EFFECTS OF OXYGENATED DIESEL FUELS ON IN-CYLINDER COMBUSTION AND SOOT-FORMATION PROCESSES

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Blending oxygen-containing compounds ("oxygenates") with diesel fuel can lead to reduced soot and NOx emissions, as well as reduced fuel consumption. The detailed mechanisms that cause such reductions are not well understood. For instance, the literature contains conflicting results as to whether overall blend oxygen content is the only important parameter in determining the soot-reduction potential of a given blend, or if oxygenate molecular structure or other variables also play significant roles. To begin to resolve this controversy, in-cylinder measurements of direct luminosity (DL) coupled with heat-release and efficiency analyses were made using three oxygenated blends. For comparison purposes, results also are presented for a 45-cetane non-oxygenated blend of two $C_{16}H_{34}$ primary reference fuels (CN45). The DL image sequences show the evolution of regions of high soot concentration and temperature throughout the combustion event. A 1200-rpm, moderate-load operating condition was studied using a modern-technology, 4-stroke, heavy-duty DI diesel engine that has been modified to provide extensive optical access into the combustion chamber. Injection timing was optimized independently for each fuel such that the engine always operated at peak efficiency.

In an attempt to isolate molecular structure effects on ignition, combustion, and soot-formation processes, the overall oxygen contents of two of the three oxygenated blends were matched at 26 wt% by blending with $C_{16}H_{34}$ primary reference fuels. Combustion phasing also was matched by adding an ignition improver to the lower-cetane blend. The first blend, denoted GE80, was composed of 80 vol% tri-propylene glycol methyl ether and 20 vol% heptamethylnonane. The second blend, denoted BM88, was composed of 88 vol% di-butyl maleate, 7 vol% *n*-hexadecane, and 5 vol% ethylhexyl nitrate ignition improver. Whereas no dramatic differences between ignition or combustion processes between blends are evident from the DL images, spatially-integrated DL data (used as a measure of the amount of in-cylinder soot) are twice as great for BM88 as for GE80. Although further experiments are required, these initial results suggest that overall oxygen content may not be the only important parameter in determining the soot-reduction potential of an oxygenated blend.

The third oxygenated fuel had an oxygen content of 50 wt% and a cetane number < 5 such that glow plug (GP) assisted ignition was essential for stable engine operation. The fuel, denoted M100, was composed of methanol and 95 ppmv of a commercially-available corrosion-inhibiting additive. The M100 data show significant departures from the traditional diesel combustion features exhibited by CN45. Whereas CN45 readily autoignites at the conditions studied, M100 does not. The GP-assisted ignition of M100 was found to be strongly dependent on GP temperature and proximity to a fuel jet. The DL images show that M100 ignition occurs at the GP, followed by combustion propagation first to the two jets straddling the GP, then to the adjacent two jets, and finally to the last two jets emanating from the 6-hole, centrally-located injector nozzle. Three spikes in the apparent heat release rate are observed to correspond to these pair-wise jet ignition events. Spatially-integrated DL image data suggest that in-cylinder soot concentrations during M100 combustion are at least 2 orders of magnitude lower than those during CN45 combustion. Peak heat release rates during M100 combustion are only half of those achieved during the premixed burn phase of CN45 combustion, resulting in noticeably quieter engine operation.

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Relevance to Overall DOE Objectives

- **Challenge: Diesel-cycle engines are highly efficient, but have difficulty meeting emissions targets (esp. soot and NOx)**
- **Motivation: Oxygenates can provide significant benefits to diesel engine emissions and efficiency by**
  - **reducing soot emissions,** esp. at high loads & retarded timings {Litzinger et al., Choi et al., Miyamoto et al., ...}
  - **reducing NOx emissions by enhancing EGR tolerance,** higher power density at smoke limit {Miyamoto et al.}
  - **increasing efficiency by reducing in-cylinder radiative heat transfer** {Flynn et al.}
  - **may help enable ultra-efficient aftertreatment strategies**
- **Objective: Understand oxygenate effects on in-cylinder combustion and emissions-formation processes**

Research Questions: Oxygenated Diesel Fuels

- **Does oxygen content alone determine soot-reduction potential of an oxygenated blend?**

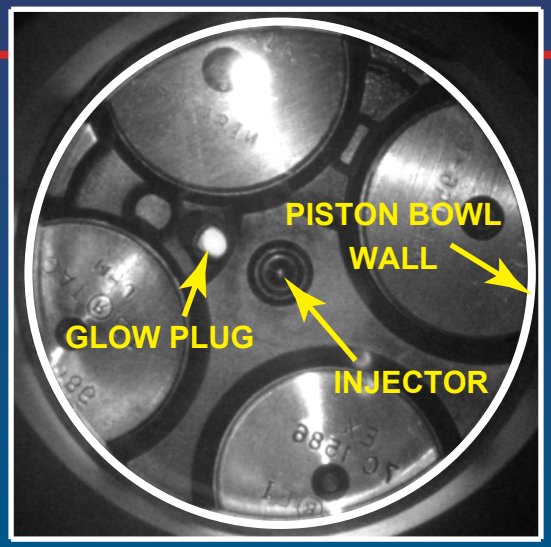
- **Other potentially-important effects:**

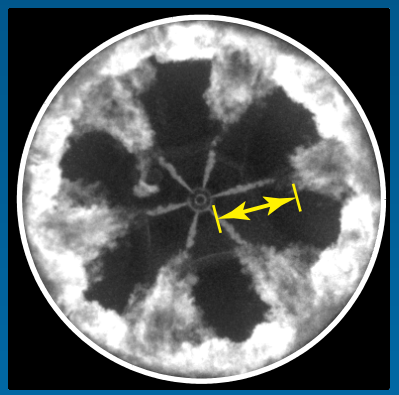
  - combustion phasing: ignition delay, duration of combustion
  - molecular structure: *e.g.*, ethers *vs.* esters *vs.* alcohols
  - chemical-kinetic effects: rxn intermediates affect soot
  - lift-off length: affects fuel/air premixing, soot formation
  - thermophysical properties: distillation curve, liquid length
  - fuel-injection equipment: rate shape, malfunctions
  - engine operating conditions: load, EGR rate, ...

- **Many studies of oxygenated diesel fuels have been conducted, many conflicting results**

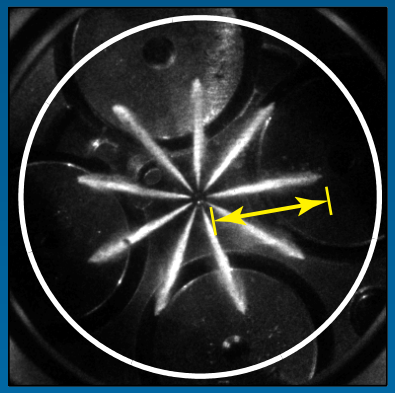
Unique Capabilities

- **Some important variables are *very difficult (if not impossible) to measure in all-metal engines***
  - **lift-off length**
  - **liquid length**
  - **injector malfunction**





lift-off length



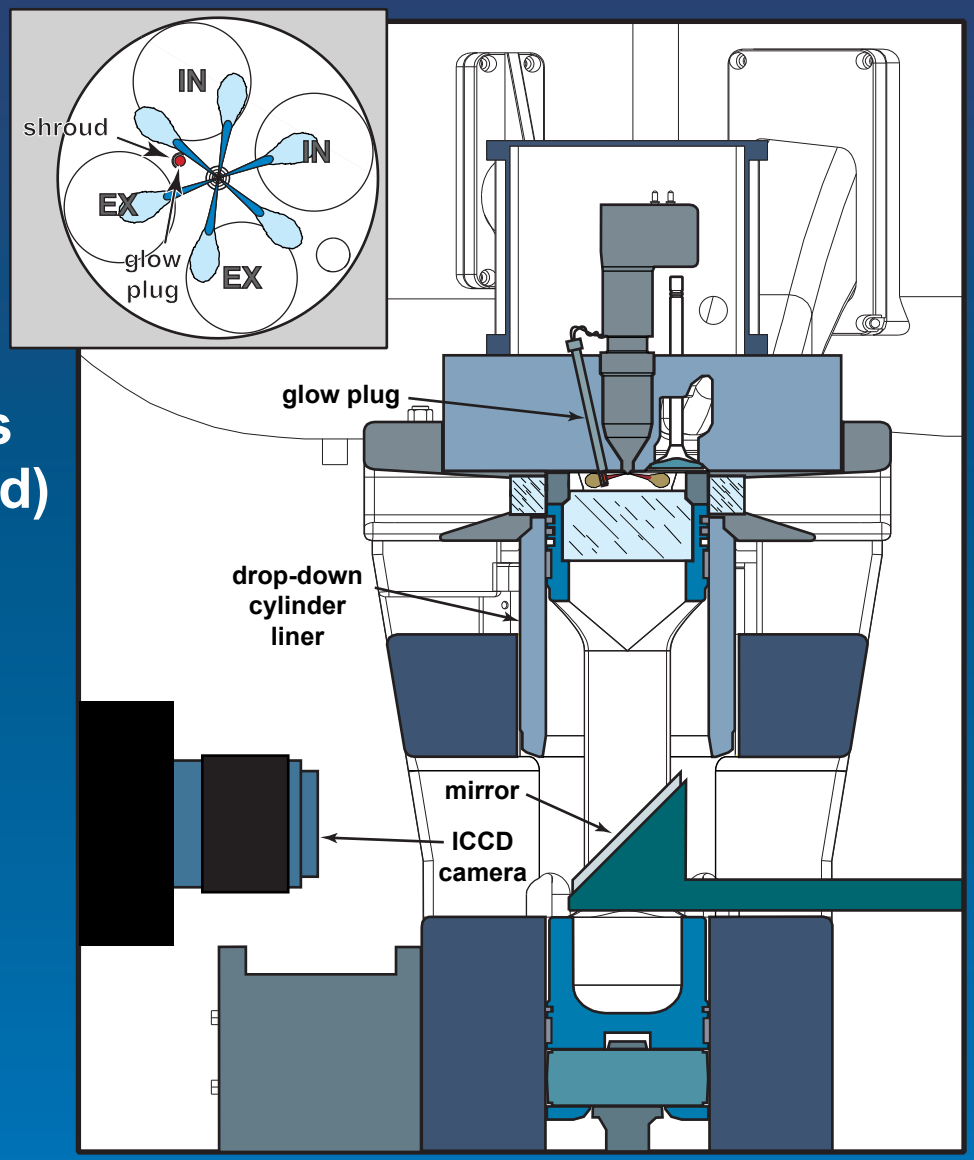
liquid length

injector malfunction

- **These variables can affect emissions as much as an alternative fuel**

Sandia/Caterpillar Optical Engine

- **Specifications**
  - single-cylinder, 4-stroke DI diesel, based on Cat 3176/ C-10 HD truck engine (1.72 liter displacement)
  - operating envelope same as production engine (skip-fired)
  - glow plug ignition-assist
- **Approach**
  - apply laser/imaging (and traditional) diagnostics
  - proven valuable for under-standing diesel combustion
  - study limiting cases of fuel effects on in-cyl. processes



Fuels and Operating Parameters

- **Fuels**
  1. hydrocarbon fuel for baseline characterization (CN45)
  2. 50 wt% oxygen, low-cetane fuel requires glow plug (M100)
  3. 26 wt% oxygen, typical-cetane ether blend (GE80)
  4. 26 wt% oxygen, typical-cetane di-ester blend (BM88)

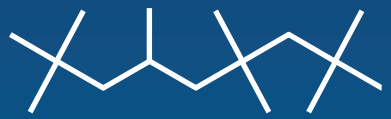
  → combustion phasing matched

- **Operating parameters**
  - 1200 rpm, 8.00 bar gross IMEP (moderate speed and load)
  - motored TDC conditions: 900 K, 60 bar, 23 kg/m^3
  - injection timing adjusted for maximum gross indicated torque (MGIT)

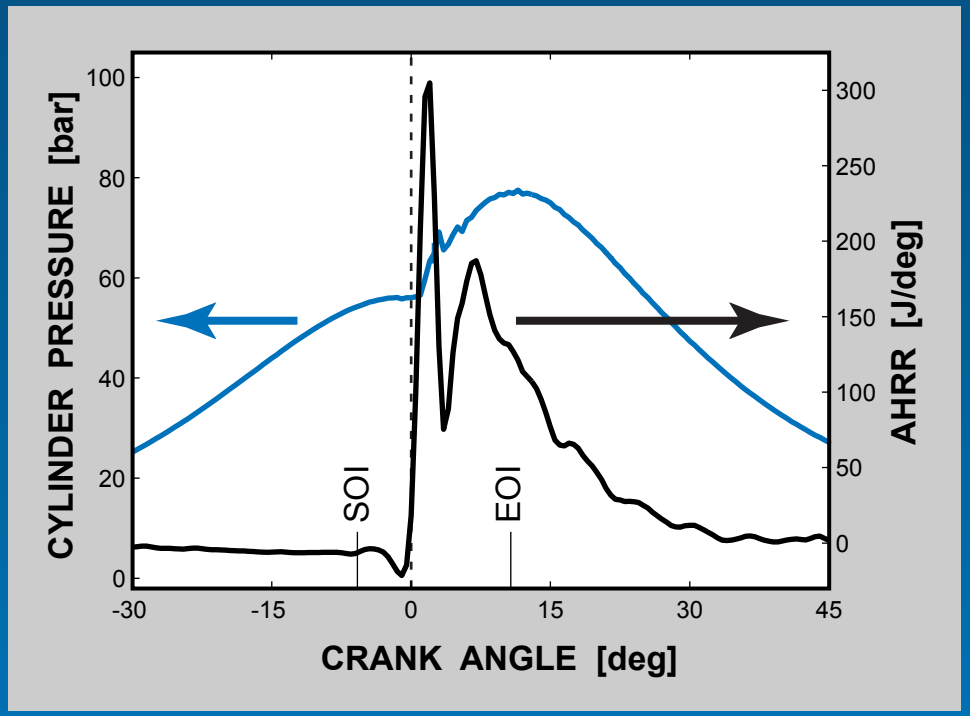
Baseline Engine Characterization Using CN45

- CN45 is two-component blend of $C_{16}H_{34}$ hydrocarbons
  - *n*-hexadecane (NHD)

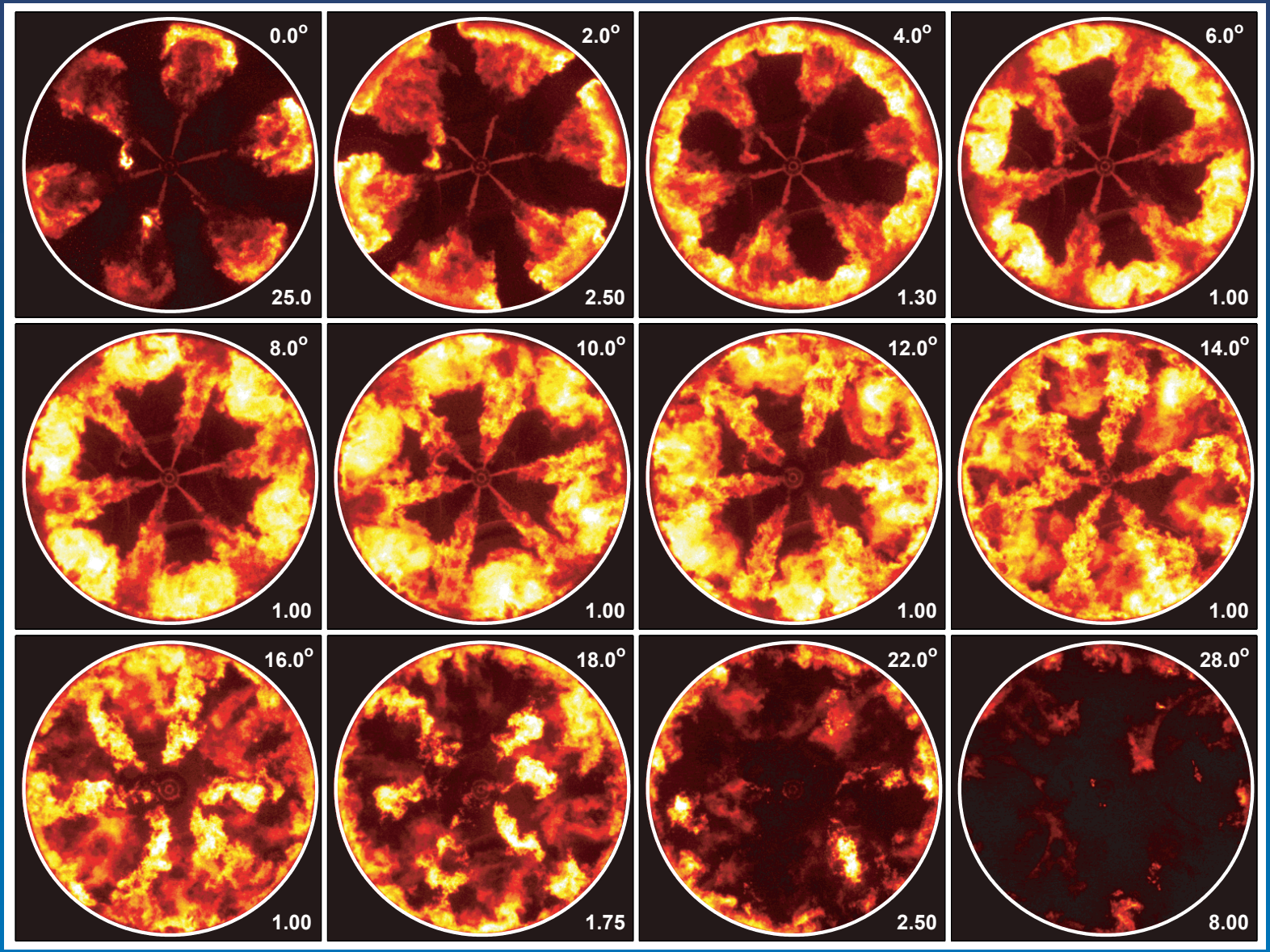
  - 2,2,4,4,6,8,8-heptamethylnonane (HMN)



- Engine and injector performance representative of production hardware
  - classic features of diesel combustion are evident
  - no post-injections or other problems with fuel-injection system

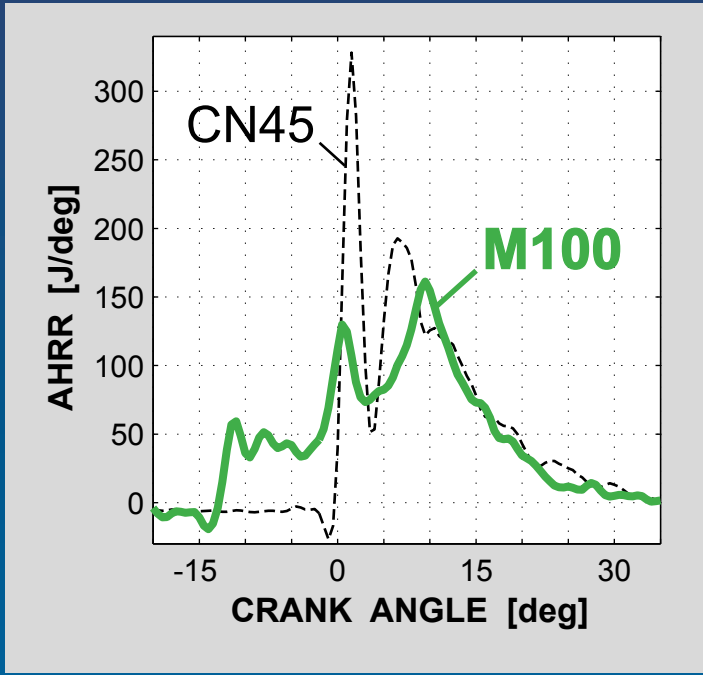


CN45 Direct Luminosity Image Sequence



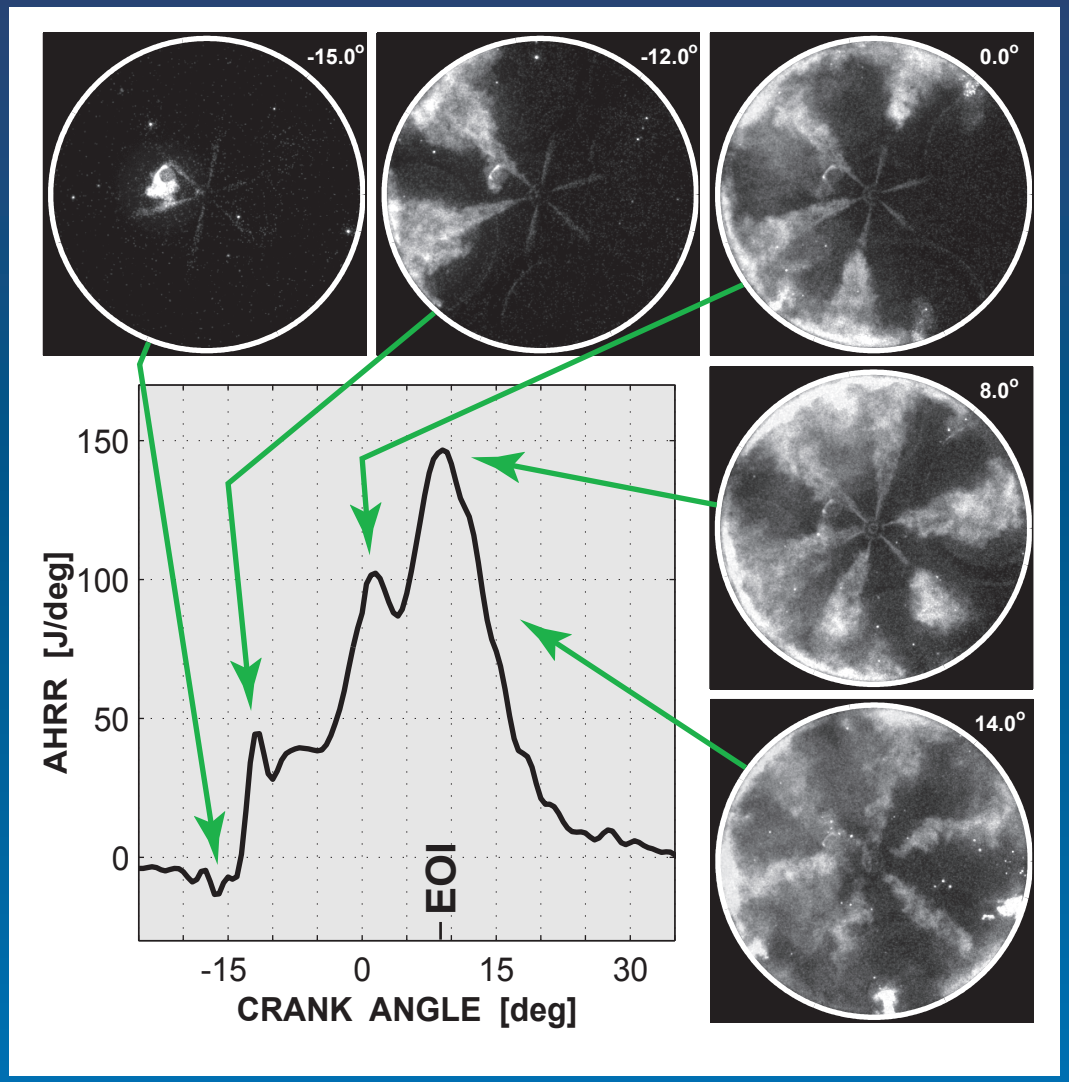
Glow Plug Assisted Ignition & Combustion of 50 wt% Oxygen, Low-Cetane Fuel

- Upper limit on oxygenation, lower limit on cetane number → neat methanol
- Proper glow plug temperature and orientation are critical for achieving stable operation
- M100 AHRR is significantly different from typical diesel
  - multiple spikes in M100 AHRR appear to be a new observation — what causes them?
  - perhaps surprisingly, peak AHRR for M100 (CN < 5) is half that of CN45 → much quieter engine operation



Explanation of Peaks in M100 AHRR Profile

- Jets ignite in pairs, each ignition event produces a local peak in AHRR
  - single jets ignite rather than pairs < 20% of time
  - combustion always propagates in sequence from glow plug ignition site
- Efficiency same as CN45
- Detailed results in SAE 2001-01-2004



Oxygenated Blend Properties

- **Highly-oxygenated, typical-cetane fuel blends**

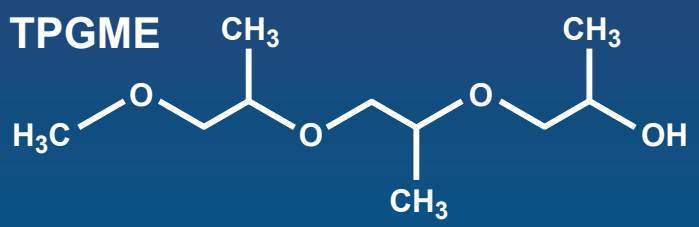
  - GE80 blend:

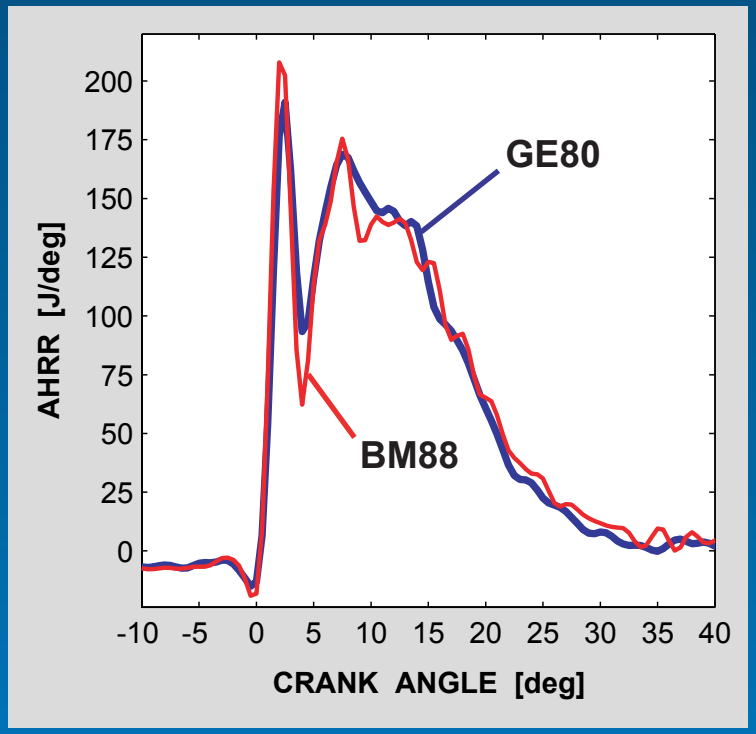
  - 80.0 vol% tri(propylene glycol) methyl ether (TPGME)
    20.0 vol% $C_{16}H_{34}$ (HMN)
  - 25.8 wt% oxygen in blend
  - injection timing adjusted for MGIT

  - BM88 blend:

  - 88.0 vol% di-butyl maleate (DBM)

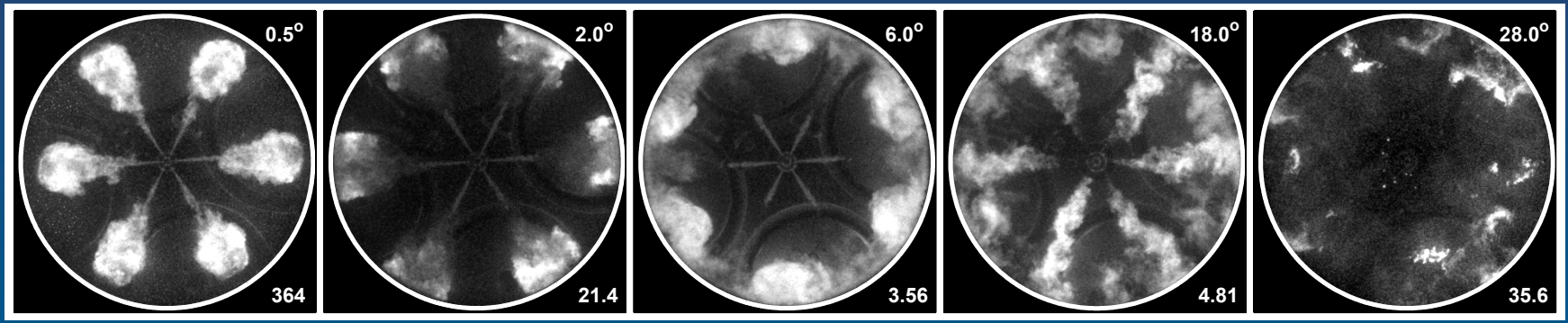
    7.0 vol% $C_{16}H_{34}$ (NHD)
    5.0 vol% 2-ethylhexyl nitrate (EHN)
  - 26.5 wt% oxygen in blend
  - combustion phasing matched to GE80



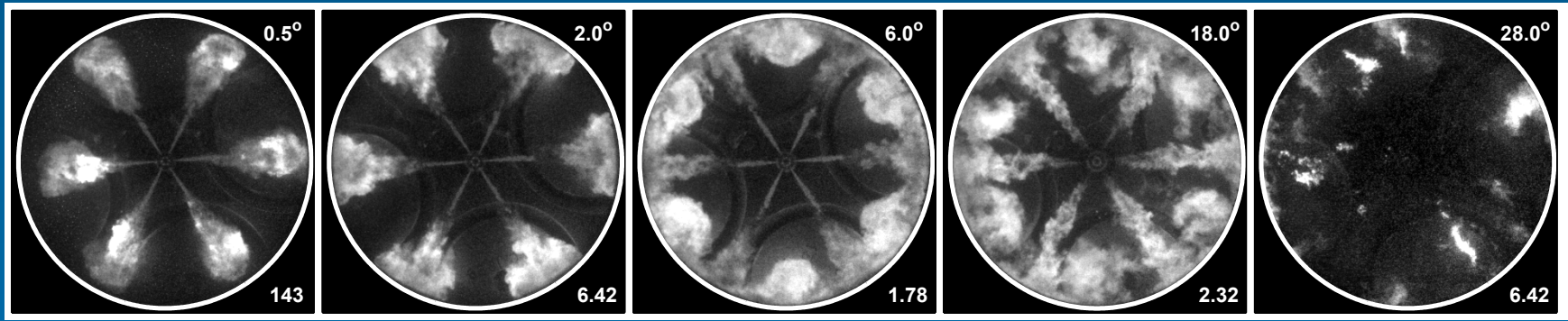


GE80 & BM88 Direct Luminosity Sequences

- **GE80 blend**



- **BM88 blend**

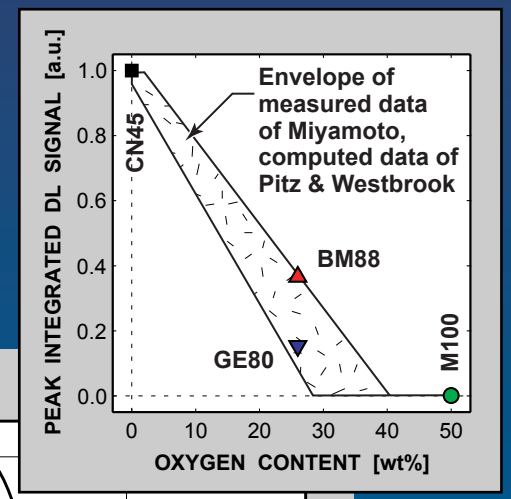


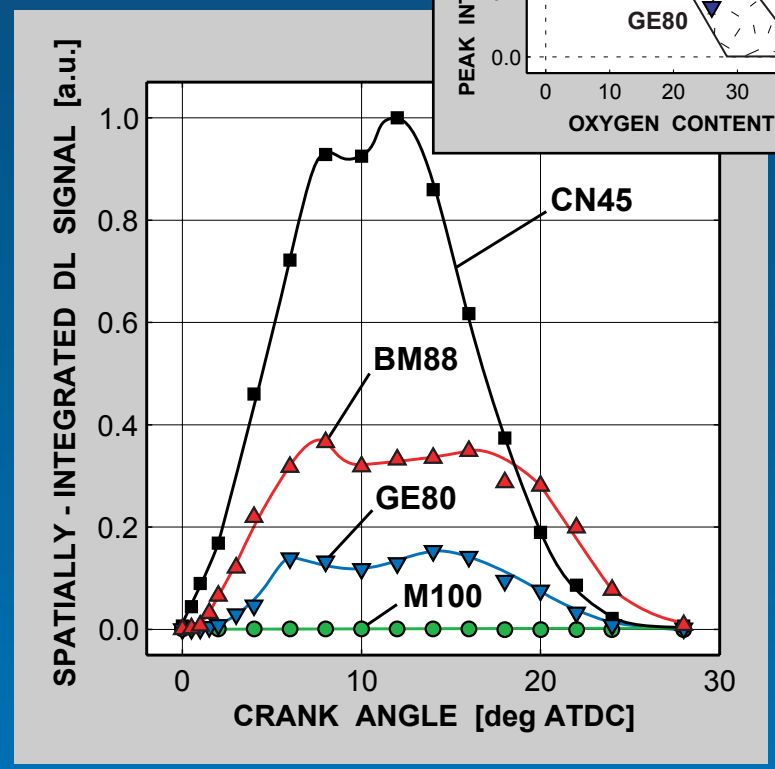
- **General combustion features very similar; larger signal from BM88 blend**

Spatially-Integrated DL Signal Shows Effects of Fuel Oxygenation on In-Cylinder Soot

- Integrated DL signal level provides a measure of amount of hot, in-cylinder soot

- Peak integrated DL levels decrease with fuel oxygenation in same manner as
  - measured engine-out emissions (Miyamoto et al.)
  - soot precursor concentrations from detailed chemical-kinetic calculations (Pitz, Westbrook, et al.)





Plans for Coming Months

- **Remainder of FY01**
  - measure lift-off lengths, liquid lengths for each oxygenated blend (in addition to tasks originally proposed for FY01)
  - initiate in-cylinder LII to study evolution of soot-formation zones for each oxygenated blend
- **FY02 Proposed**
  - add di-ethyl adipate to oxygenate test matix (match combustion phasing, oxygen content ➔ DL imaging, efficiency, lift-off length, liquid length)

  - complete experiments using in-cylinder LII to study soot evolution for each oxygenated blend
  - study glow plug assisted ignition and combustion of low-cetane hydrocarbon fuel

Outside Collaborations

- CIDI Oxygenates Screening Project: Dave Naegeli, Southwest Research Institute
  - final oxygenate selection in October 2000
- Accelerator Mass Spectrometry: Bruce Buchholz, Lawrence Livermore National Laboratory
  - do some fuel constituents produce more soot than others?
- LII Diagnostic for Exhaust PM: Pete Witze, Sandia National Laboratories (California)
  - relates in-cylinder processes to engine-out emissions
- Chemical Kinetics of Alt. Fuel Combustion: Pitz and Westbrook, Lawrence Livermore National Lab
  - development of detailed mechanisms for oxygenates

Acknowledgments

- **Mark Musculus (SNL)**
  - was post-doc, now in charge of Sandia/Cummins lab
  - began transition just after beginning of this FY
- **Tom Briggs (Caterpillar)**
  - very instrumental in helping obtain production fuel-injection system components and other hardware
- **Glen Martin (UIUC)**
  - doctoral candidate, will conduct thesis research in alt. fuels lab (advisor is Prof. Chia-Fon Lee)
  - began work at Sandia on March 12, 2001