Alcohol fuels for spark-ignition engines: performance, efficiency and emissions effects at mid to high blend rates for binary mixtures and pure components

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Abstract

The paper evaluates the results of tests performed using mid- and high-level blends of the low-carbon alcohols methanol and ethanol in admixture with gasoline, conducted in a variety of test engines to investigate octane response, efficiency and exhaust emissions, including those for particulate matter. Additionally, pure alcohols are tested in two of the engines, in order to show the maximum response that can be expected in terms of knock limit and efficiency as a result of the beneficial properties of the two alcohols investigated. All of the test work has been conducted with blending of the alcohols and gasoline taking place outside of the combustion system, i.e. the two components are mixed homogeneously before introduction to the fuel system and so the results represent what would happen if the alcohols were introduced into the fuel pool through a conventional single-fuel-pump (dispenser) approach.

While much has been written on the effect of blending the light alcohols with gasoline in this way, the results present significant new findings with regards to the effect of the enthalpy of vaporization of the alcohols in terms of particulate exhaust emissions. Also, in one of the tests, two mid-level blends were tested in a highly-downsized prototype engine, these blends being matched for stoichiometry, enthalpy of vaporization and volumetric energy content. The consequences of this are discussed and the results show that this approach to blend formulation creates fuels which behave in the same manner in a given combustion system; the reasons for this are discussed.

One set of tests using pure methanol alternately with cooled exhaust gas recirculation and with excess air shows the significant increase in thermal efficiency that can be expected as the blend level is increased. The effect on nitrous oxide emissions is shown to be similarly beneficial, this being primarily a result of the enthalpy of vaporization of the alcohol cooling the charge coupled with the lower adiabatic flame temperature of the alcohol. However, whereas it is normally a beneficial characteristic in spark-ignition combustion systems, one disadvantage of a high value of enthalpy of vaporization is shown in another series of tests in that, in admixture with gasoline, it is a driver on flash boiling of the hydrocarbon component in the blend in direct injection combustion systems. In turn this causes the particulate emissions of the engine to increase quite markedly over those for ethanol-gasoline blends at the same stoichiometry. The paper shows for the first time the dichotomy of the potential efficiency improvement with the challenge of particulate control. This effect poses a challenge for the future introduction and use of such high blend rate fuels in engines without particulate filters. Although it must be stated that the overall particulate emissions of the methanol-gasoline blend are lower than for gasoline, the effect is only present at extremely low load, and that there is a likelihood that particulate filters will be adopted in production vehicle anyway, nullifying this issue.

1. INTRODUCTION
The two light alcohols, methanol and ethanol, have been investigated by numerous authors either as pure fuels for internal combustion engines (ICEs) or in admixture with gasoline. As pure fuels they were proposed as an alternative to gasoline for reasons of energy security at least as long ago as 1907 [1]. Most commonly they can be configured as binary mixtures of one of the alcohols with gasoline, or sometimes jointly together as ternary mixtures. This paper discusses the case of the pure alcohols and binary blends at mid- and high-level, and uses a variety of engines to investigate the response of these fuels in terms of knock limit, efficiency and emissions.

Modern gasoline commonly contains 5% ethanol (so-called ‘E5’), in a bid to improve energy security and to reduce the fossil CO2 impact of the fuel. Additionally E10 is now being introduced in Europe and the United States, in order to extend these advantages, and there are waivers in place to permit the use of up to 15% ethanol in gasoline (agreed by the US Environmental Protection Agency) [2,3]. Furthermore, in Europe up to 3% methanol is permitted as a blend component in gasoline as well, within an overall oxygen concentration limit of 3.7% by mass [4]. These low blend rate levels have been adopted as part of the worldwide fuel charter and are consequently considered to be fully commercialized and hence will not be studied in detail in this work. Instead mid- and high-level blends are investigated, ‘mid-level’ being defined herein to be 15-30% of the alcohol by volume and ‘high-level’ anything above that volumetric percentage, up to and including the pure alcohol. In reality, blend rates of 85% have successfully been used for both of the low-carbon-number alcohols in specific markets and trials (including Brazil, which has traditionally used varying rates of ethanol in its gasoline, up to and including hydrous pure ethanol), but the present work seeks to clarify certain responses of the fuels in modern spark-ignition (SI) combustion systems utilizing exhaust gas recirculation, lean combustion operation and/or direct injection.

All of the results discussed in the present work relate to the use of alcohol blend fuels in a single fuel delivery system. Dual-fuelling, or so called ‘octane-on-demand’, where a low-octane base fuel is used for most operating conditions, with a second, high-octane fuel being introduced as and when necessary to suppress knock, has been investigated with various fuel introduction methods [5-8]. The light alcohols are generally favoured in such advanced combustion systems, and these approaches can extend the benefit of the alcohol and displace a proportionally larger amount of fossil fuel. They also permit the reduction of fuel processing for the hydrocarbon component, with naphtha being one possible choice for this, and with this comes the potential to significantly reduce the energy used in refining and thus the well-to-tank carbon intensity of the fuel [9]. Such approaches will not be discussed here, the focus of this paper being blends created outside the engine’s fuel system, it thus requiring only one such handling system. However, many of the results presented in these studies by other workers do use blends of the alcohol with a low-octane base fuel for initial testing or derive an equivalent in-cylinder octane number after the fuels have been introduced [10]; consequently much can be deduced from these studies in terms of how the alcohols increase the knock resistance of pure hydrocarbons, especially when the alcohol is port-fuel-injected and the effect of its enthalpy of vaporization is reduced (see also the discussion on ‘Direct-injection Octane Number in Section 3 below) [6].

Ethanol is the commonest alcohol used in SI fuels. It can be made from biological sources which give rise to energy security and net greenhouse gas (GHG) reduction advantages; growing plants for fuel use within a nation’s borders addresses the former, while the airborne CO2 absorbed and trapped within a part of the fuel lifecycle addresses the latter. Ethanol is also an extremely good SI fuel: it has very high octane numbers, high octane sensitivity2, a high laminar burning velocity (LBV) and low adiabatic flame temperature [11]. Consequently it can support high compression ratios (CRs) and high levels of boost pressure for high Otto cycle efficiency [12], and can also operate very efficiently with higher rates of cooled exhaust gas recirculation (EGR) than conventional hydrocarbons can support. These advantages increase in a direct-injection (DI) combustion system, where its very high enthalpy of vaporization in conjunction with its low stoichiometric air-fuel ratio (AFR) generates significant charge cooling which can either be used to increase volumetric efficiency or knock resistance, or both. Furthermore, since it only has two carbon atoms and a single carbon-carbon bond, it does not directly form particulate matter easily; experiments relating to this will be returned to in Section 5, below.

1 In this paper the term ‘EXX’ refers to a binary mixture of ethanol in gasoline of volume percentage XX ethanol, and ‘MXX’ is used as the corresponding case for a binary mixture of methanol in gasoline.

2 Sensitivity, S = RON-MON, where RON and MON are the Research and Motor octane number respectively.
All of these advantages apply to methanol too, only more so (with certain provisos which will be discussed later), it having a higher enthalpy of vaporization, a lower stoichiometric AFR and, being the single-carbon alcohol, no carbon-carbon bonds. Methanol can also be made from biological sources (as 'wood alcohol'), but importantly it is very easily synthesized from any carbonaceous feed stock generally via a gasification-to-syngas approach. It can also be made directly from CO2 and hydrogen, opening up the eventual possibility of carbon-free energy being used to extract CO2 from air and this being used to fix hydrogen in a fully renewable liquid fuel, without the feed stock limitation concerns of ethanol production with its biomass limit, for example [13-18]. Recently researchers have shown the feasibility of its formation directly from air in a combined carbon-capture-and-synthesis process, which brings the possibility of a truly practical liquid renewable fuel even closer [19].

As a result of the hydrogen bonding characteristic provided by their OH characteristic group, both methanol and ethanol are infinitely soluble in water; as a consequence historical research has been undertaken on various alcohol-water blends [20]. This has also been suggested as one approach to octane-on-demand [21]. Such an approach could be seen as a potential extension to simple water injection as is being commercialized by BMW [22]. The use of an alcohol mixed into the water, or metered in in some manner if the water is harvested on board, again as proposed in several forms by BMW [23], presents some advantages in terms of avoiding the freezing of water, and bioorganism suppression. As such, some of the complication of tank heating could be avoided and the knock-suppressant system could be made to work immediately at low temperatures; a 50-50 mixture of methanol and water has a freezing point of -40°C, while a 30-70 mixture provides -20°C [24]. Varying the concentration of methanol in such 'anti-detonant injection' fluids, as they were termed when used at take-off in piston aero engines [25], could be controlled automatically either in separate-fuel octane-on-demand applications or in systems where water is mixed with gasoline just before injection. The infinite miscibility of the alcohol in water is a clear enabler for this. While further investigation of this approach is beyond the scope of the present paper, it does suggest an interesting potential direction of research.

However, there are disadvantages to the alcohols, many born of their OH characteristic group. They have low vapour pressures in their pure form but, when they are mixed with hydrocarbons, the fact that the resulting mixtures do not follow Raoult’s Law means that they then have very high ones. They possess hydrophilic tendencies, which particularly at low blend rates can lead to phase separation when relatively small amounts of water are absorbed into a mixture. Thus care must be taken to ensure that any alcohol used for blending with gasoline is fully dried and that water is kept out of the fuel supply and storage system. In the case of ethanol, because it forms an azeotrope with water (at 4.4% water by volume) this gives rise to high process energy requirements in its manufacture. Conversely the very low vapour pressures of the pure alcohols can give rise to startability issues in this case, although DI has been known to be capable of mitigating this problem for some time [26]. They are also more aggressive to fuel system materials than hydrocarbons, but countermeasures have been known and understood for this for some time [27].

More contentious than the above is the fact that methanol is toxic, although the level of its toxicity is similar to gasoline and diesel, albeit manifesting in a different form. As well as being an intoxicant, ethanol is toxic in large amounts too, and for this reason both have habitually been mixed with gasoline as a denaturant. Additionally, small amounts of additives can be used to denature them, with one – denatonium benzoate, or ‘Bitrex’, the bitterest material known – capable of making them so bitter as to be unbearable at concentrations of as low as 10 ppm [28, 29]. However, it is interesting to note that regardless of its toxicity, the US Environmental Protection Agency conducted significant research into methanol safety and concluded that if the whole US light-duty fleet switched from gasoline to this alcohol then deaths and property loss attributable to the fuel would reduce by at least one order of magnitude [30, 31]. This is primarily due to the low flammability index of methanol in its liquid form, and the opposite problem that gasoline has with unintended ignition.

As discussed above, many researchers have investigated synthesizing methanol using CO2, with the potential to extract this from the atmosphere and combine it with hydrogen from water electrolysis. When all of the process energy is carbon-free, this results in a non-fossil-carbon liquid energy carrier made from limitless feed stocks [13-18]. Audi have recently promoted a similar process with methane, which they term e-gas [32]; Specht et al. [33] have also shown how this permits storage of renewable energy in the gas grid, which for some countries is, in terms of energy capacity, significantly greater than the daily usage amount. The approach therefore decouples renewable energy from peaks and troughs of generation and usage.
Pearson and co-workers discussed how the approach of Specht et al. could be extended by making liquid fuels, so that renewable energy can then be stored and used in the liquid as well as the gaseous fuel system [17]. This opportunity has driven the blending and pure fuel investigations discussed here. As a further potential, methanol can also be part of a significant pathway to the synthesis of higher hydrocarbons, albeit with a concomitant reduction in the energy carried, opening up the opportunity to decarbonize transport by providing a blend component which is of similarly low carbon intensity. Such approaches have recently been reviewed by French and co-workers [34] and are shown in outline in Figure 1.

![Diagram of fuel synthesis pathways](Image)

**Fig. 1: Potential pathways to decarbonized liquid transport (see also [34])**

However, the reduction in process efficiency arising from the onward synthesis of methanol to hydrocarbons, and thus the resulting increase in the amount of primary renewable energy required to provide the same amount of delivered fuel energy, combined with the loss of potential engine efficiency entailed using a hydrocarbon fuel versus the original alcohol (see later), makes investigation into methanol combustion important; the same observation can be made for ethanol against the backdrop of the biomass limit on the manufacture of this fuel.

The paper will show that significant improvements in thermal efficiency are possible when alcohols are used in SI combustion engines compared to using hydrocarbon fuels with octane numbers in the range currently employed in most non-premium fuels, including when such an engine is configured with a compression ratio (CR) significantly higher than can normally be tolerated by a hydrocarbon gasoline-type fuel, or when it is highly boosted. This will be shown by tests in a variety of research engines using pure methanol and ethanol, and various mixtures of these alcohols in binary blends with gasoline at the mid level (c. 15-20% v/v) or high-level (c. 85% v/v). The paper will also discuss the effect of gasoline-alcohol mixtures on particulate emissions from DI combustion systems. Emissions are not speciated to aldehydes, although this is a significant issue in terms of the pollutant-forming mechanisms of alcohol combustion, and likely to become more so. While not wanting to ignore this issue, it is believed that changes in catalyst formulation will be sufficient to address it, since oxidation of these molecules is easier than the reduction of oxides of nitrogen (NOx), and one of the advantages of alcohol combustion is lower NOx output than for hydrocarbon fuels.

Thus in order to orient the reader, the remainder of this paper comprises four main sections and conclusions:

**Section 2** focuses on tests of a highly-downsized multi-cylinder engine optimized for gasoline in which the performance- and efficiency-enhancing attributes of the alcohols are investigated. This section also shows that when configured for equivalent stoichiometry, alcohol-gasoline blends can perform fundamentally identically in the same combustion system when operated under the same conditions.
Section 3 details tests of pure methanol in two different spark-ignition combustion systems: one is a conventional one originally designed for gasoline, the other a modification of a diesel engine to spark ignition and high-EGR operation. The purpose of this section is to show how much extra efficiency can be realized when an engine is configured to better match what methanol is capable of delivering.

Section 4 describes tests of two equal-stoichiometry blends in a production SI engine, and shows that again the such fuels effectively perform identically. It also describes knock tests showing the performance of the equal-stoichiometry blends and also that methanol itself has the highest knock limit of the pure fuel blend stocks tested.

Section 5 describes engine-out emissions tests in a direct-injection engine in which some difference is discovered in the particulate performance of the equal-stoichiometry blends. This is shown to be dependent on load and a hypothesis is put forward as to what may be causing this. It is acknowledged here that the use of a gasoline particulate filter will effectively eliminate this issue, although the phenomenon is one which would undoubtedly benefit from extra study.

2. BINARY GASOLINE-ALCOHOL BLEND TESTS IN THE ULTRABOOST EXTREME DOWNSIZING DEMONSTRATOR ENGINE

In order to investigate some of the potential of alcohol-gasoline mid- and high-level blends, a series of tests was conducted in the Ultraboost extreme downsizing demonstrator engine. These utilized an external boosting system with and without cooled exhaust gas recirculation (EGR) in order to accurately control the intake charge conditions delivered to the engine.

The ‘Ultra Boost for Economy’ project was a collaborative project part-funded by the UK Technology Strategy Board (now Innovate UK) with eight partners: Land Rover were the lead, the others comprising Lotus Engineering, GE Precision Engineering, Shell Global Solutions, CD-adapco, the University of Bath, Imperial College and the University of Leeds. It is discussed in depth elsewhere [35], but in brief the engine was a 2.0 litre in-line 4-cylinder unit designed to reproduce the torque curve of the Jaguar Land Rover AJ133 5.0 litre naturally-aspirated (NA) V8 engine while operating on commercial 95 research octane number (RON) gasoline. A successful target of the project was to demonstrate a vehicle-level CO2 reduction of 35% (by using dynamometer test results in a vehicle simulation package). The final engine was supercharged and turbocharged, but an intermediate-level engine was operated with a facilitated charging system at the University of Bath, where all of the project test work was conducted. Table 1 presents brief specifications of the engine in this externally-boosted (or ‘UB100’) specification.

<table>
<thead>
<tr>
<th>Table 1: Specifications of the Ultraboost extreme downsizing demonstrator engine in externally-boosted configuration, as used for fuels testing [35]</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>General architecture</strong></td>
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<tr>
<td><strong>Construction</strong></td>
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<tr>
<td><strong>Firing order</strong></td>
</tr>
<tr>
<td><strong>Bore</strong></td>
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<tr>
<td><strong>Stroke</strong></td>
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<tr>
<td><strong>Swept volume</strong></td>
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<tr>
<td><strong>Combustion system</strong></td>
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<tr>
<td><strong>Compression ratio</strong></td>
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<td><strong>Valve gear</strong></td>
</tr>
</tbody>
</table>
During the main programme the engine was used for an extensive series of fuel tests, the results of which for all but the mid- and high-level alcohol blends are discussed in detail in a series of other publications [36-38]. In the work reported here, the alcohol blends shown in Table 2 were tested. The results will be compared to those for conventional 95 and 98 RON gasoline, and with the Ultraboost control ‘base fuel’. This was a commercial gasoline sold as 95 RON fuel, but with some octane giveaway (see Table 2). While the 98 RON fuel did not contain ethanol, both of the 95 RON fuels were E5 blends; however, all three were production fuels of EN228 standard and so for the purposes of this paper they are considered gasolines and not gasoline-alcohol blend fuels.

Table 2: Specifications of the gasoline and binary alcohol-gasoline fuels tested in the Ultraboost extreme downsizing demonstrator engine

<table>
<thead>
<tr>
<th>Fuel Name</th>
<th>RON</th>
<th>MON</th>
<th>S</th>
<th>Volumetric LHV (MJ/l)</th>
<th>Stoichiometric Air-Fuel Ratio (:1)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Base</td>
<td>97</td>
<td>85.3</td>
<td>11.7</td>
<td>31.29</td>
<td>14.18</td>
</tr>
<tr>
<td>95 RON Pump</td>
<td>95.1</td>
<td>85</td>
<td>10.1</td>
<td>31.51</td>
<td>14.19</td>
</tr>
<tr>
<td>98 RON Pump</td>
<td>98.7</td>
<td>86.5</td>
<td>12.2</td>
<td>31.57</td>
<td>14.45</td>
</tr>
<tr>
<td>M15</td>
<td>99.8</td>
<td>86.1</td>
<td>13.7</td>
<td>29.56</td>
<td>13.25</td>
</tr>
<tr>
<td>E20</td>
<td>99.6</td>
<td>85.7</td>
<td>13.9</td>
<td>29.81</td>
<td>13.3</td>
</tr>
<tr>
<td>E85</td>
<td>107.4</td>
<td>89.5</td>
<td>17.9</td>
<td>22.65</td>
<td>9.68</td>
</tr>
</tbody>
</table>

The two mid-level blends, E20 and M15, were chosen for different reasons: E20 represents a maximum blend in the region of what could be made using ethanol derived from biomass in Europe and the US, given concerns about food supply and indirect land-use change (ILUC); M15 represents a blend which is in common use in China, the methanol generally being made from coal as a means of improving that nation’s energy security. However, in Table 2 also note that these two blends are coincidentally matched for air-fuel ratio and also for volumetric lower heating values (LHVs). This phenomenon has been discussed by several different researchers [39-43] and will be returned to in a later publication discussing further tests conducted with three-component gasoline-ethanol-methanol (GEM) blends matched for stoichiometry.

Results of spark loops for E20 and M15 at the same boost and speed conditions are shown in Figures 2 and 3, compared to that of the base fuel. The conditions for Figure 2 were an engine speed of 2000 rpm and intake plenum conditions of 40°C and 130 kPa gauge. For Figure 3 the corresponding values are 3000 rpm, 60°C and 140 kPa gauge with 10% cooled EGR. Both conditions (referred to as test points A and D later in this paper) therefore represent high load conditions, as shown by the BMEP evident in the figures.
Immediately apparent from these sets of data is that the two alcohol blend fuels perform identically. Part of the reason for the comparable performance will undoubtedly be that the two mid-level blends (which are defined on a volumetric basis, as discussed above) actually contain the same molar concentration of the respective alcohol in the mixture – approximately 40%. This is obviously a much
higher number than the volumetric blend rate and illustrates the effect of the light alcohol molecules in the much heavier bulk hydrocarbon, as has been discussed by Pearson et al. [44]. The pure alcohols possess similar octane numbers and thus in the gaseous state, as found in a combustion system, they would be expected to perform in the same manner.

Also apparent in the data is that the two alcohols perform markedly better than the base fuel (measured at 97 RON, as shown in Table 2). At the same spark advance, and since fixed plenum pressure and temperature were used, the improvement in efficiency is due to an increase in volumetric efficiency due to the greater enthalpy of vaporization of the alcohols (together with minor benefits due to their reduced heat transfer and an increased molar expansion ratio). Since the curves end at the KLSA, the improvement due to octane number is additive to this effect.

Calculating the enthalpy of vaporization based on a volume basis (as discussed by Chupka et al. [45] shows that the two blends have near-identical values in the region of 311.6-314.0 kJ/l (M15 being 0.7% higher) although the value for the mixture is also dependent on the composition of the gasoline (for which 280 kJ/kg has been used here)\(^3\). Since this is a direct injection engine, matching the enthalpy of vaporizations would also be expected to equalize the performance between the blends, which appears to be the case here. It is acknowledged that the enthalpy of vaporization varies with temperature, as discussed by Chen and Stone [46], and that detailed liquid-vapour equilibria and distillation data are required to understand the evaporation of the whole mixture properly. Nevertheless, since the plenum pressure and temperature conditions were held constant during these tests, comparison between the fuels is valid. Further discussion on the enthalpy of vaporization of the components and the resulting effect on particle emissions is made in Section 5, below.

During this sequence of tests to compare the fuels four operating points were determined that were representative of different operating regimes. They were selected so that all of the fuels in the full fuel test regime that the Ultraboost engine was performing within the main project could be operated so that the advantages of higher octane values could be ascertained. The other test results have been reported elsewhere [36-38]. The test points used are shown in Table 3.

### Table 3: Test points for Ultraboost engine testing

<table>
<thead>
<tr>
<th>Test Point</th>
<th>Engine Speed (rpm)</th>
<th>Load Condition</th>
<th>EGR (%)</th>
<th>Boost Pressure (bar)</th>
<th>Plenum Temperature (°C)</th>
<th>Exhaust Back Pressure (bar)</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>2000</td>
<td>High</td>
<td>0</td>
<td>1.3</td>
<td>40</td>
<td>0.45</td>
<td></td>
</tr>
<tr>
<td>B</td>
<td>2000</td>
<td>High</td>
<td>10</td>
<td>1.5</td>
<td>40</td>
<td>0.45</td>
<td>Boost pressure increased to compensate for presence of EGR</td>
</tr>
<tr>
<td>C</td>
<td>3000</td>
<td>Mid-High</td>
<td>10</td>
<td>1.4</td>
<td>60</td>
<td>0.7</td>
<td>Mimics supercharged operation</td>
</tr>
<tr>
<td>D</td>
<td>3000</td>
<td>Mid-High</td>
<td>10</td>
<td>1.4</td>
<td>60</td>
<td>1.2</td>
<td>Mimics turbocharged operation</td>
</tr>
</tbody>
</table>

In Table 3 the phrase ‘boost pressure increased to compensate for presence of EGR’ refers to the fact that the plenum pressure was increased so that the rate at which oxygen was ingested by the engine was the same for points A and B; effectively the same BMEP was targeted at KLSA. Point C targeted a back pressure at the exhaust manifold outlet typical of a supercharged engine while point D targeted a back pressure representative of a turbocharged one. The higher exhaust back pressure of test point

\(^3\) Note that there is an alternative view that mass-based enthalpy of vaporization should be used, as proposed by Zhou et al. [48]. Adopting this approach, E20 would have an enthalpy of vaporization of 417.4 kJ/kg and M15 421.9 kJ/kg; i.e. using this calculation approach that of M15 is 1.1% higher. Note also that these values are approximately 50% higher than the value of 280 kJ/kg used for the gasoline.
D was intended to reduce the knock limit of the engine with respect to point C. For more information on the rationale behind choosing these test conditions, see [36-38].

As described above at each point a spark loop was conducted with the relative air-fuel ratio (AFR) held at \( \lambda = 1 \) (i.e. the stoichiometric AFR) and the boost conditions were held constant (i.e. pressure, temperature and EGR rate were not varied), but torque and therefore brake specific fuel consumption (BSFC) and brake thermal efficiency (BTE) could change.

The results for torque from the tests with the base fuel, 95 RON pump gasoline and the two mid-level blends (E20 and M15) are shown in Figure 4. E85 is also shown and will be discussed later. What is apparent in these results is that in terms of torque output for the fixed intake conditions both of the mid-level blends perform better than the gasolines, which might be expected given their higher octane values shown in Table 2. It can also be seen that within experimental error they essentially perform identically, in line with the blending rules established in [39,44]. Thus mid-level blends in which the octane numbers are increased over those readily achievable with conventional gasoline (in the manner discussed by Anderson and co-workers [47]) offer the potential to improve engine efficiency while permitting renewable energy to be introduced into the fuel pool.

BSFC and BTE data is shown in Figures 5 and 6. The BSFC results show the expected trend: because of their lower LHV the alcohols record significantly higher BSFCs, but in terms of efficiency they beat the two gasolines shown.

![Fig. 4: Results for torque for two standard gasolines and three binary alcohol blends, at fixed intake conditions. Ultraboost research engine, operated at MBT ignition timing. E20 and M15 have matched stoichiometry, enthalpy of vaporization and octane numbers, and essentially perform identically](image)

![Fig. 5: Results for brake thermal efficiency for two standard gasolines and three binary alcohol blends, at fixed intake conditions. Ultraboost research engine, operated at MBT ignition timing](image)
In Figure 5 the slight differences between the BTEs for the fuels when producing the same torque with the same LHV is considered to be within experimental error. Since this engine had a relatively low CR of 9.0, albeit capable of being very heavily boosted and habitually operated at 35 bar brake mean effective pressure (BMEP) on gasoline [35], the data for this fuel suggests that significant improvements in BTE could be realized for mid- and high-alcohol blends and pure components if an engine with significantly higher CR could be used. Such a situation is discussed in the next section.

3. EXPERIMENTS INTO EFFICIENCY IMPROVEMENTS AND ENGINE LOAD CONTROL UTILIZING PURE METHANOL

3.1 Experiments with spark-ignition base engines

As discussed above, thanks to a variety of interesting properties the light alcohols have the potential to increase the power and efficiency of SI engines. While the previous section investigated blends of the alcohols with conventional gasoline, Ghent University has operated several engines on M100 as part of a research stream into utilizing the desirable characteristics of methanol combustion in optimized engines, while also investigating different strategies for load control that are enabled by those properties as well. Other studies using methanol in SI engines have shown that the potential improvement depends on the degree to which an engine can be biased towards alcohol-only operation while still maintaining flex-fuel functionality. To investigate the potential, operation on a commercial 95 RON gasoline and pure methanol was compared in two NA port-fuel injection (PFI) engines: a production-type 4-cylinder Volvo engine and a research-type single-cylinder Audi engine [49]. The specifications of these engines are given in Table 4.

Table 4: Test engine specifications

<table>
<thead>
<tr>
<th>Engine type</th>
<th>Volvo 1.8 l</th>
<th>Audi/NSU</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinders</td>
<td>4 in-line</td>
<td>1</td>
</tr>
<tr>
<td>Valves</td>
<td>16</td>
<td>2</td>
</tr>
<tr>
<td>Valvetrain</td>
<td>Double overhead camshaft</td>
<td>Overhead camshaft</td>
</tr>
<tr>
<td>Bore</td>
<td>83 mm</td>
<td>77.5 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>82.4 mm</td>
<td>86.4 mm</td>
</tr>
</tbody>
</table>

Note that both of these engines were originally designed for operation on gasoline, and as such have relatively low compression ratios appropriate for using this fuel.
Displacement | 1783 cc | 407.3 cc  
Compression ratio (CR) | 10.3:1 | 10.17:1 (results Section 3)  
| | 13.1:1 (results Section 4)  
Fuel system | PFI | PFI  
Aspiration | NA | NA  
Engine control unit (ECU) | MoTeC M800 | MoTeC M4  

The use of the Volvo production engine in this work was partly to demonstrate the ease with which widespread automotive technology can be modified to accept high alcohol blends, thus easing any potential evolution of the transport system in this direction.

A well-known advantage of using methanol in SI engines is the increase in maximum achievable engine load. In PFI engines this is mainly a consequence of the elevated knock resistance of methanol, but the high degree of charge cooling as the fuel is injected leads to increased volumetric efficiency as well. These factors provide a relative power increase of more than 10% as the results obtained with the Audi engine shown in Figure 7 demonstrate.

![Fig. 7: NA single-cylinder Audi engine: maximum torque when operated on gasoline (open symbols) and methanol (closed symbols)](image)

In DI engines a combination of the extremely high enthalpy of vaporization of alcohols together with their relatively low stoichiometric AFRs means that the possibility to reduce charge temperature at full load provides a significant potential development stream in line with the megatrend in the automotive industry towards downsized, DI SI engines [35]. The degree to which alcohols provide increased knock resistance in such combustion systems is the subject of much research at present [50-53]. Table 5 quantifies the potential charge cooling effect of several alcohols and also lists a ‘direct-injection octane number’ (DON) as defined by other researchers [52].

Table 5: Properties of alcohol fuels and gasoline. Data taken from [52,54].

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Methanol</th>
<th>Ethanol</th>
<th>Propanol</th>
<th>Butanol</th>
<th>Gasoline</th>
</tr>
</thead>
<tbody>
<tr>
<td>Heat of Vaporization (kJ/kg&lt;sub&gt;fuel&lt;/sub&gt;)</td>
<td>1170</td>
<td>930</td>
<td>693</td>
<td>583</td>
<td>440*</td>
</tr>
<tr>
<td>Stoichiometric AFR</td>
<td>6.5</td>
<td>9</td>
<td>10.5</td>
<td>11.3</td>
<td>14.4</td>
</tr>
<tr>
<td>Heat of Vaporization (kJ/kg&lt;sub&gt;stoichiometric mixture&lt;/sub&gt;)</td>
<td>180.0</td>
<td>103.3</td>
<td>66.0</td>
<td>51.6</td>
<td>30.6</td>
</tr>
<tr>
<td>Heat of Vaporization per unit mass of stoichiometric mixture relative to gasoline (:1)</td>
<td>5.9</td>
<td>3.4</td>
<td>2.2</td>
<td>1.7</td>
<td>1</td>
</tr>
<tr>
<td>Research octane number (RON)**</td>
<td>106</td>
<td>107</td>
<td>104</td>
<td>98</td>
<td>95</td>
</tr>
<tr>
<td>Motor octane number (MON)**</td>
<td>90</td>
<td>91</td>
<td>89</td>
<td>83</td>
<td>85</td>
</tr>
</tbody>
</table>
Direct-injection Octane Number (DON)** [52]

| DON | 119 | 122 | 108 | 98 | 95*** |

*Mid-point of values given in [52] for Eurosuper 95 RON E0, with 10% ethyl tert-butyl ether (i.e. no ethanol was present)

** For the alcohols, derived from Figure 6 of reference [52]

*** Derived from Figure 7 of reference [52] and an assumed motor octane number (MON) of 85 (i.e. the European minimum value)

In Table 5, the values shown for propanol and butanol are those for the normal alcohols (i.e. propan-1-ol and n-butanol-1-ol respectively). The values for DON, as reported in [52], are derived from the data given in that work and included in order to show the outright potential of the alcohols in DI combustion systems.

In addition to its potential to increase performance and provide a route to greater efficiency through increased engine downsizing, methanol also enables relative BTE gains of up to 10% (see Figure 8) even with an engine which was originally optimized for operation on gasoline. This is partly explained by the higher LBV of methanol; the reduced in-cylinder heat transfer losses compared to gasoline operation are another contributing factor. Not only does the charge cooling due to methanol evaporation reduce the unburned mixture temperature, but the high heat capacity of methanol’s combustion products also reduces the flame and exhaust gas temperatures compared to gasoline; these results mirror those for E85 reported in [54]. At high loads, the knock resistance of methanol ensures that optimal values for ignition timing can be retained, which is also helpful for efficiency. It is readily apparent that optimization of an engine to make better use of the improved qualities of alcohols over a conventional non-premium gasoline would improve this situation further; principal among the factors which could be adjusted would be CR.

As mentioned above, the lower peak combustion temperature of methanol leads to a reduction in engine-out NOx. Figure 9 shows that the values measured on the single-cylinder engine were consistently 5-10 g/kWh lower on methanol compared to gasoline. No significant changes in carbon monoxide (CO) emissions were observed, although some authors report that the oxygenated nature of alcohols can cause more complete combustion and thus reduced CO emissions [55], due partly to the fact that they can be described as being already partially oxidized as a result of the oxygen atom present in the alcoholic OH group defining this family of chemicals.

![Fig. 8: Brake thermal efficiency at part load for the NA 4-cylinder Volvo engine. Constant brake torque of 20 Nm (diamonds), 40 Nm (triangles) and 80 Nm (circles). Open symbols for gasoline and closed symbols for methanol. Stoichiometric fuelling, throttled load control](image)
In terms of specific CO\(_2\) emissions, a reduction of more than 10% was observed on methanol, as shown in Figure 10 for the four-cylinder Volvo engine. In addition to the improvement in performance of the combustion system when operating on the alcohol, this is partly due to the fact that lower alcohols produce less CO\(_2\) per unit of energy contained (68.4 g/MJ for methanol when compared to a typical value of 74 g/MJ for gasoline, or more than 7% less). Another reason is the higher BTE when using methanol. Emissions of unburned hydrocarbons (HCs) are not reported since flame ionization detectors (as used in this work) are reported to have a slow response time to oxygenated species [56,57].

The elevated LBV and wide flammability limits of methanol offer some alternative options for load control, again beyond what can be achieved with straight hydrocarbon fuels. Two such strategies are wide-open throttle (WOT) lean-burn operation and WOT EGR operation. These were compared against the conventional throttled stoichiometric operation on the single-cylinder engine [58]. These strategies respectively employed variable mixture strength or stoichiometric mixtures and variable amounts of external EGR to control load while the throttle position was fixed (and preferably wide open to the benefit of minimum pumping work).

Clearly, there would be varying demands on the exhaust after treatment (EAT) system for any engine adopting these strategies, but they are interesting for a number of reasons, the main ones being the reduction of throttling losses, which is beneficial for part load efficiency, and a reduction in heat transfer and endothermic dissociation losses thanks to the lower in-cylinder temperatures associated with dilution. Unfortunately, the application of excess air or EGR also renders the combustion increasingly
unstable and less isochoric due to reduced burning rates. A fuel with wide flammability limits and high LBV (in turn providing elevated EGR tolerance) such as methanol will be less prone to the negative side-effects of any charge dilution strategy. Measurements on the single-cylinder engine indicated that EGR levels up to 30% could be applied before the coefficient of variance (CoV) of indicated mean effective pressure (IMEP) exceeded the threshold value of 10% used, whereas for gasoline operation this limit on CoV of IMEP was found to be at only 10% EGR. For the lean-burn strategy, the combustion stability limits were $\lambda=1.5$ and $\lambda=1.25$ on methanol and gasoline respectively [58].

Figure 11 illustrates some of the key differences between the load control strategies under consideration. The pumping loops for the lean burn and WOT EGR strategies are considerably smaller than for conventional load control via the throttle due to the absence of those throttling losses. Also visible on the diagram is the adverse influence of air and EGR dilution: the combustion itself is less isochoric, the effect possibly being greater for EGR operation than for lean burn. Figure 12 shows that both alternative strategies lead to relative improvements in indicated thermal efficiency (ITE) of the order of 5% thanks to reduced throttling, cooling and dissociation losses. These are in addition to any improvements due to operating the engine on methanol over its performance on gasoline.

Fig. 11: Indicator diagram for operation with different load control strategies at 1500 rpm and 25 Nm for the Audi engine. Dotted line is conventional throttled case, dashed line is WOT EGR case and solid line is WOT lean case

Fig. 12: Indicated thermal efficiency for a fixed brake torque of 25 Nm for the Audi Engine. Diamonds for throttled case, squares for WOT EGR case, triangles for WOT lean case

3.2 Experiments with a light-duty diesel engine converted to spark ignition
After this series of investigations using a single-cylinder SI engine operating on pure methanol, the strategy employing cooled EGR at WOT was further investigated on a turbocharged four-cylinder engine. This was done because the fact that stoichiometric operation coupled with EGR dilution supports the use of a simple and robust three-way catalyst makes this load control strategy very attractive. This 4-cylinder research engine was based closely on a Volkswagen Type AXR 1.9 litre turbocharged diesel engine in order to provide the high swirl rate that was desired.

In converting the engine a similar approach was taken to that reported in [59]. It retained its compression ratio piston of 19.5:1, because the crank train of the engine was not changed, and also retained the high-swirl intake port and diesel piston bowl optimized for diesel combustion. These features were considered more appropriate for EGR dilution [59], because of its elevated levels of mixture turbulence. They increased the burn rates sufficiently to allow throttleless operation with the EGR strategy down to 3 bar brake mean effective pressure (BMEP) without excessive cyclic variability. For comparison, when operating on methanol with the single-cylinder Audi engine the corresponding lower load limit on cyclic variability was 6 bar BMEP. A standard ignition system was used together with port fuel injection; more details on this engine are to be found in [59].

For this work the engine was mapped from 1000 to 4000 rpm in 500 rpm increments, and at each speed in steps of 25 Nm up to the full load point. This resulted in 62 test points, to provide a fine grid of test data to produce performance maps such as is shown in Figure 13. Here it can be seen that the high CR helped to produce a peak BTE of 42%. At the same time the specification rendered full-load operation on standard commercial 95 RON gasoline impossible due to heavy knock. Arguably the revised configuration of the engine was closer to that which would be arrived at if full optimization of a spark-ignition engine was undertaken to take full benefit of the properties of light alcohols, although it could still be argued that its CR was too high. The advantage of this was shown at part load, though, the absence of throttling losses and the benefits associated with lower in-cylinder temperatures enabling relative efficiency improvements of up to 20% compared to conventional throttled operation.

The high levels of EGR dilution at these loads (up to 50%) also reduced the engine-out NOx emissions to extremely low levels (see Figure 14). These results demonstrate that methanol can be used in dedicated SI engines to yield diesel-like efficiencies with emission levels comparable to, or lower than, those achieved when using gasoline. The primary reason for the very low NOx results in Figure 14 in comparison to Figure 9 is because of the ability of the engine to operate with very levels of EGR dilution due to the use of methanol, the high CR and high tumble. Thus development of a fully-optimized engine could be expected to produce yet higher efficiencies due to lower friction from crank train components suitable for the lower cylinder pressures than the diesel base engine reaches, and reduced heat losses from what would likely be a lower CR than 19.5:1, coupled with a more-favourable surface area-to-volume ratio from a combustion chamber developed for SI combustion rather than for diesel (where very high swirl rates are a dominant feature).
The technologies employed in realizing the improvement in efficiency demonstrated when optimizing for a high-blend or pure alcohol fuel are essentially the same as those used in production gasoline engines now. The importance of this is that when combined with flex-fuel engine control strategies, calibrations can be developed which still permit the use of gasoline (with its much lower octane numbers and enthalpy of vaporization) in the vehicle, albeit with lower performance. This obviates any issues of range anxiety (such as is the case with electric vehicles or, on its take up, molecular hydrogen fuel) during the transition to high-alcohol fuels. The miscibility of alcohols with gasoline in the same fuel system means that the vehicle on-cost will be small to provide this complete flexibility and reassurance for the customer.

4. PERFORMANCE AND EMISSIONS OF BINARY GASOLINE-ALCOHOL BLENDS IN A PRODUCTION SPARK-IGNITION ENGINE

In this piece of work, the performance and engine-out emissions of two binary gasoline-alcohol blends corresponding to the value of stoichiometry of E85 were examined in a 4-cylinder 1.8 l PFI production engine. In parallel, a single-cylinder engine with high CR was also used for a preliminary study of the knock behaviour of these blends. The measurement results are compared with those when operating on commercial gasoline and neat methanol and ethanol in order to demonstrate the potential of these blends as a fossil fuel alternative.

The composition and properties of the two blends are shown in Table 6. Here ‘Blend A’ represents idealized ‘normal’ E85 whereas the equivalent stoichiometry methanol-gasoline ‘Blend D’ contains 57 % v/v methanol. These are therefore considered to be iso-stoichiometric blends, and they were configured in the same way as discussed in previous sections. Blend D (M57) has 1 % v/v methanol more than in the study of Turner et al. [60] because of a difference in the stoichiometric AFR of the gasoline used for blending in this section; nevertheless the same blending rules were used to determine it.

Table 6: Properties of the iso-stoichiometric binary blends tested in a 4-cylinder 1.8 l PFI production engine

<table>
<thead>
<tr>
<th>Fuel blend</th>
<th>Blend A</th>
<th>Blend D</th>
</tr>
</thead>
<tbody>
<tr>
<td>Component ratios (%)</td>
<td>G15 E85</td>
<td>G43 E0</td>
</tr>
<tr>
<td>Oxygen content [% m/m]</td>
<td>23.34</td>
<td>22.54</td>
</tr>
<tr>
<td>Gravimetric LHV [MJ/kg]</td>
<td>29.22</td>
<td>29.53</td>
</tr>
<tr>
<td>Volumetric LHV [MJ/l]</td>
<td>22.82</td>
<td>22.59</td>
</tr>
<tr>
<td>AFR_{stoich} [kg/kg]</td>
<td>9.72</td>
<td>9.73</td>
</tr>
</tbody>
</table>
Stoichiometric operation was employed throughout these tests in order to maximize the pollutant conversion rate of a three-way catalyst.

4.1 Performance

Figure 15 shows the BTE for all blends at a constant load of 40 Nm (2.82 bar BMEP) for a range of engine speeds. The hypothesis that all iso-stoichiometric blends have similar BTEs is confirmed here as all the values fall within the range of experimental uncertainty. Furthermore, this statement is valid for all loads tested here.

![Graph showing Brake thermal efficiency of Blend A (E85) and Blend D (M57) as a function of engine speed for a fixed brake torque of 40 Nm (2.82 bar BMEP) when tested in a 4-cylinder 1.8 l PFI production engine.]

Figure 16 displays the comparison with gasoline, methanol, ethanol and a mean value for the two binary blends for 40 and 80 Nm, labelled ‘GEM mean’. When compared to gasoline, it is clear that the binary blends show significant efficiency gains. The mean value for the binary blends is similar to the BTE of pure ethanol. Pure methanol clearly still has superior performance, which might be expected from the results already discussed in Section 4.

![Graph showing Brake thermal efficiency when operating on various fuels as a function of engine speed for different fixed brake torques of 40 Nm (2.82 bar BMEP) (dashed lines) and 80 Nm (5.64 bar BMEP) (solid lines) when tested in a 4-cylinder 1.8 l PFI production engine.]

BSFC does not depend on mixture composition as seen on Figure 17, primarily because of the near-identical LHV of the binary blends. Again, this might be expected from the discussion on BTE. While the binary blends display similar BTE to pure ethanol, their BSFCs are less penalized than pure methanol. This is shown in Figure 18 in which a comparison of the BSFCs of gasoline, methanol, ethanol and a mean value for the binary blends for 40 and 80 Nm is shown. Despite the better efficiency on binary blends, this engine will consume ~32% more fuel blend than when it is running on gasoline on a volume basis. This difference will be smaller for modern highly downsized and pressure-charged engines with DI in which the properties of alcohols will have greater benefits; similarly the
The in-cylinder pressure measurements can be used to obtain information regarding the combustion process in the engine, in terms of heat release and mass fraction burned (MFB). In Figure 19, the heat release rates of the iso-stoichiometric binary blends are shown, as calculated from the in-cylinder pressure measurements. As can be seen in the figure, the heat release rates are close to each other, again as might be expected. As a result, the MFBs for the different blends are very similar. The ignition delay (defined here as 0-2% MFB), the 0-10% and 0-50% MFB durations are plotted in Figure 20 as a function of engine speed, showing the similar burning velocities of the two blends at these operating conditions.

Fig. 17: Brake specific fuel consumption of the blends as a function of engine speed for a fixed brake torque of 40 Nm (2.82 bar BMEP) when tested in a 4-cylinder 1.8 l PFI production engine

Fig. 18: Brake specific fuel consumption as a function of engine speed for different fixed brake torques of 40 Nm (dashed lines) and 80 Nm (solid lines) when tested in a 4-cylinder 1.8 l PFI production engine
Fig. 19: Heat release rates of two iso-stoichiometric gasoline-alcohol blends for an engine speed of 2000 rpm and a fixed brake torque of 40 Nm (2.82 bar BMEP) when tested in a 4-cylinder 1.8 l PFI production engine

Fig. 20: Ignition delay (0-2% burned), 0-10% and 0-50% burn duration of two iso-stoichiometric gasoline-alcohol blends as a function of engine speed for a fixed brake torque of 40 Nm (2.82 bar BMEP) when tested in a 4-cylinder 1.8 l PFI production engine

4.2 Emissions

In this section, NOx emissions are shown and discussed for the two high-blend fuels tested. Figure 21 compares the engine-out NOx emissions for the two high-blend fuels, gasoline and pure methanol at a load of 40 Nm. As can be seen, the highest NOx emissions were found when operating on gasoline and the lowest NOx emissions were given on methanol. All of the NOx emissions for high-blend fuels are somewhere between gasoline and methanol. The lower combustion temperature of the alcohol fuels are responsible for the lower NOx emissions since most NOx is produced by the thermal mechanism which is very dependent on the maximum temperature reached. The lower NOx emissions at lower engine speeds are hypothesized to be the result of elevated levels of internal EGR since the vacuum in the intake due to the use of conventional throttling for load control is considerable at this low engine load of 40 Nm. For the two alcohol-gasoline blends it can be seen that there is an increase in NOx emission with increased gasoline content in the mixture. This variation with gasoline content and thus total alcohol concentration for all other measurements could be ascribed to a slight variation in flame temperature. It is considered that further research in this areas would be warranted.
Fig. 21: NOx emissions as a function of engine speed for gasoline, methanol and two iso-stoichiometric gasoline-alcohol blends as a function of engine speed for a fixed brake torque of 40 Nm (2.82 bar BMEP) when tested in a 4-cylinder 1.8 l PFI production engine

4.3 Knock behaviour

For the Volvo 4-cylinder engine at the low loads tested no knock occurred during the measurements on all of the fuels and thus MBT timing could be set for every load and engine speed. From previous work it is expected that the two binary blends would have very similar knock behaviour [39,40,44].

To investigate the hypothesis that such blends exhibit quasi-constant RON and MON via their knock resistance, Blends A and D and their individual components (pure methanol, ethanol and gasoline) were tested in a single-cylinder research engine with a high CR. The properties of this test engine are listed in Table 3 above (i.e. that used for the work reported in Section 3). At an operating point of 25 Nm (BMEP = 7.71 bar) and 2000 rpm, ignition timing was advanced until an intermediate knocking condition was obtained. In addition to the RON 95 gasoline (which was used as the gasoline component to formulate the blends) a RON 98 gasoline was also tested. The results of this experiment are shown in Figure 22. As can be seen, the blends have similar knocking behaviour, resulting in the same ignition timing at incipient knock. Furthermore, the blends display the same ignition timing as pure ethanol. As discussed, the M57 blend was configured to be equivalent to E85 and so the fact that their performance is so close to that of pure ethanol is to be expected because the molar concentrations of the alcohol in each blend is similar\(^5\). Having said this, pure methanol still displays superior knock resistance to all of the other fuels.

\(^5\) By mole fraction, E85 is approximately 94% ethanol and M57 is approximately 84% methanol.
5. PARTICULATE EMISSIONS FROM HIGH-BLEND ALCOHOL FUELS IN A DIRECT-INJECTION SPARK-IGNITION ENGINE

Despite the fact that significant activity has been undertaken investigating the performance of iso-stoichiometric blends in engines and vehicles, to date particle number (PN) emissions from these blends have not been evaluated in a DI engine. In this section, particulate emissions from a single-cylinder DI engine operating on E85 and M56 fuels and a base gasoline were measured.

5.1 Fuels tested

For this experiment, E85 and M56 were splash-blended with a base gasoline, their composition being shown in Table 7, together with their predicted dry vapour pressure equivalent (DVPE).

Table 7: Composition of the iso-stoichiometric fuel blends tested in the single-cylinder DI engine

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Gasoline (%v/v)</th>
<th>Ethanol (%v/v)</th>
<th>Methanol (%v/v)</th>
<th>Predicted DVPE* (kPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gasoline</td>
<td>100</td>
<td>0</td>
<td>0</td>
<td>62</td>
</tr>
<tr>
<td>E85</td>
<td>15</td>
<td>85</td>
<td>0</td>
<td>39</td>
</tr>
<tr>
<td>M56</td>
<td>44</td>
<td>0</td>
<td>56</td>
<td>87</td>
</tr>
</tbody>
</table>

*Prediction derived from a UNIFAC model [61].

The base gasoline for these blends was a CEC RF-02-03 specification gasoline supplied by BP. This gasoline has no oxygenate components present in it, and its properties are shown in Table 8.

Table 8: Composition of the base CEC RF-02-03 gasoline test fuel

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td></td>
<td>97.0</td>
</tr>
<tr>
<td>MON</td>
<td></td>
<td>87.7</td>
</tr>
<tr>
<td>Density @ 15°C</td>
<td>kg/L</td>
<td>0.7439</td>
</tr>
<tr>
<td>DVPE</td>
<td>kPa</td>
<td>60.0</td>
</tr>
<tr>
<td>Aromatics</td>
<td>% v/v</td>
<td>29.0</td>
</tr>
<tr>
<td>Olefins</td>
<td>% v/v</td>
<td>1.8</td>
</tr>
<tr>
<td>Saturates</td>
<td>% v/v</td>
<td>69.2</td>
</tr>
<tr>
<td>Carbon</td>
<td>% m/m</td>
<td>86.74</td>
</tr>
<tr>
<td>Hydrogen</td>
<td>% m/m</td>
<td>13.26</td>
</tr>
<tr>
<td>Gross Calorific Value</td>
<td>MJ/kg</td>
<td>46.19</td>
</tr>
<tr>
<td>Net Calorific Value</td>
<td>MJ/kg</td>
<td>43.38</td>
</tr>
<tr>
<td>IBP</td>
<td>ºC</td>
<td>28.8</td>
</tr>
<tr>
<td>T90</td>
<td>ºC</td>
<td>166.6</td>
</tr>
<tr>
<td>FBP</td>
<td>ºC</td>
<td>200.8</td>
</tr>
</tbody>
</table>

5.2 Expected fuel effects on PN emissions

It has previously been noted [62] that AFRs rich of stoichiometric increase particulate emissions. This is true of ethanol, but the increase in particulate matter (PM) emissions rich of stoichiometric for ethanol is very small, and compared to gasoline is effectively a dramatic reduction (E10 showing a greater than order of magnitude reduction in PM emissions compared with straight gasoline) [63]. This reduction is thought to be due to the fact that the presence of oxygen in the fuel molecule reduces the concentration of intermediate species that are important to the formation of precursors to soot [64].

As methanol is added to fuel, its vapour pressure increases, as can be seen by the change in predicted DVPE in Table 7. High vapour pressures can result in the flash-boiling of the fuel on injection, leading to very poor mixture preparation. This poor mixture preparation would be expected to lead to high levels of particulate emissions being observed when methanol is blended with gasoline, as is the case for M56.

Flash boiling occurs when the fuel evaporates so quickly on injection that it essentially does so as it leaves the injector in an “onion skin” manner, with the outer layers evaporating first, regardless of their
composition. This is known to occur in DI engines [65], and is the result of rapid boiling of a liquid (in this case fuel), occurring as a liquid jet is injected into a volume with a pressure lower than the saturation vapour pressure of the liquid. In this case the liquid is rapidly depressurised, and the liquid becomes superheated and consequently thermodynamically unstable, regaining its stability by flash boiling.

5.3 Test engine and particulate measurements

The engine for these tests was a single-cylinder engine with a central spray-guided direct-injection combustion system based on the Jaguar AJ133 5.0 litre V8 engine [66]. This research engine is described more fully by Leach [61] and it represents a modern DI SI configuration. The engine was fitted with a titanium piston with a steel blanking plate, and the relevant engine specifications are shown in Table 9.

Table 9: Single-cylinder DI engine parameters

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bore (mm)</td>
<td>89</td>
</tr>
<tr>
<td>Stroke (mm)</td>
<td>90.3</td>
</tr>
<tr>
<td>Cylinder capacity (cc)</td>
<td>562</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>11.1</td>
</tr>
<tr>
<td>Fuel injection pressure (bar)</td>
<td>150</td>
</tr>
</tbody>
</table>

PN emissions were measured using a Cambustion DMS500, which is fully described by Reavell et al. [67]. A Wiebe filter was used to mimic the effect of the PMP legislatively compliant protocol [68] for measuring PN emissions, and this method has been shown to be representative of legislative tests [69], although this was not a legislatively compliant test.

5.4 Results

For these experiments the engine was run at the fixed operating point shown as in Table 10. Here the engine was run with fixed injection timing, so it should be noted that injection timing amongst other parameters can have a big impact on PN emissions some work looking at the effect of injection timing on PN emissions on this engine has been previously done by Murad et al. [70]. The engine was run with open-loop AFR control with $\lambda = 0.9$ and $1.01$, and at low load and medium load (2.6 and 4.9 bar IMEP). $\lambda = 1.01$ was chosen to avoid any small rich mixture excursions which are known to have a large effect on the particulate matter emissions from non-oxygenated fuels [62]. Because of this, these rich excursions tend to dominate drive cycle PM results, hence the relevance of testing at $\lambda = 0.9$.

Table 10: Engine operating conditions for model fuels

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>IMEP (bar)</td>
<td>2.6 and 4.9</td>
</tr>
<tr>
<td>Inlet air temperature (°C)</td>
<td>40</td>
</tr>
<tr>
<td>Coolant temperature (°C)</td>
<td>60</td>
</tr>
<tr>
<td>AFR ($\lambda$)</td>
<td>0.9 and 1.01</td>
</tr>
<tr>
<td>Engine speed (rpm)</td>
<td>1500</td>
</tr>
<tr>
<td>Start of ignition (°BTDC)</td>
<td>35</td>
</tr>
<tr>
<td>Start of injection (°BTDC)</td>
<td>280</td>
</tr>
</tbody>
</table>

The particulate emissions from the fuels at light load (2.6 bar IMEP) are shown in Fig. 23. It can be seen from these results that the trend predicted above is clearly demonstrated here – with a significant increase of particulate emissions from E85 to gasoline to M56. E85 gives essentially particle free combustion at light load regardless of relative AFR, which is significant. One repeat (that of M56) was managed in the experimental sequence (which was done in a random order), and it can be seen that M56 gives repeatable PN emissions, leading to confidence in these results. In general, other testing on this engine shows good repeatability with PN emissions.

It is also seen that the levels of PN emissions from the base gasoline are higher than E85, but lower than M56, suggesting that the presence of ethanol at this load condition reduces PN, but methanol acts to increase PN. This could be explained by the flash boiling phenomenon described above, where the
methanol is flashing, leading to a poorly-prepared mixture, and hence an increase in PN emissions, despite a higher level of oxygenates. Alternatively, at rich conditions, large amounts of fuel will need to be injected at high oxygenate content levels to maintain $\lambda = 0.9$, looking at the $\Delta H_{\text{vap}}$ of methanol and ethanol (159 and 92 kJ/kg stoichiometric mixture respectively), large amounts of local cooling would be expected upon injection even without flash boiling. This may lead to incomplete mixture evaporation, hence worse mixture preparation and higher PN emissions. This is supported by the larger standard deviation of the M56 results (compared to E85), suggesting a less homogeneous mixture. It must be noted that the volume percentages of the two alcohols in the respective mixtures are not the same, though. It could be that M85 would have low PN emissions, or that as methanol is removed from the fuel, the effect is similarly eliminated, and the factors that cause oxygenate fuels (in general) to reduce PN emissions discussed above become dominant with only ethanol present, with the PN consequently being reduced relative to the gasoline levels. In addition, it is acknowledged that the particulate emissions of different gasoline formulations can vary widely. Overall this suggests that more work would be justified to gather the change in PN emissions as methanol proportion is changed.

![Figure 23: PN emissions from gasoline, E85 and M56 fuels at 2.6 bar IMEP for two different fuelling conditions ($\lambda=1.01$ and 0.9). Error bars correspond to $\pm \sigma$.](image)

Of particular interest is that the effect of $\lambda$ shows a significant increase in PN emissions from gasoline (as would be expected) and M56, but there is almost no difference in PN emission between E85 at $\lambda = 1.01$ and $\lambda = 0.9$. The presence of oxygen in the fuel molecule is clearly having a significant effect here, despite the need to inject more fuel on a volumetric basis, which might lead to worse mixture preparation and hence higher PN emissions. This shows that from a PN perspective, E85 is a very promising fuel, and even rich mixture excursions, which are inevitable on any drive cycle (with more ‘aggressive’ drive cycles having more such excursions), do not have a significant effect on PN emissions from E85. However, a similar study of ethanol proportion in gasoline would be justified, since in theory in flex-fuel vehicles any ethanol concentration (up to the maximum permitted in the blend) could be present in the tank.

Figure 24 shows the PN emissions from E85, M56 and gasoline at a higher load (4.9 bar IMEP). Here the trends shown at light load are repeated, although now M56’s PN emissions are lower than that of the base gasoline. This may be because at higher cylinder pressures, either less flash boiling is occurring or the higher pressures are promoting spray evaporation more generally, leading to the factors which cause oxygenate fuels to reduce particulate emissions in ethanol to dominate in methanol too. Again the effect of $\lambda$ on E85 is minimal for the same reasons as discussed above. The same observation with regards to the range of particulate emissions from different gasoline compositions that is made above must also be made, together with the fact that the widespread adoption of gasoline particulate filters will render any issues discovered here largely null anyway.
Fig. 24: PN emissions from gasoline, E85, and M56 fuels at 4.9 bar IMEP for two different fuelling conditions (λ=1.01 and 0.9). Error bars correspond to ±σ

Overall, these results show that using oxygenated fuels will not significantly impact the PN emissions witnessed from GDI engines, and some of them can significantly decrease the PN emissions observed. At light load, a slight increase in PN emissions may be observed with blend fuels with high methanol content, and this could be due to methanol promoting flash boiling, alternatively the very high latent heat of vaporisation might be leading to poor local mixture formation on injection. As the load increases the results show that these methanol blend fuels will give lower particulate emissions than gasoline, which is thought to be due to the effect of flash boiling reducing, the presence of oxygen in the molecules then reducing the number of particulate precursors formed in combustion. At both light and intermediate load high ethanol content in the fuels results in significantly lower PN emissions compared to the reference gasoline, again because the presence of oxygen in the molecules reduces the number of particulate precursors formed during combustion. Of course PN emissions are not solely a function of oxygenate content, but are also significantly influenced by a wide range of other parameters including base gasoline composition [61,71]. Here the engine has been run fully warm and the widely-documented effect of cold start dominating PN emissions has not been captured [69]. A more comprehensive study would be needed to validate this more thoroughly.

6. CONCLUSIONS

This paper has shown that the light alcohols, methanol and ethanol, can be used in mid- and high-blend fuels to improve the efficiency of spark-ignition engines and thus can help to move towards a more decarbonized transport network. Furthermore, pathways exist to enable fully-decarbonized hydrocarbon fuels to be synthesized from methanol (albeit with an associated energy loss). While ethanol production using biological sources is restricted by a biomass limit which varies from region to region, no such restriction exists for methanol production because it can be manufactured straightforwardly from any carbonaceous feed stocks using chemical processes.

As far as the use of these alcohols in binary blends with gasoline at mid- and high-level is concerned, the paper has shown that:

6.1 When configured to have the same stoichiometry, blends of gasoline and ethanol and of gasoline and methanol behave in an identical manner in SI combustion systems. This is due to fixing the stoichiometric AFR resulting in matched lower heating values, heats of vaporization and molar concentrations in the charge, in turn leading to matched octane numbers due to the extremely close RON and MON of the two alcohols.

6.2 The two high-blend matched stoichiometry fuels, E85 and M57, effectively exhibited the same knock performance as pure ethanol in a high CR single cylinder test engine. This is due to the very high molar concentration of the alcohols in their respective blends, being approximately 90% and thus dominating any negative effects of the hydrocarbon components present.
6.3 The use of the light alcohols in SI combustion systems permits significant improvements in thermal efficiency which, due to the fact that they can be manufactured using biological or zero-carbon processes, will have benefits in terms of the demands placed on such future energy systems.

6.4 In direct injection combustion systems, methanol blends have a tendency to increase particulate number emissions whereas those with ethanol do not. This is a new finding. It only occurs at light loads, and increasing load reduces the methanol blend particulate number results to values less than gasoline. It is surmised that this is a result of the very high enthalpy of vaporization and lower boiling point of the methanol component causing flash boiling and thus incomplete combustion of the hydrocarbon components. Increasing methanol concentration may also reduce the effect; the expected widespread adoption of particulate filters because of the general such challenges of gasoline fuels will of course, nullify it. The particulate-forming characteristics of different gasoline compositions will also affect any results. Overall, more research is warranted in this area.

6.5 The miscibility of the alcohols with gasoline, and the results shown here, present a method by which vehicles and fuels can co-evolve towards the complete decarbonization of transport via the use of liquid energy carriers; the current economic viability of the personal transport system is based on the ease with which liquids can be stored and distributed. This potentially has profound implications for future energy and transport policy, since it does not require a revolution to be undertaken by any of the major stakeholders in the area.

When used in their pure forms, the paper has shown that:

6.6 The alcohols provide much higher knock limits than for conventional non-premium gasoline, and this in turn increases the thermal efficiency of engines in which they are used. This has been shown in test engines with port-fuel-injection systems, which were also suitable for gasoline use.

6.7 When an SI engine can be configured to make more complete use of the beneficial characteristics of the alcohols in SI combustion systems, thermal efficiencies higher than those that can typically be achieved by current diesel engines can be realized. More-optimal development of such engines is expected to yield further benefits, leading to the possibility to extend the use of renewable energy in transportation because of increased gasoline displacement.

6.8 When operated on methanol, such high-CR engines allow load control using cooled EGR or excess air to a much greater degree than is possible using gasoline. This is due to the higher LBV of the alcohol. At the same time significantly lower engine out NOx can be shown, which is due to the lower adiabatic flame temperature coupled to the high enthalpy of vaporization reducing the overall cycle temperature.

6.9 The use of identical technologies for pure alcohols and gasoline means that engines can be optimized for the high-efficiency alcohol fuel while being protected to still be able to operate on conventional non-premium gasoline. While there would be expected to be a concomitant reduction in performance when using the hydrocarbon fuel, this removes the issues of range anxiety prevalent with electric vehicles (and likely to be the case with hydrogen fuel as and when it is first introduced). This will permit the gradual evolution of the system as discussed above, with significant benefits in terms of the viability of the approach.

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ABBREVIATIONS

AFR Air-fuel ratio  
BMEP Brake mean effective pressure  
BSFC Brake specific fuel consumption  
BTE Brake thermal efficiency  
CO Carbon monoxide  
CO₂ Carbon dioxide  
CoV Coefficient of variation  
CR Compression ratio  
DI Direct injection  
DON Direct-injection octane number  
DVPE Dry vapour pressure equivalent  
EAT Exhaust after treatment  
ECU Engine control unit  
EGR Exhaust gas recirculation  
GEM Gasoline-ethanol-methanol  
HC Hydrocarbons  
ICE Internal combustion engine  
ILUC Indirect land use change  
IMEP Indicated mean effective pressure  
ITE Indicated thermal efficiency  
MON Motor octane number  
NA Naturally-aspirated  
NOx Oxides of nitrogen  
LBV Laminar burning velocity  
LHV Lower heating value  
MFB Mass fraction burned  
PFI Port fuel injection  
PM Particulate matter  
PN Particle number  
ppm Parts per million  
RON Research octane number  
SI Spark-ignition  
WOT Wide open throttle  
ΔH_vap Heat of vaporization  
λ Lambda (relative air-fuel ratio)  
%m/m Molar percentage  
%v/v Volume percentage  
%w/w Mass percentage

REFERENCES


