Fuels as Enablers for Alternative Mode of Combustion

David E. Foster
Phil and Jean Myers Professor
Engine Research Center
University of Wisconsin - Madison

ERC Research Symposium: Future Fuels for IC Engine
June 6-7, 2007
Simplified Global Statements

• Key to LTC:
  – Achieve appropriate mixing of fuel and oxidizer prior to the ignition chemistry progressing to auto-ignition, which is to occur within some designated time during the cycle

• Many different scenarios have been proposed for achieving this
  – HCCI, PCCI, MK, DCDC, CAI, ...

• These different scenarios are really different approaches to mold the engine operation around the fuel’s physical and auto-ignition characteristics
  – LTC is ultimately controlled by ignition kinetics (which depend on fuel characteristics)
### Example: Impact of Fuels on LTC

#### Fuel Properties

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Description</th>
<th>RON</th>
<th>MON</th>
</tr>
</thead>
<tbody>
<tr>
<td>n-butane</td>
<td>99.5 % purity n-butane C₄H₁₀</td>
<td>91.8</td>
<td>89</td>
</tr>
<tr>
<td>PRF 91.8</td>
<td>Blend of primary reference fuels, n-heptane (C₇H₁₆); and iso-octane (2,2,4 tri-methyl-pentane) C₈H₁₈</td>
<td>91.8</td>
<td>91.8</td>
</tr>
<tr>
<td>BIN-1</td>
<td>Blend of indolene-1&lt;sup&gt;a&lt;/sup&gt; (research gasoline) and n-heptane</td>
<td>94.1&lt;sup&gt;b&lt;/sup&gt;</td>
<td>86.8&lt;sup&gt;b&lt;/sup&gt;</td>
</tr>
<tr>
<td>BIN-2</td>
<td>Blend of indolene-2&lt;sup&gt;a&lt;/sup&gt; (research gasoline) and n-heptane</td>
<td>93.0</td>
<td>86.2</td>
</tr>
<tr>
<td>PRF 70</td>
<td>Blend of primary reference fuels, n-heptane (C₇H₁₆); and iso-octane (2,2,4 tri-methyl-pentane) C₈H₁₈</td>
<td>70.0</td>
<td>70.0</td>
</tr>
</tbody>
</table>

<sup>b</sup> Estimated values
HCCI Operating Ranges ($\phi$)

HCCI Operating Ranges Change with:
- Temperature
- Speed
- Fuel Type

SAE 2002-01-2830
Pressure and Heat Release Profiles PRF 70

PRF 70 at 900 rpm, $\phi = 0.25$

SAE 2002-01-2830
Reassessment of HCCI Operating Ranges

Kalthatgi - Octane Index: $OI = (1-K)\times RON + K \times MON$ (SAE 2001-01-3584 & 3585)

<table>
<thead>
<tr>
<th>Fuel</th>
<th>RON</th>
<th>MON</th>
<th>S</th>
<th>OI</th>
<th>CA10</th>
<th>OI</th>
<th>CA10</th>
</tr>
</thead>
<tbody>
<tr>
<td>BIN 2</td>
<td>93</td>
<td>86.2</td>
<td>6.8</td>
<td>91.74</td>
<td>-2.17</td>
<td>89.03</td>
<td>-1.19</td>
</tr>
<tr>
<td>n-Butane</td>
<td>91.8</td>
<td>89</td>
<td>2.8</td>
<td>91.28</td>
<td>-4.09</td>
<td>90.17</td>
<td>1.76</td>
</tr>
<tr>
<td>PRF 91.8</td>
<td>91.8</td>
<td>91.8</td>
<td>0</td>
<td>91.8</td>
<td>-2.02</td>
<td>-</td>
<td>N/A</td>
</tr>
<tr>
<td>BIN 1</td>
<td>94.1</td>
<td>86.8</td>
<td>7.3</td>
<td>92.74</td>
<td>1.02</td>
<td>89.84</td>
<td>0.91</td>
</tr>
</tbody>
</table>

Intake Temperature 380K
Engine Speed 600 rpm
Equivalence Ratio 0.20

Intake Temperature 380K
Engine Speed 1800 rpm
Equivalence Ratio 0.22
Correlation between Chemical Composition and LTHR

Even in the case of same Research Octane Number Fuels, the heat release rates are different because of…

(1) The LTHR characteristics of paraffins
(2) Inhibitor effects of aromatics and some naphthenes and olefins
Correlation between Chemical Composition and HTHR

1000rpm
IMEP530kPa

Chemicals that advance HTHR

Chemicals that delay HTHR

SAE 2005-01-0138

n-paraffins
iso-paraffins
aromatics
naphthenes
olefins

m-Xylene
Cyclopentane
Toluene
Di-isobuthylene
Cyclohexane
4Methyl1pentene
iso-Octane
2Methylpentane
n-Pentane
n-Hexane
n-Heptane

University of Wisconsin -- Engine Research Center
Correlation between Chemical Composition and HTHR

1000rpm
IMEP530kPa

- m-Xylene (K)
- Cyclopentane (B)
- Toluene (J)
- Di-isobuthylene (H)
- Cyclohexane (F)
- 4Methyl1pentene (C)
- iso-Octane (I)
- 2Methylpentane (D)
- n-Pentane (A)
- n-Hexane (E)
- n-Heptane (G)

- aromatics
- naphthenes
- olefins
- iso-paraffins
- n-paraffins

SAE 2005-01-0138

University of Wisconsin -- Engine Research Center
Using Mixture Pre-conditioning to Control HCCI
Injection and Valve Timings

- Injection: DI or PI
- Pre-DI
- Pre-DI SOI
- Compression
- Expansion
- Exhaust
- Induction
- NVO

Legend:
- IVC
- EVC
- IVO
- BDC
- eTDC
- fTDC

Crank angle [CAD after fTDC]

-180 - 180
0
118
180
285
360
420
540

35
30
25
20
15
10
5
0

SAE 2007-01-0219
SAE 2007-01-0227
Experimental Pre-DI Timing Results

- Changes SOC attributed to the reformation of the fuel and heat release during the NVO period
- NMEP stays constant with changing SOC

SAE 2007-01-0219
There appears to be a correlation between the quantity of energy release during the negative valve overlap and the change in the pumping work.

- Suggests thermal (temperature) effect.
Species Formations – pre-DI Timing

70° beTDC

30° beTDC

20° beTDC

Crank angle [CAD after eTDC]

Crank angle [deg after eTDC]

Species conc. [ppm]

Qchem [J/deg]
Further Demonstration of the Impact of Fuel Reformation on LTC Phasing Intake Charge Heating System

- The thermocouples denoted $T_{g1}$-$T_{g3}$ measure the temperature of the gas at the center of the surge tanks.
- The gas in the surge tanks and all pipes upstream of the intake runner are maintained at a uniform and fixed intake temperature.
- The temperature of the charge in the intake runner can be varied by allowing heat transfer to the surroundings.
- At most we can make $T_{in}$ 50°C lower than the upstream temperature.

SAE 2005-01-3742
Premixed Fueling (PRF 87)

Heat release results for conditions where CA 50 = 5-6 deg ATDC

Cylinder Pressure and Heat Release Rate

IMEP vs Actual Engine Inlet Air Temperature (T_{in}°C)

CA50 vs Actual Engine Inlet Air Temperature (T_{in}°C)
GC Mass Spec. Data (PRF Fuel)

Mass Spectra for PRF at Various Upstream Heating Conditions

- $T_{g1} = T_{g2} = T_{g3} = 275 \, ^\circ C$
- $T_{g1} = T_{g2} = T_{g3} = 285 \, ^\circ C$
- $T_{g1} = T_{g2} = T_{g3} = 290 \, ^\circ C$
- $T_{g1} = T_{g2} = T_{g3} = 295 \, ^\circ C$

**Sample Retention Time (min)**

**Abundance**

- 2-Propanone
- 2-Methyl-2-Propenal
- 2-Methyl-2-Propanal
- Propanal
- Butanal
- 2-Butanone
- 2,2-Dimethylpropanal
- 4,4-Dimethyl-2-pentene
- 2-Propenal

SAE 2005-01-3742
Pre-DI Impacts HCCI via:

• Thermal conditioning
  – Energy release

• Reforming the fuel
  – Preconditions the charge composition

• Both have an impact!
Does “Diesel Type” Fuel Exhibit Similar Sensitivities?
Confidence in Data

CO Production Baseline

![Graph showing CO (g/kg-fl) production as a function of ignition delay (ms) from Start of Command with markers for different EU and US standards and ignitions.](Image)
Can the Paradigm be Inverted?

- Experiments and simulation show the important coupling between the ignition characteristics of the fuel with the temporal and spatial evolution of thermodynamic state space within the cylinder

- Options:
  - Identify operating conditions where LTC can be achieved and incorporating those situations into the engine operating map
    • Most likely near term application of LTC
  - Know the ignition characteristics of the fuel and match the engine operating characteristics to facilitate LTC
    • Evolution of above approach – engine control
  - Tailor a fuel to more closely match the achievable engine operating characteristics
    • Expand operating range via fuel modification
    • What would be a good fuel – engine combination?
- Alternate fuels for tar sands, shale oil, coal liquification yield fuels that are more diesel like than gasoline like.
Proposed Fuel and Engine Characteristics for Versatile LTC Operation

• Engine Characteristics
  – Valve train flexible
  – Direct Injection
  – Variable pressure intake
  – Intake mixture dilution
  – Intake charge cooling

• Fuel Characteristics
  – Moderate to high volatility
  – Low Cetane number
  – Low Octane number

Can these characteristics be tailored through the appropriate blend of napthenes, olefins and iso-parafins?

SAE 2007-01-0191 “Effects of Fuel Property Changes on Heavy Duty HCCI Combustion” - Diesel LTC load range increased with a CN of 23~32
Thank you very much