66 Homogeneous Charge Compression Ignition Combustion and Fuel Composition

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Homogeneous charge compression ignition, HCCI, combustion has potentials to deliver high efficiency and negligible cycle-to-cycle variations, while keeps NOx and particulate emissions at very low levels in comparison with conventional SI and CI combustion concepts. Since HCCI combustion is an auto ignited combustion, fuel structure has direct impact on its auto-ignition performance. In this research, by mixing iso-octane and n-heptane, the auto-ignition nature of fuels with different research octane number, RON, were simulated and analysed using a single-zone engine combustion model with detailed chemical kinetics and convective heat transfer loss. The effects of internally recirculated engine exhaust gas, IEGR, as a potential control strategy was also calculated.

Key words: HCCI, RON, EGR, chemical kinetics, auto ignition, combustion simulation

1. INTRODUCTION

The Homogeneous Charge Compression Ignition (HCCI) combustion is a combustion process that combines features of SI and CI combustions. In a HCCI engine air and fuel are mixed homogeneously prior to ignition, and then ignited by compression from the piston motion. The entire bulk mixture auto-ignite almost simultaneously throughout combustion chamber without obvious flame propagation. It is widely accepted that HCCI combustion is controlled by the chemical kinetics of the air/fuel mixture with relatively little influence of turbulence and mixing. This allegation has been supported by spectroscopic study performed by Noguchi[1], and obtained results indicated that radical's appearance was in a specific sequence. In comparison, all radicals appear at the same time spatially distributed though the flame-front in SI combustion. It is clear that the auto ignition initiated HCCI combustion is controlled by the chemical reaction mechanism. Our research results indicated that the fuel structure and both thermal and chemical quality of the engine charge consisted of air, fuel and residual burned gas strongly influence the performance of auto ignition[2]. In order to investigate the auto ignition behaviour of commercial fuels, which has research octane numbers (RON) somewhere between iso-octane and n-heptane, we developed a new combustion reaction chemical mechanism for the mixture of iso-octane and n-heptane. By varying the percentage of iso-octane contained in the mixture, the auto-ignition of fuels with different research octane number, RON, was simulated and analysed.

2. KINETICS AND SIMULATION MODEL

In order to analyse the auto ignition behaviour of a fuel with various RON, a new reaction mechanism, which is capable to predict the ignition performance of the mixture of iso-octane and n-heptane, has been developed in house. It is based on the detailed kinetics of n-heptane and iso-octane[3],[4], and consists of consists of 1087 species, 4392 reactions and a complete NOx chemistry. The RON is defined as the percentage in volume of iso-octane in the mixture of the two.

Figure 1 shows a comparison of ignition delay between calculated results using the newly developed mechanism and experimental results of pure iso-octane, RON of 100, at various pressure conditions. Figure 2 shows the predicted ignition delays and experimental results of RON of 100, 80 and 0 at a constant pressure of 41 ± 1bar. The test data were obtained via shock tube experiments[5],[6]. The predicted ignition delays were calculated using the Senkin application in the Chemkin III package[7] with the developed mechanism. The equivalence air/fuel ratio (λ) for both results is 1. The calculated results agree well with experimental ones at various pressure and temperature conditions. Both cool flame and negative temperature behaviour, typical characteristics of n-heptane, were well reproduced by the newly developed mechanism. It shows that the newly developed reaction mechanism for a mixture of iso-octane and n-heptane is capable of predicting ignition behaviour of a reference fuel at various RON.

3. ENGINE SIMULATION RESULTS

The engine parameters input into the calculations are: bore 80.5 mm, stroke 88.2 mm, connecting rod length 129.75 mm with a displacement of 0.45 litre. An un-throttled condition with a volumetric efficiency of 100% has been assumed. The IEGR is assumed to be trapped via suitable valve timing employed in our early experimental investigations using a fully variable valve train system (FVVT)[8].

The thermal conditions of the engine combustion chamber throughout the study were simulated using the Aurora application from the Chemkin III modelling package. It considered the combustion chamber as a single-zone with a variable volume according to the slider-crank relationship. The gaseous mixture that the combustion chamber being charged was assumed as homogeneous. The heat transfer was calculated by Woschni's correlation[9], and a temperature of 500K was assumed for the combustion chamber wall. Each simulation started at the beginning of compression stroke and finished at the

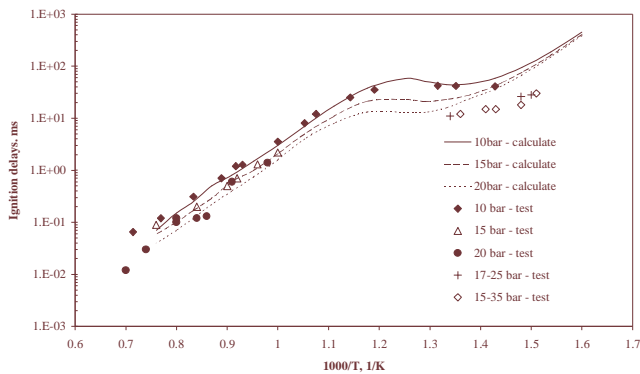end of expansion stroke with the time step of 1° crank angle.

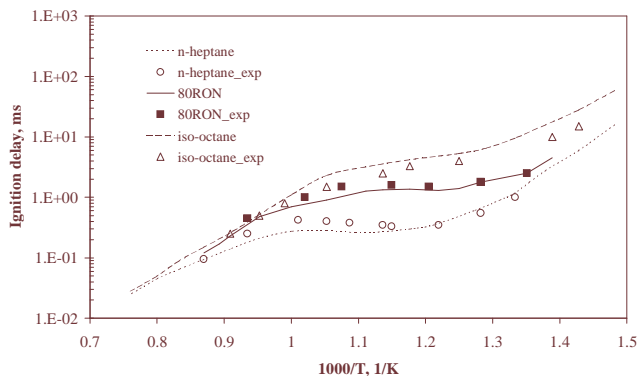*Fig.1 Auto ignition delay of iso-octane*

Fig.2 Auto ignition delay of the mixture of iso-octane and n-heptane with varying RON

3.1 Auto Ignition Timing and RON

Figure 3 shows a series of calculated cylinder pressure versus engine crank angle at various RON. Figure 4 shows the ignition timing of the fuel with various RON. The engine operation parameters employed in the calculations are: compression ratio 10.5, speed 2000rpm, equivalence air/fuel ratio λ=1. The initial temperature and pressure of the air/fuel mixture throughout the calculation are 520K and 1atm, respectively. These are equivalent to the temperature and pressure of the inlet charge at the beginning of compression stroke. It can be seen that the auto ignition timing is a function of RON. A fuel with low RON ignites significantly earlier than that with high RON, although there is a little difference in ignition timing in the range of 75<RON<95. This is because of the influence of cool-flame reactions of the n-heptane contained in the fuel with lower RON, which accelerates the start of main ignitions. As RON increases, iso-octane, which has a single-stage reaction characteristic, begin to dominate the mechanism and the contribution from cool-flame reduces. When RON is higher than 75, the contribution from cool-flame reaction is virtually override by the single-stage reaction, no obvious differences can be found. However, there is a clear difference between pure iso-octane which has a RON of 100 and the mixture contains even a small quantity of n-heptane, RON of 95 for example. This is obviously due to the contribution from n-heptane and its

cool-flame combustion characteristics. The energy released during the initial stage of reaction from n-heptane improves both thermal and chemical environment and accelerates the start of auto ignition of iso-octane.
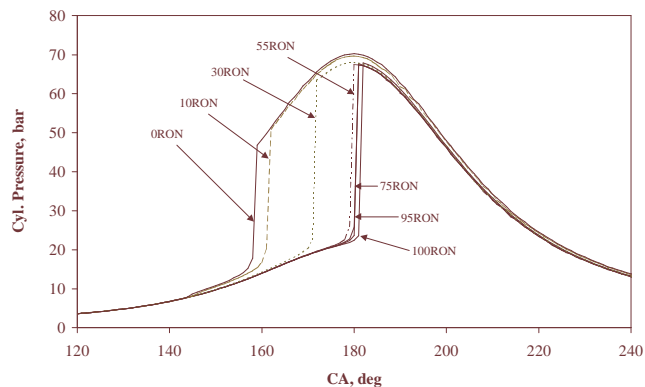

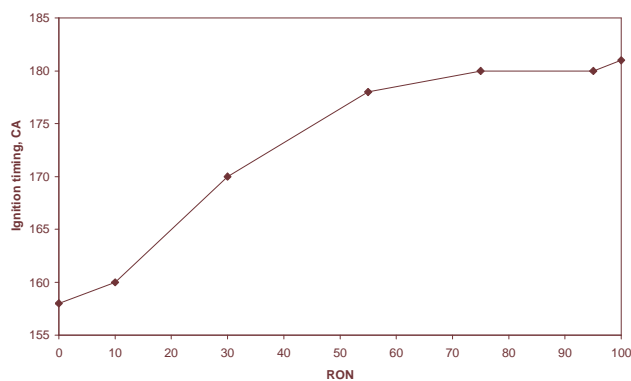*Fig.3 Cylinder pressure with various RON*

Fig.4 Ignition timing vs. RON

3.2 Effects of Air/Fuel Ratio

The natural of auto ignition combustion ensures that the HCCI can burn much leaner air and fuel mixture than conventional SI strategy. An iso-octane and n-heptane mixture with a RON of 95 is representative to commercial gasoline. The effect of air to fuel ratio on such reference fuel was calculated and shown in Figure 5. The engine parameters and the temperature and pressure of the air and fuel mixture used are same with previous calculations. It can be seen that a lean mixture ignites earlier than a rich one. There is a non-linear relationship between the two. When the air/fuel mixture becomes too lean, no obvious advances can be found. This may because of the high heat capacity of the fuel, which directly affect the thermal energy obtained by the air/fuel mixture during compression process.

Figure 6 shows the calculated specific heat capacity of the air/fuel mixture at the initial conditions with varying air/fuel ratio. When the air/fuel mixture contains more fuel, its overall heat capacity is high. More thermal energy is required to raise the temperature of the mixture to the level to start the auto ignition. In order to overcome the activation energy to initiate the combustion, further compression is needed. When the mixture is lean, the overall heat capacity reduces, and the thermal energy

contained by the mixture increases during the compression process. Consequently, the air/fuel mixture can overcome its activation energy earlier, and ignition advances. Further dilutes the air/fuel mixture with air, the increase rate in thermal energy slows done. The resulted advancing effect on ignition timing is reduced, and ignition timing becomes constant.
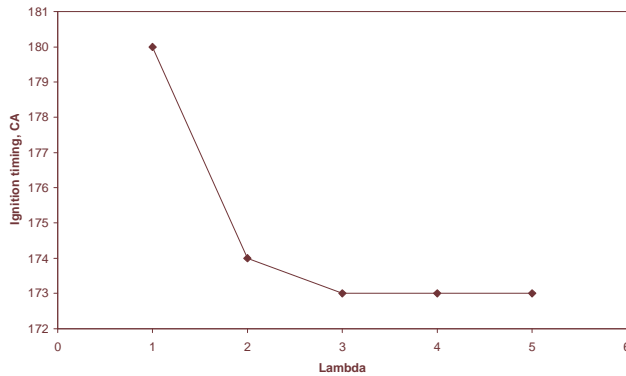

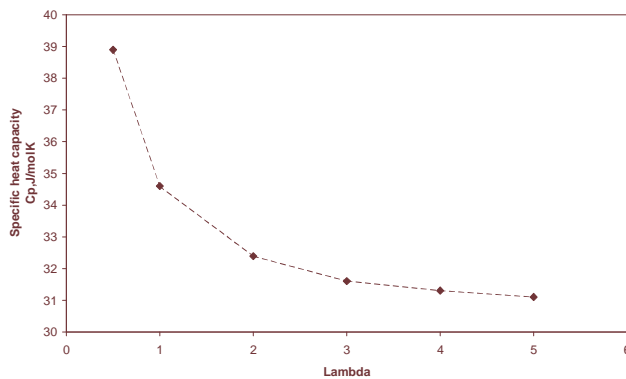*Fig.5 Auto ignition timing at 95 RON with various AFR*

Fig.6 Specific heat capacity and enthalpy of the air/fuel mixture with various AFR

3.3 Effects of Engine Speed

Figure 7 shows the auto ignition timing of the fuels with 95 RON and 55 RON, respectively. It can be seen that the ignition is retarded as engine speed is increased. The relationship is virtually linear. This is because the chemical reaction rates are independent from engine speed. There is a clear difference between different RON. The fuel with low RON ignites earlier. In addition, the engine speed appears to have more effect on the fuel with low RON than those with high ones. The gradient of 55 RON is greater than that of 95 RON. Again, this is because of the contribution of cool-flame. First, fuel with low RON has high influence from cool-flame reactions. Second, cool flame needs certain time to react, and the time is independent from engine speed. The high the engine speed, the more crank angle is needed before main ignition occurs, and the main ignition is further retarded in terms of engine crank angle.

3.4 Effects of IEGR

The internal exhaust gas recirculation (IEGR), obtained via trapping burnt gases through FVVT appears to be a feasible method for HCCI combustion control. The IEGR is a hot burned gas that consists mainly of CO_2, H_2O, N_2, and O_2. Some other partial burned and combustion reaction intermediates are also contained but in much lower concentrations in comparison. When such hot gas is mixed with freshly introduced air and fuel mixture, it has two effects[10]. One is thermal effect due its high temperature. When the hot IEGR is mixed with cool air/fuel mixture, it improves the temperature of the entire inlet charge. The other one is chemical effect due to the different chemical species the IEGR contains. Different gaseous species have different thermal heat capacity profile against temperature and chemical reactivity towards combustion reaction. Their effects on cylinder temperature history and fuel auto-ignition are different. The effect of IEGR on auto ignition, in fact, is a combination of the two.
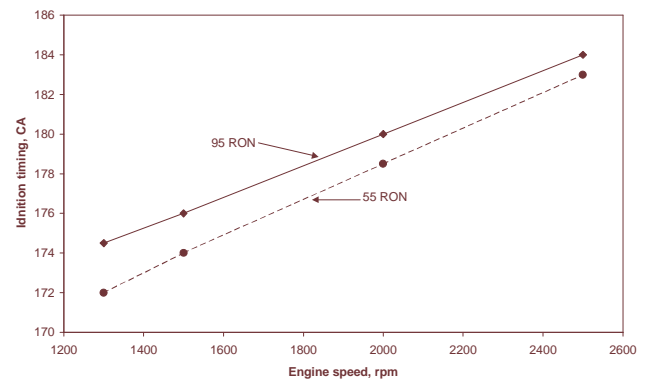

Fig.7 Auto ignition timing of 95 RON and 55 RON at various engine speeds

Figure 8 shows the calculated effect of the IEGR on auto ignition timing obtained from the fuels with a RON of 95. The engine parameters are same with previous calculations. The temperature of air and fuel mixture, and the IEGR are assumed as 298K and 873K, respectively. The IEGR input into the calculation is assumed as burned gas only. Its quantity being introduced into the engine charge is based on volume percentage. The mixed temperature of the IEGR and fresh air/fuel charge is estimated assuming the mixing of the ideal gasses. The temperature of the mixture of air, fuel and IEGR is calculated through enthalpy conservative concept. It can be seen that IEGR introduction improves the auto ignition. More IEGR introduction advances ignition timing. There is a minimum limit, 60% in this case, no ignition occurs below it. This is because the more IEGR at constant temperature being introduced into the engine charge, the high the temperature of the entire charge. It improves the thermal condition of the charge and therefore advances the auto ignition.
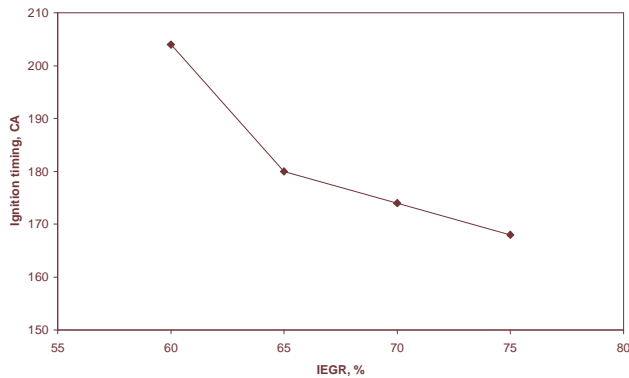
Fig.8 IEGR effect on auto ignition timing

CONCLUSIONS:

The detailed chemical kinetic mechanism developed for the mixture of iso-octane and n-heptane is capable to predict auto-ignition timings of a reference fuel with varying RON at various pressure and temperature conditions.

The fuel with lower RON ignites easier than the fuel with higher RON. This is due to the effect of cool-flame contributed by n-heptane.

A lean air/fuel mixture ignites earlier than a rich one. There is a non-linear relationship between the two. When the mixture becomes too lean, no obvious advances can be found.

The auto ignition timing is linearly related to the engine speed. As engine speed increases, the auto ignition is retarded.

The introduction of IEGR improves the auto ignition. More IEGR advances ignition timing. The relationship is non-linear. There is minimum limit, no ignition occurs below it.

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