Computational study on the ignition timing of HCCI combustion in IC engines fuelled with methane

A COMPUTATIONAL STUDY ON THE IGNITION TIMING OF HCCI COMBUSTION IN IC ENGINES FUELLED WITH METHANE

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ABSTRACT

Engines with Homogeneous Charge Compression Ignition (HCCI) combustion offer a number of benefits over conventional SI and CI combustions, such as low NOx emission, negligible cycle-to-cycle variation, higher combustion efficiency at part load than SI counterpart at part load, and low soot emission. Unlike SI and CI engines, where combustion is directly controlled by the engine management system, the combustion in HCCI engines is controlled by chemical kinetics only. Sophisticated strategies for ignition timing and rate of heat release control over wide engine operation range need to be developed. Using SENKIN chemical kinetics simulation package developed by Sandia, the effect of a number of engine operation parameters on the ignition timing of HCCI combustion has been calculated. Results were analysed and reported in this paper. It has been found that a high inlet temperature can be used to initiate the HCCI combustion, but EGR and air/fuel ratio appears to be the potential practical methods for ignition timing and engine load control.

INTRODUCTION

Homogeneous charge compression ignition, HCCI, combustion is a combustion process, which utilises homogeneous air/fuel mixture, but combustion is initiated by fuel self-ignition. Unlike conventional SI and CI combustions, HCCI needs no centralised combustion initiation, and the entire charge gives a parallel energy release throughout the entire charge. The advantage of such auto-ignition and simultaneous combustion nature is that the combustion limit towards leaner air-fuel mixture and the tolerance to EGR can be significantly extended. The low heating value of lean mixtures and the high heat capacity of EGR can lower the peak temperature of combustion, thus reduce NOx emission. Up to 95% reduction in NOx emission has been obtained experimentally [1,2,3].

Over the past two decades, a number of technologies have been developed to initiate the HCCI combustion in both 2 and 4-stroke engines with various fuels [4], but non could maintain such combustion over entire engine operation range, and smooth the much too high peak cylinder pressure. These difficulties are directly linked to the ignition timing management and the rate of heat release. Unlike SI and CI where the start of ignition and the rate of heat release are directly controlled by the engine management system, in HCCI, these two parameters are controlled by the chemical kinetics of combustion reaction only. Therefore, a good understanding into the mechanism of HCCI combustion is essential for future control strategy development.

In this report, a simplified engine combustion model with detailed chemical kinetics, named as SENKIN developed by Sandia [5,6], has been employed to simulate the HCCI combustion inside an IC engine combustion chamber. The effects of a number of engine operation parameters, such as inlet mixture temperature, air to fuel ratio, compression ratio, engine speed and EGR on the timing of fuel auto-ignition have been calculated. Results were shown and analysed in this paper.

SIMULATION MODEL

The simulation software employed in this investigation is SENKIN chemical kinetics simulation package developed by Sandia. It computes the time evolution of a homogeneous reacting gas mixture in a closed system. The model accounts for finite-rate elementary gas-phase chemical reactions, and also performs kinetic sensitivity analysis with respect to the reaction rates. The main assumptions of the program are:

- single-zone model of combustion chamber,
- uniform mixture composition and thermodynamic properties,
- adiabatic compression and expansion.

Research studies on primary reference fuels indicated that the auto-ignition behaviour of a fuel depends largely upon its composition, molecular size and structure. Methane exhibits certain oxidation characteristics that are different from other hydrocarbons, since more energy is required to break its C-H bond. It is more difficult to be ignited. In order to investigate the extreme conditions of fuel auto-ignition in HCCI combustion, methane has been selected as the fuel for this research. The chemical kinetics adopted into this simulation is consisted of 53 species and 325 reactions [7].

IGNITION TIMING OF HCCI COMBUSTION

Principally, the combustion of any organic compound always proceeds via a radical reaction mechanism. The characteristics of such reactions are that radicals, once formed, are generally found to be less selective in their attacks on other species, and further more, once initiated, reactions then proceed with great rapidity due to the establishment of fast, low energy requirement chain reactions. To analyse such reaction behaviour, the following engine parameters have been assumed and input into the model: air is 21% O_2 and 79% N_2; engine compression ratio is 15:1; equivalent air/fuel ratio, λ, is 1.0; inlet temperature of the air/fuel mixture is 519K; engine speed is 1800rpm; and no EGR and/or residual burned gases contained in the fuel/air mixture.

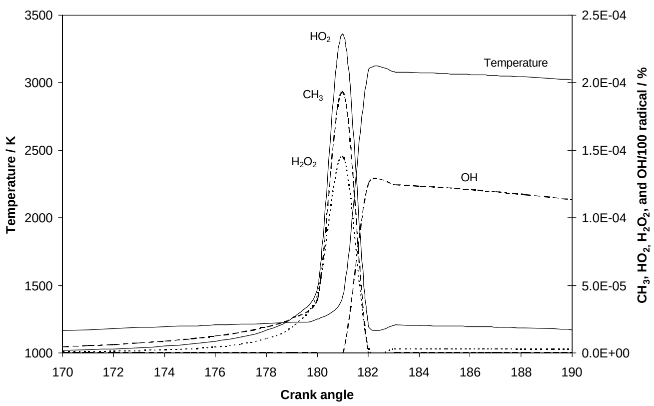

Fig.1 Fractions of typical reactive radicals

The calculation started at the beginning of compression stroke and finished at the end of expansion stroke. The interval between each calculation is 1^o of crank angle. Figure 1 shows the obtained correlation among some typical active radical and reaction intermediate CH_3, HO_2, H_2O_2 and OH. It can be seen that at crank angle of 181, H_2O_2 declines, while OH radical increases sharply. The dissociation of H_2O_2 to OH appears to be one of the key reactions to establish a pool of OH radical and initiate HCCI combustion. At the same crank angle, cylinder temperature begins to increase sharply. Obviously, the combustion starts. The time that the fraction of H_2O_2

radical reaches its peak level appears to be a good indication of the starting time of main combustion when methane is fuelled, which is 181°CA in this case.

EFFECTS OF ENGINE PARAMETERS ON IGNITION TIMING

Effect of Inlet Temperature: Using high inlet temperature to initiate combustion is a common approach to HCCI combustion [8]. To analyse the effect of inlet temperature on the ignition timing of HCCI combustion, a series of inlet temperature have been introduced into the model while other engine operation parameters remained unchanged. Figure 2 shows the calculated pressure curves. It can be seen that the higher the inlet temperature, the earlier the cylinder pressure increase occur. There is a critical temperature, which is 489K in this case, below it, no obvious combustion occurring.

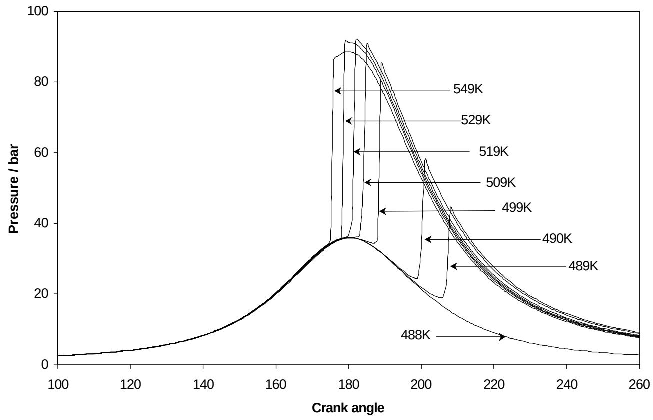

Fig.2 Cyl. pressure at varying inlet temperature

By judging the ignition timing from the occurrence of H_2O_2 peak concentration, the effect of inlet temperature on combustion ignition timing is obtained and shown in Figure 3. It can be seen that the ignition timing depends upon the inlet temperature of air/fuel mixture. Higher inlet temperature advances the auto-ignition timing. There is a critical minimum inlet temperature, below it, the ignition timing becomes infinite and no ignition occurs.

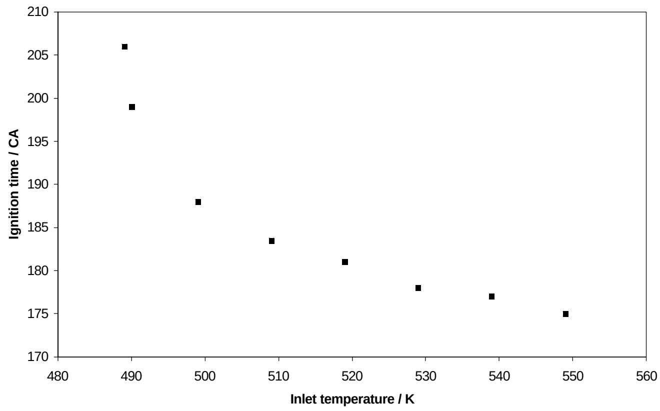

Fig.3 Effect of inlet temperature on ignition timing

Effect of Air to Fuel Ratio: Unlike conventional SI combustion, the potential ratio of air/fuel mixture can be significantly extended towards fuel lean when HCCI combustion is employed [9,10]. This is mainly due to its fuel self-ignition natural. Figure 4 shows the calculated ignition timing of the HCCI combustion with varying λ. The inlet temperature during the calculation remains constant at 490K, and other engine parameters remain the same with previous calculations. Again, a non-linear relation between ignition timing and λ has been found. Leaner air/fuel mixture, in general, results in earlier ignition.

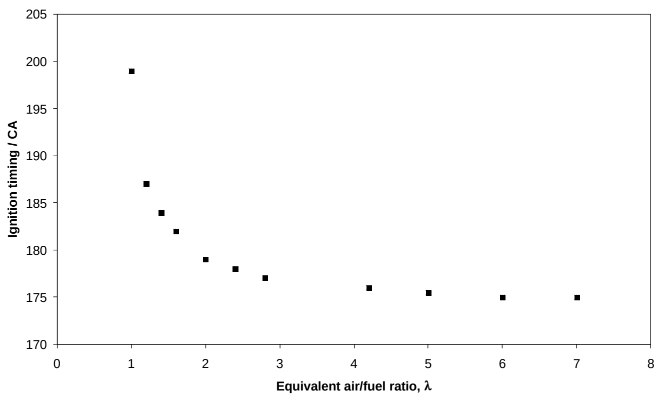

Fig.4 Effect of air/fuel ratio on ignition timing

Effect of Compression Ratio: A higher compression ratio increases the charge temperature rises during compression process and therefore advances the start of ignition of the HCCI combustion [8,11]. Figure 5 shows the calculated relationship between compression ratio and ignition timing. The inlet temperature for the calculations was 490K, and equivalent air to fuel ratio, λ, was set to 2.0. Other engine operation parameters were remaining the same with previous calculations. It can be seen that higher compression ratio results in higher thermal energy, and therefore earlier ignition.

Effect of EGR: Experimentally, two HCCI combustion control strategies with EGR have been investigated: trapping hot internal EGR inside the engine combustion chamber [3], and adding cool external EGR into engine fresh charge [12].

Trapping hot residual EGR increases the temperature of entire engine charge when it is mixed with fresh air/fuel mixture inside the combustion chamber. Therefore, by tuning the quantity of residual EGR, the ignition timing of HCCI combustion can be adjusted. Figure 6 is cited from an experimental study with infinitively variable Active Valve Train (AVT) system [3], and showed the effect of trapped EGR on HCCI combustion.

Figure 7 shows the calculated cylinder pressures with varying percentage of internal hot EGR. The EGR introduced into the calculation was assumed to be consisted of burned gas only, which is: 5% of CO_2, 15.5% of H_2O, 79% of N_2 and 0.5% of O_2. The temperature of the hot internal EGR is assumed to be 700K, and of the inlet air/fuel mixture is room temperature 298K. The λ of the air/fuel mixture is 1.0. The engine compression ratio for the calculation is

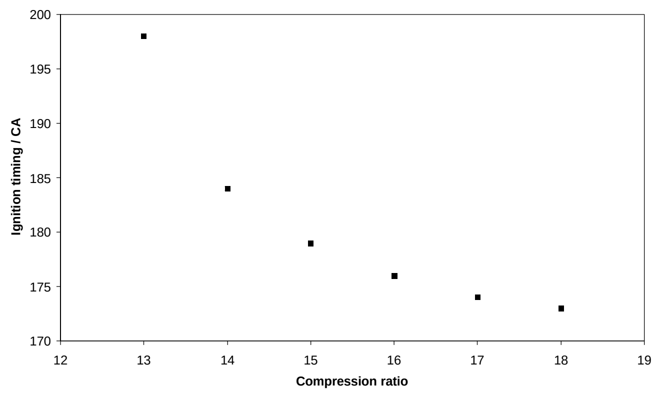

Fig.5 Effect of compression ratio on ignition timing

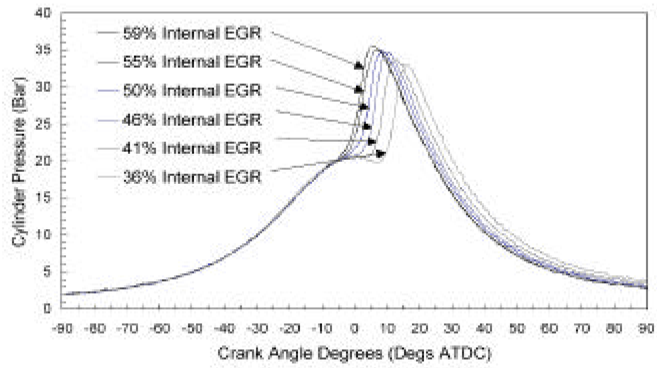

Fig.6 Cylinder pressure trace data for HCCI with different quantities of internal EGR [3].

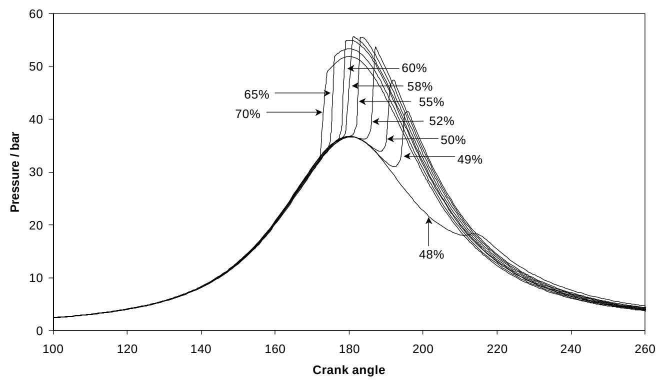

Fig.7 Calculated pressure with varying EGR

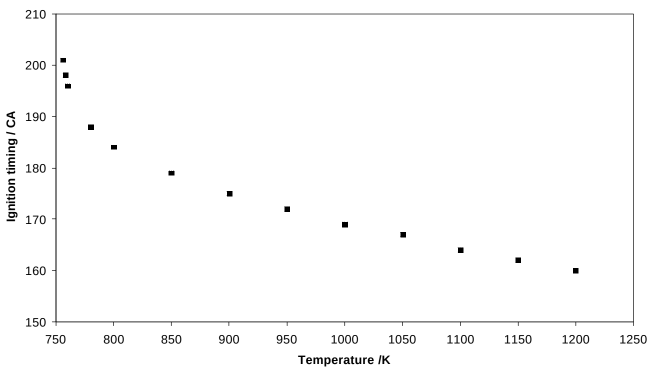

Fig.8 Effect of EGR temperature on ignition timing

15:1. Similar to the results of experimental studies, the starting time of sharp increase in cylinder pressure advances as EGR quantity increases. In other words, high amount of hot internal EGR results in earlier ignition.

Trapped hot EGR is consisted mainly of burned gases at high temperature. It therefore should have two different effects on HCCI combustion, which can be defined as the thermal effect due to its higher temperature and the chemical effect due to its chemical composition [13,14]. To investigate its thermal effect, another sets of calculation have been carried out. The quantity of the EGR during the calculation is fixed at 50%, but its temperature is varying from 750K up to 950K. Figure 8 shows the relationship of ignition timing and the temperature of EGR. It can be seen that the higher the EGR temperature, the higher the temperature of air-fuel and residual gas mixture, therefore, the earlier the ignition. Similar to the effect of inlet charge temperature, a critical EGR temperature also exists, which is 756K in this case, blow it, no combustion ignition occur except partial burn.

The chemical effect of EGR on ignition timing of HCCI combustion was calculated by fixing the temperature of overall air-fuel and residual EGR mixture at 540K, while varying the quantity of EGR contained. Figure 9 the calculated fuel ignition timing via the quantity of EGR. It can be seen that the combustion is delayed due to the addition of EGR. The higher the percentage of EGR contains, the later the combustion occurs. 75% of EGR is about the limit, no combustion occurs above.

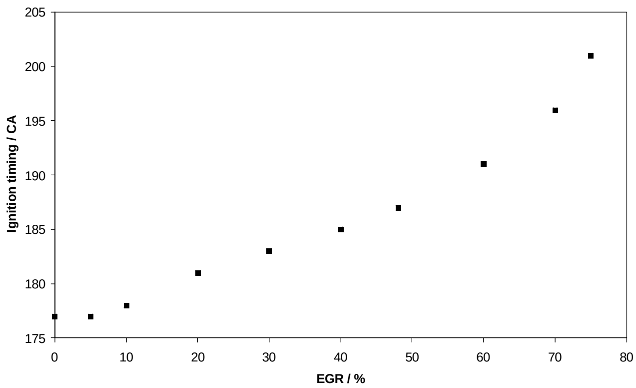

Fig.9 Effect of EGR quantity on ignition timing

CONCLUSION

1. The ignition timing of HCCI combustion is closely linked to the concentrations of a number of active radicals. Typical radicals are CH_3, HO_2, H_2O_2, and OH. The dissociation of H_2O_2 to OH appears to be one of the key reactions to establish a pool of OH radical and initiate HCCI combustion. Therefore, the timing of fuel auto-ignition can be judged by the timing when H_2O_2 concentration reaches its peak level.
2. Higher inlet charge temperature results in higher thermal energy in the charge at late stage of compression. When the thermal energy reaches the level to overcome the activation energy of the fuel, auto-ignition occurs. Therefore, a critical minimum inlet temperature exists, below it no combustion can be initiated.
3. A leaner air/fuel mixture, in general, advances the ignition timing of HCCI combustion.
4. High compression ratio increases the charge temperature uprising during compressing process and therefore advances the ignition of HCCI combustion.
5. The ignition timing of HCCI combustion in relation to engine crank angle is affected by engine speed. It is retarded when engine speed increases.
6. Hot EGR has two different effects on the ignition of HCCI combustion, thermal effect and chemical effect. Higher EGR temperature increases thermal energy of engine charge and advances ignition timing. The various chemical species inside the EGR dilute the combustible air/fuel mixture and influence combustion ignition delays.

7. High inlet temperature can be used to initiate the HCCI combustion, but EGR and air/fuel ratio appear to be the potential practical methods for ignition timing and engine load control. Further investigations are needed on heat release rates from these potential methods.

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