Future fuels for road transport

How can future fuels for IC engines contribute to sustainable road transport?

Paul Hellier, Nicos Ladommatos, Hamisu Dandajeh, Ioannis Efthymiopoulos, Aaron Eveleigh, Midhat Talibi

UnICEG University of Brighton 20th December 2016
1. Why engineer fuels?
2. Fuels from waste coffee grounds
3. Fuels from CO$_2$
4. Fate of fuel oxygen
5. Fuels from micro-algae
6. Fuel effects on PM toxicity
7. ‘Smart’ fuels
Defining fuels

Cooperative Fuels Research engine

1928

2016
What has been required of liquid fuels?
What is expected of future fuels?

Fossil fuels

Current biofuels

Advanced biofuels
Fuel molecular structure

Diesel

Gasoline

O

H

O

H

O

O

O

O
Fuels from carbon dioxide?

\[ \text{OH} + \text{O}=\text{C}=\text{O} \rightarrow \text{di-n-butyl carbonate} \]

Inorganic base catalyst

Di-n-butyl carbonate

Oxygen content (mol/mol)

<table>
<thead>
<tr>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>5-nonanone</td>
<td>Butyl valerate</td>
<td>DnBC</td>
</tr>
</tbody>
</table>

Constant injection
Constant ignition

What happens to fuel oxygen?

Oxygen bond type

Designer fuels from micro-algae

Light
CO$_2$ (flue gas)
Nutrients
(waste water)

2 – 3 µm

Triglycerides

IPP (C5) $\leftrightarrow$ DMAPP (C5)

geranyl diphosphate (C10)

farnesyl diphosphate (C15)

sterols, phytol, carotenoids

isoprene

limonene

linalool

citronellene

chemical conversion

IP$ightarrow$S

LS

GES

GDH

CJFS

geraniol

geranial

farnesene
Geraniol

Nerol

Linalool

Citronellol

3,7-dimethyloctan-1-ol

Geranial (Citral-A)

Citral dimethyl acetal

Geranyl acetate

Menthol

Citronellene

Farnesene

Squalene

cis vs trans

Alcohol group position

Degree of saturation

Functional group

Alkenyl chain length

Combustion phasing

- Constant injection
- Constant ignition

No. of double bonds
2(E,E) 2(E,Z) 1(E) 0

- OH→=O

Ignition delay (CAD)

Geraniol, Nerol, Citronellol, 3,7-d-1-o, Geranyl a, Geranial, Cda, Citronellene, Menthol, Farnesene, Squalene, Ref. diesel

C15, C30
Decrease in saturation or alkyl chain length → increase in ignition delay

Permits internal H abstraction and isomerisation across a double bond

Why is ignition delay important?

Premixed burn fraction

Premixed burn fraction → peak heat release rate

Duration of ignition delay → premixed burn fraction → peak heat release
NOx emissions

Particulate mass

Increased ignition delay → increased NOx + reduced particulates
Peak heat release rate

Ignition delay → time of peak heat release → heat transfer
NOx emissions

Ignition delay → heat release rates → NOx emissions
Alkyl chain length $\rightarrow$ viscosity $\rightarrow$ fuel air mixing $\rightarrow$ fuel pyrolysis

Alkyl chain saturation $\rightarrow$ soot precursors $\rightarrow$ soot formation

**Total particulate mass**

- Geraniol
- Nerol
- Citronellol
- 3,7-d-1-o
- Geranyl a.
- Geranial
- Cda
- Citronellene
- Menthol
- Farnesene
- Squalene
- Ref. diesel

Constant injection
Constant ignition

$6 \text{ DB}$

$6 \text{ mPa.s}$

No fuel bound oxygen
How toxic is PM?

- PAHs adsorbed on particle surface.
- Gas phase PAHs.

Can future fuels be ‘smart’?

- On-board ozonisation of 1-hexane.
- HCCI shows SOC advance with fuel ozone treatment.
- Same bulk fuel but altered ignition quality.

Conclusions

- Develop improved fuels through design of molecular structure.
- Routes of fuel production (biological/chemical) are an opportunity to exploit effects of fuel molecular structure.
- Fuel molecular structure determines ignition delay:
  - Alkyl chain length and saturation, oxygenated functional groups.
  - Sub-molecular structures have consistent impact.
- Emissions of NOx are primarily driven by ignition delay.
- PM toxicity changes with fuel composition.
Thank you for listening

Questions?

p.hellier@ucl.ac.uk