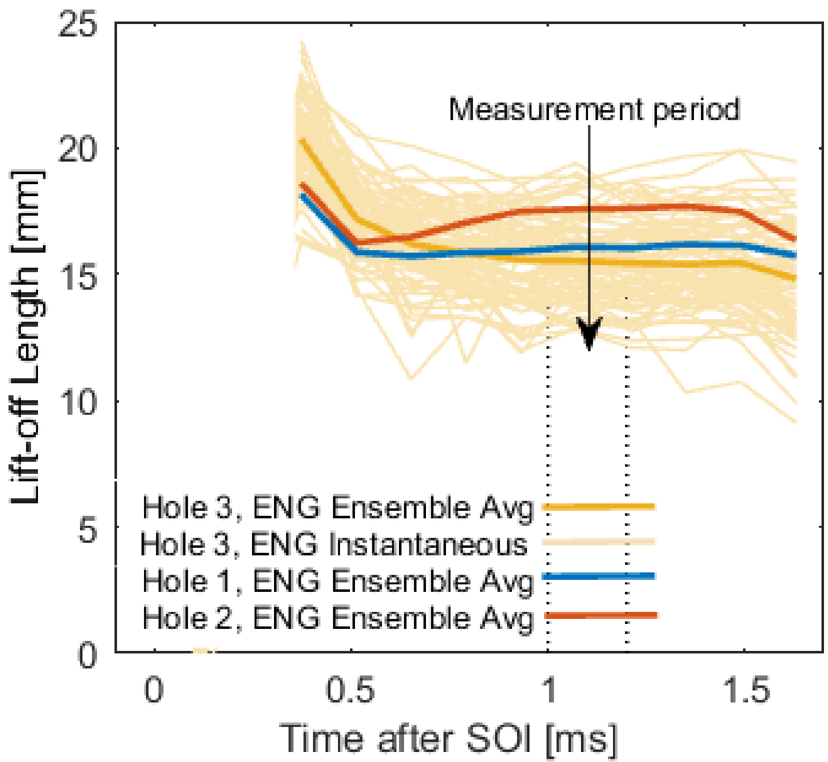
- ECN-standard non-reacting (0% O_2) conditions limited to 15.2 kg/m^3 ambient-gas density (100% N_2) in engine; available vessel data are 22.8kg/m^3 only
- Bowl-wall effect is apparent near 50 mm, and initial engine penetration is slower than expected – could be due to hole-to-hole variation, fuel system bias

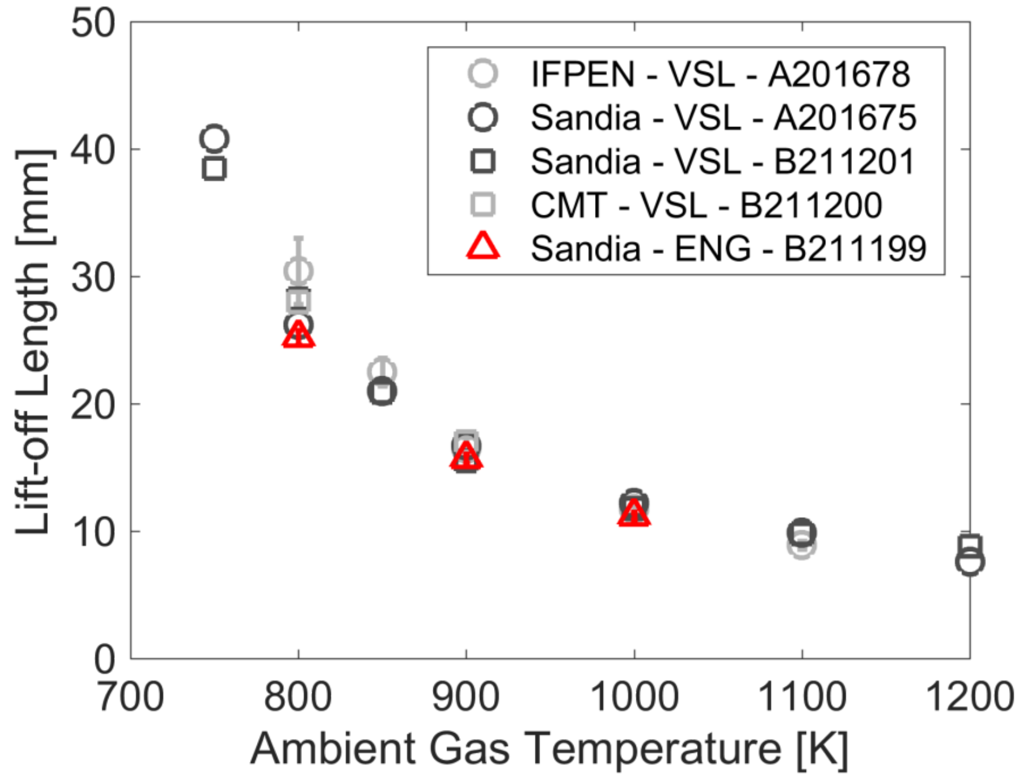




Spray B lift-off length in engine generally agrees with vessels within experimental uncertainty

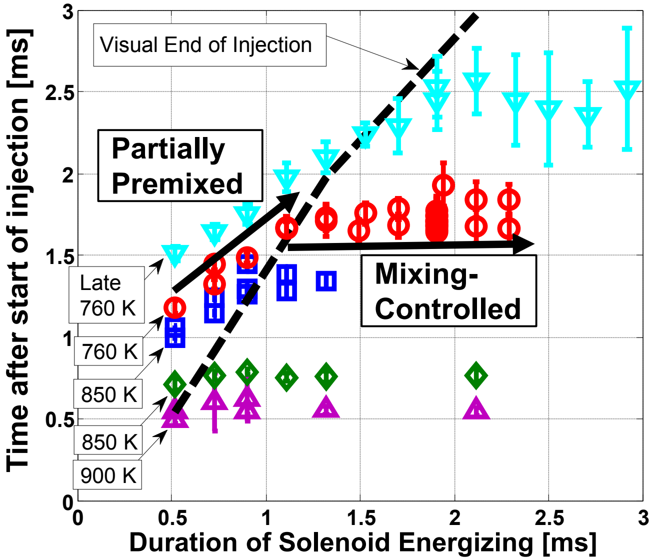
- Initial lift-off length is 3-5 mm longer than quasi-steady value, with some hole-to-hole variation in the ensemble-averaged quasi-steady length
- Ensemble-averaged liftoff lengths measured in the engine fall within experimental uncertainty with Spray B in the vessels, and are generally somewhat shorter than for Spray A

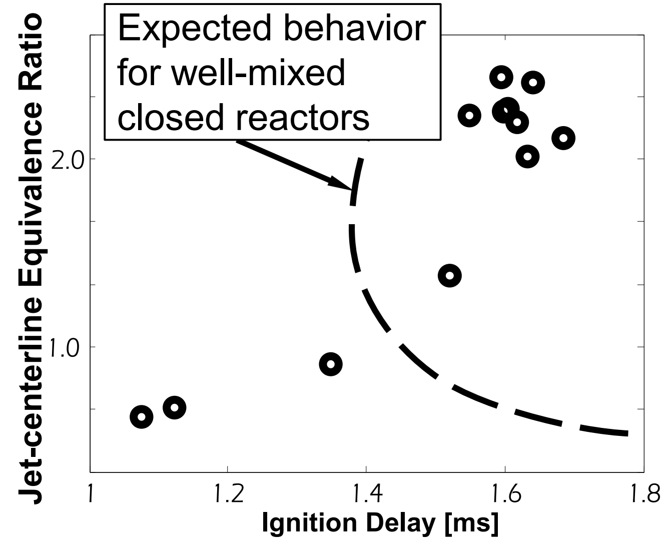




FY15 – Partial premixing: ID increases w/ injection duration; can't be explained by mixture fraction

- Simple ensemble-average 1-d mixing models good for penetration, mixing, & lean ignition
  - One apparent limitation: failure to predict delayed ignition with increasing injection duration for partially premixed conditions
- Mixing correlations: igniting mixtures are richer with longer injection duration & ID
  - Counter to well-mixed ignition kinetics expectations – **scalar dissipation effect?**





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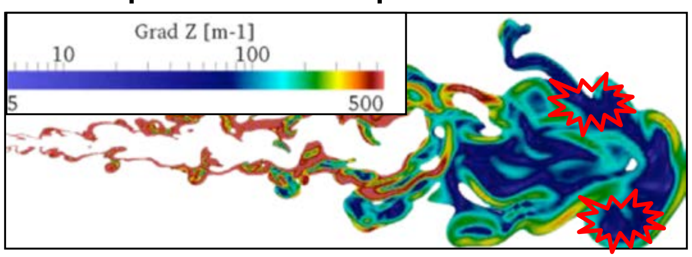
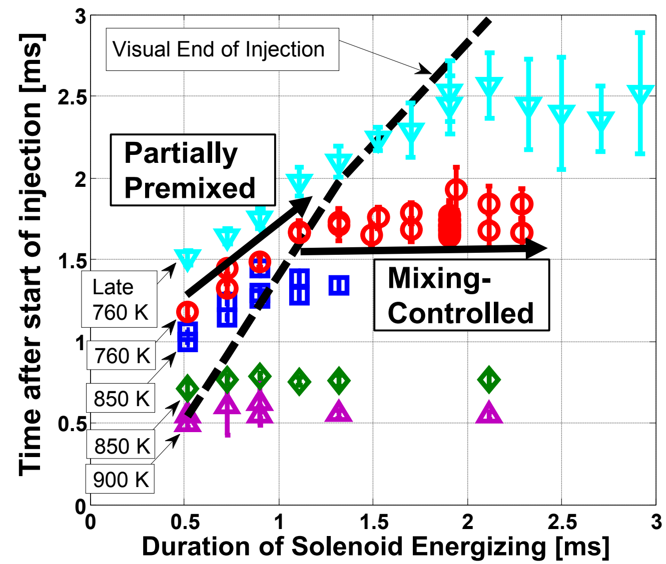
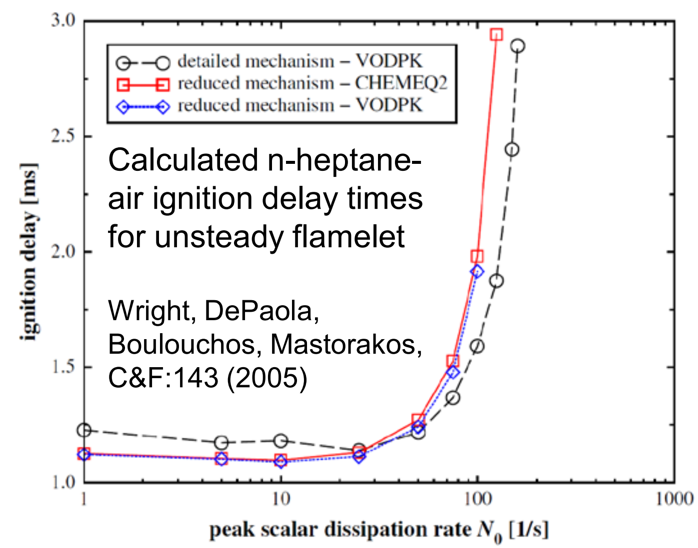
- Mixing correlations: igniting mixtures are richer with longer injection duration & ID
  - Counter to well-mixed ignition kinetics expectations – **scalar dissipation effect?**
- LES: low scalar dissipation at experimental ignition sites

(Oefelein, DOE Merit Review, 2014)



What is the role of scalar dissipation (gradients) with partial premixing? Can it be used to control ignition?

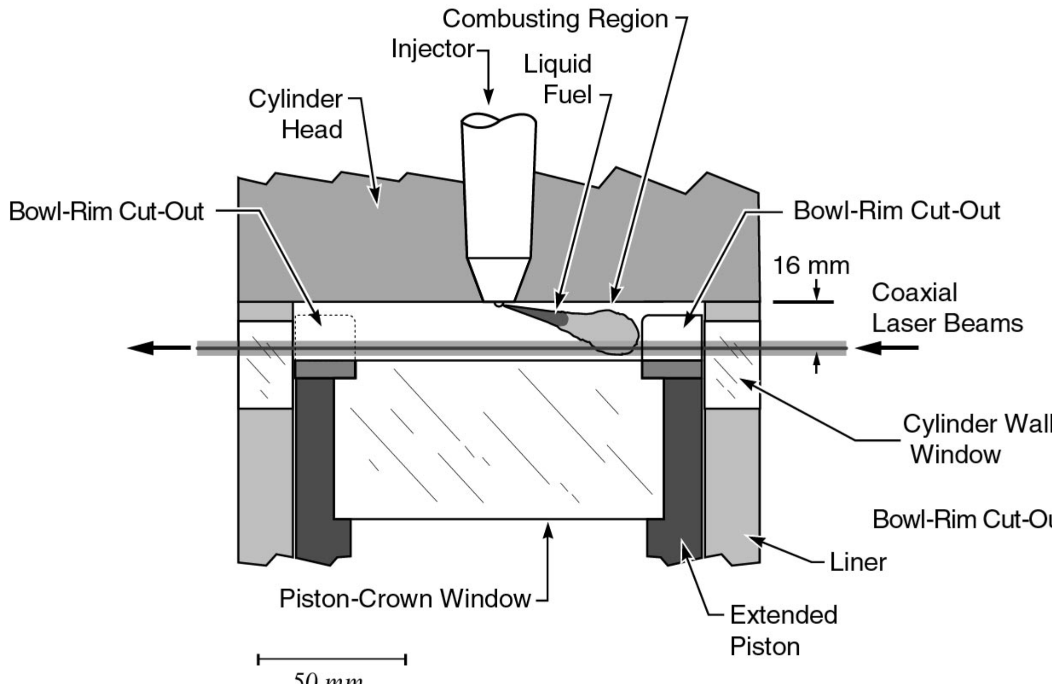




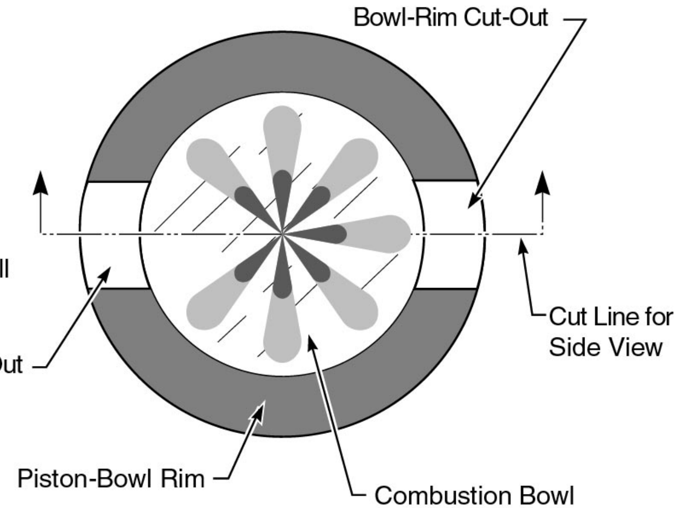
② Measuring scalar dissipation directly requires high resolution, but beam steering blurs images

- Can get scalar dissipation at low pressure from scalar imaging (e.g., fuel concentration), but need high resolution (<100 μm)

Can we achieve high enough resolution when the gradients to be measured cause strong beam steering that blurs images?



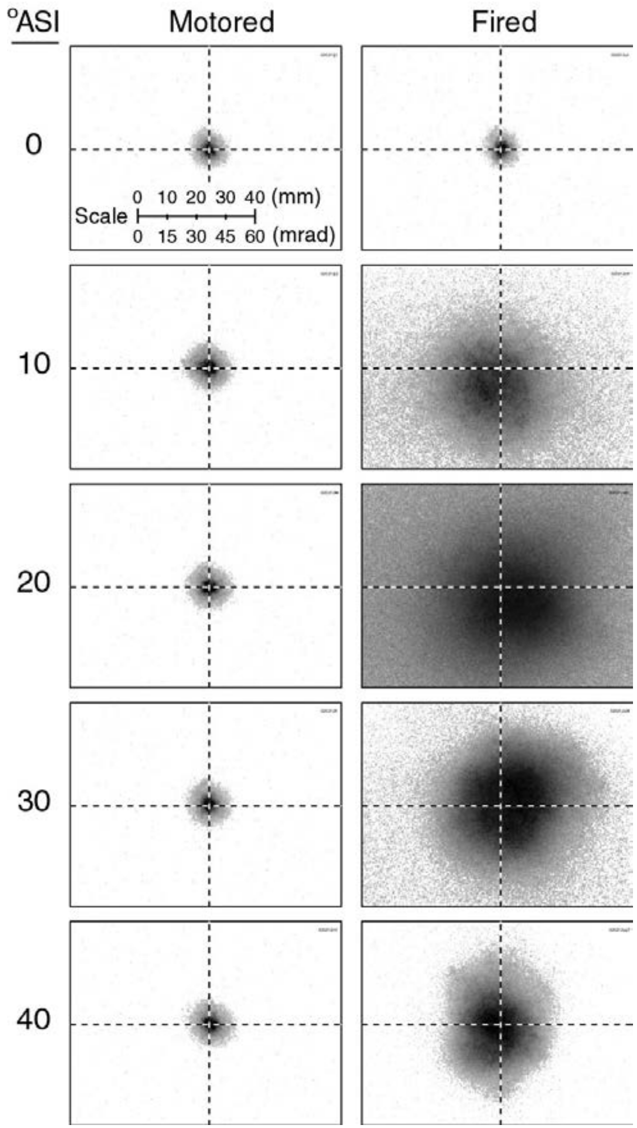
Side View of Combustion Chamber



Top View of Piston

② Previous work on laser extinction for measuring in-cylinder soot revealed strong beam steering

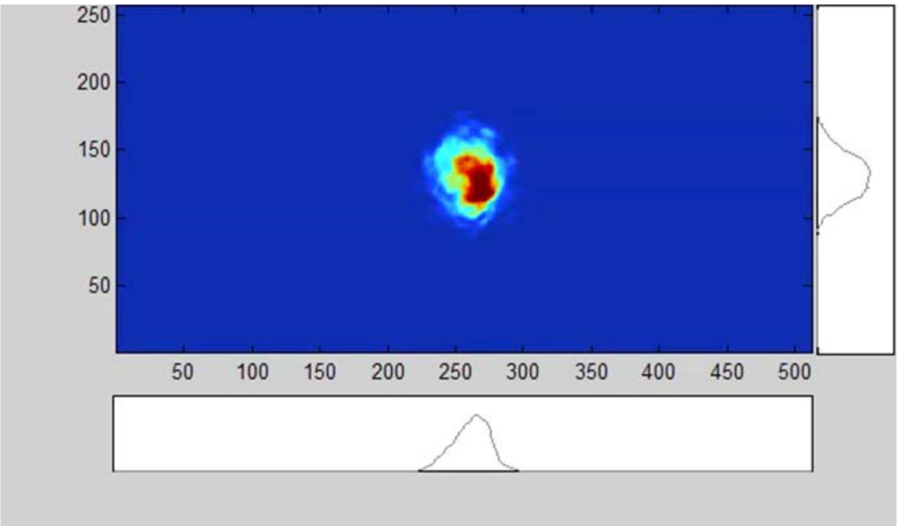
- Motored operation: diameter of laser beam passing through jet remains relatively constant
- Fired operation: index of refraction gradients widen the beam, with a full angle divergence of up to 60 mrad
  - (background level increases due to combustion luminosity)
- Laser beam steering would thicken a ~100μm sheet to 1.3mm – **too thick!**
- Signal steering could increase the 40μm image resolution to as much as 4mm across the cylinder radius – **too wide!**
- Conclusion: We can't use direct scalar / fuel-concentration imaging at engine pressures to measure scalar dissipation



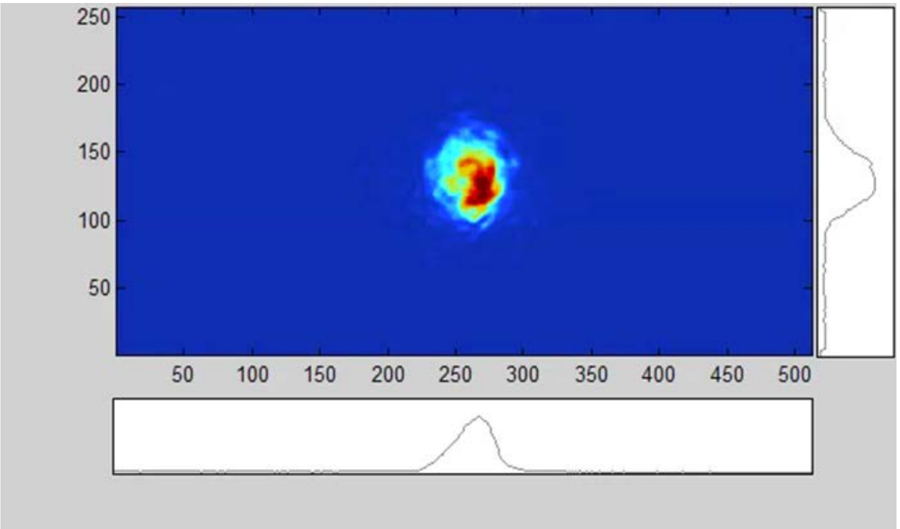
② If scalar dissipation increases beam spreading, then use it as an indirect line-of-sight measurement

- Solution: Turn the beam-steering "problem" into the solution to measure scalar dissipation – steered beam width depends on scalar dissipation, so beam width is a measure of scalar dissipation
- Proof of concept: HeNe laser beam passing laterally through diesel jet
  - No fuel injection: beam width increases slightly during compression
  - With fuel injection: larger beam width = higher scalar dissipation
- Future work: develop methodology to quantify line-of-sight integrated scalar dissipation from beam width measurements

No Fuel Injection



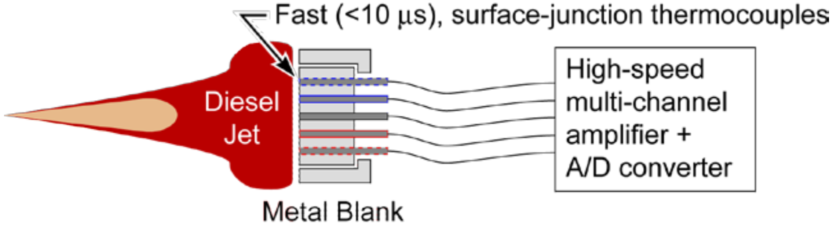
With Fuel Injection

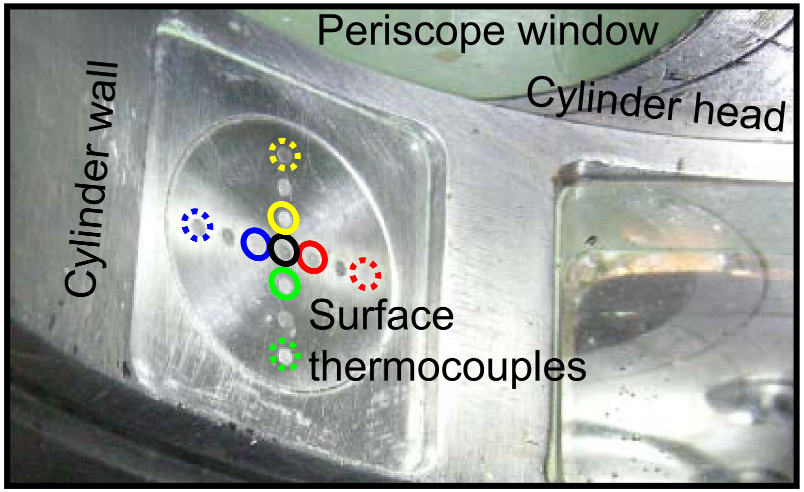


FY15: Two new heat-transfer diagnostics: Conventional thermocouple and IR thermometry

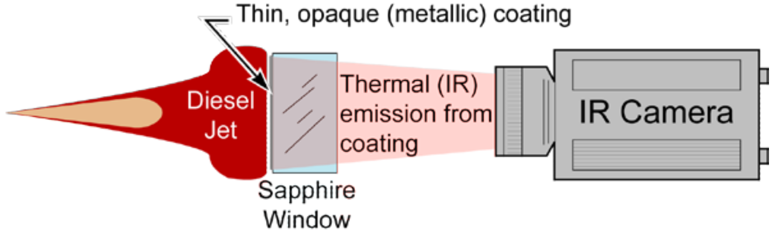
Conventional Thermocouple	IR Thermometry
Collab. w/ Terry Hendricks, Sandia NM	Collab. w/ Marcis Jansons, Wayne State

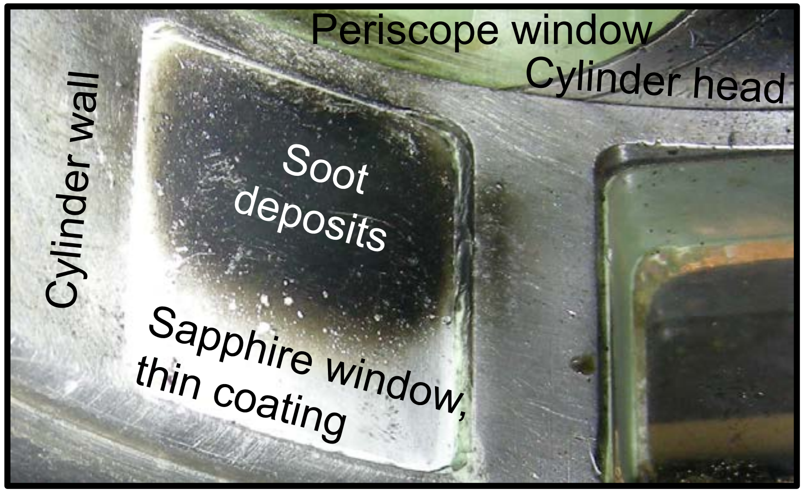
- Surface-junction thermocouple array with fast (10 μs) time response provide multiple point measurements of temperature & heat transfer





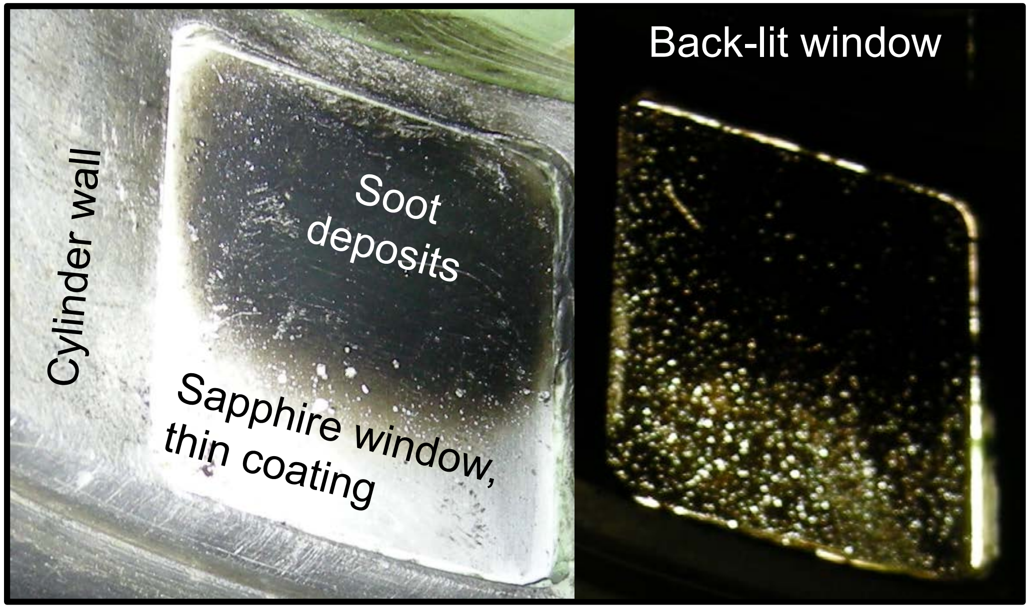
- Thin, opaque (metallic) coating on combustion side of window, IR camera views surface through window for 2-D temperature & heat transfer





Update: IR thermometry data has sufficient signal, but pinholes in coating; identified alternative

- Initial IR imaging: signal is strong even with fast exposure (10 μs)
  - Good S/N even before jet impingement on the window
- Many pinholes in coating transmit IR emission from combustion

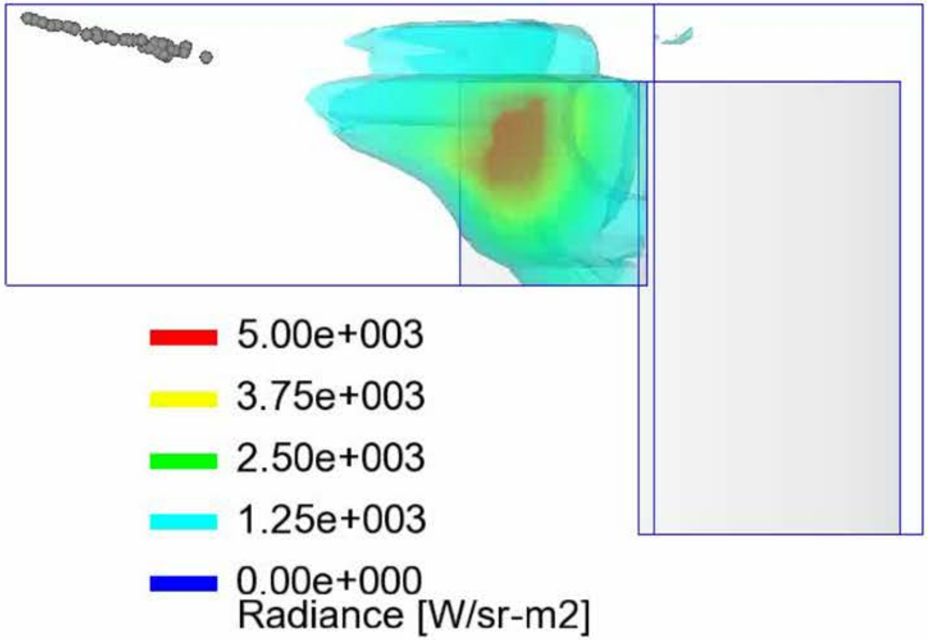


- After much development work in collaboration with Wayne State University on various coating options, a commercial metal oxide black coating with broadband emissivity exceeding 95% has been identified
  - Windows are currently being coated and will be available for testing in FY16/17
- Future work: evaluate/characterize new coating & use measurements to understand how in-cylinder flow/combustion affects heat transfer and fuel efficiency

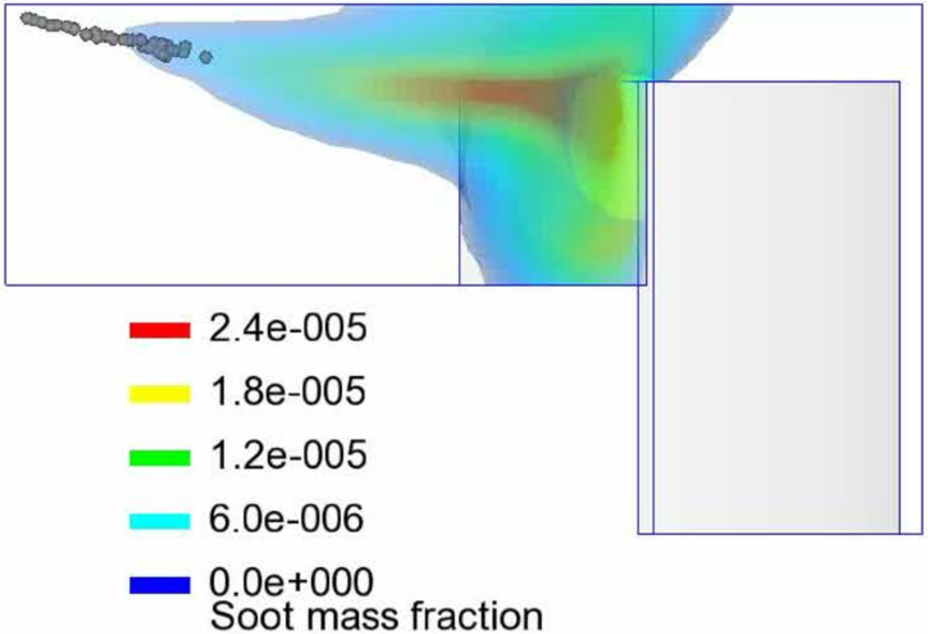
④ UW: Can widely-used soot luminosity imaging be useful for validating CFD-model soot predictions?

- Even with laser diagnostics, quantitative experimental in-cylinder soot data for model validation are difficult to acquire and/or only available for limited regions
- Experimental soot luminosity data are easily acquired, but are well known to be strongly biased to hot soot, i.e., soot luminosity ≠ soot mass fraction
- Can we use CFD model predictions to develop general guidelines for converting soot luminosity distributions to in-cylinder soot mass distributions?

<u>Left: CFD-Predicted Soot Luminosity</u>



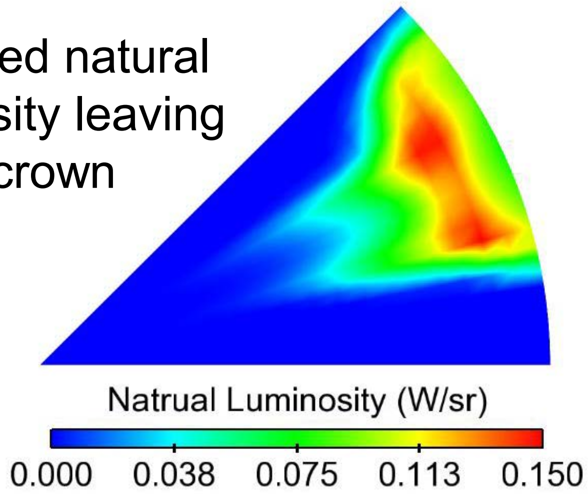
<u>Right: CFD-Predicted Soot Mass Fraction</u>



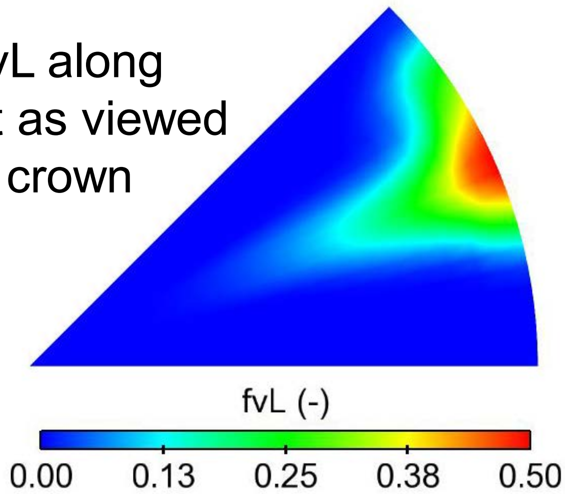
CFD soot LOS model converts soot mass to luminosity to compare with experimental imaging

- CFD soot line-of-sight (LOS) model:
    - Calculates cell-by-cell radiant emission from soot
    - Accounts for absorption/emission by soot in cells along the camera LOS
    - Corrects for high-speed camera spectral sensitivity
- CFD predictions quantify how LOS-integrated soot mass (product of volume-fraction and path-length, fvL, on left) relates to the luminosity signal (on right)
- CFD luminosity prediction also allows direct comparison to experimental soot luminosity images for model validation

Predicted natural luminosity leaving piston crown



Predicted fvL along line-of-sight as viewed from piston crown

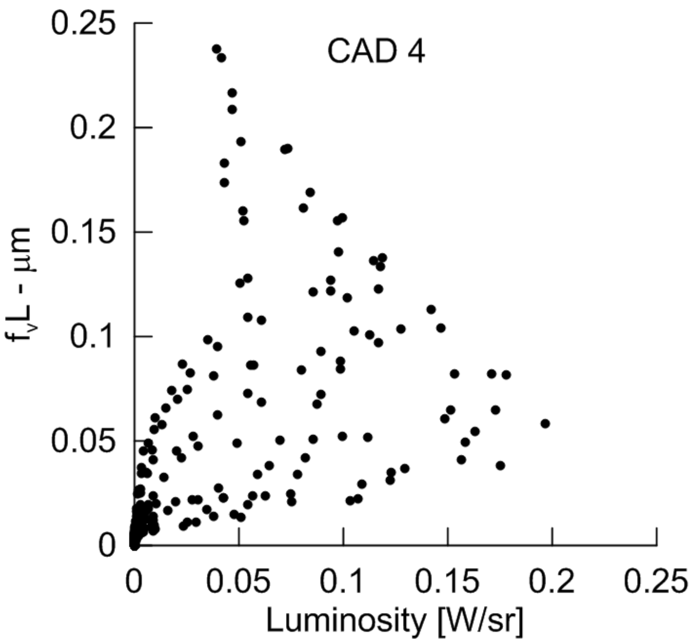


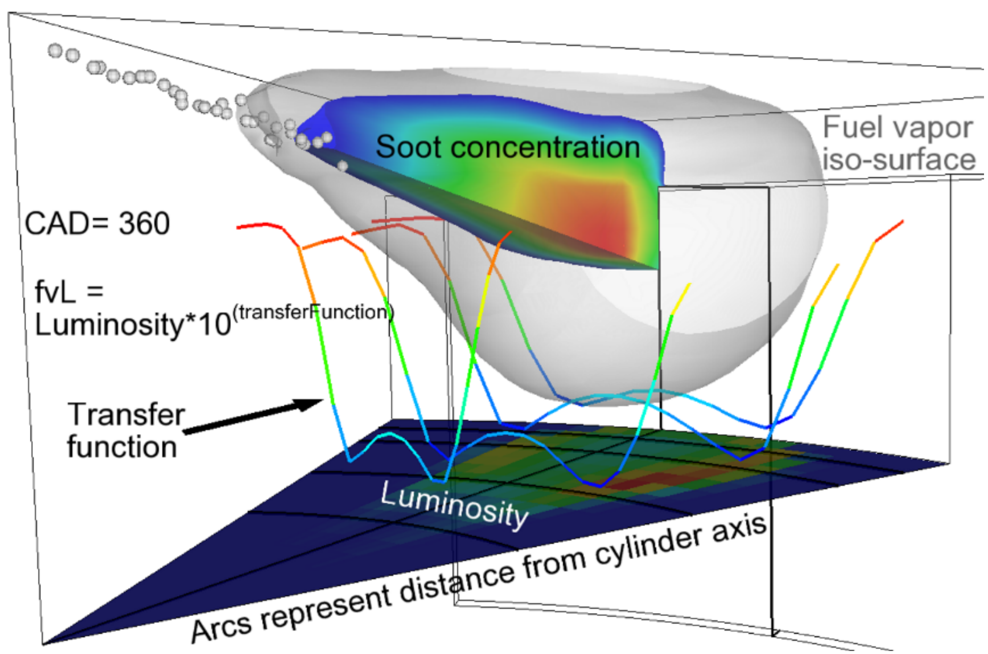
④ In addition to using luminosity for model validation, "omega" transfer function converts luminosity to fvL

- CFD predictions show wide scatter between soot fvL and luminosity throughout domain
  - No universal scaling factor to convert luminosity to fvL, but ...
- ... transfer function (TF) of the form

  $fvL = Luminosity * 10^{TF}$

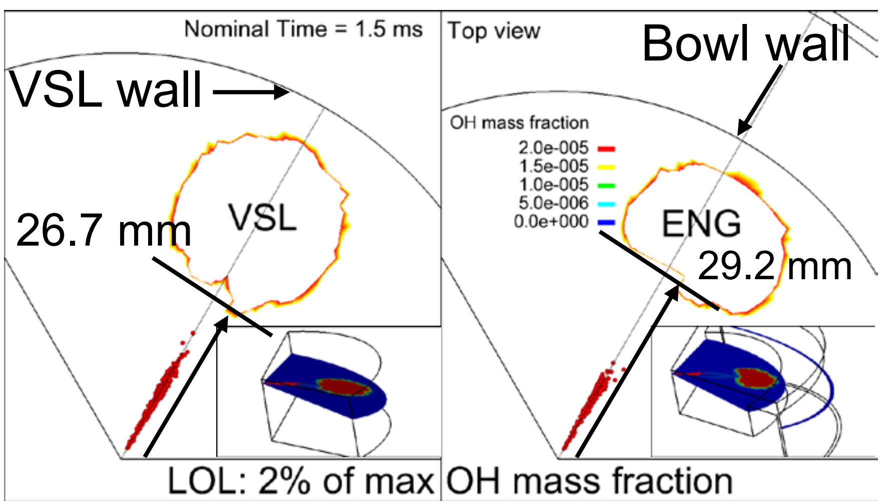
  has characteristic "omega" shape
  - Low at hot jet periphery, higher at cool center and mixed products
- Transfer function provides guidance to convert expt. luminosity images to fvL

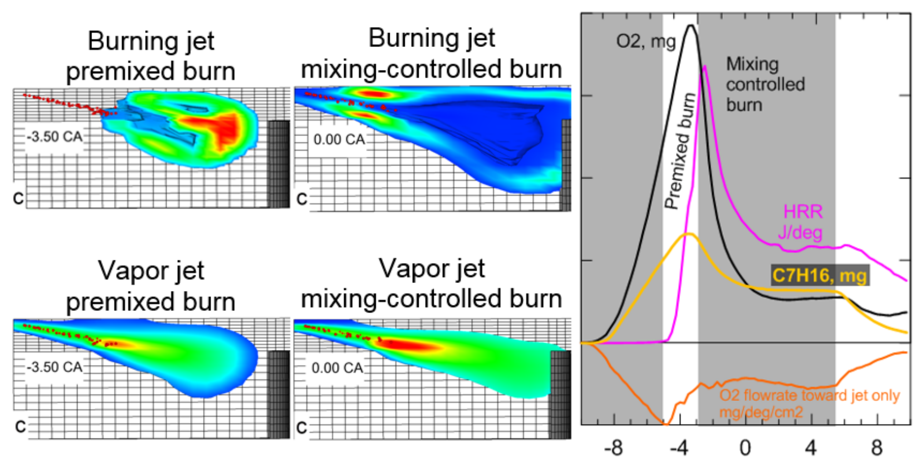




Other UW: Spray B CFD engine/vessel comparisons, In-depth CFD post-processing for jet mixing insight

- Kiva Spray B modeling shows compares engine (ENG) & constant-volume vessel (VSL)
  - Similar liquid length trend, ignition delay, 900K lift-off length, vapor-fuel penetration
  - Different liquid length absolute value, pressure rise (reacting), and 800K lift-off length
- CFD post-processing tools developed to gain insight into mixing processes during injection
  - Premixed burn reduces **O_2 flow toward jet** (~entrainment)
  - **O_2** & **fuel** within jet boundary are steady during mixing-controlled combustion, limiting **HRR** to nearly constant level



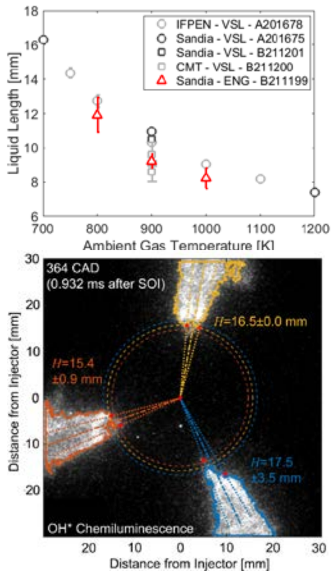


Remaining Barriers/Future Plans: Multi-injection conceptual model, heat-transfer, improve models

- Continue building a conceptual-model understanding of multiple-injection processes for both conventional diesel and LTC
  - Multi-injection schedules (pilot, post, split) deployed by industry
  - Identify mechanisms and critical requirements (injector rate-shaping, dwell, duration, etc.) to improve emissions and efficiency
  - Quantify the role of scalar dissipation in ignition/combustion and pollutant-formation/destruction processes
- Determine how combustion design affects heat transfer and efficiency
  - Measure spatial and temporal evolution of heat transfer across range of combustion modes and in-cylinder geometries; correlate to progression of in-cylinder combustion processes
- Gain fundamental insight from both experiments and models
  - Continue to refine 3-D analysis tools and apply them to end-of-injection mixing/ignition processes, multiple injections, heat transfer

Heavy-Duty Combustion and Modeling Summary

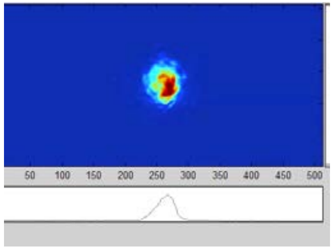
1



(SNL) New engine in-cylinder Spray B liquid length, vapor penetration, ignition delay, and lift-off generally agree well with constant-volume vessel data; slower than expected vapor penetration could be due to hole-to-hole variation or fuel system bias; detailed uncertainty analysis, including sensitivity analysis relative to reference condition to reduce uncertainty, aids model validation

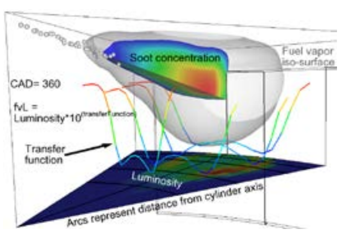
2

3



(SNL) Progress on development of laser dispersion diagnostics for quantitative in-cylinder scalar dissipation measurement and development of robust coatings for IR heat transfer imaging diagnostics

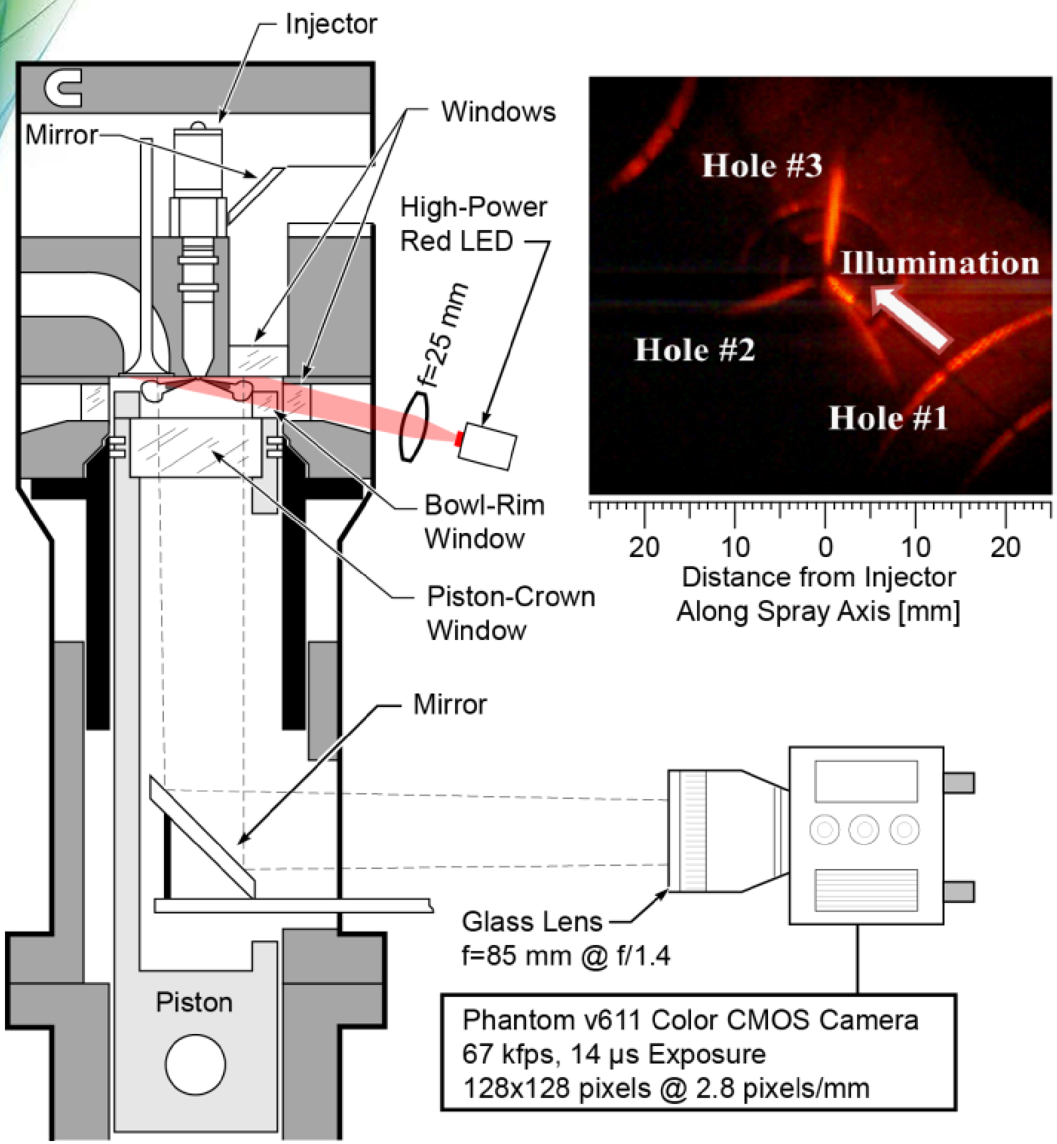
4



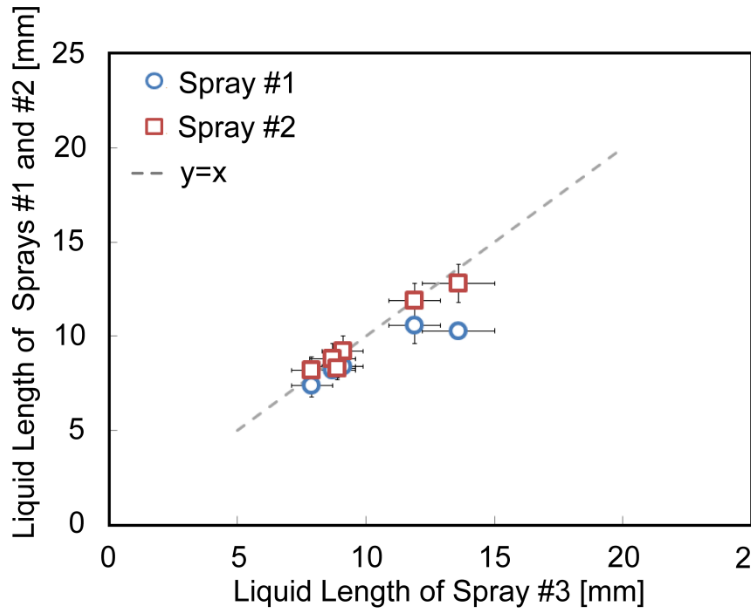
(UW) Developed new insight on validation of soot models by comparing predicted and measured soot luminosity, including transfer function; also progress on Spray B and post-injection modeling

Technical Back-Up Slides

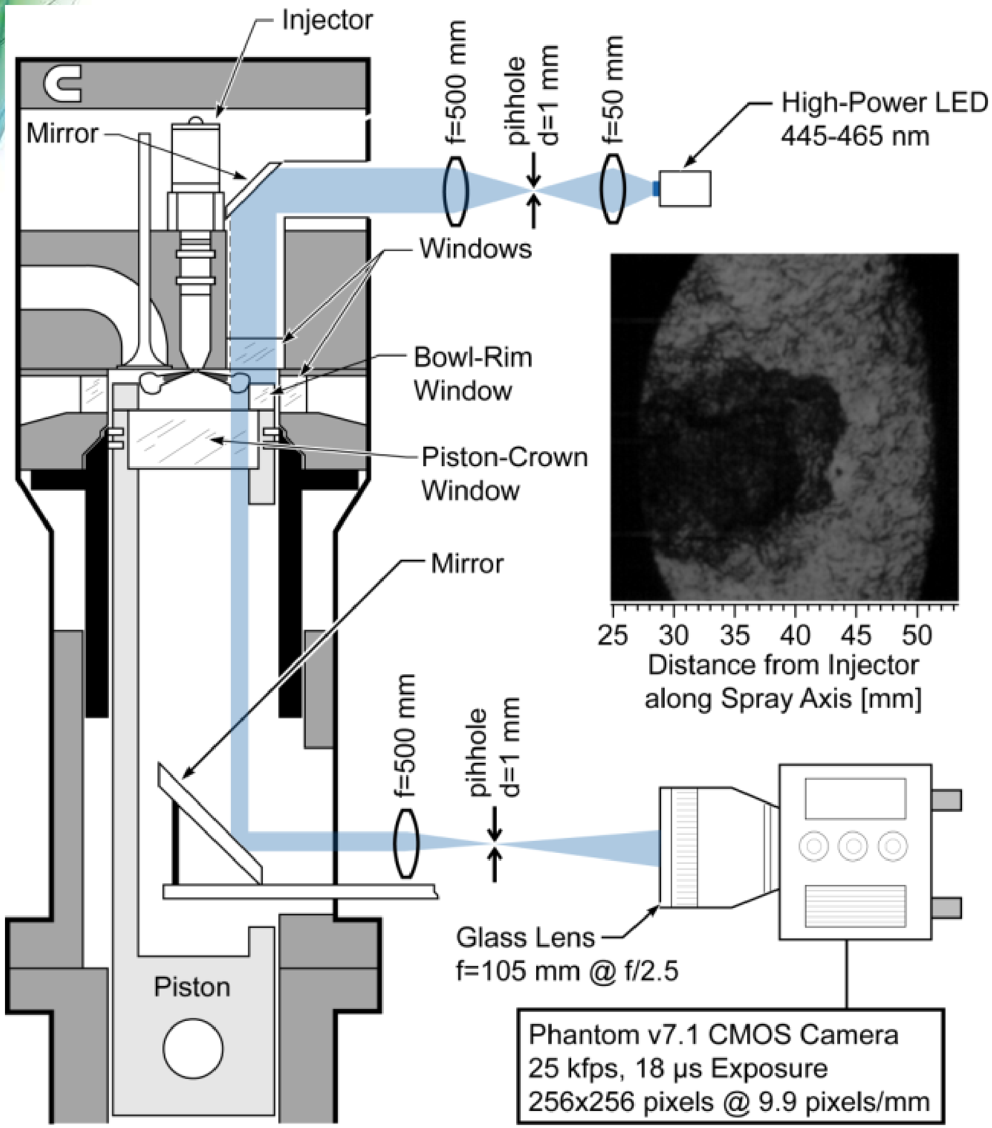
① Liquid length measured by Mie-scatter imaging with high-speed LED illumination

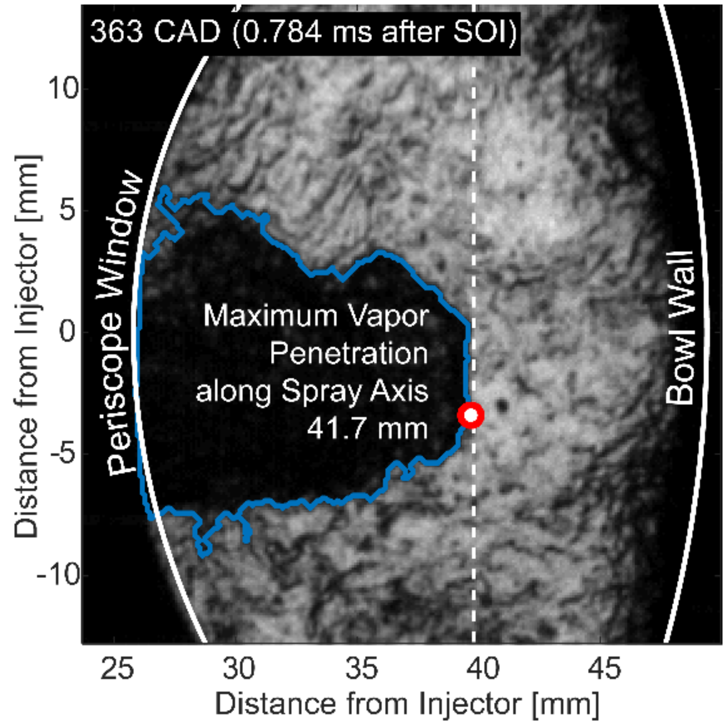


- Illumination targets spray from ECN hole #3
- All three sprays are imaged when possible for hole-to-hole comparisons



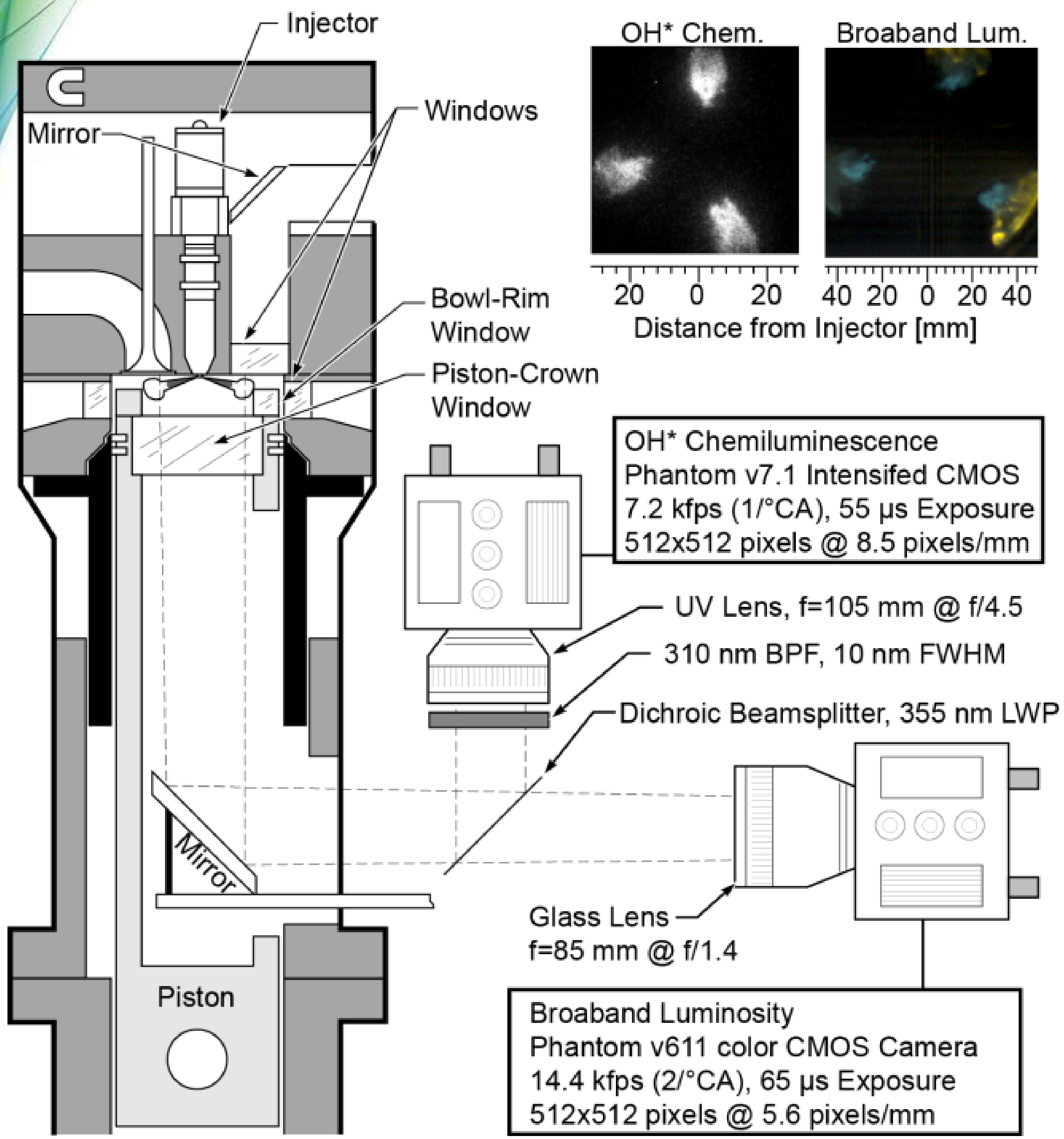
① ECN-standard schlieren imaging through exhaust-valve window for vapor penetration (26-50 mm)

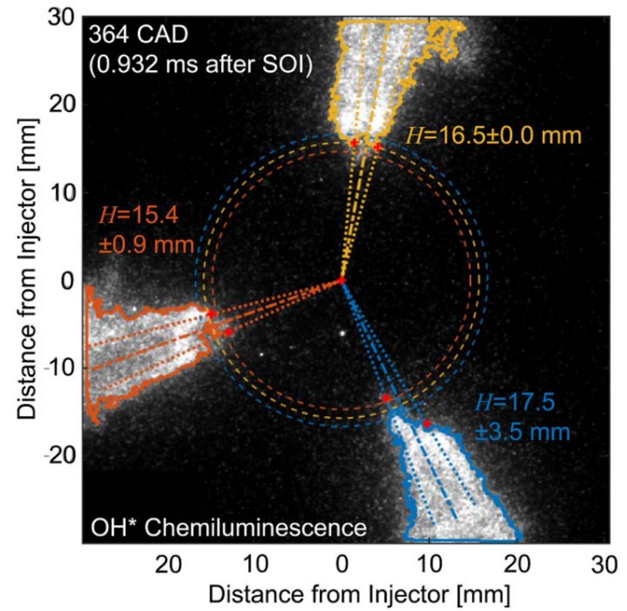


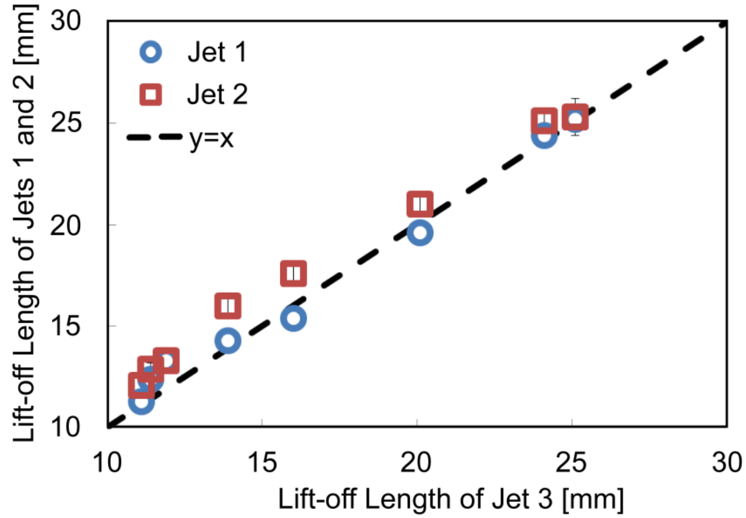


- Hole #3 is ECN standard, but only Hole #1 has pass-through optical access for schlieren in engine
- IR imaging of hot vapor-fuel emission (FY15 AMR) provides penetration for all three holes

① ECN-standard OH-chemiluminescence for lift-off length, some variation among holes







① Quantified uncertainty analysis provides method to reduce bias errors using reference/sensitivities

- "Bias" errors are systematic offsets that can be caused by boundary condition errors, differences among facilities/ techniques, calibration, etc.
  - Beyond precision errors ("scatter" in data), total uncertainty includes bias
- Bias errors are difficult to quantify, but can be reduced through sensitivity approach using reference state

$$S_i = \frac{log(f_i/f_0)}{log(x_i/x_0)}$$

$$U_{S_i} = 2({b_{S_i}}^2 + {s_{S_i}}^2)^{1/2}$$

$$A = \left(\frac{f_i}{S_i}\frac{\delta S_i}{\delta f_i}\right) = \frac{1}{log(f(x_i)/f(x_0))}$$

$$B = \left(\frac{f_0}{S_i}\frac{\delta S_i}{\delta f_0}\right) = \frac{-1}{log(f(x_i)/f(x_0))}$$

$$C = \left(\frac{x_i}{S_i}\frac{\delta S_i}{\delta x_i}\right) = \frac{-1}{log(x_i/x_0)}$$

$$D = \left(\frac{x_0}{S_i}\frac{\delta S_i}{\delta x_0}\right) = \frac{1}{log(x_i/x_0)}$$

$$\left(\frac{b_{S_i}}{S_i}\right)^2 = A^2\left(\frac{b_{f_i}}{f_i}\right)^2 + B^2\left(\frac{b_{f_0}}{f_0}\right)^2 + C^2\left(\frac{b_{x_i}}{x_i}\right)^2 + D^2\left(\frac{b_{x_0}}{x_0}\right)^2 + 2AB\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{f_0}}{f_0}\right) + 2AC\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{x_i}}{x_i}\right) + 2AD\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{x_0}}{x_0}\right) + 2BC\left(\frac{b_{f_0}}{f_0}\right)\left(\frac{b_{f_i}}{f_i}\right) + 2BD\left(\frac{b_{f_0}}{f_0}\right)\left(\frac{b_{x_0}}{x_0}\right) + 2CD\left(\frac{b_{x_i}}{x_i}\right)\left(\frac{b_{x_0}}{x_0}\right)$$

**** For details, see SAE 2016-01-0743***

Example: Liquid Length

$$LL = A_1 {d_o}^{A_2} {C_a}^{A_3} {\rho_a}^{A_4} {T_a}^{A_5} \Delta P^{A_6}$$

Variable Name	Mean	Bias	b_X/X
Liquid Length, f_0 [mm]	9.2	0.4	0.0435
Liquid Length, f_i [mm]	12.8	0.4	0.0312
Density target x_0, 22.8 kg/m^3	22.62	0.2	0.0088
Density target x_i, 15.2 kg/m^3	15.29	0.2	0.0132

Variable Name	evaluated	$\left(\frac{b_{S_i}}{S_i}\right)$
S_i	-0.84	...
$A^2\left(\frac{b_{f_i}}{f_i}\right)^2$	48.6	0.151
$B^2\left(\frac{b_{f_0}}{f_0}\right)^2$	48.6	0.102
$C^2\left(\frac{b_{x_i}}{x_i}\right)^2$	34.5	0.003
$D^2\left(\frac{b_{x_0}}{x_0}\right)^2$	34.5	0.006
Subtotal: Uncorrelated Uncertainty		±0.262
$2AB\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{f_0}}{f_0}\right)$	-80	-0.249
$2AC\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{x_i}}{x_i}\right)$	52.6	0.040
$2AD\left(\frac{b_{f_i}}{f_i}\right)\left(\frac{b_{x_0}}{x_0}\right)$	-52.6	-0.060
$2BC\left(\frac{b_{f_0}}{f_0}\right)\left(\frac{b_{f_i}}{f_i}\right)$	-52.6	-0.033
$2BD\left(\frac{b_{f_0}}{f_0}\right)\left(\frac{b_{x_0}}{x_0}\right)$	52.6	0.049
$2CD\left(\frac{b_{x_i}}{x_i}\right)\left(\frac{b_{x_0}}{x_0}\right)$	-34.5	0.008
Total: Correlated Uncertainty		±0.002

① ECN Run Conditions

Case name	SprayB	800K	1000K	15.2	13%	21%	500b	1000b
Temperature @ TDC [K]	900	**800**	**1000**	900	900	900	500	1000
Density @ TDC [kg/m^3]	22.8	22.8	22.8	**15.2**	22.8	22.8	22.8	22.8
Non-Reacting O_2 [% vol.]	7.5	7.5	7.5	0	-	-	-	-
Reacting O_2 [% vol.]	15	15	15	15	**13**	**21**	15	15
Injector rail pressure [bar]	1500	1500	1500	1500	1500	1500	**500**	**1000**
Temperature @ IVC [K]	380	340	454	400	392	396	397	390
Pressure @ IVC [bar]	2.25	2.01	2.61	1.54	2.27	2.26	2.28	2.28
Injected liquid mass [mg/cycle]	3.68	3.68	3.68	3.68	3.68	3.68	2.06	2.98
Engine speed [RPM]	1200							
Start of Solenoid Energizing [CAD]	355							
Start of Injection [CAD]	357.25							
Duration of Solenoid Energizing [^{o}CA], [μs]	5.86, 795							
Duration of Injection [^{o}CA], [μs]	11, 1500							