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

Charles J. Mueller

Combustion Research Facility

Sandia National Laboratories

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Project ID#: FT004

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:
  FY13 – $800K
  FY14 – $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

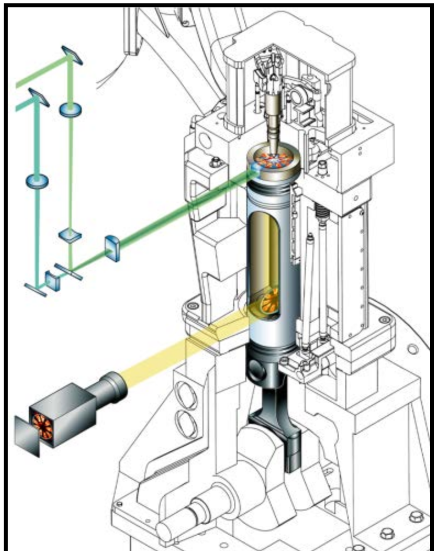
Develop the science base to enable high-efficiency, clean-combustion (HECC) engines using fuels that improve US energy security

- **Specific objectives of work since FY13 Annual Merit Review**
  - Formulate 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"
  - Analyze results from a robust, engine-based evaluation methodology for quantifying fuel effects on mixing-controlled combustion
    - Parametric study of five chemically well-characterized diesel reference fuels
  - Develop an in-cylinder diagnostic to allow soot visualization in the region above the piston bowl throughout the expansion stroke
    - To assess model validity and better understand fuel effects on soot field

Milestones

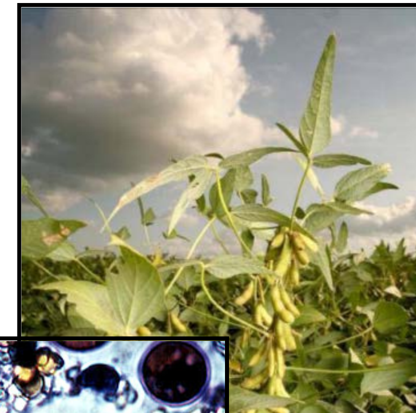
- ✓ **September 2013**
  Complete first publication from parametric study of effects of diesel reference fuels on engine combustion, efficiency, and emissions
- ✓ **December 2013**
  Demonstrate vertical-laser-sheet laser-induced incandescence imaging of in-cylinder soot with a fuel of interest
- **June 2014**
  Complete mixing-controlled combustion evaluation experiments on one or more target/surrogate fuel pairs
- **September 2014**
  Complete apparatus to evaluate fuel effects on the "Ducted Combustion Chamber" concept in Sandia's Constant-Volume Combustion Vessel
- **December 2014**
  Complete second publication from parametric study of effects of diesel reference fuels on engine combustion, efficiency, and emissions

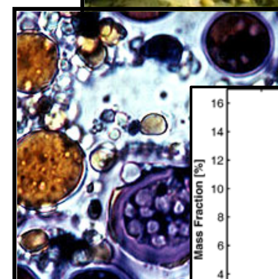
Approach

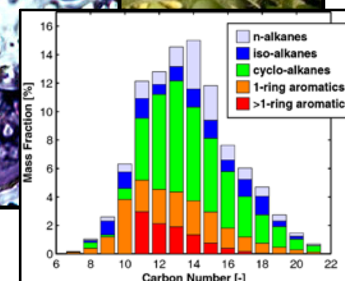


Unique and comprehensive diagnostic capabilities

Collaboration with key stakeholders







17 years of fuel-effects research

HECC engines using fuels that improve US energy security

Technical Accomplishments Summary

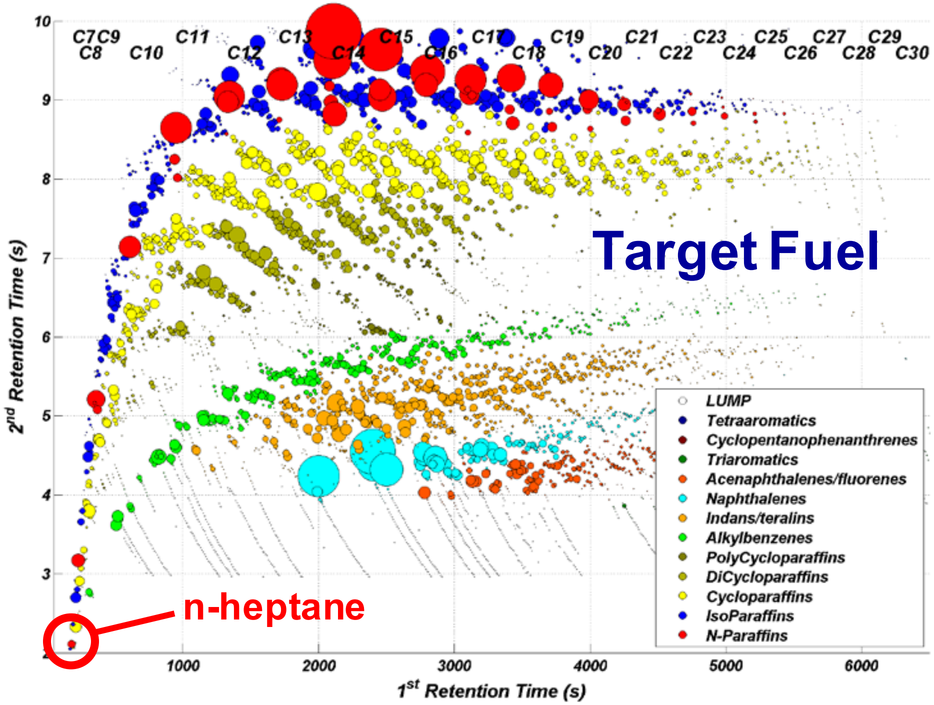
1. **Formulated a set of ultra-low-sulfur diesel surrogate fuels for engine and combustion-vessel testing**
   - Surrogates have three different fidelity levels of matching carbon bond types, ignition quality, volatility, and density to the target fuel
2. **Analyzed results from an engine-based evaluation methodology for quantifying fuel effects on mixing-controlled combustion**
   - Created and refined computational algorithms for holistic analysis of optical & conventional data, identified compelling trends
3. **Developed a vertical-sheet diagnostic to allow soot visualization in a large region above the piston bowl during expansion stroke**
   - To quantify soot-field characteristics for improved fundamental understanding and assessment of validity of CFD models
4. **Lead author of encyclopedia article entitled "Fuels for Engines and the Impact of Fuel Composition on Engine Performance"**
   - See http://onlinelibrary.wiley.com/book/10.1002/9781118354179

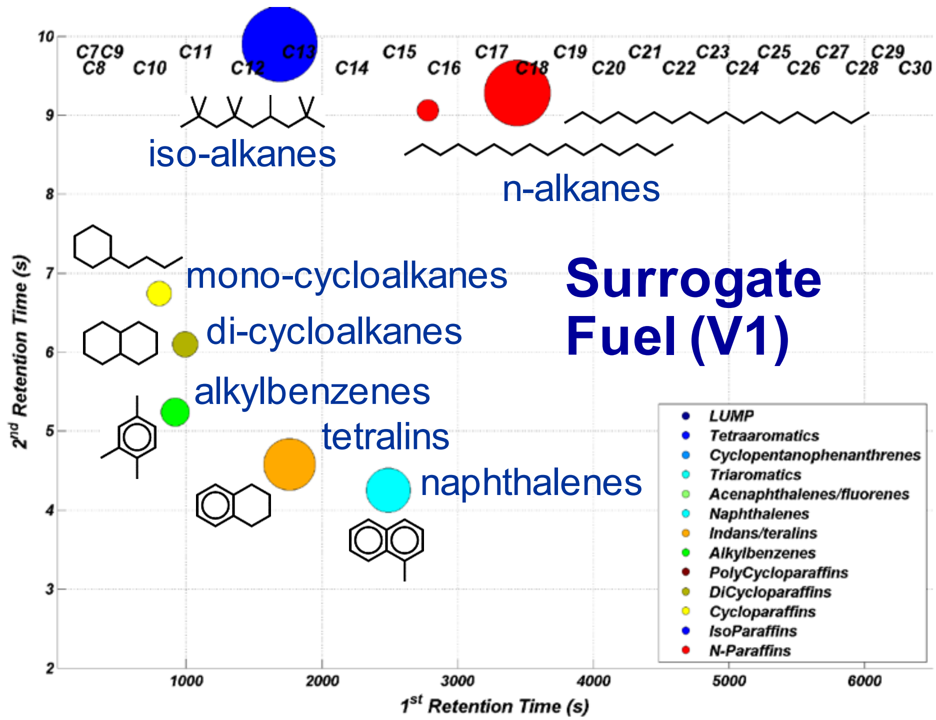
TA#1: Formulating and Testing Improved Diesel Surrogate Fuels (1 of 3)

- **Research challenge: Rigorously validated, realistic, and broadly accepted diesel surrogate fuels do not currently exist**
  - CRC Project AVFL-18/18a has addressed this issue by <u>developing and employing a methodology to formulate accurate surrogate fuels</u>
- **A desirable surrogate fuel has**
  - A simpler chemical composition than its corresponding target fuel
  - Composition and properties that are representative of the target fuel, exactly known, and computationally tractable
- **Surrogate fuels can be used as**
  - Realistic, reproducible reference fuels for conducting controlled experiments anytime and anywhere in the world
  - A necessary foundation for predictive computational engine design and optimization for evolving real-world fuels
  - Research tools for achieving a better understanding of fuel-composition and property effects

TA#1: Formulating and Testing Improved Diesel Surrogate Fuels (2 of 3)

- **Advanced compositional characterization data are essential**
  - Extensive use of 2D gas chromatography and nuclear magnetic resonance spectroscopy data from CanmetENERGY





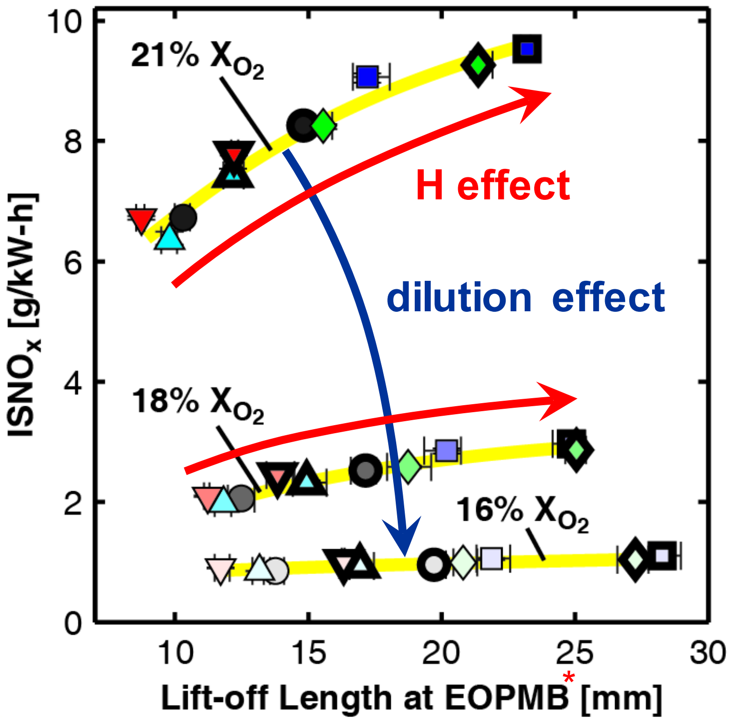
Source: Gieleciak, R. and Fairbridge, C., "Detailed Hydrocarbon Analysis of FACE Diesel Fuels Using Comprehensive Two-Dimensional Gas Chromatography," Report: CanmetENERGY CDEV-2013-2065-RT, 2013.

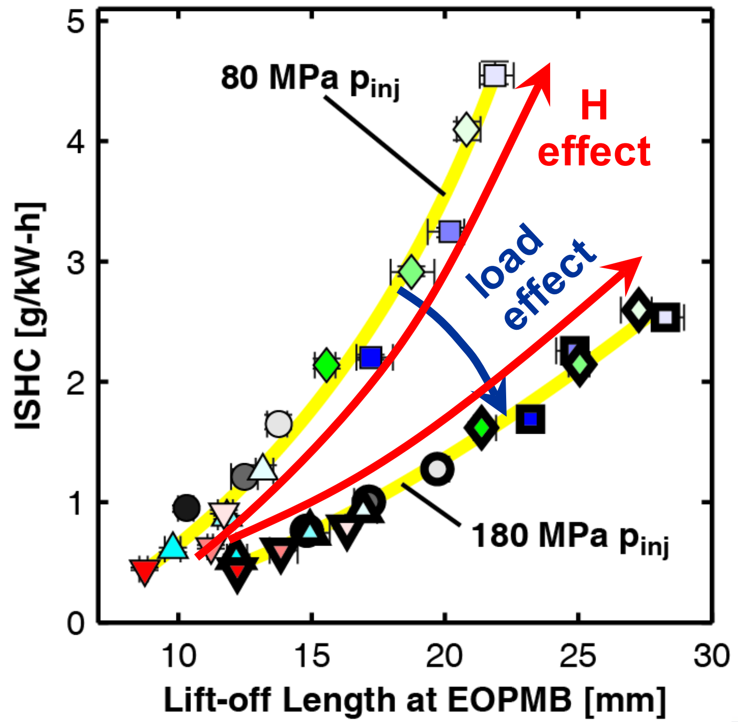
TA#1: Formulating and Testing Improved Diesel Surrogate Fuels (3 of 3)

- **Barriers that have been overcome**
  - Identifying and procuring more-representative palette compounds
    - High purity, low sulfur (esp. multi-ring), have property data, tolerable cost
  - Quantifying poly-cycloalkane content in target diesel fuel
  - Removal/prevention of ignition-accelerating contaminants
    - Silica-gel treatment, addition of anti-oxidant
  - Configuration and application of regression model
- **Current status**
  - Have formulated four surrogates for a #2 ULSD target fuel
    - V0a (4-component): Best simple surrogate proposed in the literature
    - V0b (5-component): Our best simple surrogate
    - V1 (8-component): Good trade-off between compositional fidelity and cost
    - V2 (9-component): Best composition and property fidelity
  - Treating and blending 30-L batches of the above surrogates for testing in engines & combustion vessels at US & Canadian labs

TA#2: Quantifying Fuel Effects on Mixing-Controlled Combustion

- **Research Challenge: Fuel effects on mixing-controlled CI combustion are not well understood**
  - Developed and applied an engine-based evaluation methodology
    - Uses conventional & optical diagnostics, FACE & other diesel fuels
  - Analysis codes have been written, compelling trends identified



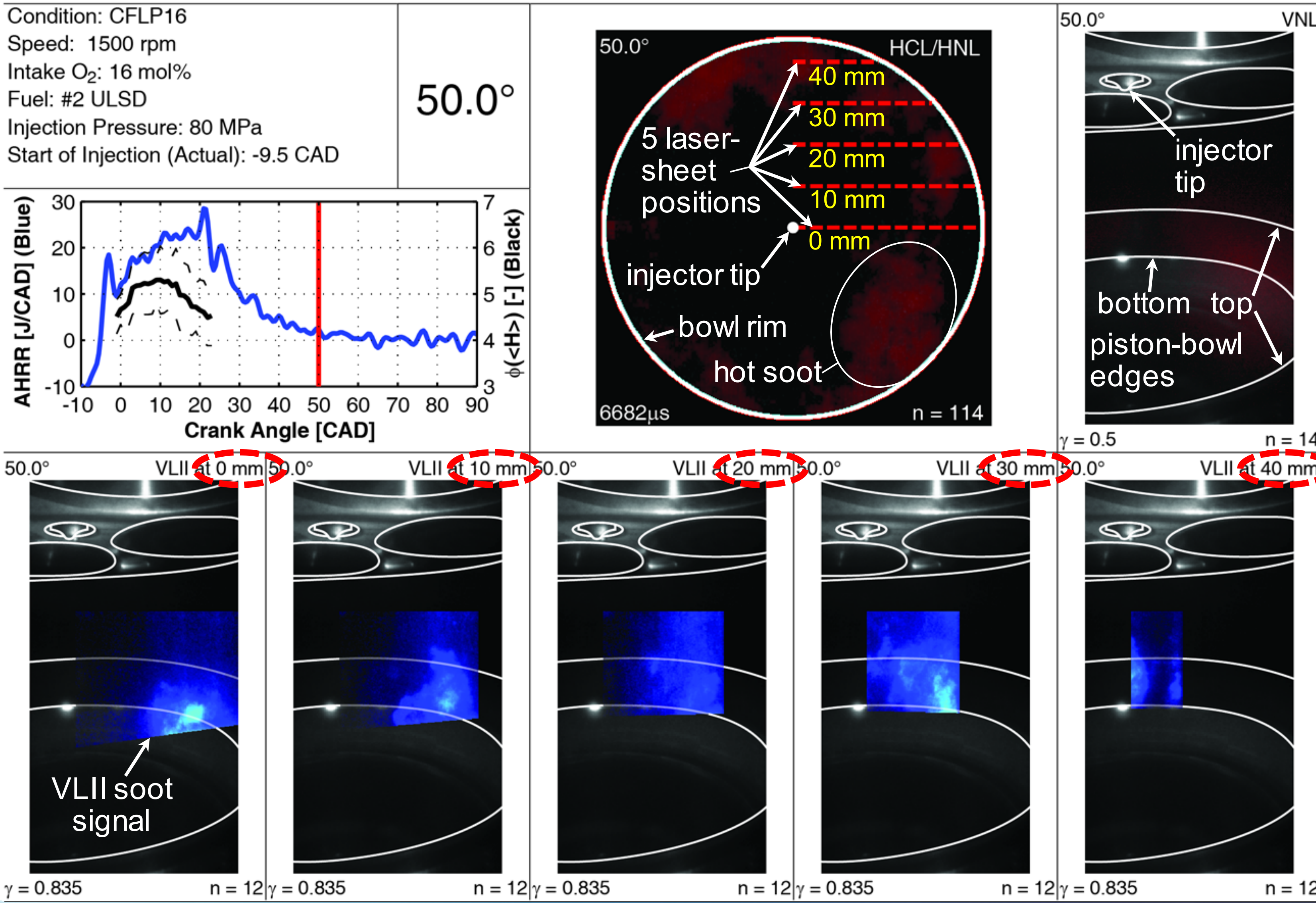


*End of pre-mixed burn

TA#3: Visualizing In-Cylinder Soot in Region above the Piston Bowl (1 of 2)

- **Research Challenge: Current models for predicting fuel effects on soot emissions are not sufficiently accurate, and there is a paucity of experimental data for determining where problems lie**
  - Diagnostic was developed to make soot-field measurements across the cylinder → can show how/where models need improvement
    - VLII = Vertical-sheet laser-induced incandescence of soot
      - New diagnostic
    - VNL = Vertical natural luminosity
    - HNL = Horizontal natural luminosity
    - HCL = Horizontal chemiluminescence of electronically excited OH radicals

TA#3: Visualizing In-Cylinder Soot in Region above the Piston Bowl (2 of 2)



Responses to FY13 Reviewers' Comments (1 of 2)

- **One or more reviewer comments were received on 33 points. The vast majority of comments were completely positive. All comments not addressed earlier that require action/clarification are addressed here.**
- **Comment: "Presentations are sometimes confusing [regarding] whether leaner lift-off is a key parameter to be targeted in all mixing control strategies…and whether it will apply to all fuels"**
  - Response: Leaner lifted-flame combustion (LLFC, i.e., combustion that doesn't produce soot) is <u>the</u> prime strategy for mixing-controlled combustion. It can be applied to any fuel, and is perhaps best suited to fuels with diesel-like ignition qualities (that also may contain oxygen).
- **Comment: "It is not clear the extent to which parameters of alternative and renewable fuels will be amenable to engineering vs. pre-determined by the feedstocks and economics of processing them. What may be more amenable to such designing could be more conventional fuels and possibly blends with renewable fuels..."**
  - Response: We agree. Oxygenate blends with hydrocarbon diesel are being studied in our LLFC research (e.g., see Eric Kurtz' presentation later in this session). Our planned future work also includes the testing of blends.

Responses to FY13 Reviewers' Comments (2 of 2)

- **Comment: "Integration with modeling efforts will help to better address the technical barriers of creating predictive tools..."**
  - Response: We co-authored a paper related to LLFC with Convergent Science Inc. during this reporting period; we are also currently partnering with LLNL, ANL, and Caterpillar to model our optical-engine results.
- **Comment: "Further work to better understand the fuel effects on mixing-controlled combustion results is essential"**
  - Response: Analysis for a 2nd publication on this topic is currently in progress.
- **Comment: "Describe more specifically how the tools being developed would be used – other than in theoretical exercises indicating that a fuel with ideal properties used in an engine optimized specifically for that fuel would not produce soot. Many alternative and renewable fuels have been promoted as beneficial when used in such purpose-built engines but such engine-fuel combinations are simply not feasible."**
  - Response: LLFC fuels are backward-compatible with existing CI engines. LLFC does not require a "purpose-built" engine or specific fuel, it only requires leaner mixtures at the lift-off length (higher inj. pressures, smaller orifices, oxygenated fuels, more boost, …).

Collaboration and Coordination with Other Institutions

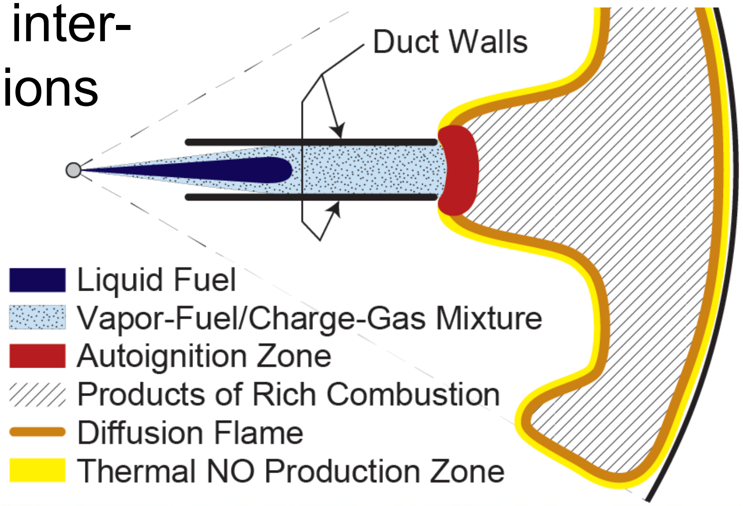
- **Combustion research conducted with guidance from Advanced Engine Combustion (AEC) working group**
  - 12 engine OEMs, 3 energy companies, 6 national labs, 6 univ's
  - Semi-annual meetings and presentations
- **Co-leading surrogate diesel fuel research conducted under auspices of CRC; participants 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
- **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

- **The new diesel surrogates have not been rigorously evaluated experimentally in engines and combustion vessels**
  - How much compositional fidelity is required to accurately match target-fuel performance in mixing-controlled combustion modes?
- **Numerical simulations have not been conducted or assessed for the new 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?
- **All of the fuel-effects data on mixing-controlled combustion (knowledge) have not yet been synthesized into a fundamental understanding of the underlying mechanisms (wisdom)**
  - Requires comprehensive analysis and hypothesis formation/testing
- **Even with oxygenated fuels, LLFC is challenging to achieve and sustain at high loads**
  - Need to consider novel in-cylinder mixing-enhancement approaches

Proposed Future Work (through FY15)

- **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 simulations, assess results**
  - To help identify and overcome barriers to truly predictive modeling
- **Synthesize results from study of fuel effects on mixing-controlled combustion into an improved fundamental understanding**
  - Identify the most important fuel-engine inter-actions governing efficiency and emissions
- **Investigate a novel in-cylinder mixing-enhancement approach for facilitating the achievement of LLFC**
  - "Ducted Combustion Chamber"



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 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**
  - Formulated a set of ultra-low-sulfur diesel surrogate fuels for engine/ combustion-vessel testing
  - Detailed analysis of fuel effects on mixing-controlled combustion data has yielded compelling trends pointing to underlying mechanisms
  - Created a new soot diagnostic to measure fuel effects on in-cylinder soot distributions and to assess soot models
  - Wrote encyclopedia article: fuel effects on engine combustion proc’s