Fuels and 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:
  FY11 – $760K
  FY12 – $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

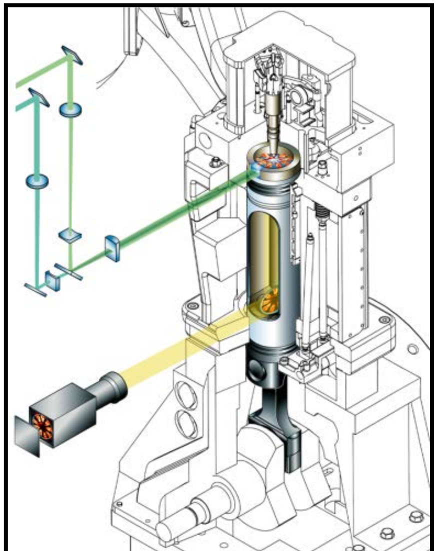
- Project lead: Sandia – C.J. Mueller (PI); C.J. Polonowski and C.E. Dumitrescu (post-docs); K.R. Hencken (part-time technologist)
- 15 industry, 6 univ., and 6 nat'l lab partners in Advanced Engine Combustion MOU
- Coordinating Research Council (CRC)
- Caterpillar Inc.

Relevance – Objectives

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

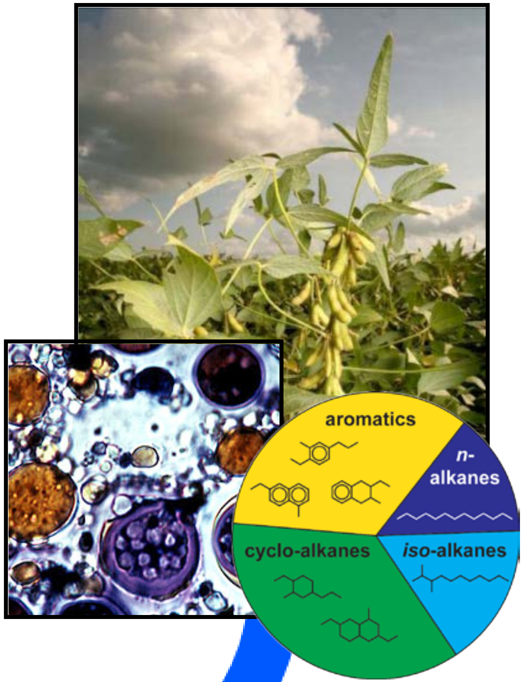
- **Specific objectives of work since FY11 Annual Merit Review**
  - Advance the state of the art of diesel surrogate fuels
    - As time-invariant reference fuels, to better understand fuel-component effects, and to enable computational engine optimization for evolving fuels
  - Quantify boundaries of Leaner Lifted-Flame Combustion (LLFC)
    - To achieve in-cylinder combustion that does not form soot
  - Develop a robust, engine-based screening technique for quantifying fuel effects on mixing-controlled combustion
    - Will be applied to characterize current and future fuels

Approach



Unique and comprehensive diagnostic capabilities

Collaboration with key stakeholders



15 years of fuel-effects research

HECC engines using fuels that improve US energy security

Approach – Milestones

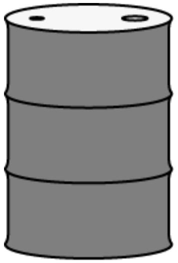
- ✓ **August 2011**
  Present paper describing 10-factor parametric study of leaner lifted-flame combustion (LLFC) with baseline #2 ultra-low-sulfur diesel fuel
- ✓ **February 2012**
  Submit to *Energy & Fuels* manuscript describing methodology that was developed and applied to create "Version 1" diesel surrogate fuels
- **August 2012**
  Complete mixing-controlled combustion screening experiments on subset of Fuels for Advanced Combustion Engines (FACE) diesel fuels
- **December 2012**
  Complete LLFC experiments with one or more oxygenated renewable fuels of interest
- **May 2013**
  Complete mixing-controlled combustion screening experiments on one or more target/surrogate fuel pairs

Technical Accomplishments Summary

1. **Co-led an international team of researchers that significantly advanced the state of the art of diesel surrogate fuels**
   - Two surrogate fuels were created using an improved technique
   - Wrote and submitted manuscript summarizing initial results
2. **Quantified soot-formation regimes for mixing-controlled combustion with baseline #2 diesel certification fuel**
   - Equivalence ratio at lift-off length appears to be key parameter
   - Showed important role of soot production near end of injection
3. **Developing a robust, engine-based screening technique for quantifying fuel effects on mixing-controlled combustion**
   - Experiment design is critical
   - Utilizes a comprehensive set of conventional and optical diagnostics

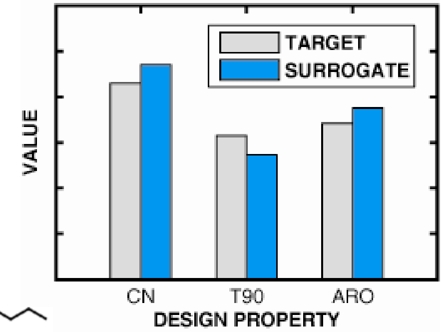
TA#1: Advanced the State-of-the-Art of Diesel Surrogate Fuels

- **Target fuel**
  - A "real" fuel with selected properties that are to be matched by a surrogate fuel

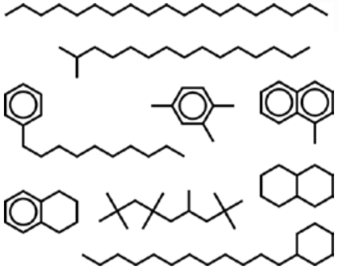


- **Surrogate fuel**
  - Fuel composed of a small number of pure compounds that is formulated to match selected properties of a target fuel

- **Design properties**
  - Selected properties of the target fuel that are to be matched by the surrogate fuel

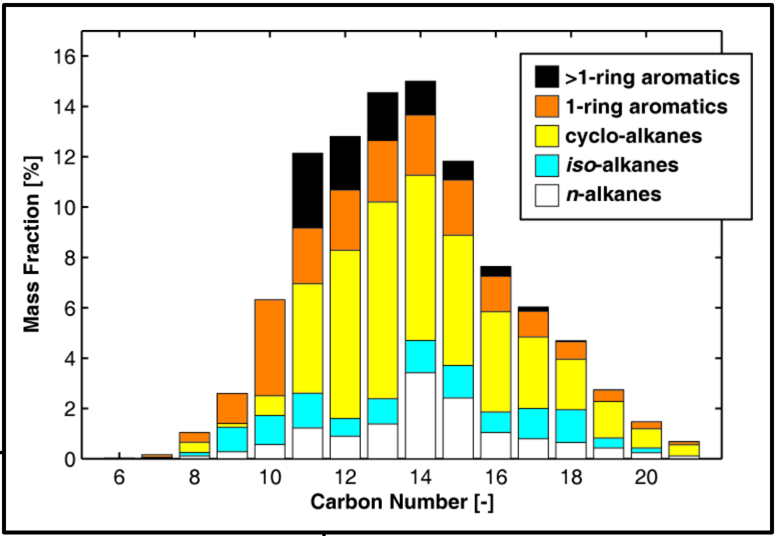


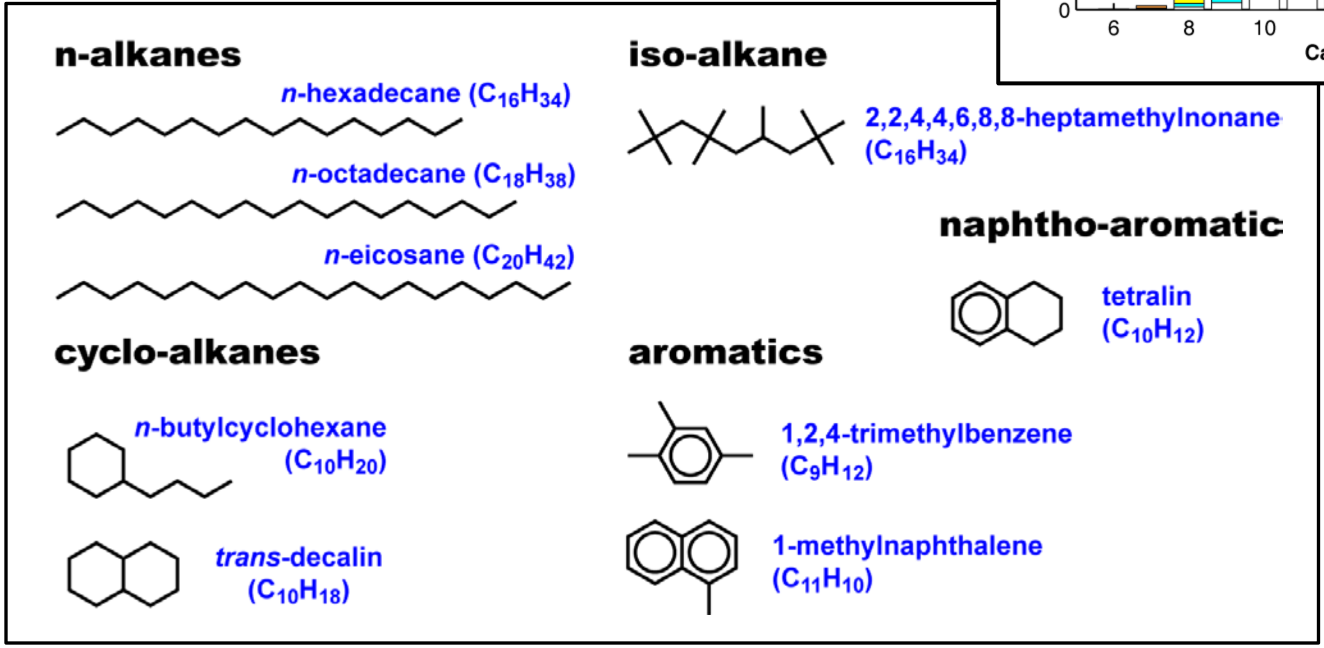
- **Surrogate palette**
  - The set of pure compounds that are blended together to create a surrogate fuel



TA#1: Advanced the State-of-the-Art of Diesel Surrogate Fuels

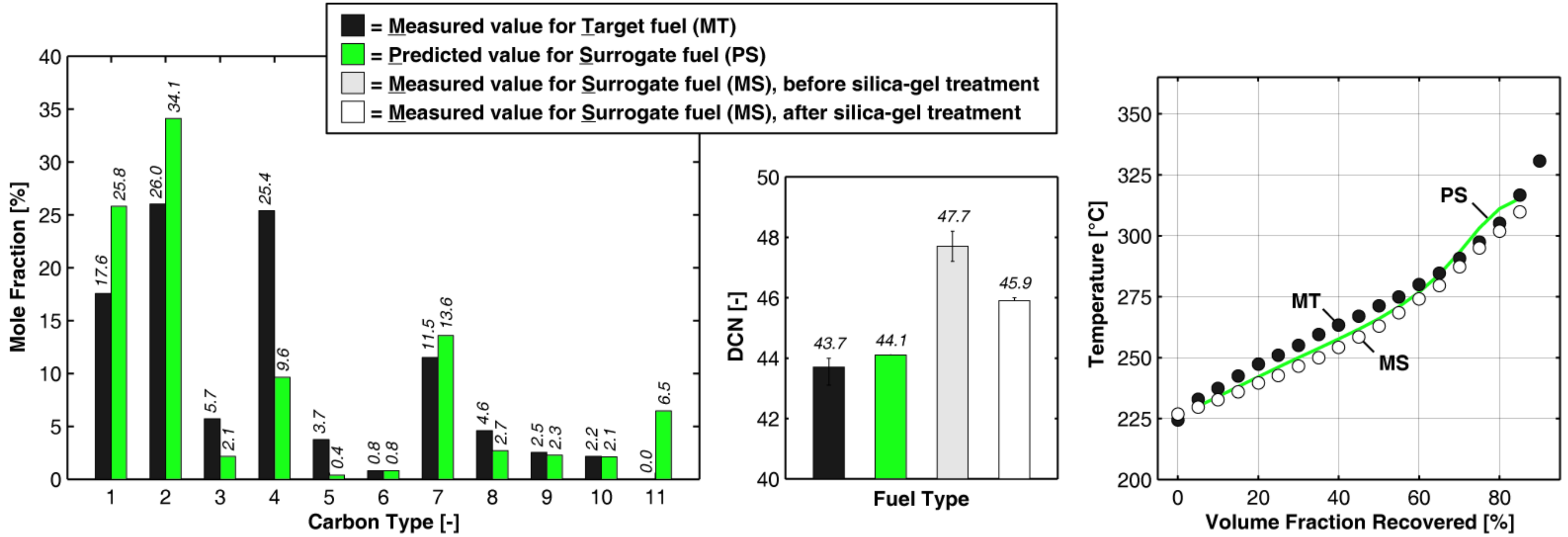
- **Used detailed target-fuel characterization data from CanmetENERGY…**
- **… to create a palette that contains all major hydrocarbon classes present in the target fuels**





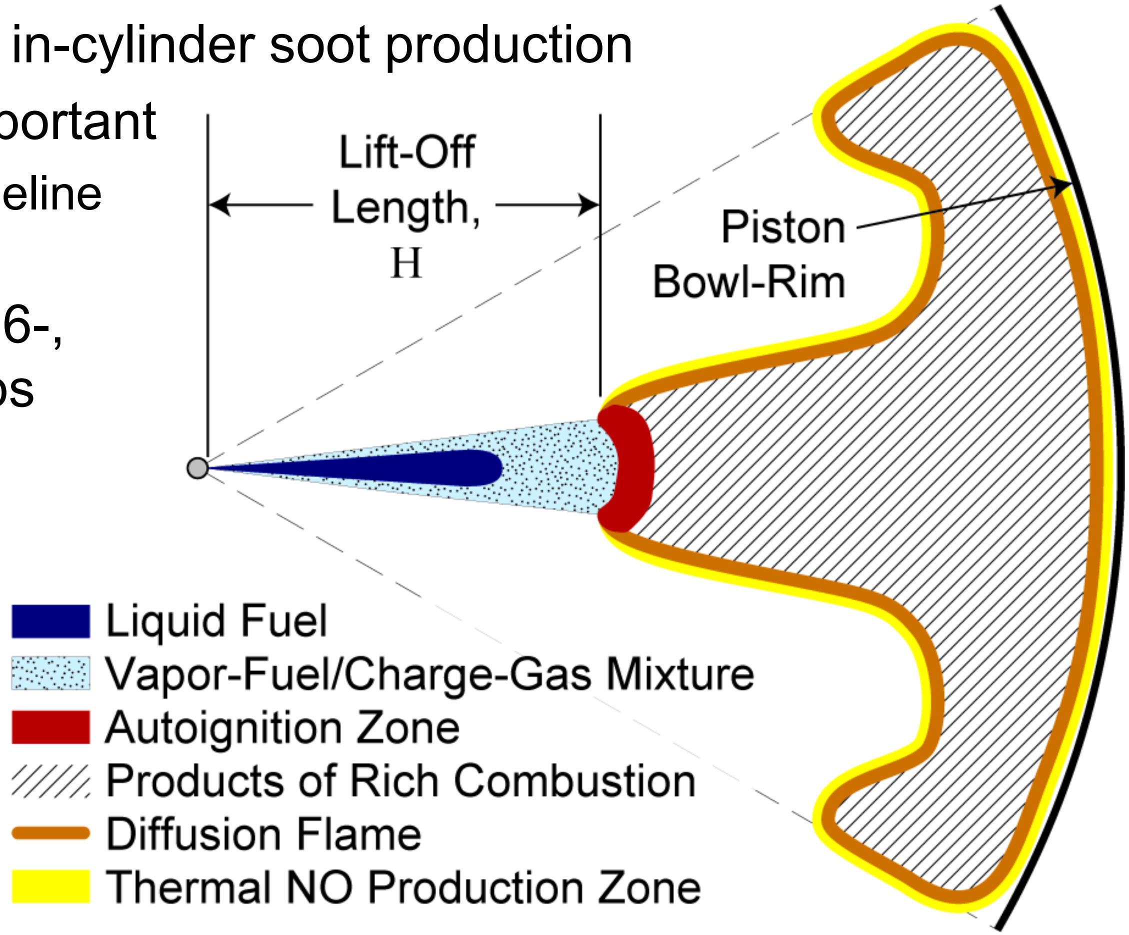
TA#1: The New Surrogate-Formulation Technique Works Well

- **Good matching of property targets was achieved**
  - 5 of 11 carbon-bond types were matched within ± 3 mol%, error in others averaged 7.3 mol%
  - Surrogate DCNs (derived cetane numbers) initially ~10% too high
    - Improved to 3.9% higher after removal of ignition-accelerating impurities
  - Surrogate advanced distillation curve points averaged 2.1% lower

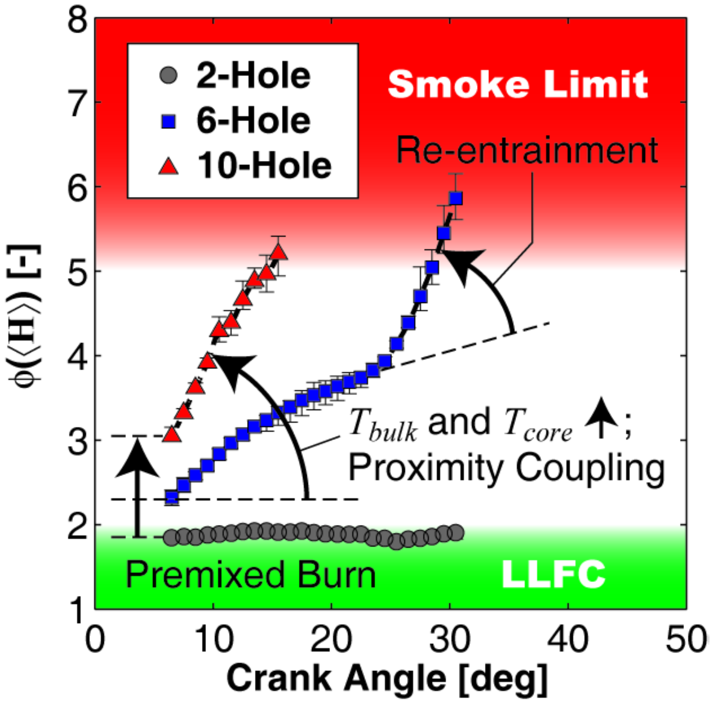


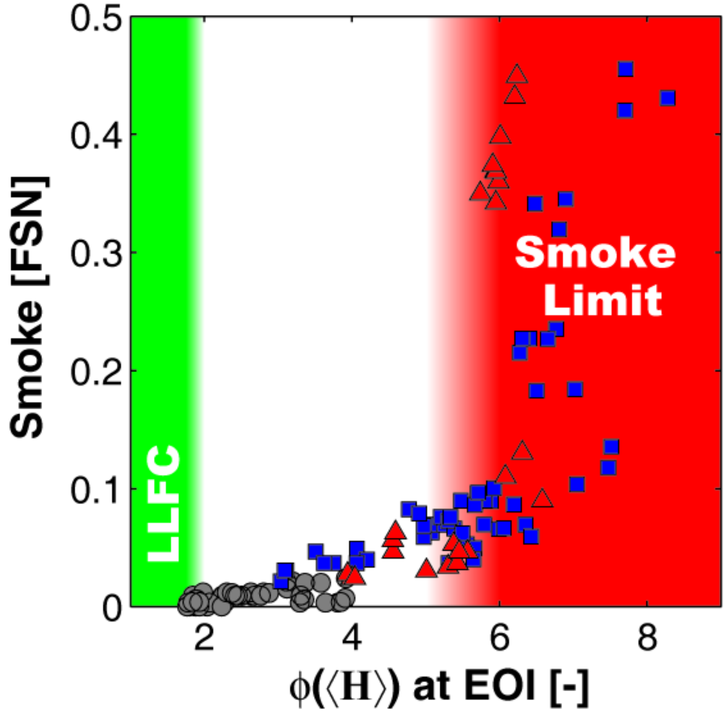
TA#2: Improved Understanding of Leaner Lifted-Flame Combustion (LLFC)

- **LLFC: Equivalence ratio at lift-off length, $\phi(H)$, is leaner (closer to stoichiometric) than for conventional diesel combustion**
  - Objective is to prevent in-cylinder soot production
  - Fuel effects can be important
    - 1st step: establish baseline with #2 diesel fuel
  - Data acquired with 2-, 6-, and 10-hole injector tips
    - 106 µm diameter
    - 240 MPa injection pressure
    - Single injection near TDC



TA#2: LLFC Is the Goal, but Smoke Can Be Acceptable Even without LLFC

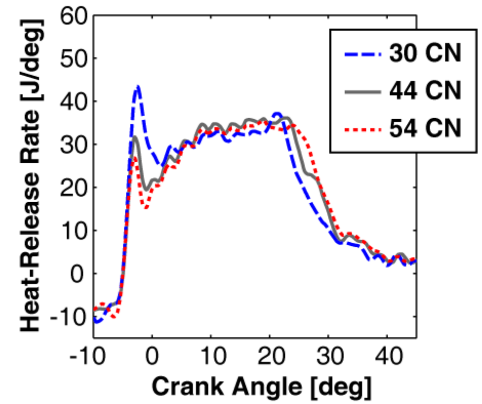


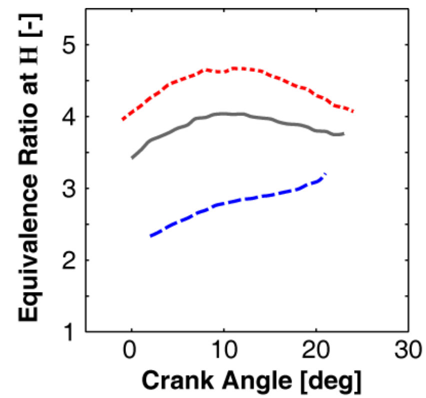


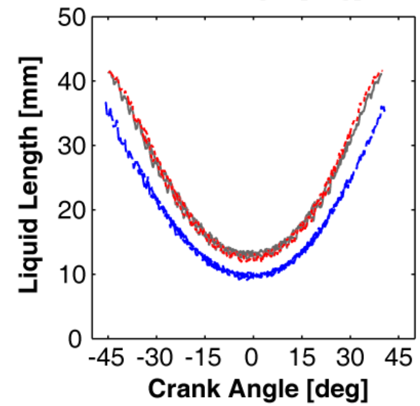
- **Three sooting regimes based on $\phi(H)$ at end of injection (EOI)**
  - $\phi(H)$ at EOI < 2 → No soot formed → LLFC
  - 2 < $\phi(H)$ at EOI < 5 → Most soot formed is oxidized before exhaust valves open → Acceptable smoke emissions
  - $\phi(H)$ at EOI > 5 → Unacceptable smoke emissions

TA#3: Quantifying Fuel Effects on Mixing-Controlled Combustion

- **Problem: Currently no robust, general technique exists for determining fuel effects on mixing-controlled combustion and emissions**
  – We are developing such a technique
- **Involves a comprehensive set of diagnostics**
  – Cylinder-pressure based: heat release, T_{bulk}, …
  – Engine-out emissions: smoke, NOx, HC, CO, …
  – Efficiency
  – Lift-off length (H) $\rightarrow$ equivalence ratio at H
  – Liquid-phase fuel penetration (“liquid length”)
  – Injection rate, soot incandescence
- **Using 2-hole tip helps avoid geometry-dependent effects such as jet-jet interactions**
- **1st application is to FACE diesel fuels**







Collaboration and Coordination with Other Institutions

- **Mixing-controlled combustion research conducted with guidance from Advanced Engine Combustion Memorandum of Understanding (MOU) working group**
  - 10 engine OEMs, 5 energy companies, 6 national labs, 6 universities
  - Semi-annual meetings and presentations
- **Surrogate diesel fuel research conducted under auspices of the Coordinating Research Council (CRC); working group includes participants from**
  - 4 energy companies, 1 Canadian + 6 US national labs, 1 auto OEM
  - Tri-weekly teleconferences, tri-annual presentations
- **Work-for-others contract**
  - Funds-in agreement with Caterpillar Inc.
  - Tri-weekly teleconferences, semi-annual meetings

Proposed Future Work (through FY13)

- **Apply the robust, engine-based screening technique for quantifying fuel effects on mixing-controlled combustion**
  - Comprehensive diagnostics: lift-off length, liquid length, emissions, efficiency, heat release, soot incandescence
  - 1st application will be to a subset of the FACE diesel fuels
  - Other potential fuels: biodiesel esters, heavy ethers
- **Engine testing of diesel surrogate/target-fuel pairs**
  - Employ new screening technique discussed above to determine whether adequate matching has been achieved
  - Explore effects of new palette compounds and/or new formulation strategies
  - Testing also planned for other experimental facilities in US & Canada
- **Conduct research focused on overcoming barriers to LLFC**
  - Employ oxygenated biofuel(s)
  - Utilize new fuel-flexible, 3000-bar, common-rail fuel-supply system

Summary

- **This research is dedicated to providing an improved under-standing of fuel effects on advanced combustion strategies**
  - Focused on overcoming DOE MYPP barriers by developing predictive tools and providing data on fuel effects
    - To achieve HECC with fuels that enhance energy security and environmental quality
  - Includes close collaboration and guidance from engine mfrs., energy companies, national labs, and academia
- **Significant technical progress has been made**
  - Created improved diesel surrogate fuels to facilitate predictive modeling and computational engine optimization for current and emerging fuels
  - Improved the understanding of LLFC, a HECC strategy that is synergistic with oxygenated domestic renewable fuels
  - Developing a robust, engine-based technique for quantifying fuel effects on mixing-controlled combustion