Fuel Effects on Mixing-Controlled Combustion Strategies for High-Efficiency Clean-Combustion Engines

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Overview

Timeline

- Project provides fundamental research to support DOE/ industry fuels-technologies projects
- Project directions and continuation are evaluated annually

Budget

- Project funded by DOE/VT:
  FY14 – $800K
  FY15 – $800K

Barriers *(from DOE/VT MYPP 2011-2015)*

- Inadequate data and predictive tools for understanding fuel-property effects on
  - Combustion
  - Engine efficiency optimization
  - Emissions

Partners

- Project lead: Sandia (C.J. Mueller, PI)
- 15 industry, 6 univ., and 6 nat'l lab partners in Advanced Engine Combustion MOU
- Coordinating Research Council (CRC)
- Ford Motor Company
- Caterpillar Inc.
- Yale University, Chevron, LLNL

Relevance

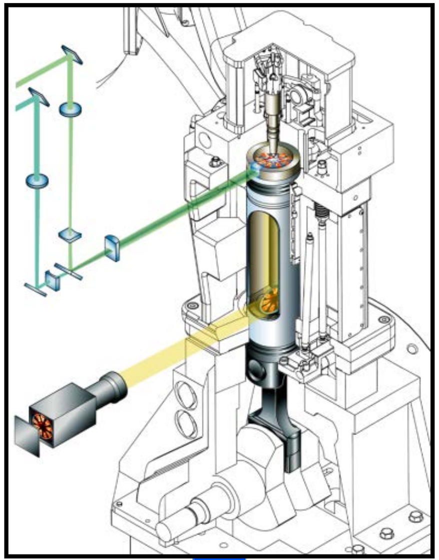
Develop the science base to enable cost-effective high-efficiency clean-combustion (HECC) engines using fuels that improve US energy security

- **Specific objectives of work since FY14 Annual Merit Review**
  - Create/distribute a set of diesel surrogate fuels for engine/vessel testing
    - Serve as co-leader of CRC Project AVFL-18a: “Diesel Surrogate Fuels for Kinetic Modeling and Engine Testing”
  - Develop an optical diagnostic to estimate total in-cylinder soot mass
    - To assess CFD model validity and better understand fuel effects on soot field
  - Evaluate the feasibility of using oxygenated fuels to achieve LLFC
    - LLFC = “leaner lifted-flame combustion” (combustion that does not form soot)
  - First-ever testing of a novel in-cylinder mixing-enhancement technique
    - Ducted fuel injection can yield LLFC with lower-cost fuels & injection systems

Milestones

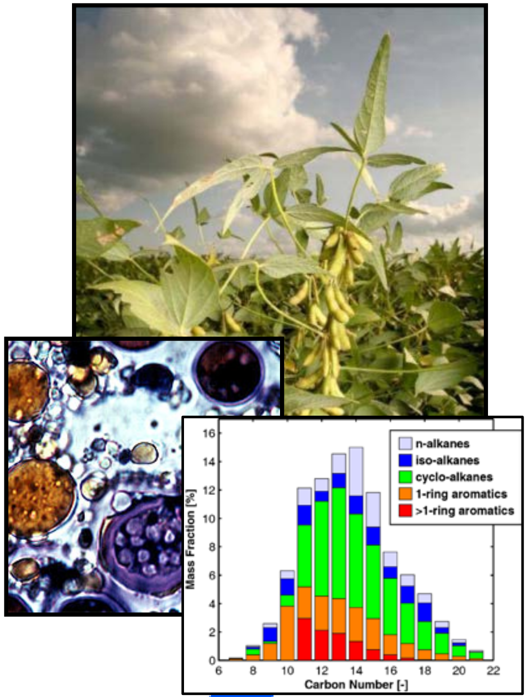
- ✓ **September 2014**
  Fabricate required hardware and evaluate the Ducted Fuel Injection (DFI) concept in Sandia's Constant-Volume Combustion Vessel
- ✓ **December 2014**
  Publish paper summarizing results of testing methyl decanoate, an "optimal" biodiesel fuel, as a means to achieve LLFC
- **April 2015**
  Publish paper describing new optical diagnostic to estimate total in-cylinder soot mass as a function of crank angle
- **September 2015**
  Publish paper describing creation and property testing of a set of diesel surrogate fuels for combustion experiments and kinetic modeling
- **December 2015**
  Summarize initial results of optical-engine testing of target and surrogate fuels

Approach



Unique and comprehensive diagnostic capabilities

Collaboration with key stakeholders

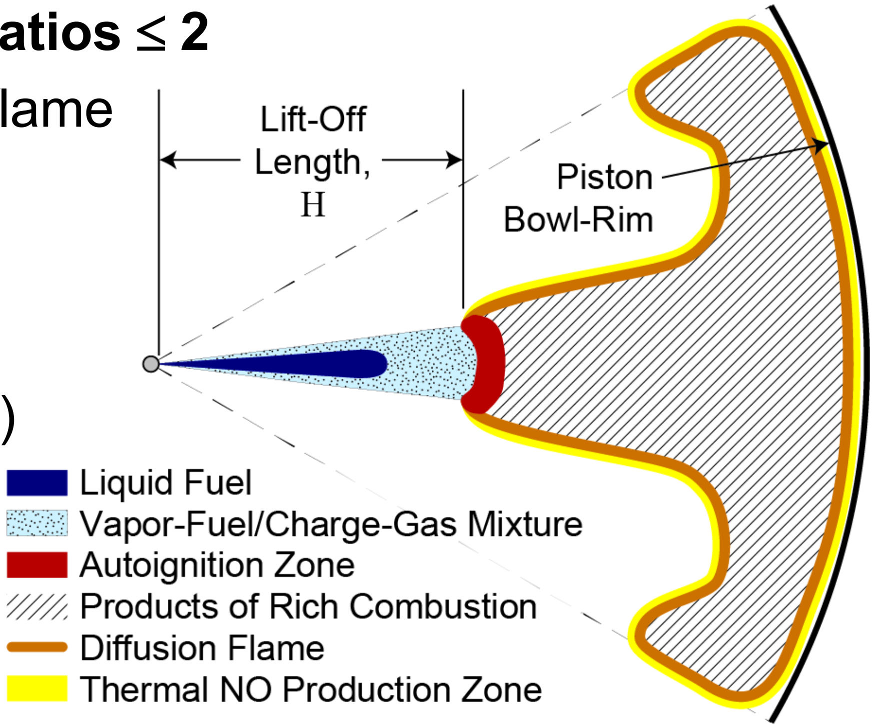


18 years of fuel-effects research

HECC engines using fuels that improve US energy security

Approach: Use New Fuels and In-Cylinder Mixing Strategies to Achieve LLFC

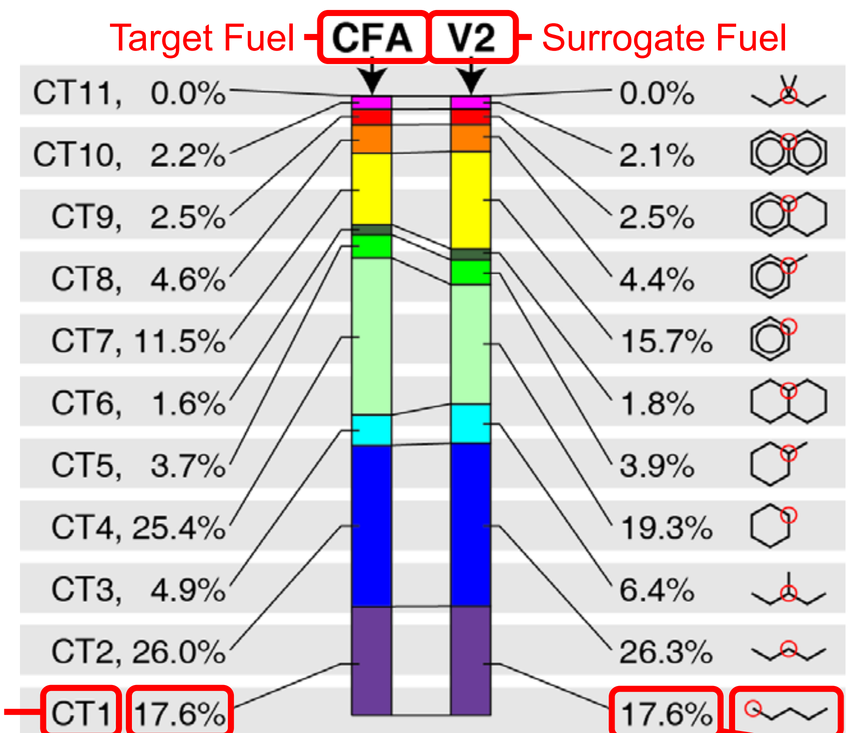
- **LLFC is mixing-controlled combustion that does not form soot because it occurs at equivalence ratios ≤ 2**
  - In autoignition zone and diffusion flame
- **Advantages of LLFC**
  - High efficiency (compression ign.)
  - No soot (soot is #2 climate forcer)
  - Easy to control (by injection timing)
  - Fuel-flexible (specs. ≈ to D2)
  - Low noise (steady heat release)
  - Less-expensive aftertreatment
- **Successful deployment of LLFC depends on appropriate**
  - Fuel properties: e.g., molecular structure, ign. quality, oxygenation, …
  - Engine implementation: e.g., injection strategy, charge preparation, …



Technical Accomplishments (TAs)

TA#1: Created and Property-Tested a Set of Improved Diesel Surrogate Fuels

- **Research challenge: Rigorously validated, realistic, and broadly accepted diesel surrogate fuels have been unavailable.**
  - CRC Project AVFL-18/18a has addressed this issue by developing and employing a methodology to create accurate surrogate fuels
- **Surrogate fuels can be used as**
  - Realistic, reproducible ref. fuels for conducting controlled exp'ts anytime/anywhere in the world
  - A req'd foundation for predictive CFD engine optimization for evolving real-world fuels
  - Research tools for achieving a better understanding of fuel-composition and property effects



Mole fraction of given CT in target fuel (from NMR spectrum) and surrogate fuel (from composition)

TA#1: Created and Property-Tested a Set of Improved Diesel Surrogate Fuels

- **Palette compounds were procured, individually silica-gel treated (to remove peroxides), and then a 30-L batch of each surrogate was blended, additized, tested, …**

Measurement	Lab	CFA	V0a	V0b	V1	V2
Composition by GCxGC-FID	CanmetENERGY	M	P M	P M	P M	P M
Composition by NMR	PNNL	M	P M	P M	P M	P M
Derived Cetane Number (DCN)	NREL	M	P M	P M	P M	P M
Peroxides	Chevron	M	M	M	M	M
ASTM D86 Distillation	SwRI	M	M	M	M	M
Advanced Distillation Curve	NIST	M	P M	P M	P M	P M
Simulated Distillation	NREL	M	M	M	M	M
Density @ 20 °C	NREL	M	P M	P M	P M	P M
Carbon	SwRI	M	P M	P M	P M	P M
Hydrogen	SwRI	M	P M	P M	P M	P M
Sulfur	SwRI	M	P M	P M	P M	P M
Net Heat of Combustion	SwRI	M	P M	P M	P M	P M
Copper Strip Corrosion	SwRI	M	M	M	M	M
Cloud Point	NREL	M	M	M	M	M
Lubricity	Chevron	M	M	M	M	M
Kinematic Viscosity	SwRI	M	M	M	M	M
Flash Point	Chevron	M	M	M	M	M
Aromatic Content	SwRI	M	P M	P M	P M	P M
Smoke Point	SwRI	M	M	M	M	M

P = predicted
M = measured

[red box] = organizations that made measurements

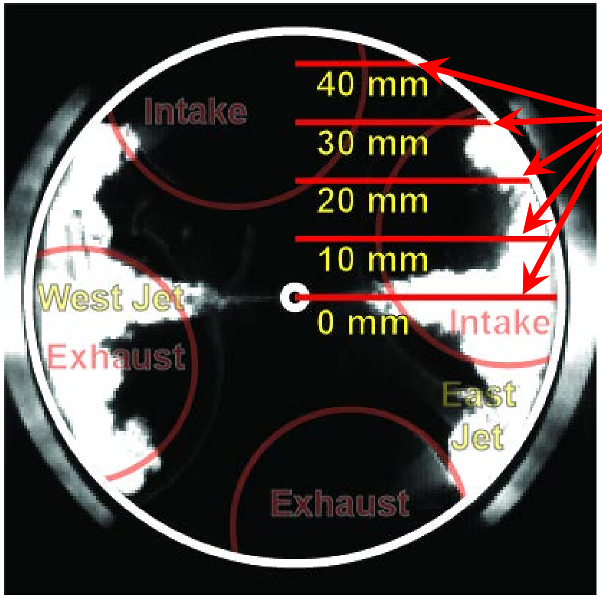
[blue box] = Chevron also completed the silica-gel treatment, as well as blending, additizing, and distributing the fuels

TA#1: Created and Property-Tested a Set of Improved Diesel Surrogate Fuels

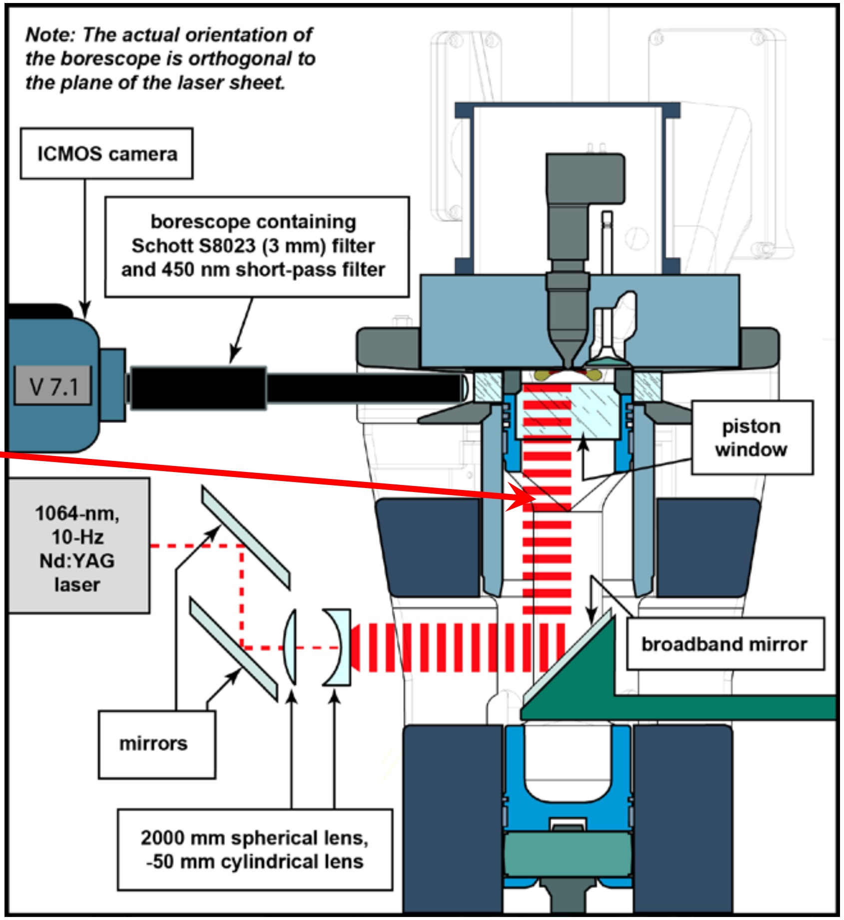
- **Palette compounds were procured, individually silica-gel treated (to remove peroxides), and then a 30-L batch of each surrogate was blended, additized, tested, …and distributed!**
  - For single-cylinder engine and combustion-vessel experiments in four separate labs
    - National Research Council (Canada)
      - HCCI engine
    - US Army Research Laboratory
      - Continuous-flow vessel
    - Sandia National Laboratories
      - Constant-volume combustion vessel
      - Optical engine (mixing-controlled combustion)

TA#2: Developed an Optical Diagnostic to Estimate Total In-Cylinder Soot Mass

- **Research challenge: A diagnostic for estimating the total in-cylinder soot mass as a function of crank angle did not exist.**
  - Cannot directly assess CFD soot models without this capability
  - A diagnostic using vertical-sheet laser-induced incandescence (VLII) has been developed

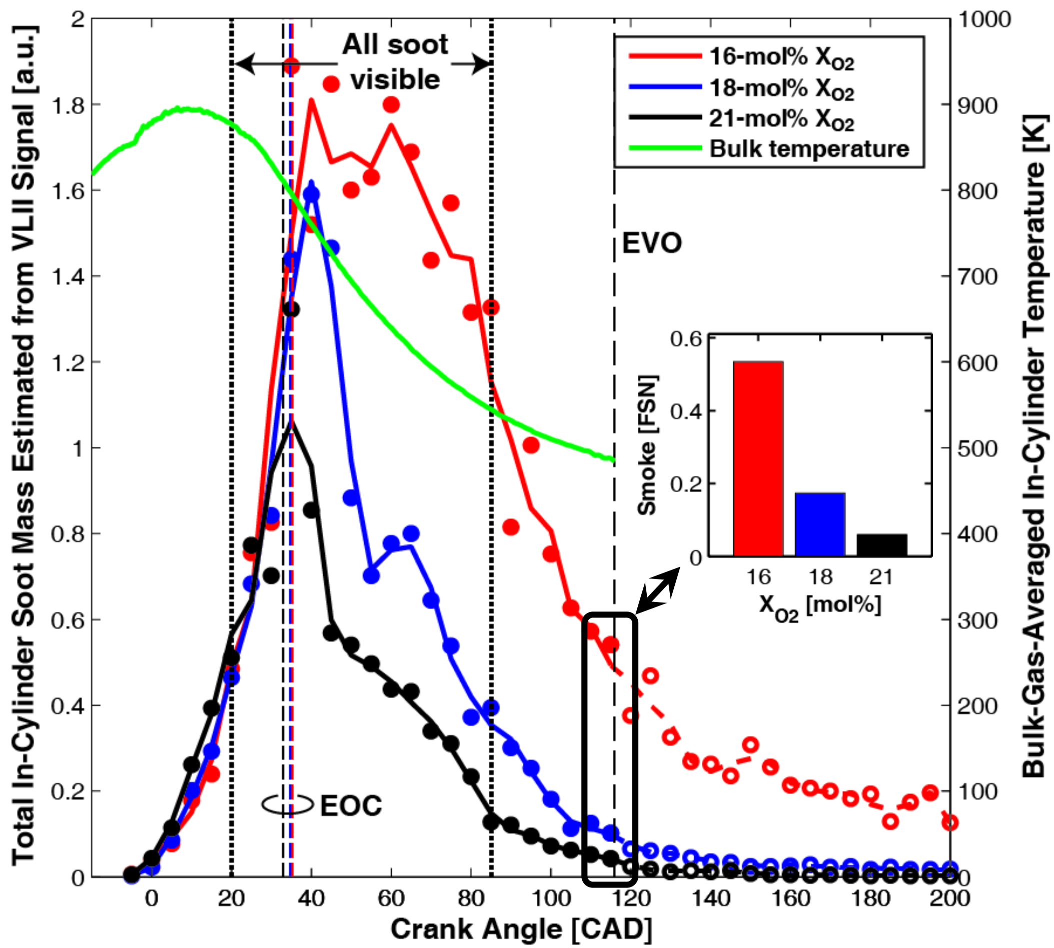


Vertical laser sheets



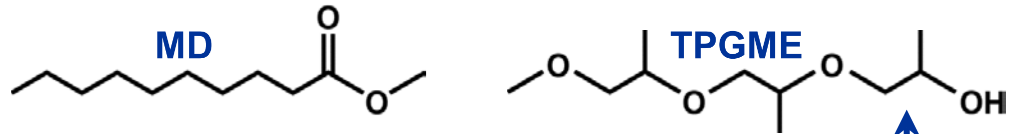
TA#2: Developed an Optical Diagnostic to Estimate Total In-Cylinder Soot Mass

- **This is a significant improvement in in-cylinder soot measurement.**
  - Trends in estimated soot mass agree with trends in engine-out smoke
  - Apparently, soot production rate exceeds oxidation rate until end of combustion (EOC)
    - I.e., in-cylinder soot mass is increasing as long as primary heat release is occurring
  - It is unclear whether this result will hold true for all fuels and operating conditions

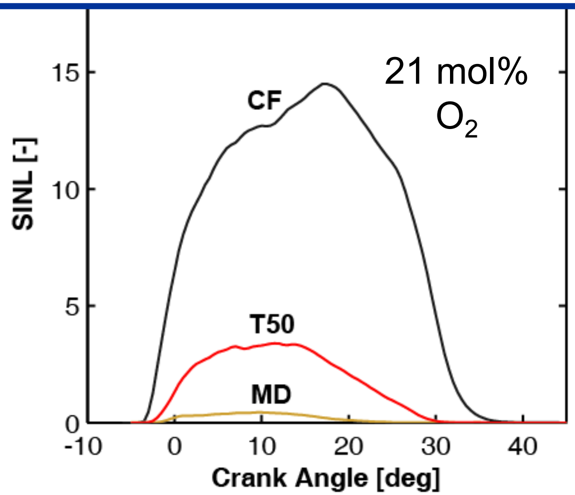


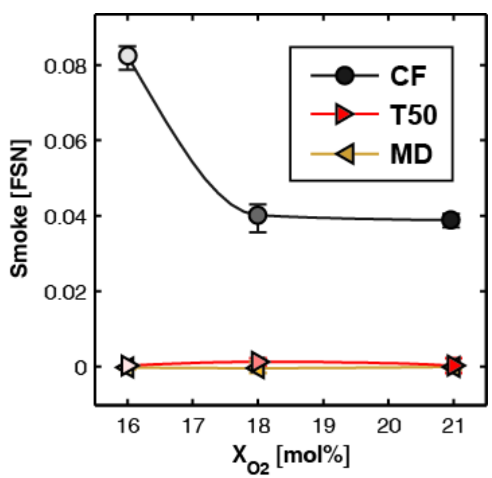
TA#3: Evaluated the Effectiveness of Using Oxygenated Fuels to Achieve LLFC

- **Research challenge: It has not been possible to achieve LLFC with conventional diesel fuel at combustion timings consistent with peak thermal efficiencies.**
  - Three fuels were tested
    - #2 ultra-low-sulfur diesel emissions-certification fuel (CF) → baseline
    - 100% methyl decanoate (MD) → an "optimal" biodiesel component
    - 50 vol% tri-propylene glycol methyl ether + CF (T50) → "realistic" oxy. blend



Initially LLFC was not achieved…but the oxygenates have zero smoke emissions!

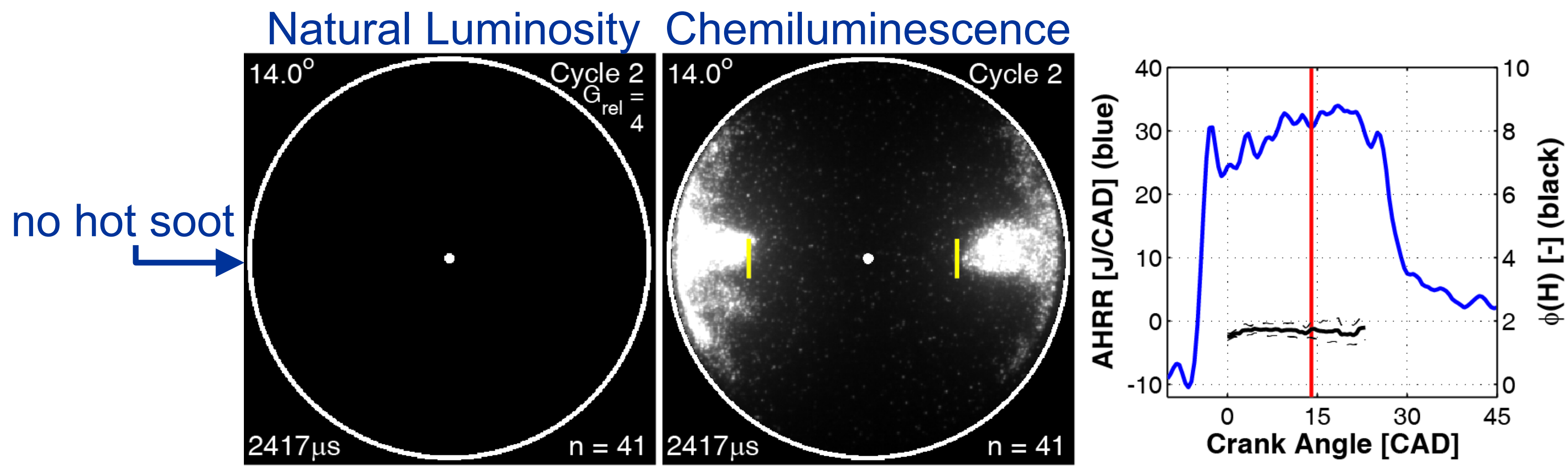




Conditions/definitions:
Single injection near TDC
Inj. pressure (P_{inj}) = 180 MPa
Injection duration = 32 CAD
Start of combust. = -5 °ATDC
Intake temp. (T_{in}) = 95 °C
SINL = spatially integrated natural luminosity
X_{O2} = intake-O_2 mole fraction

TA#3: Evaluated the Effectiveness of Using Oxygenated Fuels to Achieve LLFC

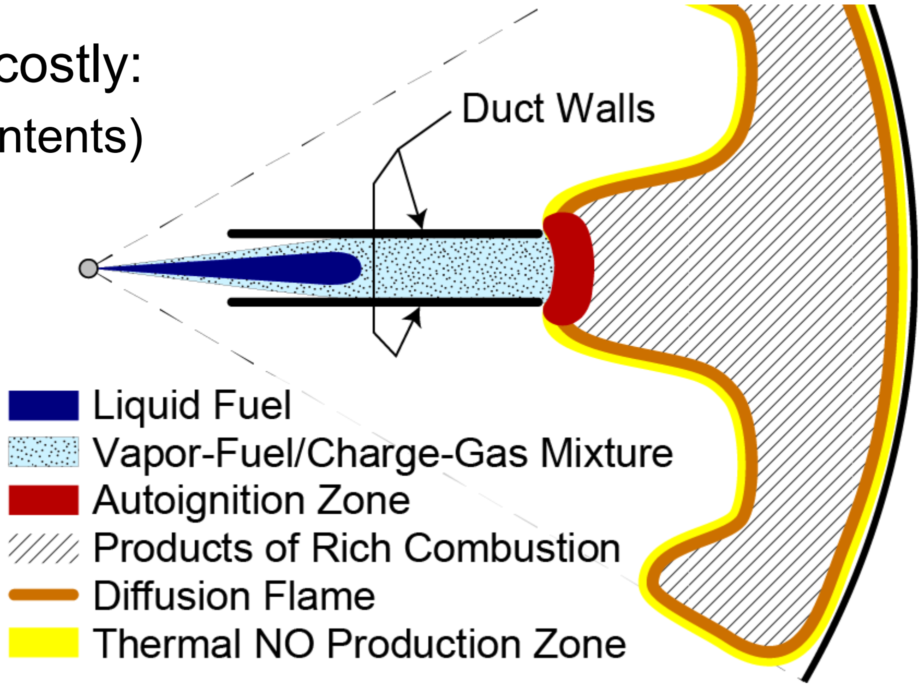
- **Ultimately, LLFC was achieved and sustained using T50 by raising P_{inj} from 180 → 240 MPa and lowering T_{in} from 95 → 50 °C.**



  - At 21 mol% O_2, comparing LLFC with T50 (240 MPa P_{inj}, 50 °C T_{in}) vs. non-LLFC with CF (180 MPa P_{inj}, 95 °C T_{in})
    - Smoke: eliminated
    - $ISNO_x$: 25% lower
    - ISHC: 60% higher
    - ISCO: 160% higher
    - Thermal efficiency: equal
    - Combustion efficiency: 0.4% lower
    - Noise: 80.9 dBA (< 87 dBA max.)
    - Ringing intensity: 0.20 MW/m^2 (<< 5.0 max.)

TA#4: Demonstrated Ducted Fuel Injection: A Novel Mixing-Enhancement Strategy

- **Research challenge: Further increases in fuel-injection pressure and fuel oxygenation are likely insufficient to provide adequate mixing to achieve LLFC – a new approach is necessary.**
  - Ducted fuel injection (DFI): Inject fuel through a tube downstream of the orifice exit to increase the velocity gradients that drive turbulent mixing of fuel and charge-gas
  - Could enable the use of less-costly:
    - Fuels (e.g., higher aromatic contents)
    - Fuel-injection equipment (e.g., lower injection pressures)
    - Aftertreatment systems
  - This is a new, largely unexplored combustion concept



TA#4: Demonstrated Ducted Fuel Injection: A Novel Mixing-Enhancement Strategy

- **Conducted the first-ever experiments proving the DFI concept.**
  - 1-week study done using Sandia constant-volume combustion vessel
  - 900 K, 22.8 kg/m^3, 21 mol% O_2, 150 MPa injection pressure, 90-μm orifice, n-dodecane fuel (i.e., Engine Combustion Network “Spray A”)

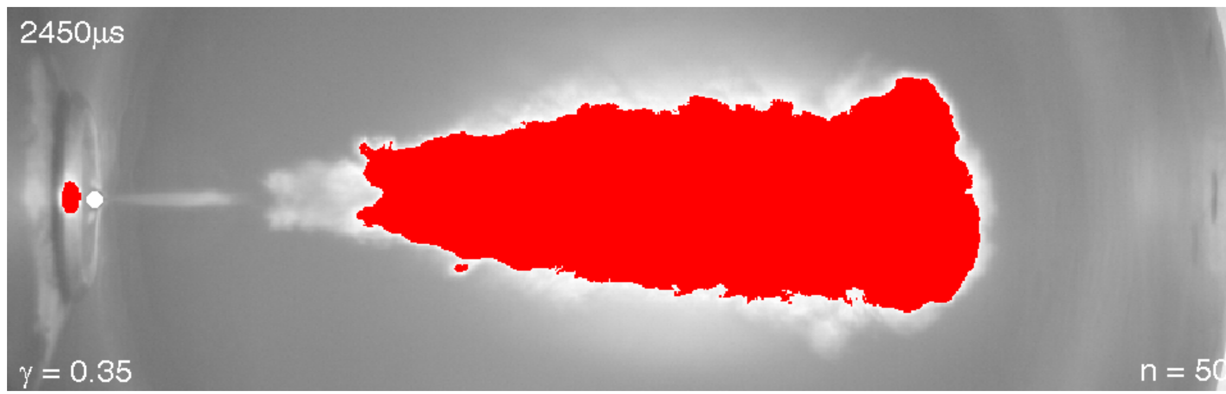
Free Jet, *Red = hot soot*

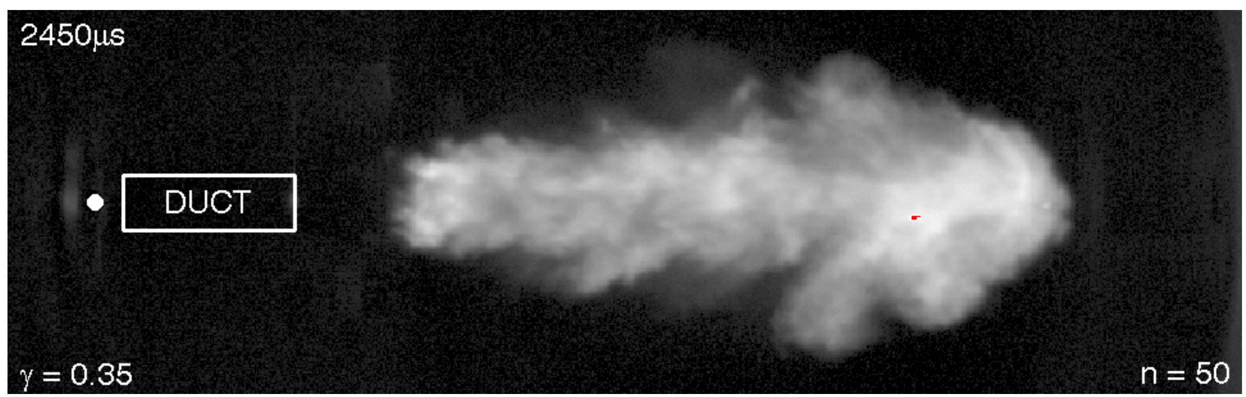
↑

Identical natural-luminosity imaging and display parameters

↓

Ducted Fuel Injection (DFI)





Responses to FY14 Reviewers' Comments

- **Comment:** "The practical application of [LLFC] appears to be quite limited due to its being dependent on tightly specified and standardized fuel parameters, which may be different for different vehicles."
  - Response: Our goal is to implement LLFC in such a way that the fuels have similar or looser processing requirements and specs (and hence cost) than #2 diesel. Ducted fuel injection is a step in this direction. For example, the aromatics spec could be relaxed because soot is not formed with LLFC via DFI. We do not see why the specs would need to be different for different vehicles.
- **Comment:** "[The] ducted [fuel injection] work should not be undertaken until there has been more analysis and modeling done."
  - Response: We did as much analysis as we could, and no "show-stopper" issues were found. We did some modeling with an industry partner, but the modelers had low confidence in the accuracy of their results with such a novel geometry, nor were they very motivated to spend effort modeling an untested concept. Experiments were conducted only after these routes were exhausted, and the experiments show that the concept works. We welcome input from the modeling community.
- **Comment:** "[T]he project has achieved numerous milestones to date but some of the key objectives, such as target and surrogate fuels, have been pursued for a number of years and remain to be completed. Such completion appears to be slated for the coming year although…presentation language is not completely clear on that."
  - Response: The surrogate and target fuels are all now available in bulk, and we have taken the time to do the work correctly. Accurate knowledge of the target fuel composition is required to make accurate surrogate fuels, but different techniques for determining fuel composition can yield different results. It took a great deal of time and effort to vet our methods. Also, procuring representative diesel compounds in high purity with low sulfur is not trivial. A good example is 1-methylnaphthalene, which is in every surrogate. We have succeeded in both of the above areas, but the path has been challenging, and the timelines have not been easy to predict or control.

Collaboration and Coordination with Other Institutions

- **Combustion research conducted with guidance from Advanced Engine Combustion (AEC) working group**
  - 12 engine OEMs, 3 energy companies, 6 national labs, 6 univ's
  - Semi-annual meetings and presentations
- **Co-leading surrogate diesel fuel research conducted under auspices of CRC; participants from**
  - 3 energy co's., 1 Canadian + 5 US nat'l labs, 1 auto OEM, US Army
  - Tri-weekly teleconferences, tri-annual presentations
- **DOE/VT FOA 239 contract to study fuel effects on LLFC**
  - Partnership with Ford Motor Co.
  - Monthly teleconferences, quarterly reporting (ended March 2015)
- **NSF/DOE collaboration with Yale University, Chevron, and LLNL**
- **Work-for-others contract**
  - Funds-in agreement with Caterpillar Inc.
  - Tri-weekly teleconferences, semi-annual meetings

Remaining Challenges and Barriers

- **Diesel surrogate fuels**
  - The diesel surrogate fuels have not yet been rigorously evaluated experimentally in engines and combustion vessels
    - How much compositional fidelity is required to accurately match target-fuel performance in mixing-controlled (and other) combustion modes?
  - Numerical simulations have not yet been conducted or assessed for the diesel surrogate fuels
    - Are such models truly predictive? If not, what are the key barriers?
    - What experimental data can be used to assess the model results?
- **Achieving LLFC via ducted fuel injection is promising but remains largely untested, and fuel effects are unknown**
  - Duct-geometry and fuel optimization are needed
  - The concept requires simulation and testing in an engine environment
- **While successful with a 2-hole injector tip, it is not known whether LLFC can be sustained with oxygenated fuel at higher-load cond's**
  - Testing with a more-representative, 6-hole tip is needed

Proposed Future Work (through FY16)

- **Diesel surrogate fuels**
  - Engine testing of diesel surrogate/target-fuel pairs
    - Determine if adequate surrogate/target matching is achieved
    - Provide well-characterized, comprehensive experimental data for comparisons to computational modeling results
  - Work with modeling groups to conduct surrogate-fuel simulations and assess results
    - To help identify and overcome barriers to truly predictive modeling
- **Refine the vertical-sheet LII diagnostic for soot-model assessment**
  - For use with target, surrogate, and/or oxygenated fuels
- **Continue development of the ducted fuel injection concept**
  - Begin duct-geometry optimization and/or fuel-effects studies
- **Conduct experiments to determine whether LLFC can be sustained at higher loads using an oxygenated fuel and a 6-hole injector tip**
  - Use T50 and/or methyl decanoate

Summary

- **Goal of this research is to provide an improved understanding of fuel effects on advanced, mixing-controlled combustion strategies**
  - Focused on overcoming DOE MYPP barriers by providing high-quality data and analyses on fuel effects
    - To achieve cost-effective HECC with fuels that enhance energy security and environmental quality
  - Includes close collaboration and guidance from energy companies, engine manufacturers, national labs, and academia
- **Significant technical progress has been made**
  - Created and property-tested a set of improved diesel surrogate fuels
    - Distributed samples for engine and combustion-vessel testing
  - Developed an optical diagnostic to estimate total in-cylinder soot mass
  - Evaluated the efficacy of using oxygenated fuels to achieve LLFC
  - Conducted first experiments proving the ducted fuel injection (DFI) concept, a novel strategy for achieving cost-effective LLFC