Mark P. B. Musculus
Combustion Research Facility
Sandia National Laboratories

FY 2010 DOE Vehicle Technologies Program Annual Merit Review
Advanced Combustion Engine R&D/Combustion Research
8:30 – 9:00 AM, Tuesday, May 10, 2011

Sponsor: U.S. Dept. of Energy, Office of Vehicle Technologies
Program Manager: Gurpreet Singh
## Heavy-Duty Combustion Project Overview

### 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/VT:
  - FY10-SNL/UW: $660/115K
  - FY11-SNL/UW: $700/115K

### Barriers
- Inadequate understanding of fuel injection, mixing, thermodynamic combustion losses, combustion/emission formation processes.
- Inadequate capability to accurately simulate these processes.

### Partners
- University of Wisconsin
- 15 industry partners in the AEC MOU
- Project lead: Sandia (Musculus)
Heavy-Duty In-Cylinder Combustion Objectives

Long-Term Objective
Develop improved understanding of in-cylinder LTC spray, combustion, and pollutant-formation processes required by industry to build cleaner, more efficient, heavy-duty engines

Current Specific Objectives:

1. SNL - Quantify oxidation of piston-bowl soot remaining from main injection by narrow included-angle post-injections
2. SNL+UW – Characterize RCCI combustion using high-speed imaging diagnostics
3. SNL+UW - Define the in-cylinder conditions that govern flame propagation / distributed autoignition combustion modes
4. UW - Compare multi-mode combustion model predictions to measurements of combustion propagation
Heavy-Duty In-Cylinder Combustion Milestones

1. (SNL+UW) Demonstrate dual-fuel system in SNL heavy-duty optical engine.
2. (SNL+UW) Characterize combustion propagation for high-efficiency dual-fuel RCCI.
3. (UW) Compare multi-mode combustion model predictions to measurements of combustion propagation.
**Approach: Optical Imaging and CFD Modeling of In-Cylinder Chemical and 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

- 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., UHC for LTC, soot in higher load conditions)

- Industrial partners provide equipment and support for laboratory activities
Accomplishments (19 slides)

Accomplishments for each of the four current specific objectives below are described in the following nineteen slides.

**Current Specific Objectives:**

1. **SNL** – Quantify narrow included-angle post-injections oxidation of piston-bowl soot from the main injection.
2. **SNL+UW** – Characterize RCCI combustion using high-speed imaging diagnostics.
3. **SNL+UW** – Define the in-cylinder conditions that govern flame propagation / distributed autoignition combustion modes.
4. **UW** – Compare multi-mode combustion model predictions to measurements of combustion propagation.
Previous data showed how post injections oxidize squish-soot, but bowl-soot remains.

- 2009 data showed that with a constant main injection, adding a post increases soot at small dwell, but decreases soot at larger dwell.
- Wide-angle (154°) injector: soot is split between bowl and squish.
- A late post-injection oxidizes soot, but only in the squish region.
- Most soot, in the piston bowl, is not affected by post injection.

How well can piston-bowl soot from the main injection be oxidized by post-injection into the bowl (narrow-angle inj.)?
Post-injections with narrow-angle provide similar soot-reduction as with wide-angle

- Narrow-angle (124°) injector yields much more exhaust soot (FSN 1.5 vs. 0.6)
- Post injection reduces soot, but only modestly (similar to 154°)

- Soot luminosity images show post-injection impinging on bowl-window and disturbing bowl-soot
  - Can significantly affect 2-color measurements
- In-cylinder 2-color KL data: considerable scatter, no clear trends.
Developed new GDI system to expand capabilities to dual fuels, premixed charge

- U. Wisc. (Reitz et al.) has shown mid-load $\eta_{th} > 50\%$ at 2010 PM/NOx in-cyl. with dual-fuel gasoline/diesel
- Presents both a modeling challenge and a diagnostic opportunity
  - Both distributed autoignition and flame propagation are possible.

- GDI side-injector system for gasoline fuels designed and installed in optical engine.
- UW modeling student (Sage Kokjohn) to visited Sandia for 8 months in FY2010/11
  - Optical diagnostic study of flame propagation / autoignition to improve model fidelity
Central Common-Rail + side-mounted GDI enable dual-fuel (RCCI) capability

- Bosch GDI (100 bar) mounted in place of side-window
  - Premixed charge of gasoline-like fuel
- 8-hole production Cummins XPI common-rail fuel injector (300-1600 bar) in cylinder head
  - Direct injection of diesel-like fuel
- Sprays illuminated using CW high-power LED white-light source through side-windows
LTC: RCCI with n-heptane & iso-octane

- No EGR
- GDI from top of view, CR in center
- High gain: cool flame visible, no soot

Fuel (net) PRF64 ($\phi=0.42$)
Intake 21% $O_2$ (EGR)
Load 4.3 bar IMEP
Intake T 90°C
Intake P 1.15 bar
GDI SOI -240° ATDC
CR SOI -57°, -37° ATDC
Speed 1200 rpm
Engine $r_c$ 10.75
Window 100 mm diam
Framing 7200 fps
Gain 500
Filter 500 nm SWP
RCCI: Fuel reactivity and $\phi$ stratification are important for managing peak heat release rate

- Common-rail (n-heptane) SOI timing sweep creates range of equivalence ratio ($\phi$) and reactivity stratification
- CA50 held constant at 2° ATDC by adjusting intake temperature
- Minimum peak AHRR: SOI= -50° ATDC
- Higher AHRR at both earlier and later SOI

**Operating Conditions**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
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</thead>
<tbody>
<tr>
<td>Engine speed</td>
<td>1200 rpm</td>
</tr>
<tr>
<td>Gross IMEP</td>
<td>4.2 bar</td>
</tr>
<tr>
<td>Intake temperature</td>
<td>73 to 100 °C</td>
</tr>
<tr>
<td>Intake pressure</td>
<td>1.1 bar abs.</td>
</tr>
<tr>
<td>Inlet oxygen concentration</td>
<td>21 vol. %</td>
</tr>
<tr>
<td>CR SOI</td>
<td>-165 to -15° ATDC</td>
</tr>
<tr>
<td>GDI SOI</td>
<td>-240° ATDC</td>
</tr>
<tr>
<td>n-heptane mass (CR)</td>
<td>36%</td>
</tr>
<tr>
<td>iso-octane mass (GDI)</td>
<td>64%</td>
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<tr>
<td>Premixed equivalence ratio</td>
<td>0.27</td>
</tr>
<tr>
<td>Overall equivalence ratio</td>
<td>0.42</td>
</tr>
</tbody>
</table>

*See back-up slide for still-image summary*
Mid-range SOI (-50° ATDC) ignites in squish and burns gradually to center of cylinder

- Likely moderate fuel reactivity and concentration gradients at ignition

**CR SOI:** -50° ATDC
- Intake Temperature: 92° C
- Global equivalence ratio: 0.42

*See back-up slide for still-image summary*
Early SOI (-145° ATDC) ignites in pockets throughout chamber and burns quickly

- Likely low fuel reactivity and concentration gradients at ignition (HCCI-like)

CR SOI: -145° ATDC
Intake Temperature: 93° C
Global equivalence ratio: 0.42
Late SOI (-15° ATDC) ignites in jets (premixed burn), some mixing-controlled combustion

- Likely strong reactivity and concentration gradients with rich jet mixtures (diesel-like)

CR SOI:
-145° ATDC
Intake Temperature: 85° C
Global equivalence ratio: 0.42

*See back-up slide for still-image summary
Focused high-power laser beam pulse creates positionable plasma for spark ignition

- Focused laser beam (~100 mJ) creates plasma (spark)
  - Can probe ignitability of mixtures to explore combustion regimes (flame propagation/distributed autoignition)
- Multiple combustion modes achievable
  - Spark Ignition
    - For study of known flame propagation regime
  - HCCI
    - For study of known distributed autoignition regime
  - RCCI
    - Combustion strategy where both autoignition and distributed autoignition are possible
**HTC: Conventional Spark-Ignition**

- GDI only, throttled, near stoich.
- Laser spark at center
- High-speed chemiluminescence

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**Cycle 2**

- Fuel: iso-octane (φ=0.95)
- Intake: 21% O₂
- Load: 4 bar IMEP
- Intake T: 30°C
- Intake P: ~0.5 bar
- Spark: -25° ATDC
- Speed: 1200 rpm
- Engine rₜ: 10.75
- Window: 100 mm diam
- Framing: 7200 fps
- Gain: 300
- Filter: 500 nm SWP

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*See back-up slide for still-image summary*
Subsequent fuel-tracer PLIF shows GDI fuel (iso-octane) is not very uniform.

<table>
<thead>
<tr>
<th>Parameter</th>
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<tr>
<td>Fuel</td>
<td>PRF57 (φ=0.35)</td>
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<tr>
<td>Intake</td>
<td>21% O₂ (EGR)</td>
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<tr>
<td>Load</td>
<td>3.7 bar IMEP</td>
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<tr>
<td>Intake T</td>
<td>90°C</td>
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<tr>
<td>Intake P</td>
<td>1.15 bar</td>
</tr>
<tr>
<td>GDI SOI</td>
<td>-240° ATDC</td>
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<tr>
<td>CR SOI</td>
<td>-345° ATDC</td>
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<tr>
<td>Speed</td>
<td>1200 rpm</td>
</tr>
<tr>
<td>Engine r_C</td>
<td>10.75</td>
</tr>
<tr>
<td>Window</td>
<td>100 mm diam</td>
</tr>
<tr>
<td>Framing</td>
<td>7200 fps</td>
</tr>
<tr>
<td>Gain</td>
<td>500</td>
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<tr>
<td>Filter</td>
<td>500 nm SWP</td>
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LTC: RCCI with n-heptane & iso-octane

- No EGR
- GDI from top of view, CR in center
- High gain: very little soot, cool flame

Fuel (net) PRF64 ($\phi=0.42$)
Intake 21% O$_2$ (EGR)
Load 4.3 bar IMEP
Intake T 90°C
Intake P 1.15 bar
GDI SOI -240° ATDC
CR SOI -57°, -37° ATDC
Speed 1200 rpm
Engine $r_C$ 10.75
Window 100 mm diam
Framing 7200 fps
Gain 500
Filter 500 nm SWP
Laser-spark to define combustion regimes

- Just before SOC, Laser spark in center of cylinder
- Center mixture does not support flame propagation

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<tr>
<td>Intake</td>
<td>21% O(_2) (EGR)</td>
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<tr>
<td>Load</td>
<td>4.3 bar IMEP</td>
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<td>Intake T</td>
<td>90° C</td>
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<tr>
<td>Intake P</td>
<td>1.15 bar</td>
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<td>-240° ATDC</td>
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<tr>
<td>CR SOI</td>
<td>-57°, -37° ATDC</td>
</tr>
<tr>
<td>Engine (r_C)</td>
<td>10.75</td>
</tr>
<tr>
<td>Window</td>
<td>100 mm diam</td>
</tr>
<tr>
<td>Framing</td>
<td>7200 fps</td>
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• Just before SOC, Laser spark near piston bowl
• Bowl-edge mixture often supports flame propagation

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<td>Filter</td>
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</table>
4 Models: flame propagation required to capture lift-off edge-flame, kinetics sufficient otherwise

- For both conventional diesel and LTC, combustion structure is virtually identical with (KIVA-G) or without (KIVA) flame propagation submodels (kinetics models are sufficient)

- Flame propagation sub-models are required to capture triple-flame structure at the lift-off location.

- Only non-negligible flame speed is in nose-like structure in near-stoichiometric region at lift-off length.
4 Models: RCCI mostly distributed autoignition, but some flame propagation locally

- For simulations of a heavy-duty engine at many RCCI conditions, the global combustion characteristics can be captured without consideration of flame propagation.

- Models predict that most of RCCI combustion is dominated by distributed auto-ignition, though flame propagation is important in some regions, depending on local conditions (e.g., equivalence ratio).

![Simulations without flame propagation model](image)
Future Plans: High-efficiency dual-fuel experiments and modeling, LTC soot, and multiple injections

- Probe in-cylinder mixing and combustion processes of high-efficiency dual-fuel operation
  - Build a fundamental understanding of in-cylinder processes that contribute to improved efficiency.
  - Incorporate insight and validation data from optical experiments exploring transitions from distributed autoignition to flame propagation to improve model fidelity

- Explore multiple-injection efficiency and emissions
  - Quantify emissions and efficiency improvements across wide parameter space to identify critical requirements
  - Use laser diagnostics (fuel-tracer, formaldehyde, and OH PLIF) to understand governing in-cylinder mechanisms

- Build understanding of in-cylinder LTC soot and PAH
  - Use multiple laser wavelengths and high-temporal-resolution imaging/spectroscopy to track PAH growth and conversion to soot
Improved understanding of in-cylinder LTC spray, combustion, and pollutant-formation to help industry build cleaner, more efficient, heavy-duty engines

1. (SNL) Narrow-angle injection: higher soot than wide-angle, but similar post-injection oxidation

2. (SNL+UW) New GDI enables RCCI, high-speed imaging shows heat release affected by reactivity gradients

3. (SNL+UW) Laser-spark ignition probe combustion regimes for understanding and model development

4. (UW) Models predict most combustion dominated by kinetics, but flame propagation important locally
Summary: Fuel reactivity and $\phi$ stratification important for managing peak heat release rate

- Over- or under-stratification results in rapid energy release.
- Early SOI: Low reactivity & concentration gradients (HCCI-like)
- Mid-range SOI: Moderate reactivity & concentration gradients (RCCI)
- Late SOI: Strong gradients with rich jet mixtures (diesel-like)
With dual-fuel injection and laser ignition, multiple known combustion modes achievable

- Combustion regimes for RCCI and other LTC (and conventional) strategies may span from flame propagation to distributed autoignition
  - Can be important for both modeling and high-efficiency operation
- Defined combustion regimes provide reference for optical diagnostics

Spark Ignition: Flame Propagation

HCCI: Distributed Autoignition
• GDI sprays (100 bar) are first, entering at top of field of view
  – Creates premixed charge of iso-octane (PRF 100)
• Common-rail sprays (600 bar) occur in two injections, emanating from centrally located injector in cylinder head
  – Direct injection of n-heptane (PRF0)
• Gives overall PRF=64
• Sprays illuminated using CW high-power LED white-light source through side-windows