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# 67 A Theoretical Study on HCCI with Diesel Type Fuels: N-heptane, Dimethyl Ether, Methyl Butanoate and Methyl Formate

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Homogeneous charge compression ignition (HCCI) offers high fuel economy and significantly reduced NO<sub>x</sub> 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. Difficulties for practical applications are controlling of ignition timing and heat release rate over wide engine operation range. In the research work reported in this paper, four various diesels type fuels: N-heptane, Dimethyl Ether, Methyl Butanoate and Methyl Formate 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.

*Key words: HCCI, chemical kinetics, auto ignition, combustion simulation, EGR, biodiesel, dimethyl ether, n-heptane*

## 1. INTRODUCTION

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 NO<sub>x</sub> 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<sup>1</sup>. In the research work reported in this paper, 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. SIMULATION MODEL

The simulation software employed in this investigation is Aurora application of Chemkin III modelling package developed by Sandia<sup>2</sup>. 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<sup>3</sup>. 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<sup>4,5</sup>:

- n-heptane: 565 species, 2540 reactions
- DME: 78 species and 336 reactions<sup>6</sup>
- methyl butanoate: 264 species and 1219 reactions
- methyl formate: 193 species, 925 reactions<sup>7</sup>

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. SIMULATION RESULTS

### 3.1 Auto Ignition

Figure 1 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 phenomenons 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 MB395K. 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 bonded H atoms, which have high isomerization rates. The  $C_7H_{15}$  radicals being produced lead to a relatively high rate of chain branching from ketohydroperoxide decomposition<sup>8</sup>, 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.

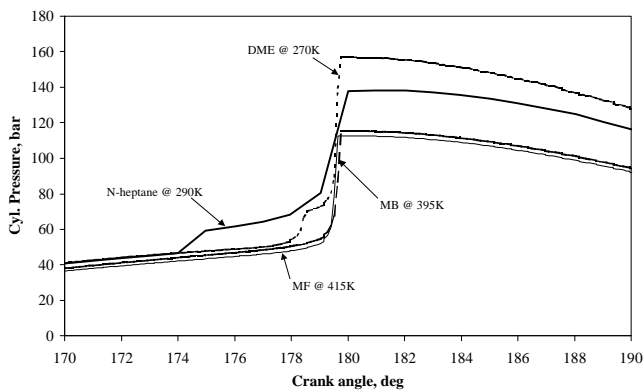


Fig.1 Cylinder pressure with various fuels at different inlet temperature of the air/fuel mixture

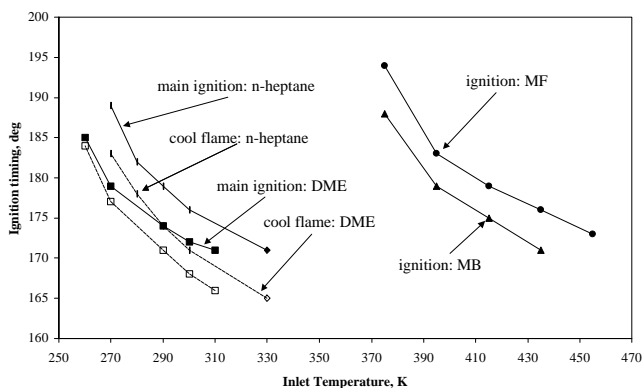


Fig.2 Effect of the inlet temperature on ignition timings

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<sup>9</sup>.

MB and MF show single stage ignition only. This is mainly due to the presence of methyl and olefinic methyl ester radicals. Unlike  $C_7H_{15}$  and peroxy radicals, these two groups of radicals lead to chain termination reactions<sup>10,11</sup>, 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.

### 3.2 Effects of Engine Parameter on Auto Ignition

**Effect of Inlet Temperature:** Figure 2 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 be 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 needed to accumulate sufficient thermal energy to initiate the main combustion.

Clearly, a non-linear relationship between inlet temperature and ignition timings exists 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 3 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 be 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 be 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.

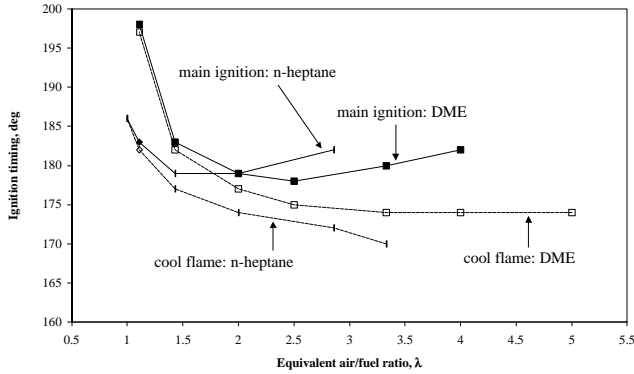


Fig.3 Effect of air to fuel ratio on ignition timings of n-heptane and DME

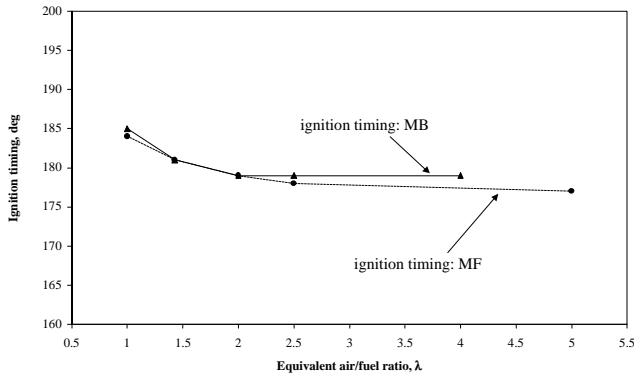


Fig.4 Effect of air/fuel ratio on ignition timings of MB, MF

Figure 4 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 5 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 6 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.

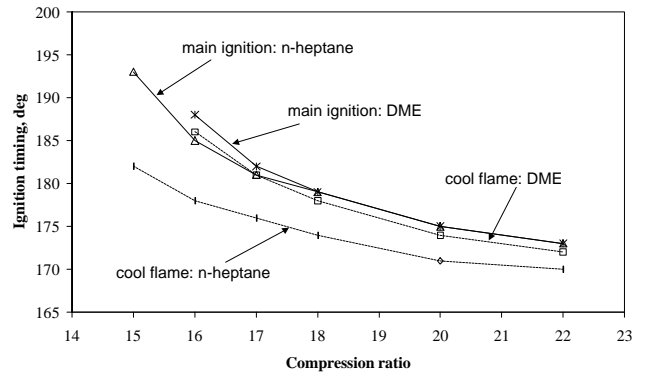


Fig.5 Effect of compression ratio on ignition timings of n-heptane and DME

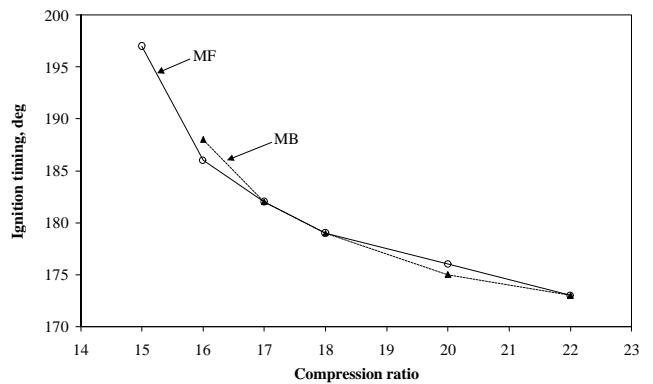


Fig.6 Effect of compression ratio on ignition timings of MB and MF

**Effect of Engine Speed:** Figure 7 shows the calculated relationship between engine speed and ignition timing of n-heptane and DME. Figure 8 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<sup>12,13</sup>, 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.

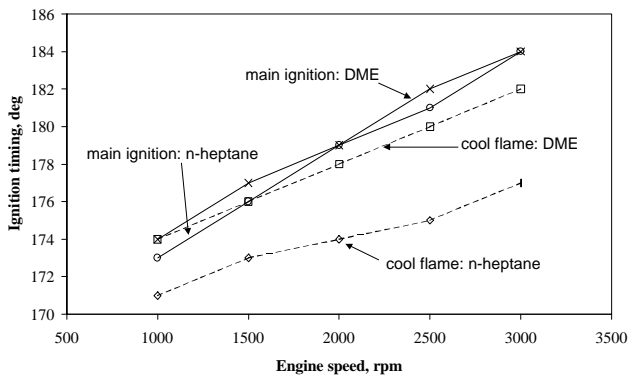


Fig.7 Effect of engine speed on ignition timings of n-heptane and DME

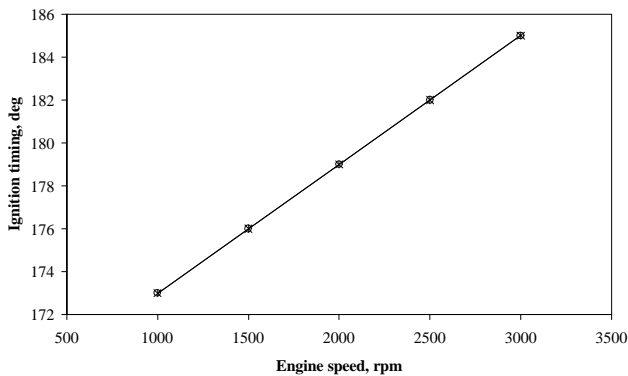


Fig.8 Effect of engine speed on ignition timings of MB and MF

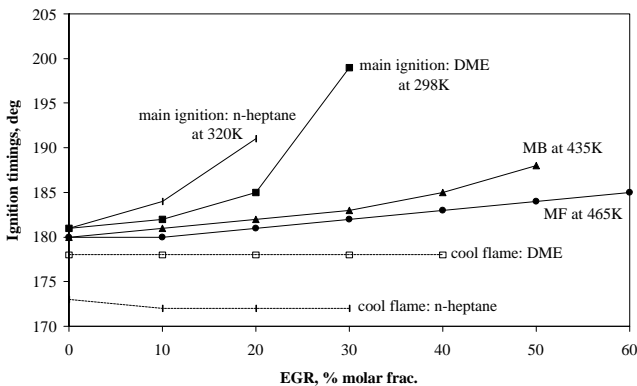


Fig.9 Effect of EGR on the ignition timing

## 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.

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