

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

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Sandia National Laboratories

FY 2015 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D/Combustion Research
11:00 – 11:30 AM, Tuesday, June 9, 2015

Sponsor: U.S. Dept. of Energy, Office of Vehicle Technologies

Program Manager: Leo Breton, Gurpreet Singh

ACE001

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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

Budget

- Project funded by DOE/VTP:
FY14-SNL/UW: \$710k/115k
FY15-SNL/UW: \$735k/99k

Barriers

From DOE VTP Multi-Year Program Plan 2011–2015:

- 2.3.A: Lack of fundamental knowledge of advanced engine combustion regimes
- 2.3.B: Lack of cost-effective emission control
- 2.3.C: Lack of modeling capability for combustion and emission control

Partners

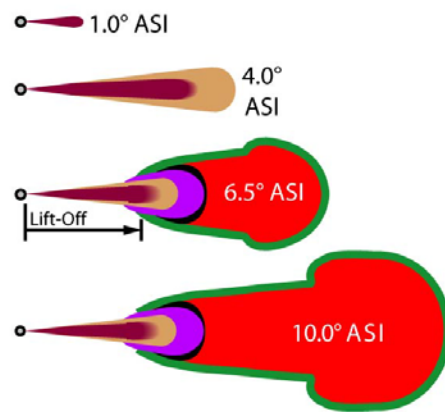
- University of Wisconsin, Delphi, Cummins, Convergent Science
- 15 industry partners in the AEC MOU
- Project lead: Sandia (Musculus)

Relevance/Objectives: HD In-Cylinder Combustion

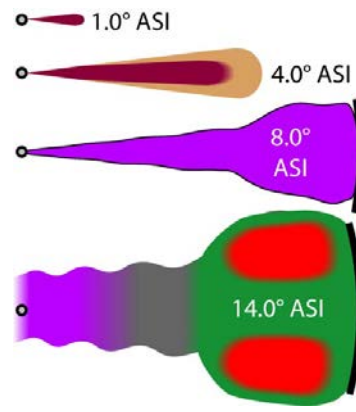
Long-Term Objective

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

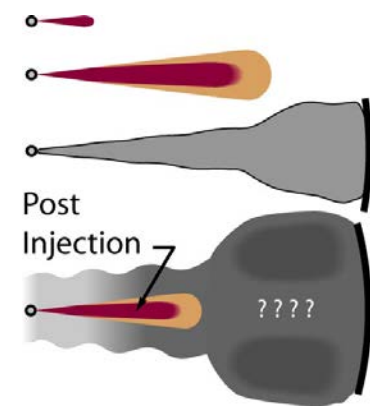
1997: Conventional Diesel
(Single Injection)



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

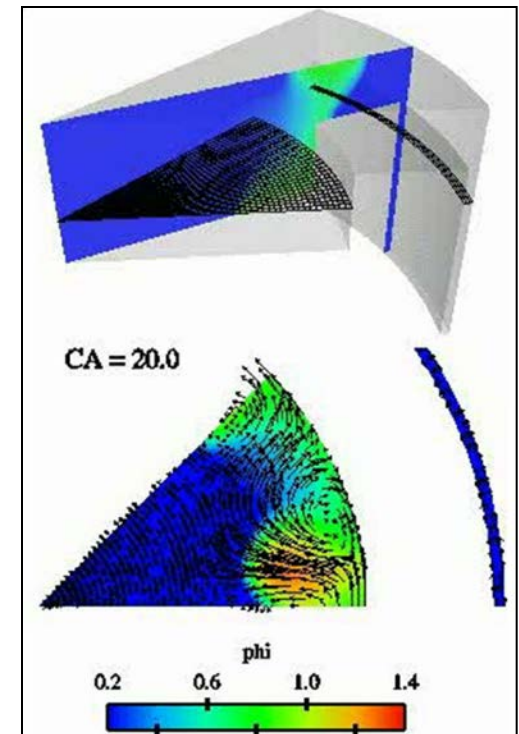
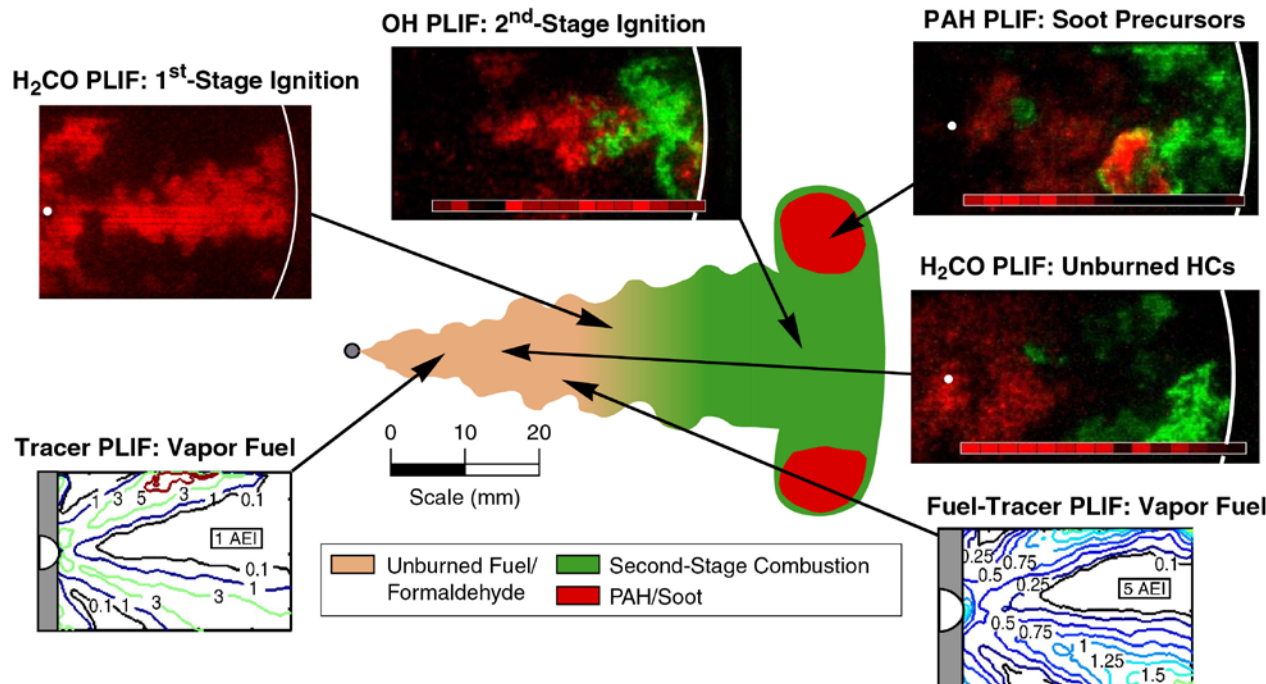
Develop the science base of in-cylinder spray, combustion, and pollutant-formation processes for both conventional diesel and LTC that industry needs to design and build cleaner, more efficient engines

Current Milestones/Objectives:

- ① SNL – Reveal fluid-mechanical processes of injection rate-shaping to control mixing
- ② SNL – Provide Spray B in-cylinder engine data for ECN
- ③ SNL – Develop/demonstrate in-cylinder surface heat transfer diagnostic capability
- ④ SNL – Improve computer-model simulation/analysis tools to complement experimental measurements

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 (e.g., LTC soot precursor modeling with Cummins/Convergent Science/UW)
- Industrial/University partnerships support laboratory activities
 - FY2015: Delphi, Cummins – continued injector support
 - FY2015: Wayne State University – IR diagnostic development



Technical Accomplishments & Progress (15 slides)

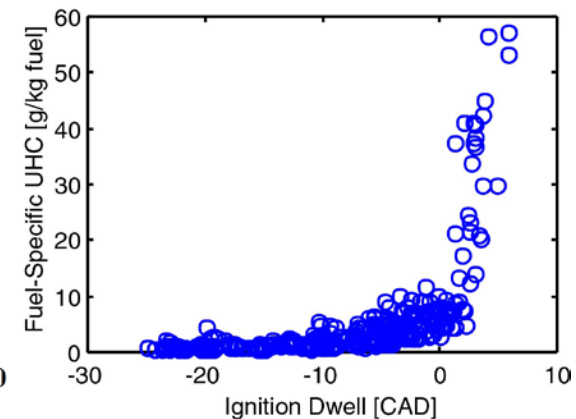
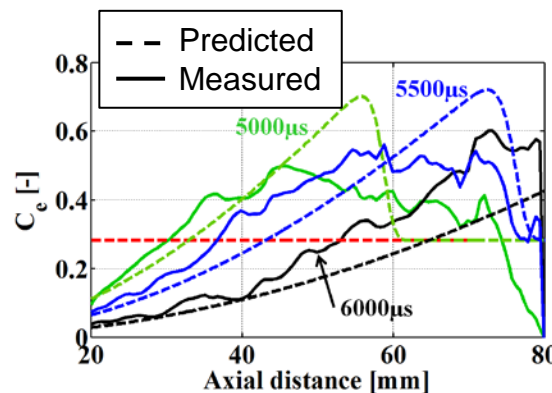
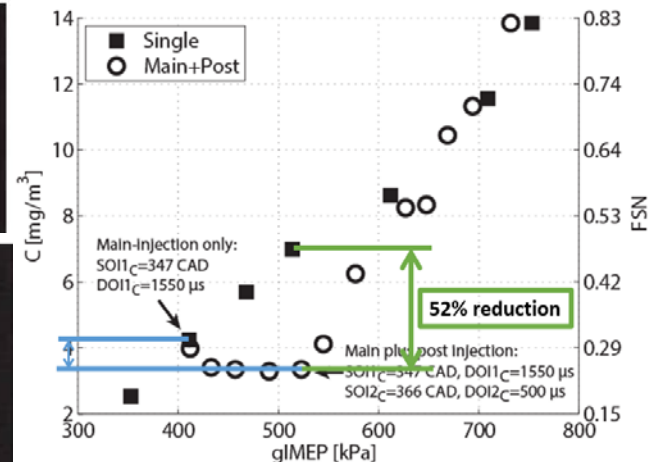
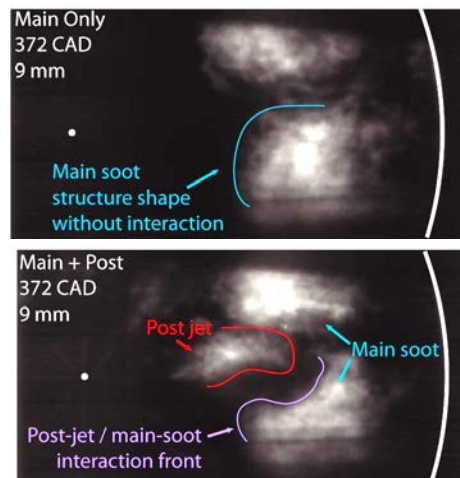
- Accomplishments for each of the four current milestones / objectives below are described in the following fifteen (15) slides

Current Milestones/Objectives:

- ① **SNL – Reveal fluid-mechanical processes of injection rate-shaping to control mixing**
- ② **SNL – Provide Spray B in-cylinder engine data for ECN**
- ③ **SNL – Develop/demonstrate in-cylinder surface heat transfer diagnostic capability**
- ④ **SNL – Improve computer-model simulation/analysis tools to complement experimental measurements**

Previous work on post- and single-injections point to importance of end-of-injection mixing

- FY13: Post-injections can reduce emissions & BSFC
- FY14: post-jet interacts with end-of-injection residual of main-injection jet
- ④ FY15: developing CFD analysis tools for insight into post-injection mechanisms
 - FY16: exp'ts to confirm
 - FY15: exp'ts on main inj.
- FY07: high UHC at long IDs for single (main) injections
 - Cause: over-mixing near injector
- FY14: PIV data confirms “entrainment wave” of increased mixing

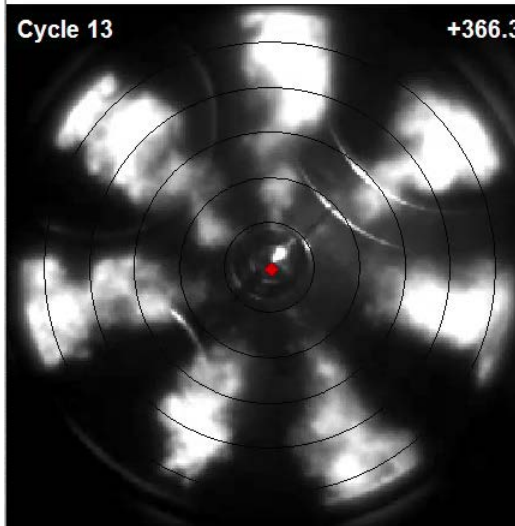
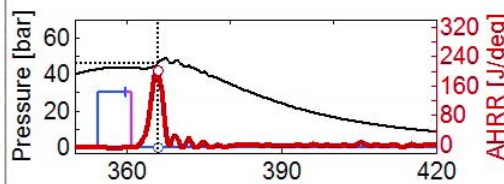


Post injections penetrate into residual mixing fields created by main injections; post-injection mechanisms depend on this residual field

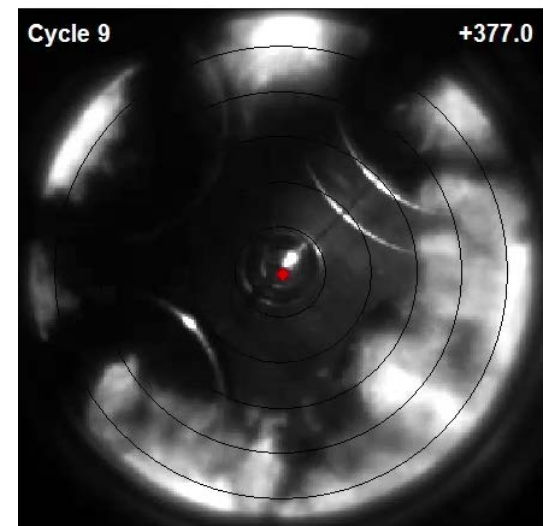
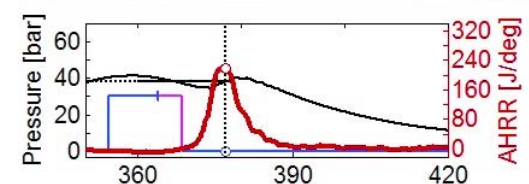
① Some conditions have gradual progression of ignition that allows higher loads at a given AHRR

- Enhanced premixing (PCI, PCCI, MK, HCCI, etc.) is interesting for reducing emissions and improving efficiency, but load is limited by peak heat-release rates (AHRR)
- Some conditions show gradual progression of ignition in the residual mixing field of the main injection, allowing higher loads at a given AHRR

800 K TDC, 1 bar gIMEP,
210 J/° peak AHRR



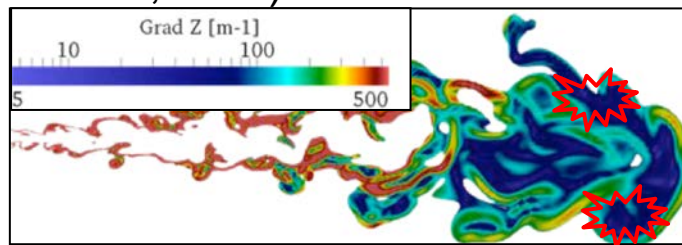
760 K TDC, 3.5 bar gIMEP,
220 J/° peak AHRR



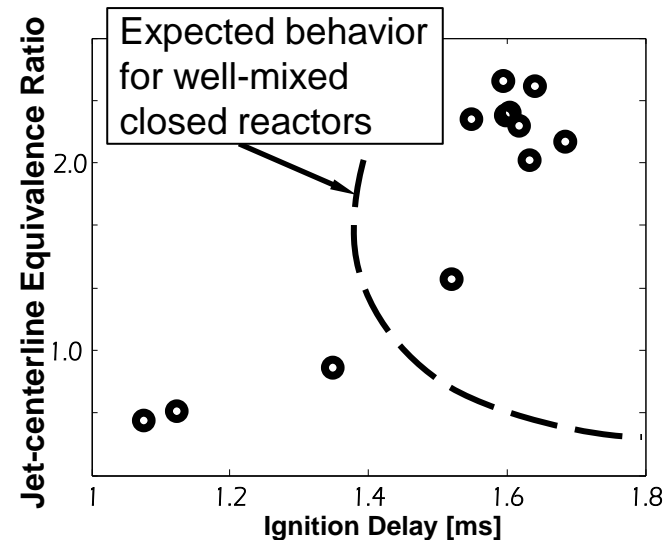
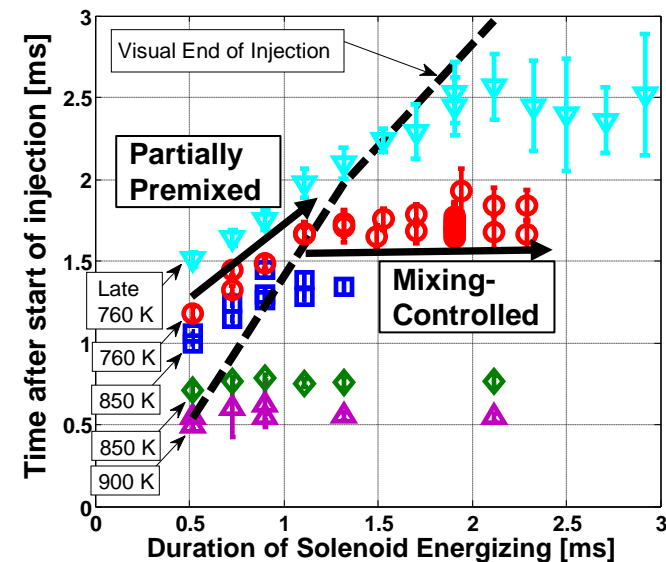
Can we tailor the mixing field created by the main injection, either for heat-release-rate control, or for better coupling with post injections?

① Partial premixing: ID increases with injection duration; can't be explained by mixture fraction

- At lower TDC temperature, ID is longer
 - For mixing controlled combustion, ignition delay is flat with injection duration
 - But, for partial premixing, increasing injection duration can delay ignition
- Ind. partner: 2nd inj. at ignition can delay too
- Mixing correlations: igniting mixtures are richer with longer injection duration & ID
 - Counter to well-mixed ignition kinetics expectations –scalar dissipation effect?
- Simulations (Oefelein, SNL): low scalar dissipation at experimental ignition sites (Skeen, SNL)



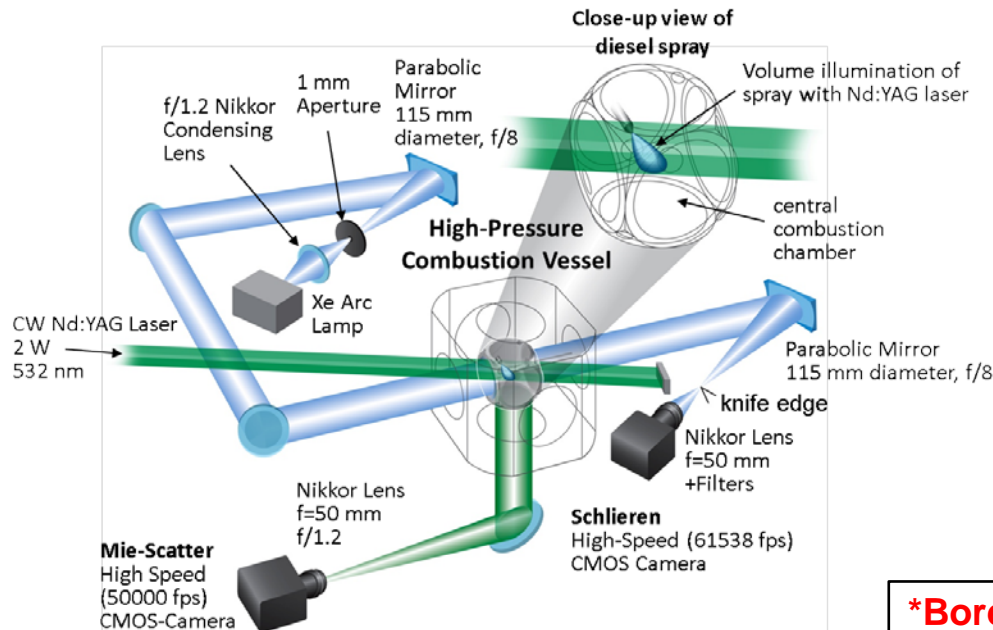
Future work: what is role of scalar dissipation with partial premixing? Can it be controlled for ignition/post-inj.?



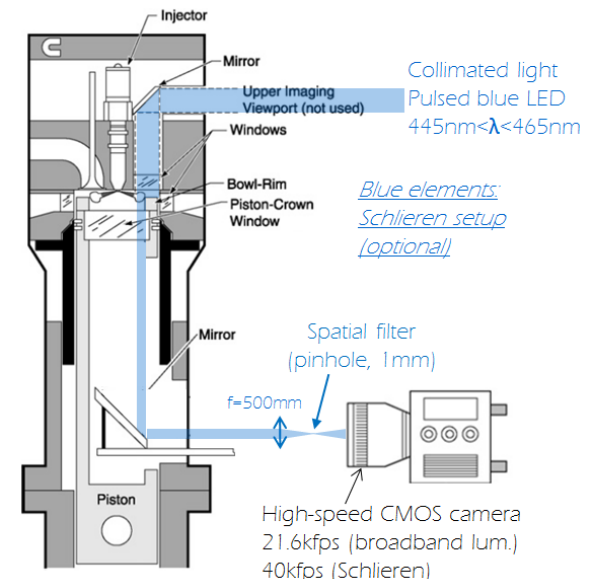
② Vapor penetration is of critical importance for ECN fuel-jet data, but requires extensive optical access

- Engine Combustion Network is a forum and database for collaboration on engine combustion
 - Initial ECN data: single-hole, constant-volume combustion vessels
 - Now adding data for multi-hole injectors and engines
 - First engines step: generate single-injection data; Next: multi-injection
- Vapor jet penetration is a critical measurement, but standard schlieren techniques require pass-through optical access

Constant volume vessel: Full pass-through optical access



Optical engine: Partial pass-through

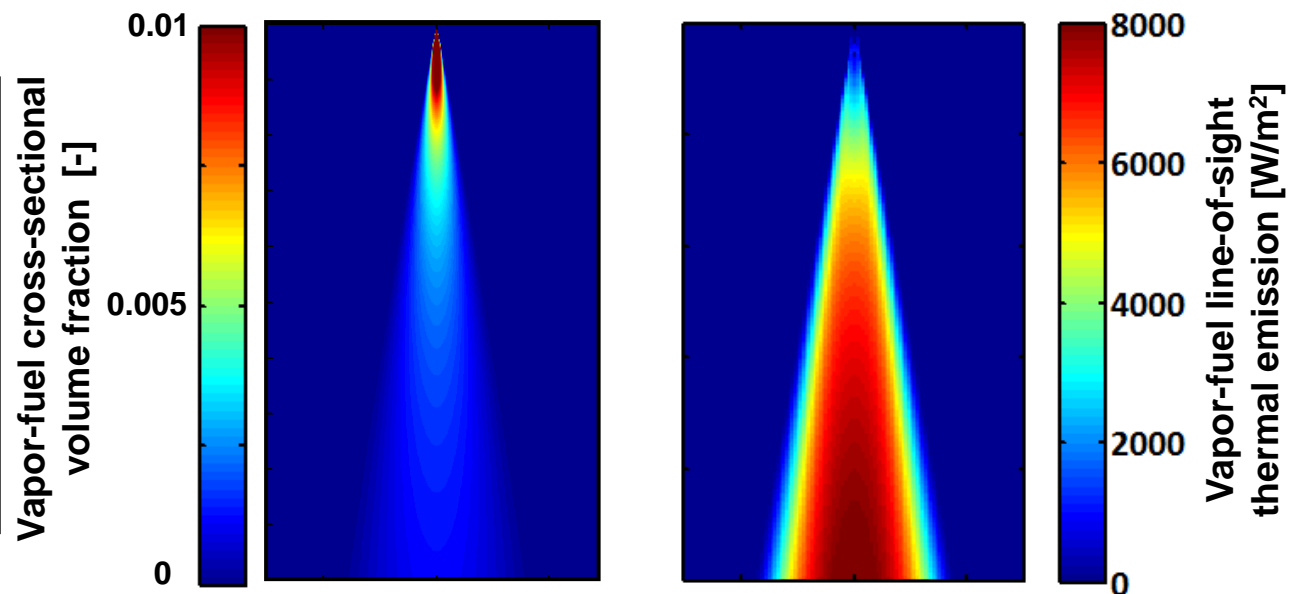


***Borescope engine: Little/no pass-through**

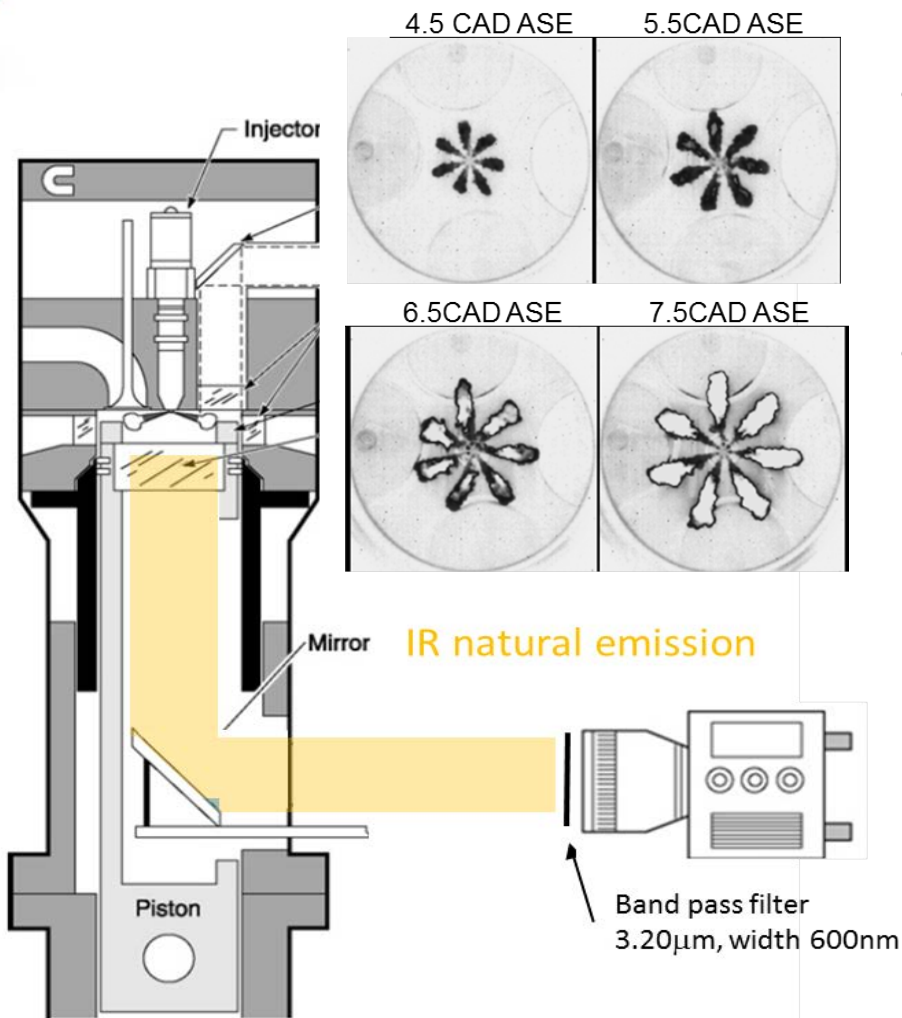
② Thermal (infrared) imaging can provide vapor-fuel penetration data with simpler optical access

- Injected fuel is quickly heated as it vaporizes and mixes with compression-heated in-cylinder gases \Rightarrow IR emission near $3.4 \mu\text{m}$
- Well-established jet-mixing and absorption / emission models (e.g., soot) can predict line-of-sight thermal emission of hot fuel
 - Vapor-fuel concentration profile is diffuse, but line-of-sight and adiabatic heating effects yield sharp-edged IR emission images
- Single window/endoscope is sufficient for vapor-fuel penetration; fused silica transmits @ $3.4 \mu\text{m}$ (expensive sapphire not req'd)

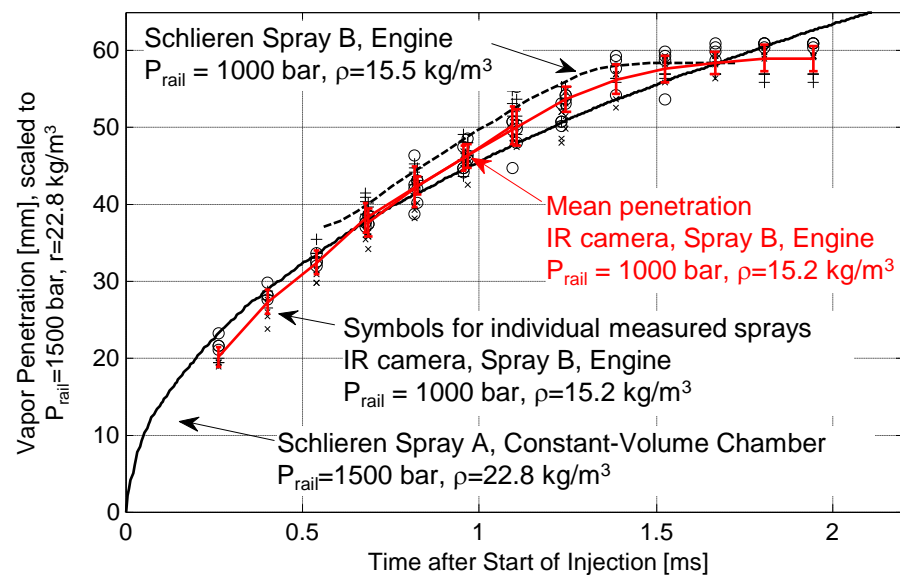
Injection of initially liquid hydrocarbon fuel into 900K ambient through 0.14 micron orifice using Naber/Siebers diesel-jet correlation and assuming adiabatic mixing



② Simple 1-camera IR penetration agrees well with schlieren; engine and chamber data comparable



- Single IR-camera setup yields well-defined vapor-jet boundaries
- IR penetration agrees with conventional pass-through schlieren measurements, and with scaled const.-vol. chamber data
- Also acquired liquid length, lift-off length, and ignition location data





③ Heat transfer is important for efficiency and/or exh. enthalpy for turbocharging/WHR, esp. LTC

- Heat transfer losses can be over 30% of input fuel energy
 - 1980's adiabatic engines using conventional combustion yielded hotter exhaust with little/no efficiency increase¹
 - Low-temperature combustion engines can benefit much more from reduced heat transfer, both increased efficiency and higher exhaust enthalpy for turbocharging, catalysts, and/or waste heat recovery²
 - Post injections can improve fuel efficiency, and one mechanism may be redistribution of combustion that reduces wall heat transfer³
- Heat transfer models need improvement/validation data
 - Predictions from cycle-simulation heat-transfer models (e.g., Woschni) vary by an order of magnitude⁴

Heat-transfer data correlated with optical flow/combustion measurements can provide better understanding and prediction of heat transfer for conventional/LTC and/or single/multiple injections

¹"Low heat rejection engines - an overview," S. Jaichandar and P. Tamilporai, SAE 2003-01-0405, 2003.

²"Thermodynamic advantages of low temperature combustion (LTC) engines using low heat rejection (LHR) concepts," J. Caton, SAE 2001-01-0312.

³"Reexamination of multiple fuel injections for improving the thermal efficiency of a heavy-duty Diesel engine," H. Osada et al., SAE 2013-01-0909.

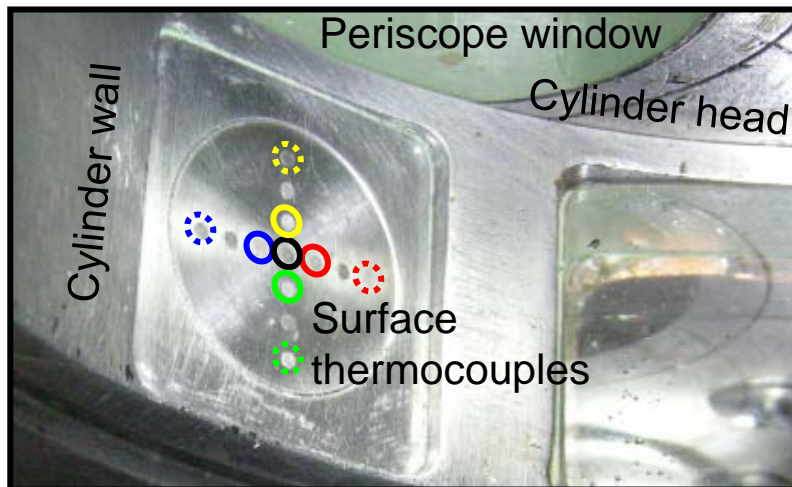
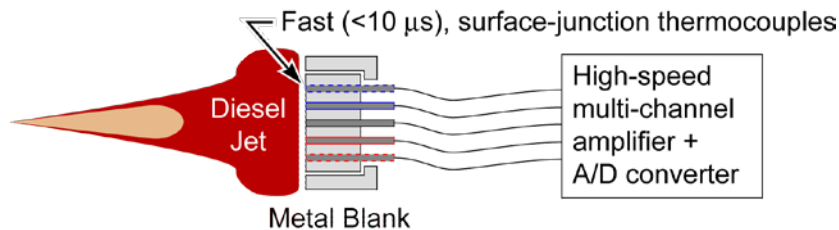
⁴"Heat transfer characteristics of conventional and high efficiency reciprocating engines," J. Caton, Paper IC10, 7th US Nat'l Comb. Meeting, 2011.

③ Two new heat transfer diagnostic developments: Conventional thermocouple and IR thermometry

Conventional Thermocouple

Collab. w/ Terry Hendricks, Sandia NM

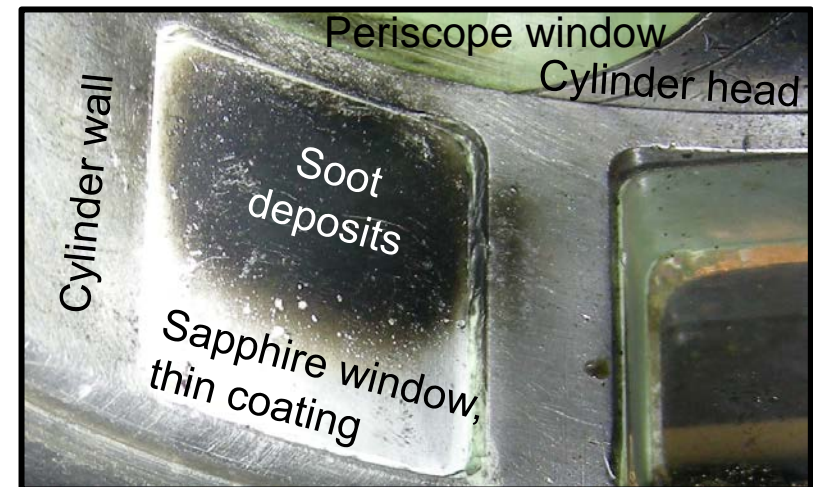
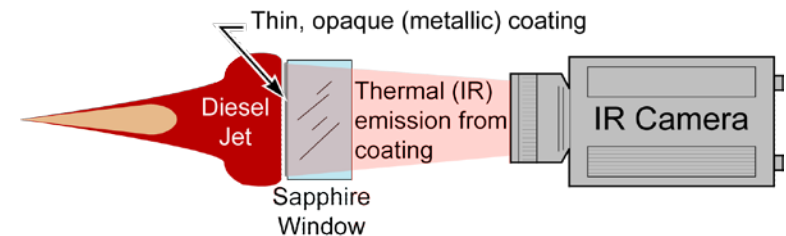
- Surface-junction thermocouple array with fast ($10\ \mu\text{s}$) time response provide multiple point measurements of temperature & heat transfer



IR Thermometry

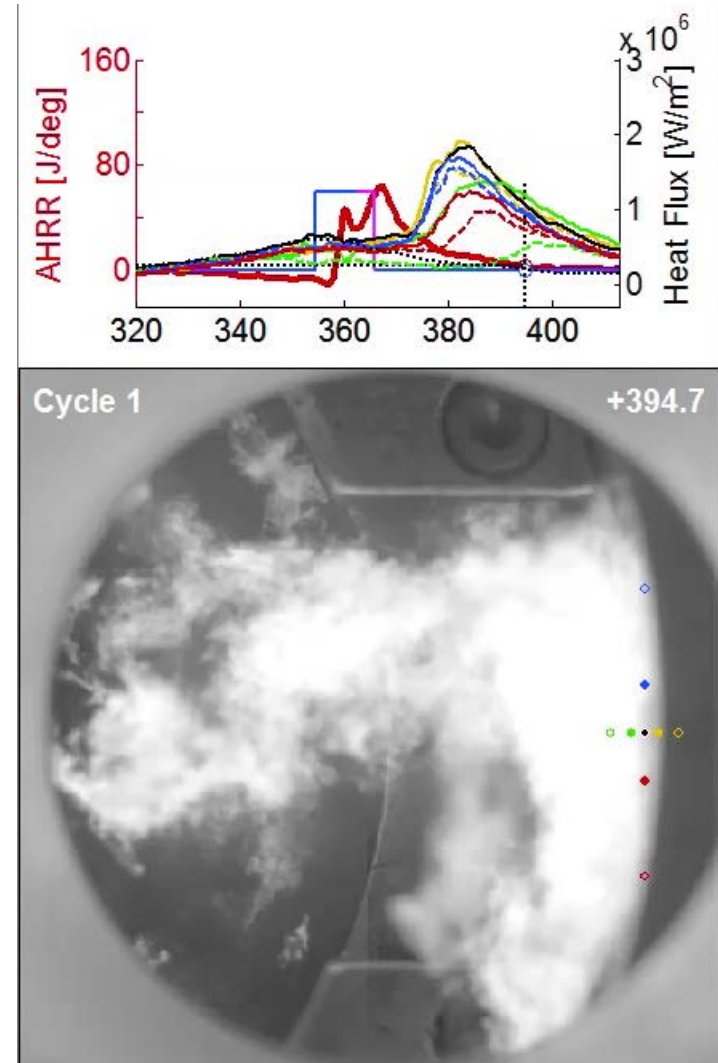
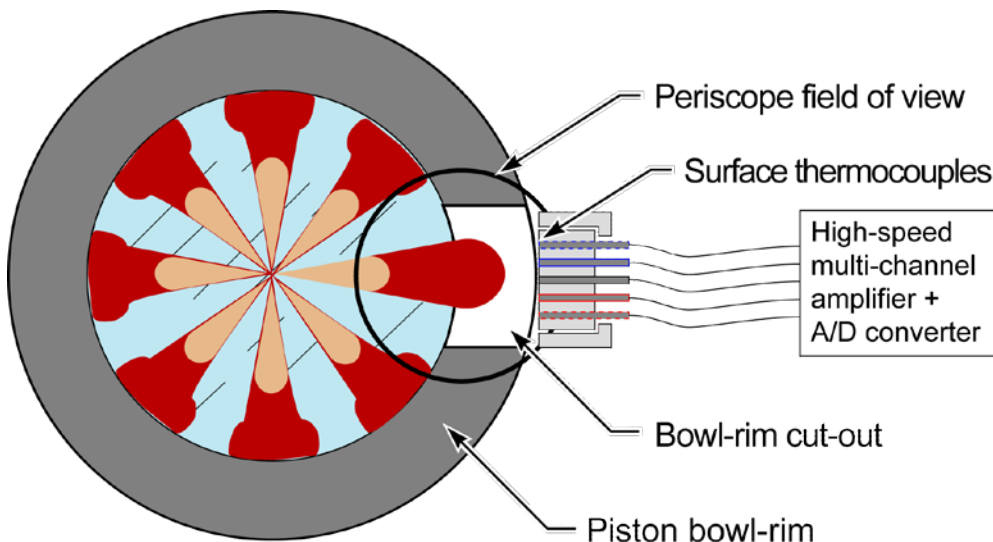
Collab. w/ Marcis Jansons, Wayne State

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



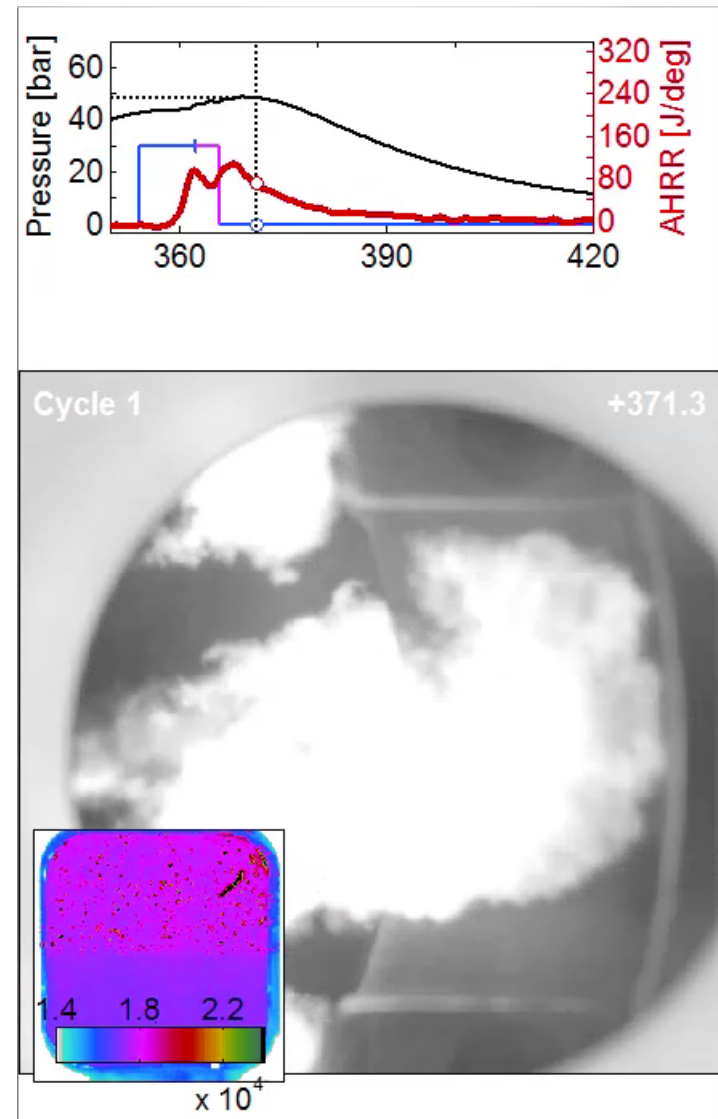
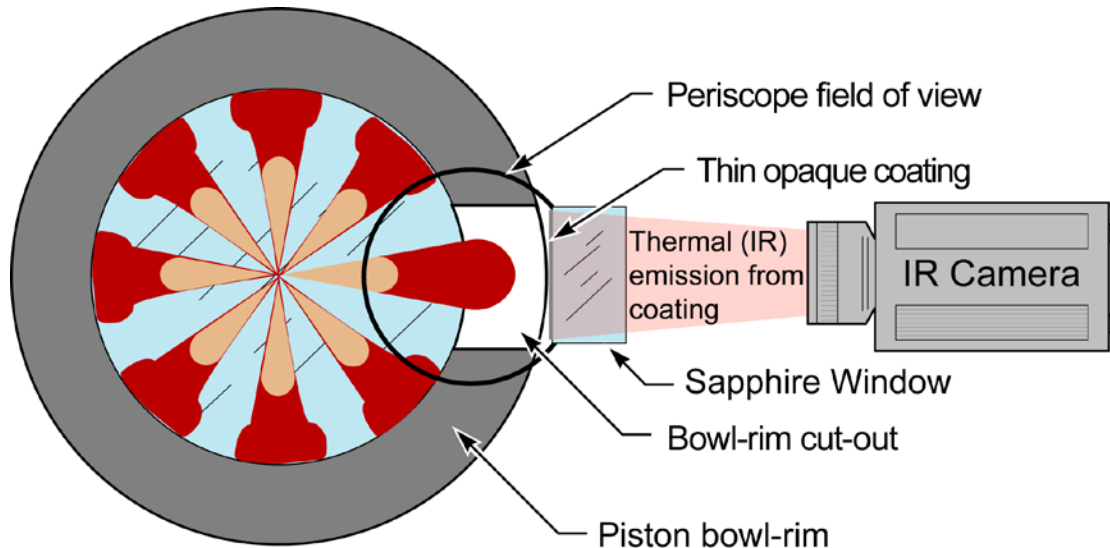
③ Preliminary thermocouple data: jet-impingent heat transfer quantified, not in phase w/ cyl. pressure

- Initial wall heat flux measurements use piston bowl-rim cut-out to allow jet to impinge on cylinder wall, with simultaneous combustion imaging
- Multiple thermocouples quantify heat transfer at jet arrival, not in phase with cylinder press. (contrast to Woschni)



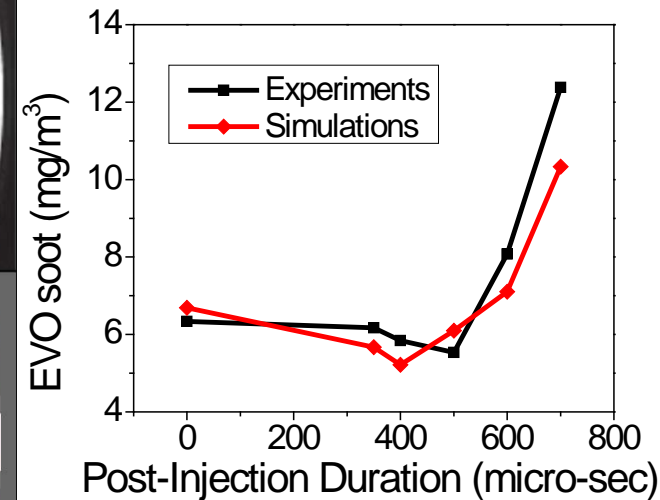
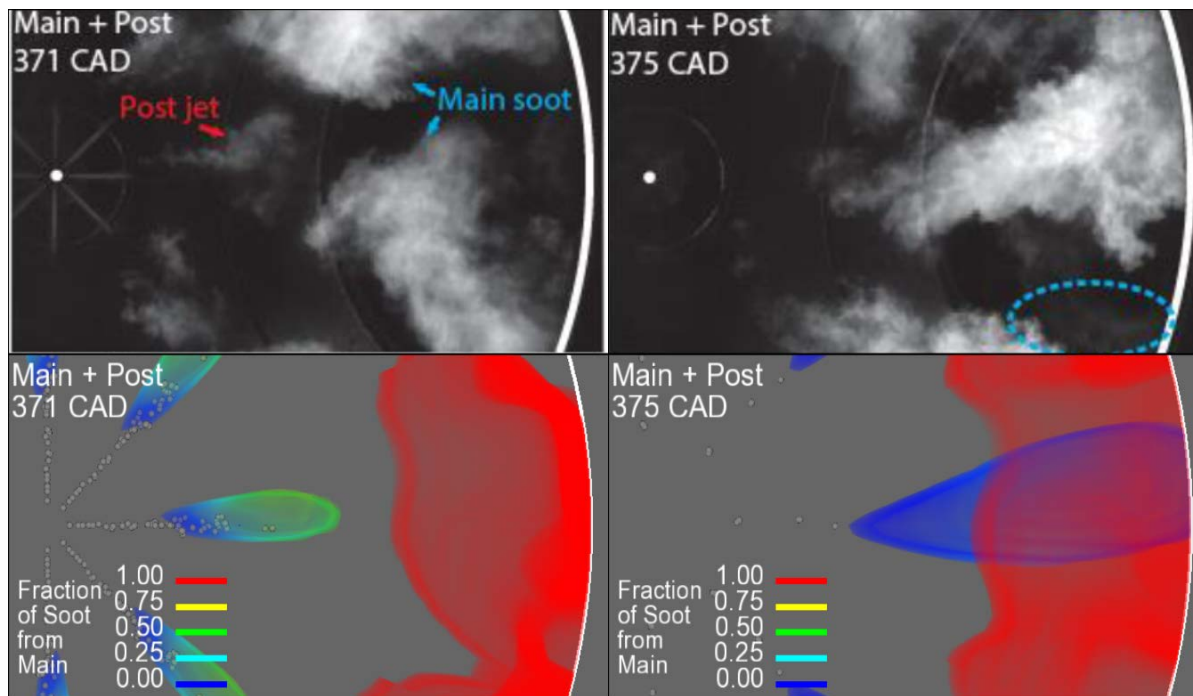
③ Preliminary IR thermometry data: sufficient signal, but pinholes in coating; needs more development

- Initial IR imaging: signal is strong even with fast exposure ($10\ \mu\text{s}$)
- Good S/N even before jet impingement on the window
- Many pinholes in coating transmit IR emission from combustion
- More development needed to maintain adhesion (thin) and opacity (thick)



Satisfactory agreement between model and exp't soot distributions supports analysis of predictions

- Model-predicted spatial and temporal distributions of soot agree well with experimental images of luminous soot and measured engine-out soot
- Appearance of post-injection soot is timed well (U. Wisc., R. Hessel)
- Model captures interaction with residual main-injection soot and reduction of engine-out soot (U. of Wisconsin, Zongyu Yue)

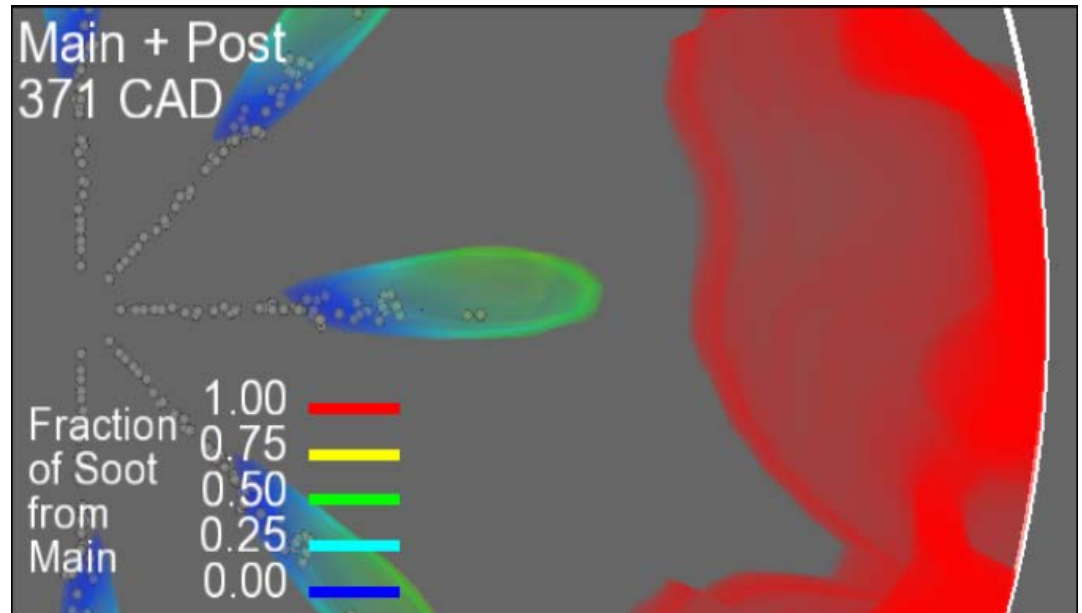


*Engine-out soot predictions from detailed chemistry combustion model with semi-detailed soot model (Yue)

*Images from characteristic time combustion model with 2-step soot model (Hessel)

In exp'ts, difficult to separate soot formation/oxidation, main/post soot \Rightarrow analyze model results

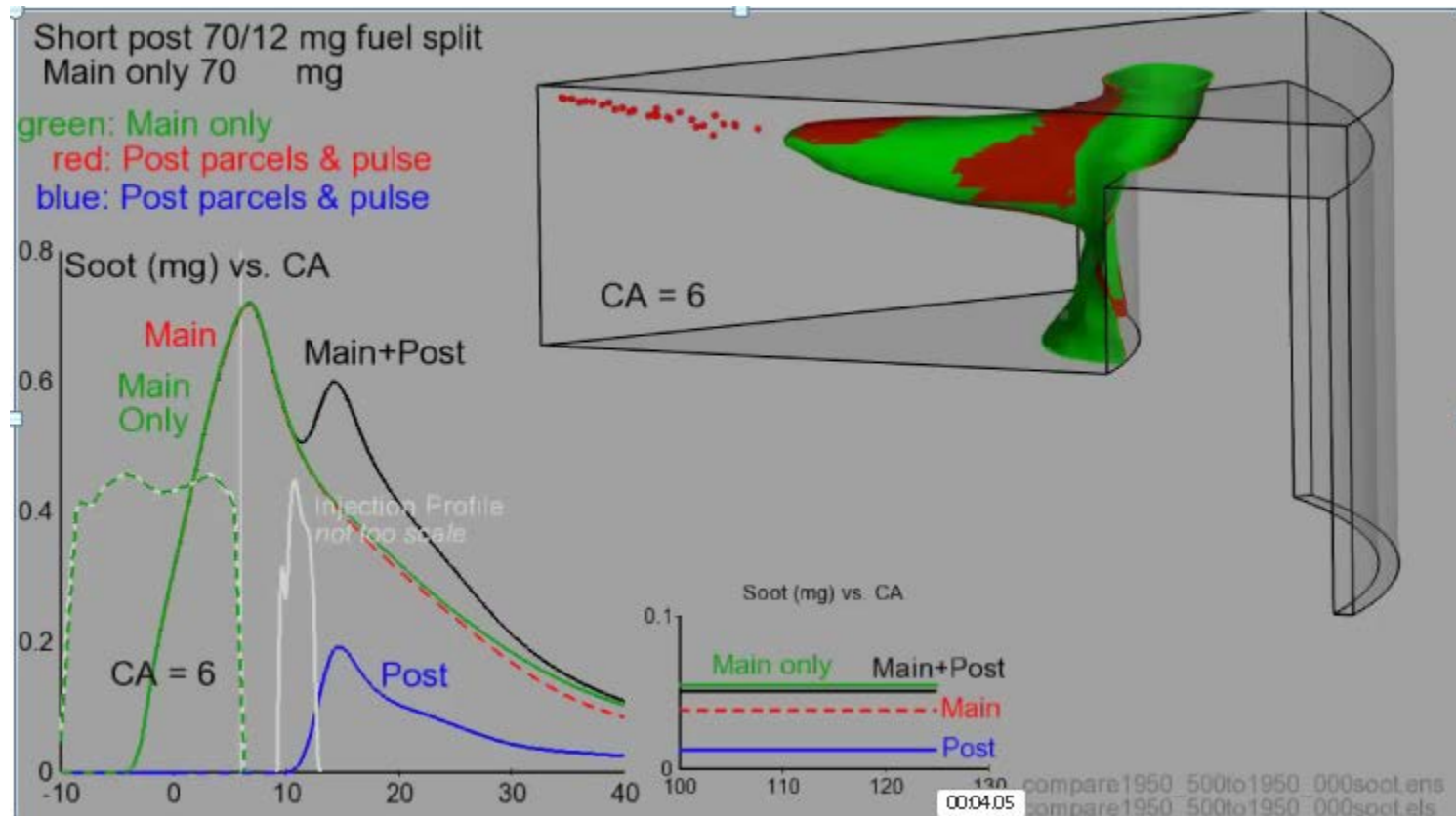
- Experiments can reveal total soot, but formation/oxidation rates are hard to separate, but models can help (FY14 report, or SAE 2014-01-1256)
- Also need model to discriminate soot contributions of main- and post-fuel
- Main- and post-injected fuel in the model can be tagged and tracked separately to quantify their contributions to the total in-cylinder soot
- Rendering shows predicted soot, color coded according to the carbon source, either main (red) or post (blue) injected fuel
- Post-soot forms partly from residual main fuel (blue + red = green)



Can 3-D analysis of the model predictions provide insight into the mechanisms by which the post-injection affects main-injection soot?

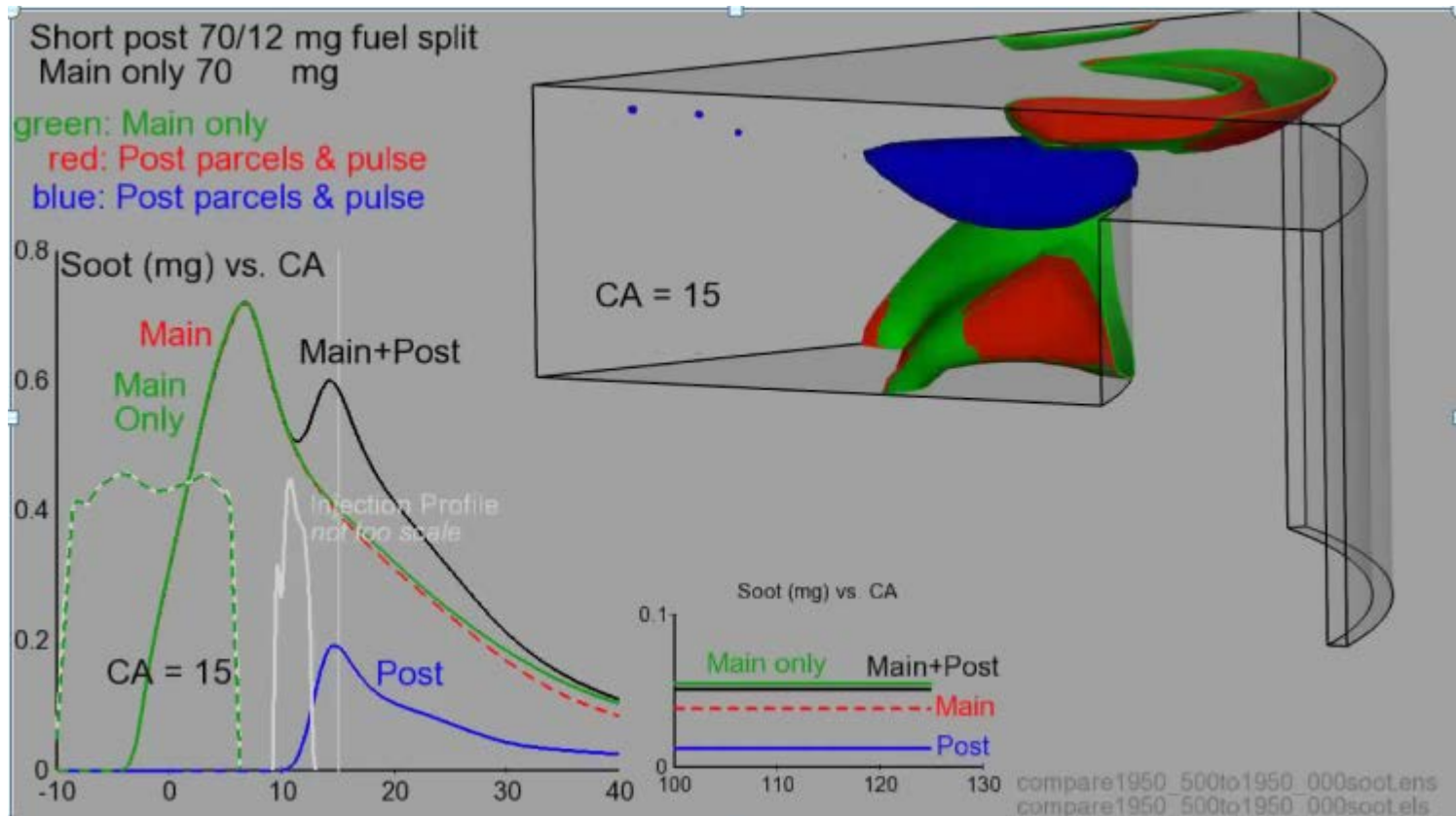
Prior to the addition of a post-injection, predicted soot resides near bowl wall, as in experiments

Case	New Color Scheme
Main-injection-only	green = soot from single injection (main)
Main+post injection	red = soot from main injection fuel
	blue = soot from post-injection fuel
	black = soot from main+post injection fuels



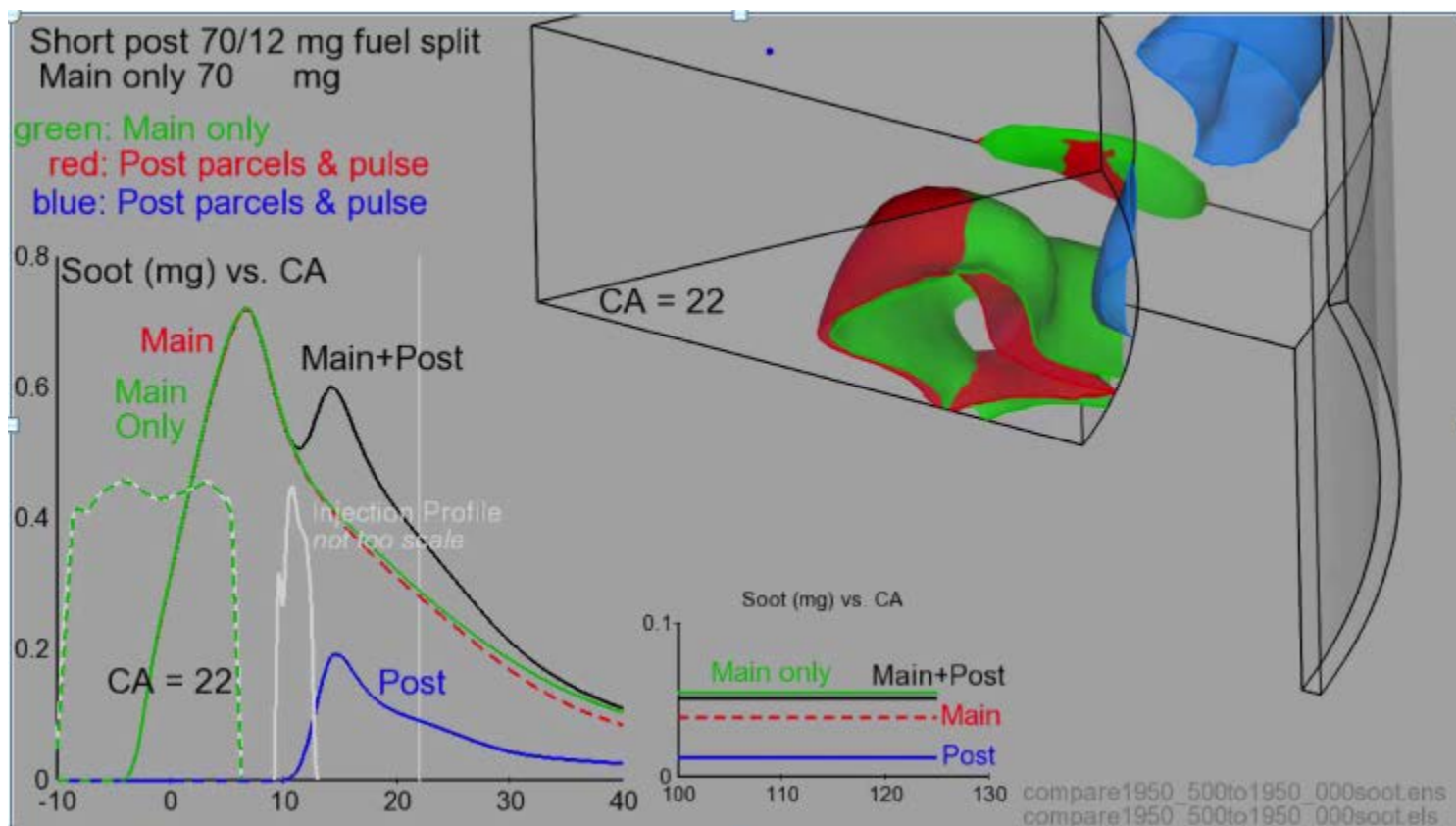
④ As post-injection penetrates, it reduces the main soot primarily by consuming main fuel

- Post injection adds fuel, so total soot (black curve) increases relative to main-injection only (green curve)
- Main soot (red curve) decreases due to lower main-fuel concentration as post-injection promotes faster combustion



④ Post-injection displaces main-injection soot cloud (red) from where it would have been (green)

- Post injection redistributes main-injection soot (red) back toward center of chamber relative to where it would have been without a post injection (green) – is this redistribution essential?
- FY16: Confirm redistribution in experiments and explore role





Remaining Barriers/Future Plans: Multi-injection conceptual model, heat-transfer, fuel-injectors

- 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



Responses to Previous Year Reviewers' Comments

Comment: *"Improvements possible regarding the connection between the work here at a fundamental level with more real-world operation ... with respect to overall engine and power-plant efficiency"*

Response: This year's work to develop quantitative heat transfer measurements opens the door for more explicit connections to efficiency beyond only using high-efficiency conditions.

Comment: *"Would like to have seen one topic fully investigated" "how simulations were improved and validated"*

Response: We focused our work this year on injection processes and efficiency (through heat transfer), and the simulation validations and improvements on post injection soot modeling were addressed.

Comment: *"Would like to hear a hypothesis as to why [post injections reduce soot], then to see a test plan to prove (or disprove) it"*

Response: This year, we used analysis of model predictions to start generating hypotheses about critical features of the post-injection interactions with soot, and have experimental plans to validate them.

Comment: *"Greater focus going forward on end-of-injection mixing should be valuable" "[spend time] understanding the sensitivity of this advanced combustion process (to control variables so that a multi-cylinder engine could find a way into production)"*

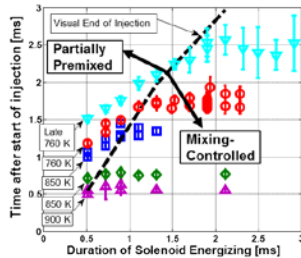
Response: Experiments this year focused on end-of-injection mixing as evidenced by ignition delay dependence on injection duration, which has fundamental implications for post-injection interactions with the main-injection field, as well as practical implications for combustion phasing control.

Comment: *"Continue building the conceptual model", "how many injection events were to be considered. The current approach appeared to focus on a main plus post injection strategy"*

Response: Developing the conceptual model is a multi-year task that will continue, and will include other multiple injection strategies as experimental and computational data are generated.

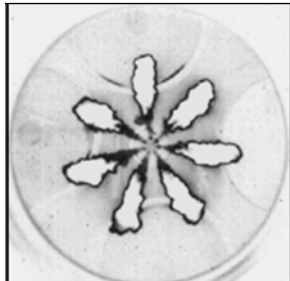
Heavy-Duty Combustion and Modeling Summary

①



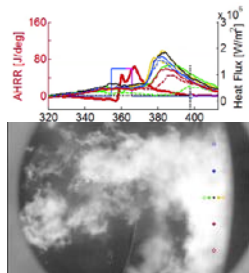
(SNL) Ignition in the residual mixtures of the main injection affected by more than mixing state – scalar dissipation (gradients)? \Rightarrow Likely affects how post injections interact with residual main injection.

②



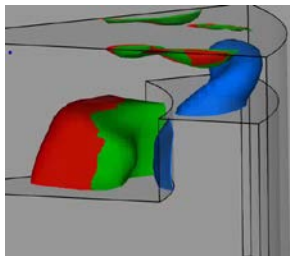
(SNL) Generated Spray-B engine data for ECN including liquid length, lift-off length, ignition/combustion luminosity, and developed new single window/camera IR vapor-fuel penetration diagnostic.

③



(SNL) Developed conventional thermocouple and IR-thermometry diagnostics for quantitative heat-transfer measurements correlated with in-cylinder phenomena for model and efficiency improvements.

④



(UW) Achieved good agreement with experimental in-cylinder and exhaust soot so that analysis of CFD predictions can add insight and help guide experiments for multiple injection conceptual model.



Recent Publications and Presentations

- "In-Cylinder Soot Precursor Growth in a Low-Temperature Combustion Diesel Engine: Laser-Induced Fluorescence of Polycyclic Aromatic Hydrocarbons," C.A.J. Leermakers, M.P.B. Musculus, Proc. Comb. Inst. 35(3):3079–86, 2015.
- "Effect of Load on Close-Coupled Post-Injection Efficacy for Soot Reduction in an Optical, Heavy-Duty Diesel Research Engine," J.A. O'Connor and M.P.B. Musculus, J. Eng. Gas Turb. Power, 136(10):101509-101509-16, May 2014.
- "Effects of EGR and Load on Soot in a Heavy-Duty Optical Diesel Engine with Close-Coupled Post-Injections for High Efficiency Combustion Phasing," J.A. O'Connor and M.P.B. Musculus, Int. J. Eng. Res. 15(4):421-443, June 2014.
- "In-Cylinder Mechanisms of Soot Reduction by Close-Coupled Post-Injections as Revealed by Imaging of Soot Luminosity and Planar Laser-Induced Soot Incandescence in a Heavy-Duty Diesel Engine," J.A. O'Connor and M.P.B. Musculus, SAE Int. J. Engines 7:673-693, July 2014.
- "A CFD Study of Post Injection Influences on Soot Formation and Oxidation under Diesel-like Operating Conditions," R.P. Hessel, R.D. Reitz, M.P.B. Musculus, J.A O'Connor, D. Flowers, SAE Int. J. Engines 7:694-713, July 2014.
- "Cinema-Stereo Imaging of Fuel Dribble after the End of Injection in an Optical Heavy-Duty Diesel Engine," W.E. Eagle and M.P.B. Musculus, THIESEL 2014 Conference on Thermo- and Fluid Dynamic Processes in Direct Injection Engines, Sept. 2014.
- "Measuring Transient Entrainment Rates of a Confined Vaporizing Diesel Jet," W.E. Eagle, M.P.B. Musculus, L-M. Malbec, G. Bruneaux, ILASS Americas 26th Annual Conf. on Liquid Atomization and Spray Systems, May 2014.
- "A Conceptual Model for Low-Temperature Diesel Combustion," M.P.B. Musculus, Invited Lecture at Eindhoven University of Technology, February 2014.
- "How Jets Get It All Mixed Up: Combustion Research Using Laser Diagnostics in Optical Engines at Sandia National Laboratories," Invited Lecture at Pennsylvania State University Seminar Series, April 2014.
- "Evaluating Temperature and Fuel Stratification for Heat-Release Rate Control in a Reactivity-Controlled Compression-Ignition Engine using Optical Diagnostics and Chemical Kinetics Modeling," S.L. Kokjohn, M.P.B. Musculus, R.D. Reitz, accepted into Combustion and Flame, April 2015.
- "Image-Based Correlation of Engine Operating Parameters with Occurrence and Duration of Diesel Fuel Injector Dribble," W.E. Eagle and M.P.B. Musculus, Oral-Only Presentation and SAE International Congress, April 2015.
- "Advanced CFD Diagnostics: Tracking Soot from Originating Fuel Sources through to EVO in a Cummins N14 Optical Engine Utilizing Post Injections," R.P. Hessel, R.D. Reitz, Z. Yue, M.P.B. Musculus, J.A. O'Connor, Oral-Only Presentation and SAE International Congress, April 2015.

Critical Assumptions and Issues

- Is low-temperature combustion a viable approach for meeting future emissions and efficiency targets?
 - Based on feedback from industrial partners, the consensus is that some level of low-temperature combustion deemed worthy of further research and development. Studies will include a range of EGR representative of uses across the industry, including strategies that use aftertreatment.
- Relevance of results depends on state-of-the-art injector technology
 - As much as possible, we work with our industrial partners to use the most modern injector technology, but issues with proprietary content can cause some lag.
- Are optical engine results fully representative of production/metal engine performance?
 - The results of previous research, as well as the use of optical diagnostic observations for developing computer models, have demonstrated that fundamental research in optical engines is relevant to production engine performance. Future partnerships with parallel metal engine experiments and more realistic optical geometries are currently being explored.