Fuels and Combustion Strategies for High-Efficiency Clean-Combustion Engines

Charles J. Mueller
Combustion Research Facility
Sandia National Laboratories

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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
HECC engines using fuels that improve US energy security

Approach

Unique and comprehensive diagnostic capabilities

Collaboration with key stakeholders

15 years of fuel-effects research
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

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<tr>
<th>n-alkanes</th>
<th>iso-alkane</th>
<th>cyclo-alkanes</th>
<th>aromatics</th>
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<tr>
<td>n-hexadecane (C₁₆H₃₄)</td>
<td>2,2,4,4,6,8,8-heptamethylnonane (C₁₆H₃₄)</td>
<td>n-octadecane (C₁₈H₃₈)</td>
<td>1,2,4-trimethylbenzene (C₉H₁₂)</td>
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<td>n-eicosane (C₂₀H₄₂)</td>
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<td></td>
<td>1-methylnaphthalene (C₁₁H₁₀)</td>
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<td></td>
<td>n-butylcyclohexane (C₁₀H₂₀)</td>
<td>trans-decalin (C₁₀H₁₈)</td>
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Mass Fraction [%]
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

Diagram:
- Lift-Off Length, $H$
- Piston Bowl-Rim
- Liquid Fuel
- Vapor-Fuel/Charge-Gas Mixture
- Autoignition Zone
- Products of Rich Combustion
- Diffusion Flame
- Thermal NO Production Zone
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, $T_{\text{bulk}}$, …
  - 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 understanding 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