A computational study on the effect of exhaust gas recirculation on auto-ignition timing of HCCI engine fuelled with N-heptane, iso-octane, ethanol and methane

63 A Computational Study on the Effect of EGR on Auto-Ignition Timing of HCCI Engine Fuelled with N-heptane, Iso-octane, Ethanol and Methane

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The homogeneous charge compression ignition, HCCI, uses compression ignition to auto-ignite a homogeneous air/fuel mixture. Using internally trapped engine exhaust gas, IEGR, as an indirect control method, HCCI offers superior fuel economy and pollutant emission reductions. Fuel structure has direct impact on its auto-ignition performance. In this research, the effect of IEGR on auto-ignition timing of four typical fuels with distinct Octane number: N-heptane, Iso-octane, Ethanol and Methane have been studied using a single zone adiabatic combustion model and detailed chemical kinetics. It was found that the introduction of internal exhaust gas recirculation, IEGR, delays ignition timing of all four fuels, but differently. N-heptane is the most sensitive fuel to IEGR, iso-octane and ethanol has a much higher endurance, while methane is somewhere in between.

Key words: HCCI, CAI, chemical kinetics, auto ignition combustion simulation

1. INTRODUCTION

Controlled auto-ignition (CAI) is a combustion strategy, which uses auto ignited homogeneous air and fuel mixture but the combustion is controlled by regulating the quantity of internally re-circulated exhaust gas (IEGR). Such combustion has grown in interest in recent years originally arising from works on 2-stroke engines now has crossed to 4-stroke[1]. The reason for the interest in 4-stroke engines stems from the fact that CAI combustion holds considerable promise as a part-load throttle-less engine control strategy which is capable of yielding superior fuel economy and significantly reduced pollutants[2]. It has been proved through our previous research results that such combustion phenomenon can be practically controlled in a certain engine operation range by controlling the quantity of EGR, using advanced active valve train (AVT) system[3]. In order to clarify the effect of IEGR on ignition timing of different fuels, typically the IEGR effect on the fuels with distinct Octane number, we performed a series of calculations using SENKIN combustion simulation software with detailed chemical kinetics. Four fuels have been investigated, these are: n-heptane with an Octane number of 0, iso-octane with an Octane number of 100, ethanol with an Octane number of 107 and methane with an Octane number of 120. It has been found that different fuel has different activation energy and therefore needs different inlet temperature to initiate the combustion, if same ignition timing is expected. IEGR delays the auto-ignition timing of all fuels interested, but the amounts of delay are very different. The difference largely depends on fuel structure and relevant Octane number.

2. METHODOLOGY

The simulation software employed in this investigation is SENKIN chemical kinetics simulation package developed by Sandia. It uses a single-zone model of combustion chamber, assumes uniform composition and thermodynamic properties inside the chamber, and computes the time evolution of a homogeneous reacting gas mixture in a closed system. The volume of the combustion chamber is engine parameter based, and varies according to a slider-crank relationship. Both compression and expansion have been considered as adiabatic processes.

The reactions introduced into the calculation are detailed chemical kinetics. For n-heptane, the mechanism consists of 565 species and 2540 reaction, iso-octane consists of 857 species and 3606 reactions, ethanol consists of 57 species and 383 reactions[4], and methane consists of 53 species and 325 reactions[5].

3. SIMULATION RESULTS

The engine parameters used by the calculations are: λ of the air/fuel mixture is 1.0, compression ratio is 10.5:1, and engine speed is fixed at 2000rpm. The air introduced into the model is assumed as 21% O_2 and 79% of N_2. The calculation started at the beginning of compression stroke and finished at the end of expansion stroke. The interval between each calculation is 1^oCA.

3.1 Auto-ignition

Figure 1 shows the calculated cylinder pressures of the four fuels. In order to ensure that the auto-ignition starts at TDC, different inlet temperature has been used as detailed in Figure 2. It can be seen that the fuel with low Octane number needs low inlet temperature to start the auto-ignition, while high Octane number needs high temperature. Such relationship is shown in Figure 3.

The distinct difference in inlet temperature requirement for fuels with different Octane number is because of the 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 and the ignition is characterised with two-stage ignition process: cool flame and main

ignition. This because of that the C_7H_{15} radicals being produced lead to a relatively high rate of chain branching from ketohydroperoxide decomposition[6], 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 done the overall reaction rate before main ignition occurs.

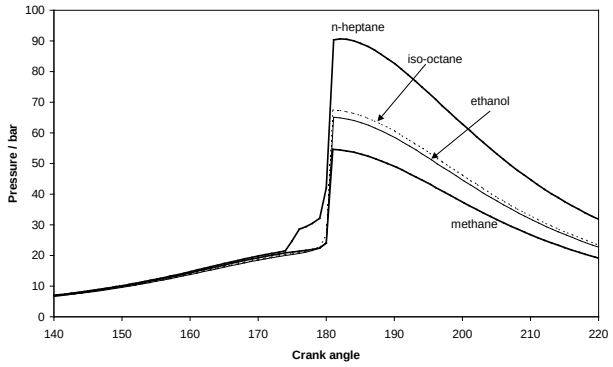

Fig.1 Cylinder pressure of n-heptane, iso-octane, ethanol and methane

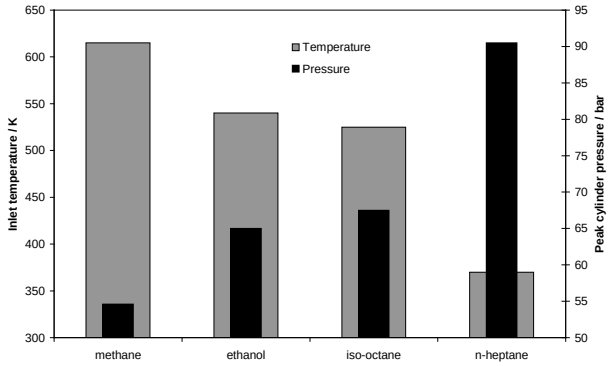

Fig.2 Inlet temperature required for auto-ignition at TDC and resulted peak cylinder pressure of n-heptane, iso-octane, ethanol and methane

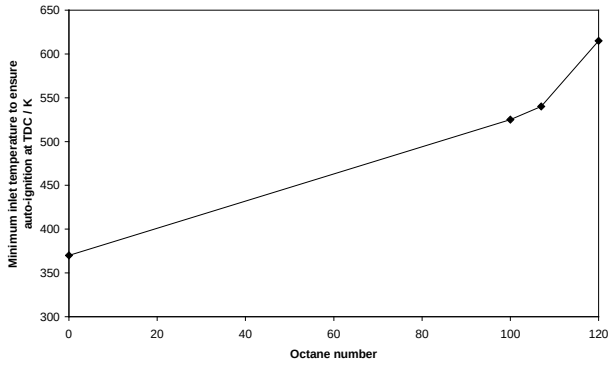

Fig.3 Inlet temperature required for auto-ignition at TDC vs. fuel Octane number

In contrast, iso-octane is a branched-chain fuel, which is consisted mainly of primary H-atom sites and one tertiary H-atom site. Although the tertiary site is easy to be abstracted, the rest primary sites are much more difficult. Therefore, the activation energy of iso-octane is much higher than that of n-heptane. At temperature below 1000K, virtually all the isomerisation pathways, which produce OH radicals, are inhibited. Therefore, iso-octane is characterised with single-stage ignition process only.

Since the C-C bonds are weaker than C-OH bond, ethanol does not displace OH group in the initiation step. The dominant initial step is $C_2H_5OH+M=CH_3+CH_2OH+M$, where M is the third body. The initiation reaction is started when the C-C bond is broken. Since the activation energy of breaking the C-C bond is slightly higher than that of abstracting primary H-atom site[7], the initiation temperature of ethanol is close but slightly higher than that of iso-octane. Ethanol has a slightly higher Octane number (107) than that of iso-octane. Its combustion is also characterised with single-stage ignition process only.

Methane exhibits certain oxidation characteristics that are different from all other hydrocarbons. It has a very high Octane number (up to 120), and is more difficult to be ignited. This is because methyl radicals generated from H atom abstraction lead chain termination reaction $CH_3+CH_3=C_2H_6$, which inhabits the overall rate of ignition. As has been calculated, the required inlet temperature for methane to start the auto-ignition at TDC is 615K, which is the highest among the fuels being analysed.

Figure 2 also shows the peak cylinder pressure with four different fuels. The difference is caused by a number of factors. Methane has the lowest energy density, when it is burned, the relatively low energy release causes lower pressure increase. Ethanol and iso-octane have a close Octane number. When a similar inlet condition being used, a similar combustion pressure profile has been observed. Although the inlet temperature of n-heptane is the lowest, the cool flame combustion may have played a significant role in improving cylinder pressure even before main combustion starts.

3.2 IEGR effect

In CAI combustion, the combustion ignition timing is mostly controlled by its chemical kinetics. Direct controlling methods are not suitable. There are a number of in-direct control methods, which have the potential of controlling the timing of auto-ignition of CAI combustion. Among them, IEGR trapped by Flexible Variable Valve-train (FVVT) system appears to be a potential method for practical applications[8].

IEGR is consisted mainly of burned gases at high temperature. Its effect on auto ignition is composed of two aspects[9,10]. One is its thermal effect due to its high temperature. When the hot internal EGR is mixed with cool air/fuel mixture, it improves the temperature of the entire inlet charge, which helps the initiation of auto-ignited combustion. The other aspect of the effect is the chemical effect due to the different chemical species it contained. Different gaseous species have different thermal heat capacity profile against temperature and

chemical activity towards combustion reaction. Their effect on cylinder temperature history and fuel auto-ignition should therefore be different. In order to simplify the calculation, but still compare the CAI potential for all four fuels, only the major burned gases are considered in this investigation, which are O_2, N_2, H_2O, and CO_2. Their concentrations were obtained from equilibrium combustion reaction.

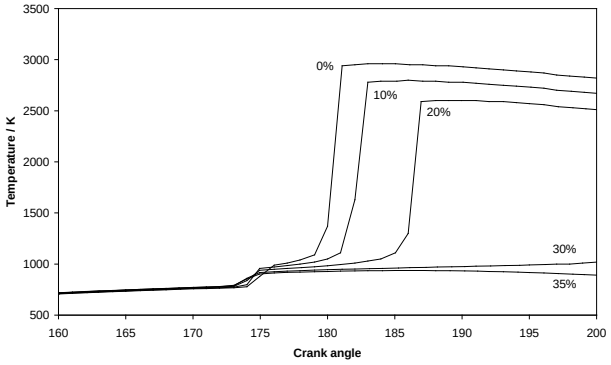

Fig.4 IEGR effect on cylinder temperature with n-heptane at inlet temperature of 370K

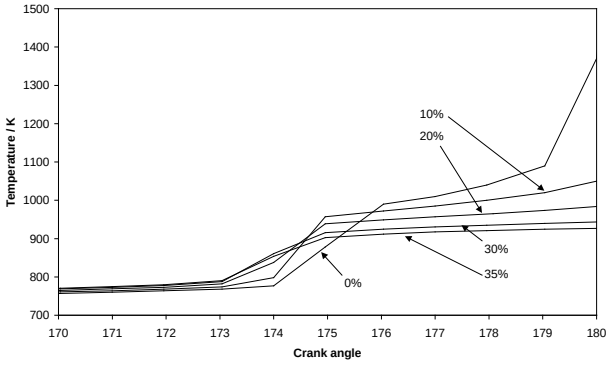

Fig.5 IEGR effect on the cool flame reaction at inlet temperature of 370K

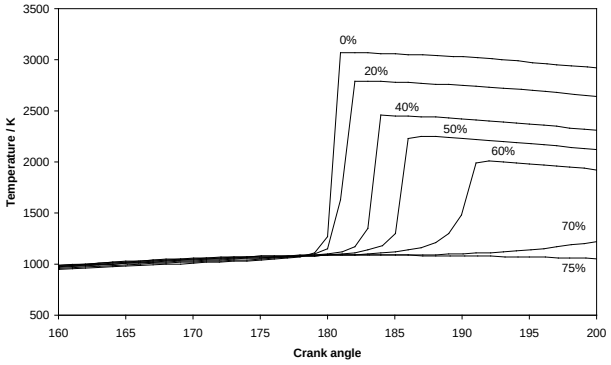

Fig.6 IEGR effect on cylinder temperature with iso-octane at inlet temperature of 525K

Figure 4 shows the IEGR effect on the auto-ignition of n-heptane, and Figure 5 shows the detailed cylinder temperature during this period of reaction. The inlet temperature of entire charge at the beginning of compression stoke is fixed at 370K. It can be seen that with more IEGR introduction, start of cool flame advances, but the induction time, which is defined as the time between start of cool flame and start of main ignition, increases, too. EGR in general has a higher heat capacity than air and fuel mixture since it contains relatively high percentage of CO_2 and H_2O. When inlet temperature remain unchanged, more IEGR introduction absorbs more heat. This reduces the temperature rise during the period of cool flame reaction and therefore retards the start of main ignition. If the temperature after cool flame period can not reach the level required by the main ignition, then main ignition fails and partial burn occurs. As a result, n-heptane has a limited IEGR endurance in comparison with other fuels with higher Octane numbers. The calculated results show that the start of main ignition is very sensitive to the quantity of EGR introduction. When EGR quantity is higher than 30% of the entire charge, no main ignition occurs.

Figure 6 shows the calculated IEGR effect on the auto-ignition of iso-octane. The inlet temperature of entire charge at the beginning of compression stoke is fixed at 525K. The effect of IEGR on auto-ignition is different from that of n-heptane. First, the EGR endurance is much higher, the maximum quantity of EGR introduction to maintain the auto-ignition is 75%, which is about twice as much as that with n-heptane. Second, the ignition delay due to EGR introduction is much shorter than that with n-heptane. With 20% EGR introduction, for example, 1^{o}CA delay with iso-octane has been observed in comparison with 6^{o}CA with n-heptane. These effects are mainly due to the fact that iso-octane has only a single stage ignition, no cool flame occurs.

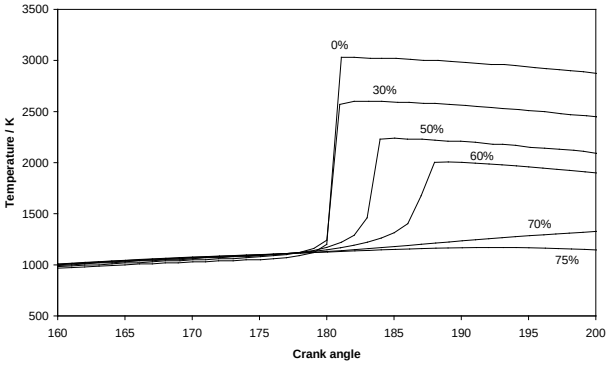

Fig.7 IEGR effect on cylinder temperature with ethanol at inlet temperature of 540K

Ethanol has a similar Octane number to iso-octane. Figure 7 shows the calculated IEGR effect on the auto-ignition of ethanol. The inlet temperature of entire charge at the beginning of compression stoke is fixed at 540K. It can be seen that ethanol, similar to iso-octane, has a very high EGR endurance up to 75% of entire charge in this case. However, with different EGR introduction, the corresponded ignition delay is different. For instance, even with 30% EGR introduction, there is no clear ignition delay with ethanol. In comparison, 1^{o}CA delay has been observed with 20% EGR introduction with iso-octane. Such behaviour is due to the fact that ethanol is an alcohol, which contains oxygen that is required for combustion. The ignition is less sensitive to IEGR[11].

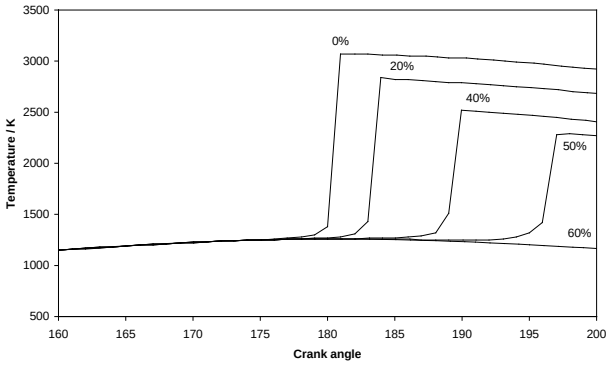

Fig.8 EGR effect on cylinder temperature with methane at inlet temperature of 615K

Methane has a very high Octane number. Figure 8 shows the calculated results of IEGR effect on the auto-ignition with methane. It can be seen that the IEGR endurance is higher than that with n-heptane. On the hand, methane has a less endurance to IEGR introduction than that of iso-octane and ethanol. The maximum EGR introduction to maintain successful ignition is 60% in this case. This is because of that the methane is a gaseous fuel, and has a different chemical structure. It does not have oxygen atom to compromise the IEGR effect like ethanol, and has methyl radicals which reacts slower in comparison with alkyl radicals in appear in iso-octane reactions. Consequently, the ignition delay is more sensitive to IEGR than iso-octane and ethanol, but less than n-heptane. With 20% EGR introduction, for example, 3^{o}CA delay comparing to 1^{o}CA with iso-octane and 6^{o}CA with n-heptane has been observed.

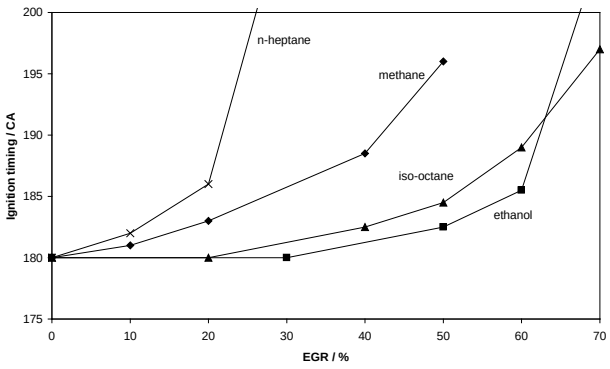

Fig.9 EGR effect on ignition timing of ethanol, iso-octane, methane and n-heptane

Figure 9 shows the IEGR effect on ignition timing of all four fuels with different Octane numbers and distinct chemical structure. It shows that n-heptane is the most sensitive fuel to IEGR introduction, iso-octane and ethanol has a much higher endurance, while methane is somewhere in the middle.

It is clear that iso-octane and ethanol have the highest EGR endurance and potentially are suitable fuels for CAI combustion application. Although n-heptane has the least endurance to EGR introduction, but its auto-ignition temperature is much lower. It may therefore have the potential to improve the CAI combustion when it is mixed with other high Octane fuels.

CONCLUSIONS:

- Fuels with high Octane number needs high inlet temperature to initiate the auto-ignition.
- IEGR delays the auto-ignition timing of all fuels. N-heptane appears to be the most sensitive fuel to IEGR, iso-octane and ethanol has a much higher endurance, methane is somewhere in between.
- Iso-octane and ethanol appear to be the suitable fuel for CAI combustion application.
- N-heptane has a very low auto-ignition temperature, it therefore have the potential to improve the CAI combustion when it is mixed with other higher Octane number fuels.
- The IEGR analysed in this computational study is consisted of major burned gases only. Further investigation on the effect of other chemical components contained in the hot IEGR should be considered in the future work.

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