Dimethyl ether and bio-diesel fuels: the potential renewable fuels for CI and NCCI combustion in internal combustion engines

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Dimethyl Ether and Bio-diesel Fuels – The Potential Renewable Fuels for CI and HCCI Combustion in Internal Combustion Engines

R. Chen, J. Patterson, N. Milovanovic
(Department of Aeronautical and Automotive Engineering, Loughborough University, UK)

Abstract: Methyl esters derived from vegetable oils, commonly known as ‘Bio-diesel’, can be used as an alternative fuel in compression ignition engines as they have very similar physical properties (for example cetane number, viscosity and density) to mineral diesel. In this study, three different vegetable oils (rapeseed oil, soya oil and waste oil) were esterified and the resulting biodiesel samples were then tested in an inline four cylinder direct injection engine, typically used in small diesel genset applications, as blends of 5% and 50% in mineral diesel, or as the pure methyl ester. The engine performance and emissions of the engine were then recorded at five load conditions and at two different speeds. The data were then compared to those obtained under the same operating conditions for mineral diesel. Homogeneous Charge Compression Ignition (HCCI) combustion employs premixed homogeneous air and fuel mixture, but the combustion is ignited by compression. It has the potential to deliver high efficiency, low NOx and particulate emissions. The auto-ignition nature ensures that the HCCI has the potential to burn different fuels. It is therefore a potential alternative technology for diesel applications. However, unlike conventional CI and SI combustion methods, the combustion process of HCCI is predominantly governed by chemical kinetics of the air/fuel mixture. It has been proved difficult to effectively controlling the ignition timing and combustion heat release rate over wide engine speed / load range over recent years of investigation. In the research work reported in this paper, four various diesel type fuels: N-heptane, Dimethyl Ether (DME), Methyl Butanoate (MB) surrogating heavy bio-diesel and Methyl Formate (MF) substituting light bio-diesel were studied using a single-zone combustion model with convective heat transfer loss and detailed chemical kinetics. The effects of different engine parameters such as recirculated exhaust gas, air/fuel ratio, intake temperature, and compression ratio on auto ignition performance were investigated.

Keywords: DME, Bio-diesel, Engine simulation, HCCI control, HCCI combustion

1. Introduction

There has been increasing research interest in alternative fuels for compression ignition (CI) engines as a consequence of legislation, or because the economics of certain areas of the world make these alternatives more attractive (Hall, Barnard et al. 1982). Of the various alternatives, Dimethyl ether (DME) and methyl esters commonly known as ‘bio-diesel’, are becoming increasingly accepted as an alternative fuel for compression ignition engines.

Dimethyl ether (DME) is an easily liquefied gas, much like propane. It can be made from almost any biomass, not just grain, even garbage. The process involves gasification of the biomass – reacting it with steam and oxygen at high temperature. The resulting synthesis gas, CO and H2, is reacted at high pressure over a catalyst to produce DME directly or methyl alcohol which is subsequently dehydrated into DME. It can also be easily made from natural gas, or coal. DME costs about the same as methanol from coal or natural gas which is much less expensive than bio-diesel (methyl esters of vegetable oils and animal fats). It is non-corrosive to metals, stable under high temperature or high humidity conditions, and has a Cetane number of over 55, with no particulates in the exhaust since it is a low molecular weight compound with no C-C bonds. It is therefore an excellent alternative diesel fuel.

Methyl esters derived from vegetable oils, commonly known as ‘Bio-diesel’, can also be used as an alternative fuel in compression ignition engines as they have very similar physical properties (for example Cetane number, viscosity and density) to mineral diesel. Bio-diesel is produced by transesterification of tri-glycerides using either an alkaline or acid catalyst. It has a number of advantages such as that can be used on existing diesel engines without expensive engine modifications, will not shorten the engine life or service periods, can usually be produced from a locally available source and its production is environmentally safe.

Homogeneous Charge Compression Ignition (HCCI) combustion employs premixed homogeneous air and fuel mixture, but the combustion is ignited by compression. It has the potential to deliver high efficiency, low NOx and particulate emissions. The auto-ignition nature ensures that the HCCI has the potential to burn different fuels. It is therefore a potential alternative technology for diesel applications. However, unlike conventional CI and SI combustion methods, the combustion process of HCCI is predominantly governed by chemical kinetics of the air/fuel mixture. It has been proved difficult to effectively controlling the ignition timing and combustion heat release rate over wide engine speed / load range over recent years of investigation.

The objective of the present research was to characterise the performance and emissions characteristics of a four cylinder DI CI engine whilst fuelled on three different types of bio-diesel fuels in order to investigate how performance characteristics vary with different source oils. An unmodified CI engine was used in order to evaluate to what extent bio-diesel can be used without engine modifications (i.e. if widespread fuelling of current CI engines is feasible).
Finally, different blends of the bio-diesels with mineral diesel were tested, as current European legislation requires that a certain percentage of diesel fuel used must in future be derived from renewable sources (2% of all transport fuel must be replaced this year, and 5.75% replaced by 2010). The most likely route to achieve this is though blending of bio-diesel with mineral diesel. The three different fuels that were tested were a rape seed oil derivative (commonly used in Europe), a soy bean oil derivative (commonly used in USA) and waste oil derivative which may be used as part of a recycling strategy. The emissions of NOx and visible smoke were focused upon in this study, as they are regarded as the main emissions of interest in CI engines. In addition, four various diesels type fuels: N-heptane, Dimethyl Ether (DME), Methyl Butanoate (MB) surrogating heavy bio-diesel and Methyl Formate (MF) substituting light bio-diesel were studied using a single-zone combustion model with convective heat transfer loss and detailed chemical kinetics. The effects of different engine parameters such as recirculated exhaust gas, air/fuel ratio, intake temperature, and compression ratio on auto ignition performance were investigated.

2. Experiment Study on Bio-diesel

2.1 Engine set-up

The engine used in this study was a Lister-Petter inline four cylinder direct injection diesel engine, typically used in small diesel genset applications. Details of the engine specification are given in Table 1.

<table>
<thead>
<tr>
<th>Engine Type</th>
<th>Lister-Petter 4x90, DI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Configuration</td>
<td>Vertical in-line 4 cylinder</td>
</tr>
<tr>
<td>Cylinder Bore</td>
<td>90 mm</td>
</tr>
<tr>
<td>Cylinder Stroke</td>
<td>90 mm</td>
</tr>
<tr>
<td>Compression Ratio</td>
<td>18.5:1</td>
</tr>
<tr>
<td>Displacement</td>
<td>2.29 litres</td>
</tr>
<tr>
<td>Rated Speed</td>
<td>1800 rpm</td>
</tr>
<tr>
<td>Rated Power</td>
<td>37.5 kW at 2100 rpm</td>
</tr>
<tr>
<td>Maximum Torque</td>
<td>143Nm at 2000 rpm</td>
</tr>
<tr>
<td>Cooling</td>
<td>Water</td>
</tr>
<tr>
<td>Breathing</td>
<td>Naturally Aspirated</td>
</tr>
</tbody>
</table>

Table 1 Engine specifications

The engine was coupled to a Heenan-Dynamatic MkII 220kW eddy current dynamometer. Torque was measured by means of a strain gauge load cell connected to the lever arm, and speed by means of a magnetic pick up that generated a voltage signal with the passing of each gear tooth of a 60 toothed wheel. Intake airflow was measured using a viscous laminar airflow meter and type 5 Cussons manometer, and inlet air depression was measured by a Druck type general purpose pressure transducer coupled to a digital readout. 'K type' thermocouples were used to record the inlet air temperature, cooling water before and after the cylinder head, exhaust gas temperature and diesel fuel temperature. Diesel fuel consumption was recorded using a gravimetric fuel measurement system. The installation is shown schematically in Figure 1.

![Fig.1 Schematic diagram of the test engine and equipment](image-url)
2.2 Fuels

Three candidate oils which have the potential to be converted into bio-diesel fuels have been studied in this research, soya oil, rape oil and waste oil. Soya, and rape oil were obtained from a local supermarket, and waste oil obtained from a university hall of residence. In order to achieve consistency between the converted bio-diesel fuels, all three oils were converted ‘in-house’ via the same reaction process. The catalyst used was sodium hydroxide; and the alcohol was methanol (99%). Agitation was maintained at 500 RPM throughout the reaction duration. Table 2 listed some of their properties in comparison with a conventional mineral diesel fuel.

<table>
<thead>
<tr>
<th>PROPERTY</th>
<th>DIESEL</th>
<th>RAPE</th>
<th>SOY</th>
<th>WASTE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cetane Number</td>
<td>47.2</td>
<td>53.5</td>
<td>59</td>
<td>63.2</td>
</tr>
<tr>
<td>Density at 15°C (Kg/m³)</td>
<td>846.2</td>
<td>880</td>
<td>885</td>
<td>877</td>
</tr>
<tr>
<td>Viscosity at 400°C (mm²/s)</td>
<td>2.69</td>
<td>4.63</td>
<td>4.546</td>
<td>5.85</td>
</tr>
<tr>
<td>LCV (kJ/Kg)</td>
<td>42026</td>
<td>39826</td>
<td>39622</td>
<td>39651</td>
</tr>
</tbody>
</table>

Table 2 Properties different test fuel.

2.3 Experimental results

Three blends of three different bio-diesel fuels were then tested. These were a 5 percent, 50 percent and 100 percent blend of Soya (S), Rape (R) and Waste (W) methyl esters, referred to as S5, S50 ,S100 , R5, R50, R100 and W5,W50 and W100 respectively. The standard diesel fuel No 2 was used for the baseline tests, and was also used to create the blends of bio-diesel in the proportions of 5 and 50 percent.

During this study, engine performance and emissions data were obtained under steady state operating conditions at five loads corresponding to no load, quarter load, half load, three quarters load and full load, and at two speeds of 1500 rpm and 2000 rpm. To ensure repeatability and consistent operating conditions, the engine was first run for approximately 10 minutes at 1500 rpm at half load until the cooling water temperature out of the cylinder head reached 80°C, and the exhaust gas temperature reached a temperature of 250°C. Once these conditions had been achieved, the engine was brought to the required test point, and allowed to settle there for 1 minute before sampling of data began.

ENGINE POWER – In order to assess any degradation in engine performance, the maximum power output of each bio-diesel blend was recorded at two different speeds. The results are expressed as a percentage of the maximum power output obtained under the same operating conditions for mineral diesel, in Table 3.

<table>
<thead>
<tr>
<th>Fuel blend</th>
<th>Rape</th>
<th>Soy</th>
<th>Waste</th>
<th>Rape</th>
<th>Soy</th>
<th>Waste</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td>1500 rpm</td>
<td>2000rpm</td>
<td></td>
<td></td>
</tr>
<tr>
<td>5%</td>
<td>98.20</td>
<td>99.33</td>
<td>98.15</td>
<td>100.35</td>
<td>98.98</td>
<td>97.43</td>
</tr>
<tr>
<td>50%</td>
<td>99.74</td>
<td>99.24</td>
<td>98.47</td>
<td>98.66</td>
<td>95.33</td>
<td>96.62</td>
</tr>
<tr>
<td>100%</td>
<td>95.67</td>
<td>92.11</td>
<td>94.53</td>
<td>89.82</td>
<td>91.30</td>
<td>95.14</td>
</tr>
</tbody>
</table>

Table 3 Maximum power at 1500 and 2000 rpm

The error in these results was calculated as 1% to account for any fluctuations in speed and torque whilst readings were taken. It can be seen that at 5% blend of any of the three bio-diesel fuels causes negligible decrease in maximum power output of the engine at both speeds, for rape and soy. A decrease in power is evident with W5 at both speeds. This may due to a later energy release that occurs with waste oil than diesel due to the heavier molecular weight of materials present.

A 50% blend also causes negligible decrease in power at 1500 rpm, but as the speed is increased to 2000 rpm, the reduction in maximum power output becomes more significant. When the engine is fuelled with the pure bio-diesel fuels, and is especially emphasised at higher speeds. At 2000 rpm, a ten percent reduction in maximum power was observed with the rape and soy derivative fuels. The differences between rape and soy were small, but it would appear that the rape derivative fuel produced a consistently higher maximum power output than soy, and on average, the engine power output was more degraded with waste oil.

Some explanation for these trends can be observed by referring to Table 4 where the measured CN for each fuel tested are presented, and to the LCV data presented in table one. Bio-diesel blends have lower energy content on a volumetric basis, and without any changes in the fuel equipment, it can be therefore expected that the power output of the engine will be lower with bio-diesel. It can be seen in table one that rape and soy have a (similar) higher energy content on a volumetric basis than waste oil, whereas the CN values for soy and waste were quite close resulting in the close values for power between soy and waste oil. Where the CN for the fuel was higher for the soy blend, then this blend had the highest power output, but where waste has a higher CN, it also had a higher power output than soy. Finally, the
seemingly anomalous result in table three where R100 at 2000 rpm had the lowest power can be explained by the much lower CN than waste resulting in a longer ignition delay.

<table>
<thead>
<tr>
<th>Fuel</th>
<th>Rape ME</th>
<th>Soy ME</th>
<th>Waste ME</th>
</tr>
</thead>
<tbody>
<tr>
<td>Diesel</td>
<td>47</td>
<td>47</td>
<td>47</td>
</tr>
<tr>
<td>5%</td>
<td>47.6</td>
<td>47.4</td>
<td>47.4</td>
</tr>
<tr>
<td>50%</td>
<td>50.6</td>
<td>51.4</td>
<td>51.2</td>
</tr>
<tr>
<td>100%</td>
<td>53.9</td>
<td>59</td>
<td>63.2</td>
</tr>
</tbody>
</table>

Table 4  Cetane numbers of each fuel and blend

It can also be noted that there is some degree of variability in this data. On the basis of CN and LCV, it is surprising that the engine performance if degraded to a greater extent with waste oil ME. This is partially due to the unquantifiable quantity of impurities in the waste oil, and also because this oil degraded quickly in the hot and humid conditions of the engine test cell, where degradation of rape and soy was not observed. It is also likely that the blends in diesel were not consistent. The mixtures were obtained through splash blending but recent research has reported that whilst this method has traditionally been considered as the best, it can lead to inhomogeneous blends. It was not possible in the present research to assess the extent to which this may have had an effect. Other fuel quality issues causing a degradation in power could be caused by fuel filter plugging, gum like deposits on injection equipment and injector cavitation, although due to the relatively short term duration of the engine tests, these effects would be small.

NOx EMISSIONS – The NOx readings are presented as brake specific NOx (BSNOx), in order to account for slight fluctuations in speed and load, and are plotted against power in Figure 2. It can be seen that for the three bio-diesels, the difference in emissions of BSNOx for 5% blends compared with diesel are so small as to be negligible, and for rape and soy the BSNOx values converge to be approximately the same at above ½ load (12kW), whilst for waste, the convergence occurs at full load. The most marked differences are observed at low loads where significant reductions in BSNOx are observed with 50% blends and pure bio-diesel. For rape and soy, BSNOx was reduced to approximately half of the diesel value with 100% bio-diesel, and significant reductions in BSNOx were also observed with 50% blend of soy. The waste oil results showed a different trend where BSNOx emissions were lowest with a 50% blend. Overall, BSNOx emissions were the lowest for soy.

Fig.2  BSNox against power for the all fuels at 1500 rpm

The results for BSNOx emissions at 2000 rpm are plotted against power in Figure 3. As before, the emissions of BSNOx converge to approximately the same values above half load, and the differences between 5% blend and mineral diesel are negligible throughout. Emissions of BSNOx are reduced to around half of the diesel value at low load for pure bio-diesel, but this time, there is a much smaller difference between BSNOx emissions levels for 50% blends which were again always lower than for pure diesel. The anomalous result for waste oil is repeated again where the 50% blend has much lower BSNOx than the pure oil.
NOx emissions are strongly related to cylinder pressure development, as higher combustion temperatures, and earlier heat release rates, and greater fuel borne oxygen content that can occur when bio-diesel fuels are used in engines. The effect of increased NOx has not occurred in these tests as the fuel system was not optimised for bio-diesel operation. It is interesting to note that found that NOx in a bio-diesel fuelled engine can be significantly reduced by an EGR system that includes an oxidising catalyst. In the present study, NOx was probably lower due to a lower maximum combustion temperature due to a higher injected particle size that reduced combustion efficiency and hence maximum combustion temperature.

The convergence of BSNOx emissions levels beyond half load is probably due to the increased viscosity of the bio-diesel fuels compared with No 2 diesel. This is confirmed to some extent that density effects are particularly important at low loads. The higher viscosity of the bio-diesel fuels would have resulted in poorer atomisation, lower spray penetration, increased cone angle, and a greater injected particle size, resulting in poorer combustion efficiency and hence lower combustion temperatures.

SMOKE EMISSIONS – The average Bosch Smoke Number from three consecutive tests for each fuel is plotted in figure five for all fuels. It can be seen that at low load (up to approximately 5 kW) there is negligible difference between the smoke emissions of any bio-diesel as compared to mineral diesel. Beyond ¼ load, the emissions of smoke are always lower than for corresponding mineral diesel operation, except for the 5% blends where there is again, negligible difference.

As the proportion of bio-diesel is increased in the blend, the emissions of visible smoke decrease, except for the waste oil blend where the results from 50% blend and pure waste oil were virtually the same. Overall, the lowest smoke emissions were always recorded with rape blends.

The smoke results are plotted for 2000 rpm in Figure 4 and 5. The results for all fuels at low load are virtually the same, but beyond no load it is apparent that the bio-diesels produce less smoke (the difference was not apparent until beyond ¼ load for the 1500 rpm case). Again, there is negligible difference for the 5% blends, and rape produced the lowest smoke levels of all the bio-diesel fuels. In fact, the visible smoke levels were so low for R100 that they were at the limit of what could be measured with the lab equipment.
Overall, W100 and W50 produced higher levels of smoke compared with the corresponding rape and soy fuels, possibly due to increased number of carbon atoms in the fuel and hence a greater degree of pyrolysis. Bio-diesels smoke reducing effect could be attributed to its displacement of aromatic and short chain paraffin hydrocarbons and its higher oxygen content compared with No 2 diesel, but it is important to note that smoke can be increased at cold start.

**Fig.5 Bosch Smoke Number against power for the all fuels at 2000 rpm.**

IGNITION DELAY – The ignition delay was calculated as the crank angle interval between start of injection and start of combustion, which was found from experimental data. Start of injection was defined as the crank angle where fuel line pressure first exceeded the nozzle opening pressure of 235 bar, and start of combustion was found from the heat release rate analysis where the cumulative heat release rate first reaches zero after a small dip coinciding with fuel injection. Start of combustion was then confirmed by checking that the second derivative of cylinder pressure with respect to volume was zero. The results for the 1500 rpm experiments are presented in Figure 6.

**Fig.6 Ignition delay at 1500 rpm.**

Ignition delay decreased as load increased for all fuels, as expected, and converged to the same shorter values as for diesel beyond three quarters load. Once again, the results for the 5 % blends were almost identical to diesel values. It can be seen that for 50 % blends and pure bio-diesel, ignition delays were increased at low loads, with the longest ignition delays being observed with waste oil blends, and the shortest with Rape. More surprisingly, is the tendency of 50% blends to exhibit longer ignition delays than the pure bio-diesel fuel. There was evidence at the longest ignition delays (for W50) for the ignition process occurring in two stages, and the extended ignition delay recorded is for the second phase of combustion that is thought to occur with the bio-diesel fuel. This is discussed further in the heat release rate section.

The results for ignition delay at 2000 rpm are presented in Figure 7. At the higher speed, differences in ignition delay are more marked than they were at 1500 rpm, and values do not converge until full load. It can be seen that ignition delay increased with the addition of bio-diesel, even in 5% blends, and the longest ignition delays were observed for
waste oil blends, and the shortest ignition delays were observed with soy. It is also particularly interesting to note that there was some evidence of a two stage ignition process for the 50 % blend of waste oil at low loads, where the rate of pressure rise first increased beyond motoring pressure, and then levelled out before increasing again which suggests that the diesel fuel ignited first, then the waste oil fuel. This is supported by the excessively long ignition delays noted for W100.

3. Theoretical Study on HCCI Combustion

3.1 Simulation Model

The simulation software employed in this investigation is Aurora application of Chemkin III modelling package developed by Sandia. The model assumes the combustion chamber as a single-zone reactor charged with homogeneous mixture, and its volume varies according to a slider-crank relationship. The heat loss is calculated from the heat transfer due to the temperature difference between gas temperature and an assumed average cylinder wall temperature of 500K using Woschni correlation. Each simulation starts at the beginning of compression stroke and finishes at the end of expansion stroke with a time step of 1° of crank angle.

The chemical kinetic mechanisms employed are:

- n-heptane: 565 species, 2540 reactions
- DME: 78 species and 336 reactions
- methyl butanoate: 264 species and 1219 reactions
- methyl formate: 193 species, 925 reactions

The engine on which the simulation is based is a single cylinder engine with a bore of 80.5mm, a stroke of 88.2mm, and a connecting rod length of 129.75mm. For all operation conditions calculated in this study, the engine is assumed un-throttled with a volumetric efficiency of 100%.

3.2 Auto Ignition

Figure 8 shows the calculated cylinder pressure of the four fuels. The engine compression ratio is 18:1, speed is 2000rpm, and equivalent air to fuel ratio, \( \lambda \), is 2. There are a number of important phenomena can be observed from the results. First and most significant observable fact is that N-heptane and DME exhibit dual stage ignition, with cool-flame (or low-temperature ignition) and main (or high-temperature) ignition. On the other hand, MB and MF undergo single stage ignition only.
Secondly, in order to auto ignite the combustion at about the same crank angle position, 180CA in this case, a different inlet temperature is needed for each fuel. DME needs the lowest temperature, 270K, while MF needs the highest, which is 415K. N-heptane requires 290K and MB 395K. In other words, the thermal energy required to start the auto ignition is in the order of: DME < n-heptane < MB < MF. DME appears to be the most suitable fuel to initiate the auto ignition combustion.

Thirdly, DME produces the highest peak cylinder pressure, while MB generates the least.

Such differences in ignition and combustion behaviour are mainly due to different fuel structure, chemical composition, and molecular size. N-heptane is long straight-chain paraffin with a series of weakly bounded H atoms, which have high isomerization rates. The C\textsubscript{7}H\textsubscript{15} radicals being produced lead to a relatively high rate of chain branching from ketohydroperoxide decomposition \cite{1}, which results in a rapid ignition. Therefore, n-heptane needs relatively low inlet temperature to start initial chemical reactions. However, a competition between the fast chain branching reactions and the relatively slow chain propagation reactions exist. This slows down the overall reaction rate, and considerably extends the induction time, which is defined as the time between start of cool flame and start of main ignition.

In comparison, DME is the simplest ether and oxygen fuel, which has a C-O-C bond instead of C-C bonds. This lowers the temperature required for main ignition. The short induction period in DME is due to the dominant role of the peroxide chemistry, which favours fast radical branching reactions thus, keeps overall reaction rate high\cite{2}.

MB and MF show single stage ignition only. This is mainly due to the presence of methyl and olefinic methyl ester radicals. Unlike C\textsubscript{7}H\textsubscript{15} and peroxy radicals, these two groups of radicals lead to chain termination reactions \cite{3,4}, and prohibit further low temperature reactions. Therefore, cool flame chemistry is considerably inhibited from MB and MF. Considerably higher temperatures are required to ignite MB and MF.

Effect of Inlet Temperature: Figure 9 shows the calculated ignition timing with varying inlet temperature. The other engine parameters remain the same with previous calculations. The start timing of cool flame of n-heptane and DME are shown in the figure, too. It can be seen that the higher the inlet temperature, the earlier the ignition starts for all four fuels. The same trends are also found with the start timing of cool flame. This is simply because of high temperature accelerates combustion reaction rates.
It is also interesting to note that the induction period for both n-heptane and DME is extended when inlet temperature increases. This may because of the start of cool flame is directly linked to the temperature of the mixture. The mixture reaches this critical temperature earlier with higher inlet temperature. However, the following main ignition is a function of the accumulated thermal energy during induction period. If cool flame starts early, the contribution from piston compression is less, and therefore, a longer time is need to accumulate sufficient thermal energy to initiate the main combustion.

Clearly, a non-linear relationship between inlet temperature and ignition timings exits for each fuel. There is an essential minimum temperature for each of the fuel. Below it, no combustion occurs.

**Effect of Air to Fuel Ratio:** Since HCCI combustion is initiated via fuel auto ignition, no centralised ignition source is required, significantly fuel lean mixtures can therefore be employed. Figure 10 shows the calculated influence of air to fuel ratio on the ignition timing of cool flame and main ignition of n-heptane and DME. It can be seen that the strength of the air/fuel mixture has rather different effects on the start of ignition timing of cool flame and main ignition. For cool flame, it appears that the leaner the mixture, the earlier the ignition starts, but the advance gradually becomes finite when the mixture becomes too lean. This may because of the fact that the start of cool flame reaction depends upon two factors: the thermal energy and the availability of oxidants the mixture contains. The more oxidant (oxygen in air) available, the easier the fuel oxidation reaction can be initiated. Hence, the earlier the ignition starts. However, excess air dilutes the air/fuel mixture, absorbs the heat generated by the compression of the piston and therefore limits the temperature upraising during compression process. This tends to retard the cool flame reaction. The observed phenomenon is a combined result between the two.

For main ignition timing, the trend of that the leaner, the earlier last only to a certain limit. Leaner than the limit, ignition timing begins to be retarded. This may also because of the two factors: the thermal energy and the excessive air the mixture contains. To start the main ignition, the mixture has to have a certain level of thermal energy to overcome the activation energy required by full-scale combustion reaction. There are two sources to supply the thermal energy: the heat energy released during cool flame reactions plus a contribution from piston compression. When the mixture is slightly lean, the thermal energy is accumulated inside the mixture. The main ignition is quickly initiated when activation energy is overcome. However, if the mixture is too lean, excess air absorbs the heat generated from cool flame reactions and piston compression. The thermal energy accumulation becomes difficult, and the main ignition is retarded.

Figure 11 shows the influence on MB and MF. Different from n-heptane and DME, MB and MF undergo a single stage of ignition only. It can be seen that the leaner mixture clearly favours the auto ignition. The leaner the mixture, the earlier the ignition starts. The advance gradually becomes finite when the mixture becomes too lean. Again, it is a combined effect between the thermal energy generated by piston compression and the availability of oxidant the mixture contains.
Effects of Compression Ratio: A higher compression ratio increases the charge temperature uprising during compression process. Figure 12 shows the calculated influence of compression ratio on the ignition timing of cool flame and main ignition of n-heptane and DME. It is interesting to see that the induction time between the two stages of ignition reduces as compression ratio increases. This is clearly due to the improvement in charge temperature at high compression ratios.

Figure 13 shows the calculated influence of compression ratio on the ignition timing of MB and MF. Again, high compression ratio improves charge temperature and therefore advances ignition timing.

Effect of Engine Speed: Figure 14 shows the calculated relationship between engine speed and ignition timing of n-heptane and DME. Figure 15 shows the ignition timing of MB and MF. It can be seen that the ignition timing of all four fuels retards as speed increases. This is because of that the start timing of auto ignition depends largely on air/fuel mixture performance and is relatively free from engine speed influences.
Effect of EGR: In our recent theoretical and experimental investigations [5,6], it has been found that the hot EGR promotes HCCI combustion via two distinct mechanisms: the thermal effect and chemical effect. Figure 9 shows the calculated effect of EGR on ignition timings by fixing the temperature of air/fuel/EGR mixture at the beginning of compression stroke at the temperature indicated in the figure, while varying the quantity of EGR. The compression ratio chosen for the calculation was 14:1. It can be seen that start timing of cool flame remains almost unchanged since the inlet temperature remains the same. However, the main ignition timing of all four fuels are significantly delayed with higher EGR introduction. In comparison, MB and MF exhibit higher tolerance to EGR in comparison to n-heptane and DME.

4. Conclusions

- Among the four fuels studied, n-heptane and DME are characterised with the two-stage ignition behaviour, while biodiesel fuels MB and MF exhibit single-stage ignition only.
- The thermal energy required to start the auto ignition is in the order of: DME < n-heptane < MB < MF.
- An essential inlet temperature is required to initiate the auto ignition. High inlet temperature advances auto ignition timing.
• Fuel lean mixture favours auto ignition, but too lean will retard the main ignition timing.
• High compression ratio advances auto ignition timing.
• The ignition timing retards as engine speed increases.
• When temperature is fixed, more EGR dilutes the entire charge and retards auto ignition timing. However, it has no clear effect on cool flame.