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A computational study into the effect of exhaust gas recycling on homogeneous charge compression ignition combustion in internal combustion engines fuelled with methane

Rui Chen *, Nesa Milovanovic

Department of Aeronautical and Automotive Engineering, Loughborough University, Ashby Road, Loughborough, Leicestershire, LE11 3TU, United Kingdom

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Abstract

Engine with homogeneous charge compression ignition, HCCI, combustion offers a number of benefits over conventional SI and CI, such as much lower NO_x emission, negligible cycle-to-cycle variation, higher combustion efficiency at part load than its SI counterpart, and low soot emissions. Unlike conventional SI and CI engines, where the combustion is directly controlled by the engine management system, the combustion in HCCI engines is controlled by its chemical kinetics only. Trapping hot internal EGR appears to be a potential technology for a practical application of this potential technology. In this paper, by using the advanced combustion simulation package SENKIN, both thermal and chemical effects of the hot EGR on HCCI combustion were calculated and analysed. It was found that the thermal energy contained in the EGR is essential for the combustion initiation, but the chemical species it contained have different effects towards both combustion ignition timing and heat release rate.

Keywords: HCCI; Combustion; Auto-ignition; Combustion simulation; Chemical kinetics; Natural gas; EGR

1. Introduction

Combustion in spark ignition (SI) engines relies on an electric discharge released between two electrodes of the spark plug to establish an initial burning kernel in a premixed homogeneous air/fuel mixture, with an overall air to fuel ratio close to stoichiometric. Because of the variation of the mixture strength within the small space between electrodes, large cycle-to-cycle combustion variations are expected. This is a fundamental problem of SI engines, due to its negative effect on engine performance and thermal efficiency [1]. After the air/fuel mixture has been ignited, the burning flame front propagates through the combustion chamber and separates the entire chamber into burned, burning, and unburned zones. The pressure and temperature of unburned gas then naturally increases as a consequence of the heat release from the burned gas. When sufficient high points were reached, another fundamental problem—knock, which is due to the self-ignition of unburned "end gas", occurs [2]. Severe knock can cause physical damage to the engine, and it can only be avoided by suppressing the end gas pressure and temperature [3]. The primary method is to drop the engine compression ratio, which further reduces SI engine efficiency. Emissions continue to be a problem. NO_x due to the high burning temperature, CO due to the relatively low oxygen availability, low efficiency results in high CO_2, and unburned HC due to incomplete combustion.

Combustion in compression ignition (CI) engines occurs via fuel self-ignition by spraying the fuel directly into the combustion chamber charged with high pressure and temperature inlets. The overall air/fuel ratios are lean, but vary locally from extremes of rich to lean, which results in higher NO_x formation in lean regions and soot formation in rich regions [4]. Exhaust gas recycling (EGR) can help to control NO_x but usually carries soot production penalty. Increased fuel injection pressure reduces soot formation by improving air and fuel mixing process, but can also increase NO_x production [5].

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,

* Correspondence and reprints.
E-mail address: r.chen@lboro.ac.uk (R. Chen).

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HCCI needs no centralised combustion initiation, and the entire charge gives a parallel energy release throughout the entire charge. The potential advantage of such auto-ignition and simultaneous combustion nature is that the combustion limit towards leaner air–fuel mixture and the tolerance to exhaust gas recycling, 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 NO_x emission. Up to 95% reduction in NO_x emission has been obtained experimentally [6–8].

Compared to SI, HCCI combustion avoids the unstable flame propagation, which results in negligible cycle-to-cycle variation [8]. At part load conditions, un-throttled engine control strategy could be employed with HCCI combustion [7,9], since the engine load can be potentially controlled with much higher air/fuel ratio and/or higher quantity of EGR than conventional SI combustion. High compression ratios are preferred by HCCI combustion due to its self-ignition nature, which can further improve the combustion thermal efficiency. A compression ratio as high as 21 : 1 has been used for gasoline fuelled HCCI combustion engines in comparison to 12 : 1 for SI [7]. As a result, up to 23% improvements in fuel economy have been reported with HCCI combustion due to complete fuel processing, using higher compression ratios, and reducing or eliminating throttle losses [10]. Fuel flexibility is also cited as a potential benefit [11].

Fuel rich zones are the main source of particulate emissions in conventional CI engines. However, with HCCI strategy, air and fuel are pre-mixed before combustion starts, very low soot emission has been be achieved with diesel fuelled HCCI combustion [12].

The phenomenon of HCCI combustion was previously only observed in 2-stroke engines. It has recently been attempted in 4-stroke engines, but could only be facilitated providing the intake air/fuel charge was pre-heated between temperatures of 50–200 °C. These have been reviewed in an early publication by the authors [13]. Recently, Lotus Engineering successfully demonstrated that HCCI could be made to work in 4-stroke engines by trapping internal exhaust gas with their active valve train (AVT) system [8]. The system needs no inlet charge pre-heating. Therefore, it offers a potential control method for HCCI combustion and brings it much closer towards practical application.

In this research, in order to analyse the mechanism of EGR effect on HCCI combustion control, a simplified engine combustion model with detailed chemical kinetics, named as SENKIN developed by Sandia [14,15], has been employed. A rather simplified gas mixture, which is consisted of burned gas only at high temperatures close to that of engine residual gas, is used as the simulated hot internal EGR. Both thermal and chemical effects of such simulated EGR on combustion ignition timing and heat release rate of the HCCI combustion were calculated. Results were shown and analysed in this paper.

2. Simulation model

2.1. Simulation software

The simulation software employed in this investigation is SENKIN chemical kinetics simulation package developed by Sandia. It uses DASAC software to solve the non-linear ordinary differential equations that describe the temperature and species mass fractions, and employs the CHEMKIN-III Utility software package, which handles the chemical reaction mechanism and species thermodynamic data.

2.2. Fuel

Methane exhibits certain oxidation characteristics that are different from all other hydrocarbons. This is because of that the activation energy required to break the C–H bond in methane is to be kilo-calories more than other hydrocarbons [16]. It has a very high Octane number (up to 120), and therefore 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.

There are a number of additional advantages of using methane as the fuel for the initial stage of HCCI study. Firstly, it is a simple fuel. Although methane is the most stable hydrocarbon fuel, which means difficult for auto-ignition, it is simple from its chemical structure point of view. The chemical kinetics of methane has been relatively well developed and can be adopted directly into this simulation. Secondly, the kinetics of methane combustion consists of only 53 species and 325 reactions [17]. The computational time is acceptable.

2.3. Methodology and assumptions

The SENKIN simulation package employed in the analysis 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 lumped model of combustion chamber. Chemical lumping presents a mathematically rigorous reduction technique that describes the kinetics of an infinite sequence of polymerisation-type reactions by a small number of differential equations developed for the moments of the polymer distribution function [18]. The target of lumping is to reduce reaction mechanism. The reduction does not merely mean simplification of the chemistry involved but rather reduction in the complexity of the mathematical form that describes the chemical transformations of a given reaction model.

HCCI combustion is initiated by fuel auto-ignition. The gas movement inside the combustion chamber and the chamber geometry design has little effect on combustion performance [13]. Assuming that the spatial variations of the gas inside the chamber are negligible, then the entire chamber can be divided into many small zones (fragments). Each single-zone can be used to represent the entire volume.

Chemical lumping with a single-zone engine combustion chamber model forms the methodology of the SENKIN simulation. It is directly adopted by this analysis. For SENKIN simulation, it is only necessary to define the compression ratio. The clearance volume is only used to scale the engine volume, by default, it has an assumed value of 1.0. The ratio of connecting rod to crank radius introduced into the calculations reported in this paper is 3.203.

Uniform mixture composition and thermodynamic properties. The gaseous mixture introduced into the simulation is assumed to be an ideal homogeneous mixture with uniform composition and thermodynamic properties. The mixture consists of the air and fuel charge with a ratio of λ and the simulated EGR (or added gases) at certain mole percentages, which is defined as:

$$y_{\mathrm{EGR}} = \frac{n_{\mathrm{EGR}}}{n_{\mathrm{air/fuel}} + n_{\mathrm{EGR}}}$$

hence,

$$n_{\mathrm{EGR}} = y_{\mathrm{EGR}} \cdot n_{\mathrm{total}}$$

$$n_{\mathrm{air/fuel}} = (1 - y_{\mathrm{EGR}}) \cdot n_{\mathrm{total}}$$

where n_{EGR} and $n_{\mathrm{air/fuel}}$ are moles of EGR (or added gases) and total moles of air and fuel charge, respectively. $n_{\mathrm{total}} = n_{\mathrm{EGR}} + n_{\mathrm{air/fuel}}$ is the total moles of entire mixture introduced into the model. It remains the same for all the calculations.

When the air and fuel charge and the hot EGR (or added gases) at different temperatures are mixed, the uniform temperature of the final homogeneous air, fuel and EGR can then be obtained as:

$$T_{\mathrm{total}} = T_{\mathrm{air/fuel}}(1 - y_{\mathrm{EGR}}) + T_{\mathrm{EGR}} \cdot y_{\mathrm{EGR}}$$

where, $T_{\mathrm{air/fuel}}$ and T_{EGR} are temperatures of the air and fuel charge and the EGR, respectively.

Adiabatic compression and expansion. The volume of the engine combustion chamber that considered in the SENKIN simulation is time-dependent and engine parameter based. It varies according to the slider-crank relationship. In order to simplify the model and center the calculations on the chemical kinetics only, both compression and expansion strokes are considered to be adiabatic processes. None of the losses, such as the heat transfers from hot gas to combustion chamber walls, heat losses in blowby, fuel trapping in crevices, etc., have been taken into account.

3. Calculated results

3.1. Effect of trapped hot EGR

Trapping hot residual burned gases (internal 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. Fig. 1 is cited from an experimental study with infinitely variable Active Valve Train (AVT) system by Lotus Engineering [3], and showed the effect of trapped hot EGR on HCCI combustion. The fuel used in the study was gasoline with an octane number of 95.

Trapped hot internal EGR consists of many gaseous chemical species, which includes the main components of burned gases, CO_2, H_2O, N_2 and O_2, partial burned gases such as CO, particular matters and unburned HCs, high temperature combustion products NO_x and possibly some combustion reaction intermediates. Different species has different heat capacity and chemical reactivity, therefore has different effect towards ignition timing and heat release rate of HCCI combustion. In order to simplify the calculation, only the major burned gases are considered in this investigation. Table 1 lists the simulated EGR considered and the heat capacity of each component. Although concentrations are extremely low in comparison with the major burned gases, the potential chemical effects of those combustion intermediates and partial burned gases on HCCI combustion can be significant due to their high chemical reactivity. These effects are currently under investigation and will be discussed in future reports.

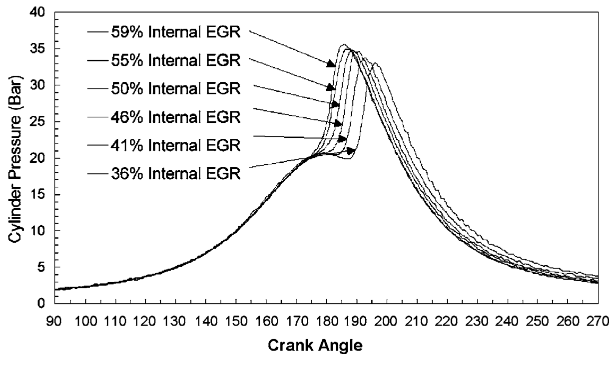

Fig. 1. Cylinder pressure trace data for HCCI with different quantities of internal EGR [8].

Table 1
EGR introduced into the simulation model

Components of EGR	Concentration (%)	Cp@1000 K ($\mathrm{cal \cdot mol^{-1} \cdot deg^{-1}}$)
CO_2	5	12.980
H_2O	15.5	9.851
O_2	0.5	8.336
N_2	79	7.815

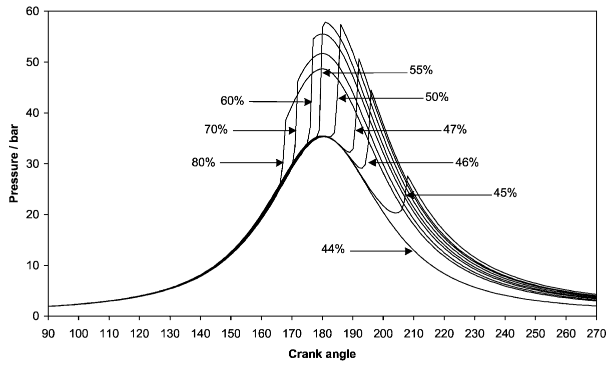

Fig. 2. Calculated cylinder pressure with varying quantity of EGR at 800 K.

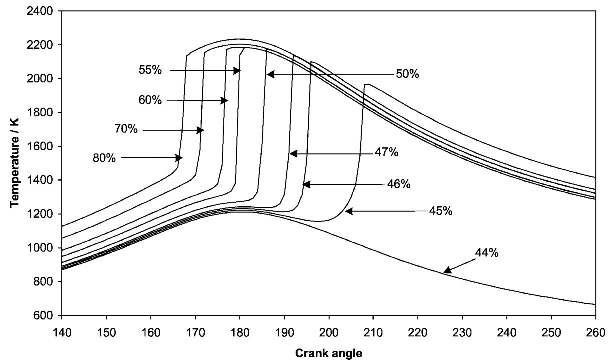

Fig. 3. Calculated cylinder temperature with varying quantity of EGR at 800 K.

Figs. 2 and 3 show the calculated cylinder pressures and temperatures with varying quantities of hot simulated EGR. The temperature of the hot EGR is assumed to be 800 K, and of the inlet air/fuel mixture is room temperature 298 K. The air, fuel and EGR are mixed before the compression process starts, and the mixture is assumed as perfect homogeneous. The λ of the air/fuel mixture is 1.0. The engine compression ratio for the calculation is 15 : 1, and the engine speed is fixed at 1800 rpm. It can be seen that although the fuel used in the calculation is different from the one used by Lotus Engineering in their experimental study, the general trend of EGR effect on HCCI combustion is agreeable. The starting time of sharp increase in cylinder pressure and temperature advances as EGR quantity increases. In other words, high amount of hot internal EGR results in earlier ignition.

Fig. 4 shows the effect of EGR on fuel auto-ignition timing obtained from the data presented in Figs. 2 and 3. The relationship between EGR quantity and its effect on HCCI combustion ignition timing is non-linear, but high percentage of EGR, in general, results in earlier combustion initiation. A critical minimum percentage of EGR exists, which is 45% in this case, below it, ignition timing becomes infinite and no combustion occurs.

Trapped hot EGR is consisted mainly of burned gases at high temperature. Its effect on the ignition timing and the heat release rate of HCCI combustion should, therefore, have two aspects. One aspect of its effect is its high temperature. When the hot internal EGR is mixed with

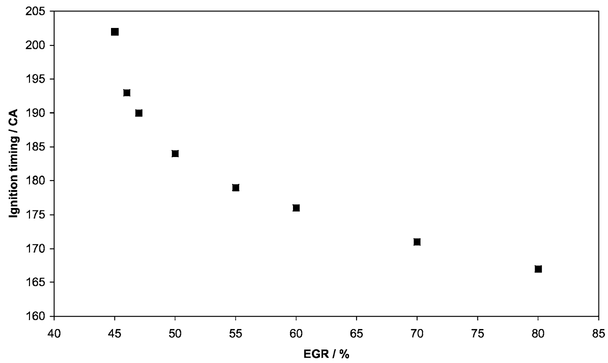

Fig. 4. Calculated effect of EGR at 800 K on the ignition timing of HCCI combustion.

cool air/fuel mixture, it improves the temperature of the entire inlet charge, which helps the initiation of HCCI combustion. This effect is similar to the inlet charge pre-heat method commonly used for HCCI combustion research. Such effect of the internal hot EGR can be named as thermal effect. The other aspect of the effect of trapped hot EGR on HCCI combustion is due to the different chemical species it contains. Different gaseous species have different thermal heat capacity profile against temperature and chemical reactivity towards combustion reaction. Their effect on cylinder temperature history and fuel auto-ignition should therefore be different. This aspect of EGR effect may be defined as chemical effect. The above observed and calculated results, in fact, should be the combination of these two.

3.2. *Thermal effect*

At higher temperature, the engine charge gives a higher thermal energy, which helps the fuel to overcome its activation energy and improves the pre-ignition chemical reactions. This part of chemical reactions is commonly regarded as the first stage ignition (cool flame). The main ignition is immediately following the first stage ignition provided that the energy produced from the first stage ignition could maintain full-scale chain branching and propagating reactions. Therefore, the combustion ignition delay relies on pre-ignition chemical reactions and reduces if the engine inlet temperature increases. One popular method of generating HCCI combustion and controlling the ignition timing is to adjust the intake air temperature. By trapping the hot internal EGR and mix it with inlet air/fuel mixture, the hot EGR can also improve the temperature of entire charge and therefore improve the auto-ignition.

To investigate the thermal effect of trapped hot EGR on HCCI combustion, another group of calculations was carried out. In order to eliminate the chemical effect due to changes in inlet mixture composition, the quantity of the EGR during the calculation was fixed at 50%. The temperature of the EGR was varied from 750 K up to 950 K. The inlet air and fuel mixture was fixed at 298 K. All other engine

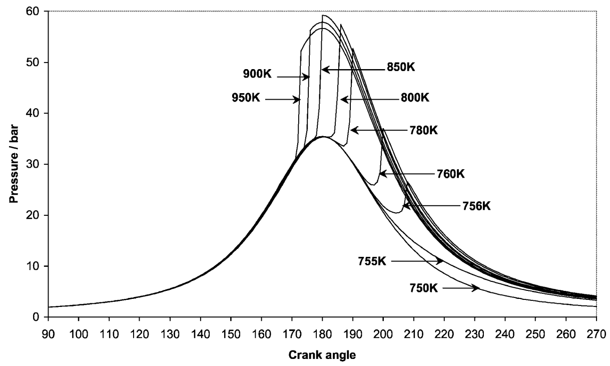

Fig. 5. Calculated cylinder pressure with 50% of EGR at varying temperature.

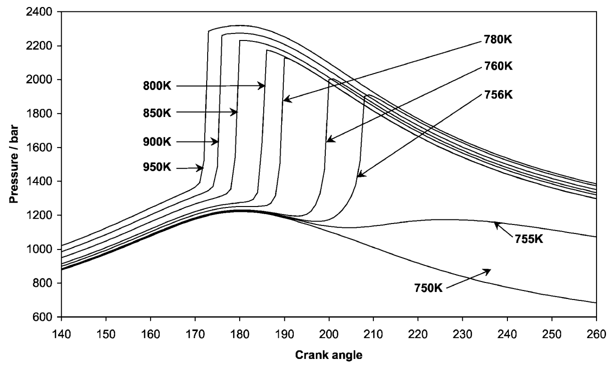

Fig. 6. Calculated cylinder temperature with 50% of EGR at varying temperature.

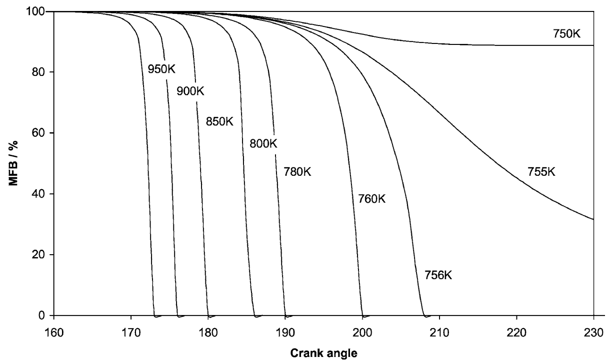

Fig. 7. Mass fraction burned with 50% of EGR at varying temperature.

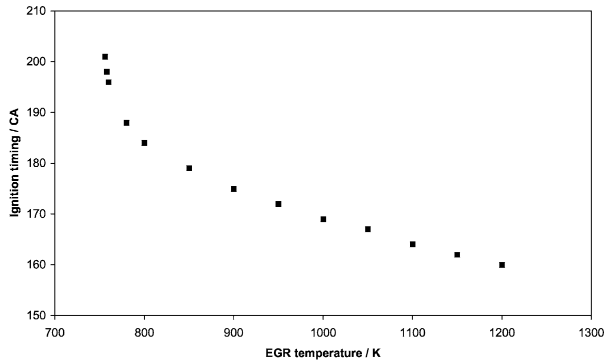

Fig. 8. Calculated effect of EGR temperature on ignition timing.

operation parameters were remaining the same with previous calculations.

Figs. 5 and 6 show the calculated cylinder pressure and temperature. Fig. 7 shows the fuel mass burned fraction.

Fig. 8 shows the effect of EGR temperature on the ignition timing of HCCI combustion. The data were obtained from the calculated results presented in Figs. 5 to 7. 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 756 K in this case, below it, no combustion ignition occur except partial burn.

3.3. Chemical effect

Each gaseous chemical species in the trapped hot EGR has different thermal heat capacity and chemical reactivity towards combustion reaction. It therefore has different effect on the history of cylinder temperature and the rate of chemical reactions. The chemical components of burned gas considered in this investigation are O_2, N_2, H_2O, and CO_2. In order to investigate their effect on fuel auto-ignition under HCCI conditions, different percentages of these gases and the simulated EGR produced from them as given in Table 1, were added into the fuel/air mixture and introduced into the calculations. These added gases were assumed to be pre-heated to a high temperature, then introduced into the air/fuel mixture to produce a perfect homogeneous engine inlet charge. The inlet temperature of the mixed inlet charge was fixed at 580 K throughout the calculation in order to separate the temperature effect. The air/fuel ratio, λ, before mixing with the added gas was equal to 1. The rest engine operation parameters were the same as in the previous calculations.

Figs. 9–13 shows the calculated cylinder temperature with varying quantity of added gases.

N_2 is the dominant species in the burned gas of an IC engine. From its chemical reactivity point of view, it is a relatively stable gas and has the least heat capacity in comparison with other major components, as given in Table 1. After mixing with the air/fuel mixture, N_2 dilutes the inlet charge, and reduces its heat capacity. The reduction in heat capacity results in slightly higher cylinder temperature uprising than air/fuel mixture only during the compression process. Fig. 11 shows the calculated cylinder temperature with varying percentage of N_2 addition. It can be seen that although the peak cylinder temperature reduces largely as more N_2 was added, the combustion ignition timing, the timing of temperature sharp increase due to combustion, were remained rather the same. In other words, N_2 seriously reduces the peak combustion temperature, but has little effect on HCCI combustion ignition timing.

Water steam has a much higher heat capacity than that of N_2, about 26% higher at 1000 K. After mixing with

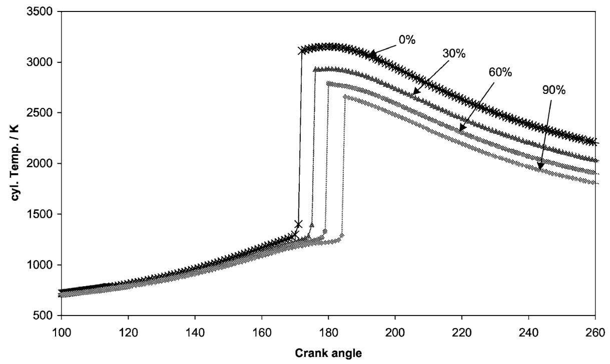

Fig. 9. Calculated cylinder temperature with varying quantity of CO_2.

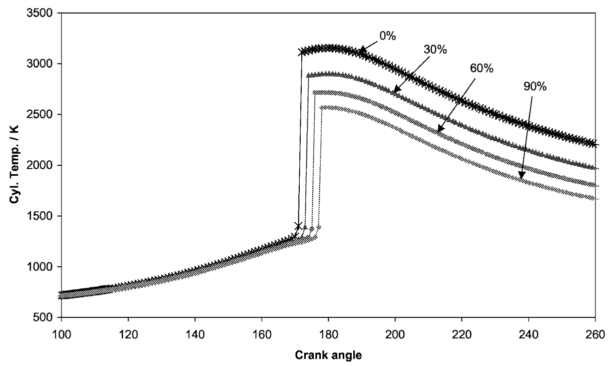

Fig. 10. Calculated cylinder temperature with varying quantity of H_2O.

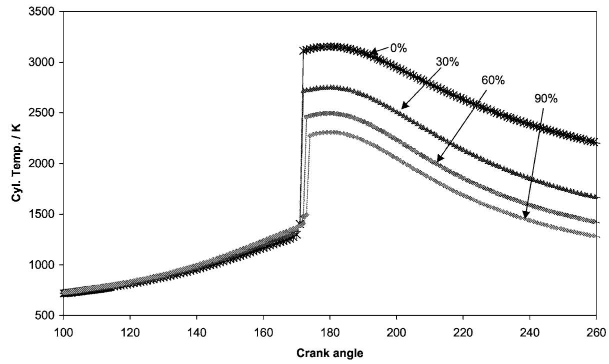

Fig. 11. Calculated cylinder temperature with varying quantity of N_2.

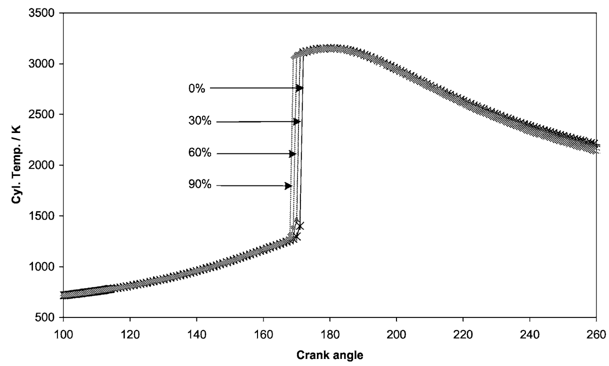

Fig. 12. Calculated cylinder temperature with varying quantity of O_2.

air/fuel mixture, the added H_2O dilutes the entire charge and also slightly increases its heat capacity. Higher heat capacity absorbs more heat energy, hence, slows down the cylinder temperature uprising during compression process, and delays the combustion ignition timing. Fig. 10 shows the temperature history with varying H_2O addition. Comparing with that of N_2 addition, H_2O has a clearer effect on the ignition timing delay. H_2O addition reduces cylinder temperature after combustion initiation as well, but the reduction is less than that with N_2 dilution. This may, again, be due to the high heat capacity of H_2O, which releases the energy it absorbed before combustion initiation and maintains the cylinder temperature high.

CO_2 has the highest heat capacity among all the gases analysed, 66.1% higher than that of N_2 at 1000 K. It increases the heat capacity of the entire charge when it is mixed with the air/fuel mixture. Fig. 9 shows the cylinder temperature history with varying CO_2 addition. The cylinder temperature uprising during compression process clearly slows down due to CO_2 addition. The ignition timing is, therefore, largely delayed. Similar with H_2O dilution, CO_2 addition reduces cylinder temperature after combustion initiation as well, but even less than that with H_2O addition.

O_2 has a heat capacity slightly higher than that of N_2. The resulted heat capacity of the entire charge with air/fuel mixture and O_2 addition is, therefore, generally unchanged. Fig. 12 shows the cylinder temperature history with varying O_2 addition. It can be seen that O_2 addition has little effect on the cylinder temperature uprising during the compression process. However, different from all other analysed gases, O_2 is part of the combustion reactant. Increasing its concentration will improve the fuel oxidation reaction, and therefore accelerate the fuel auto-ignition reactions. Fig. 12 shows the cylinder temperature history with varying O_2 addition. It can be seen that slightly advanced ignition can be obtained with increased O_2 addition. Different from all other added gases, there is no clear effect on cylinder temperature after combustion initiation when the quantity of O_2 addition is varying. This may mainly be due to the fact the combustion is advanced well before the engine top dead centre (TDC), and engine compression is making another contribution to the cylinder temperature increasing.

Fig. 13 shows the cylinder temperature with varying percentage of simulated EGR (detailed in Table 1). It can be seen that the combustion ignition delay increases and the cylinder temperature after combustion initiation drops as the quantity of the simulated EGR increases.

Fig. 14 shows the effects of different added gases with varying quantity on HCCI combustion ignition delay in comparison with the ignition delay of air/fuel mixture only. The data were obtained from the temperature traces showed in Figs. 9–13. It can be seen that CO_2 has the highest impact on ignition delay among all the gases analysed, while O_2 slightly advances the ignition timing. The ignition delay due to the addition of the simulated EGR is similar to the figure due to CO_2 addition. N_2 has negligible effect.

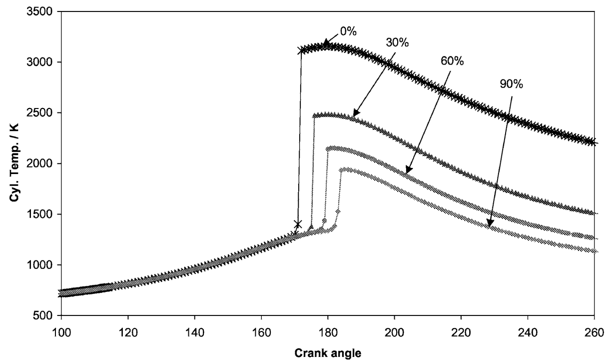

Fig. 13. Calculated cylinder temperature with varying quantity of simulated EGR.

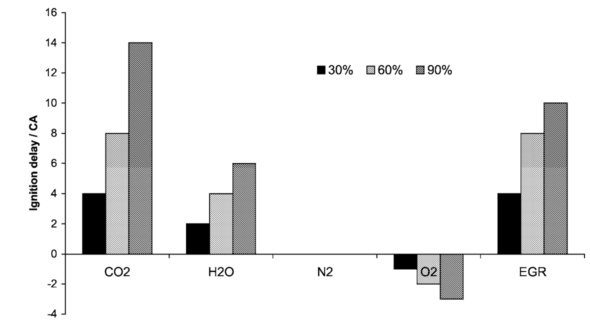

Fig. 14. Effect of added gases on ignition delay of HCCI combustion.

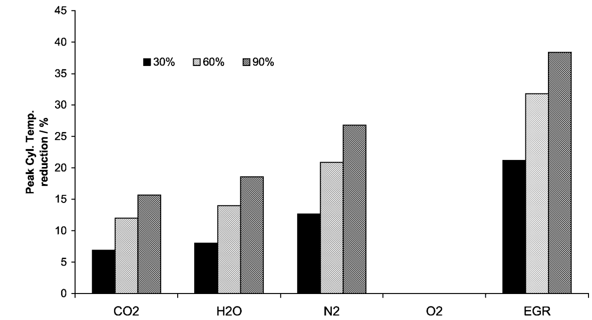

Fig. 15. Effect of added gases on peak cylinder temperature reduction.

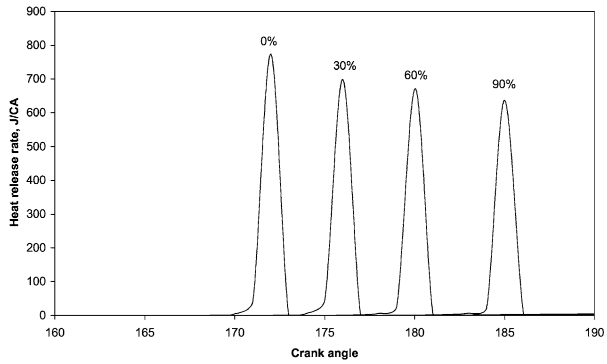

Fig. 16. Calculated heat release rate with varying quantity of CO_2.

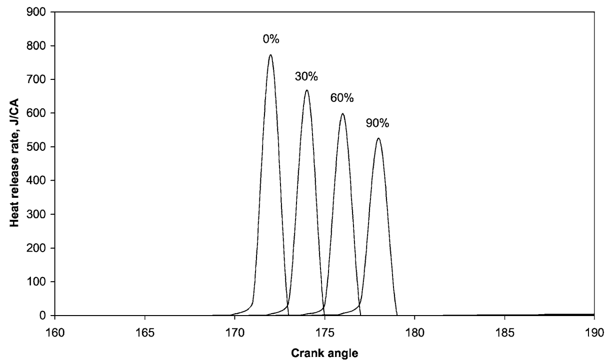

Fig. 17. Calculated heat release rate with varying quantity of H_2O.

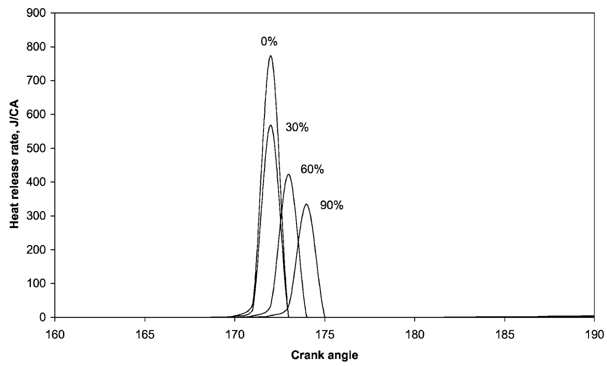

Fig. 18. Calculated heat release rate with varying quantity of N_2.

Fig. 15 shows the reduction in peak cylinder temperature due to the addition of different gases with varying quantity comparing that with air/fuel mixture only. N_2 appears to have the utmost effect on cylinder temperature reduction among all the individual gases. This is simply due to its dilution effect. Although the addition of O_2 dilutes the inlet charge as well, O_2 advances the combustion ignition. The early combustion maintains the cylinder temperature at high level, which is close to that with air/fuel mixture only. The simulated EGR has a much high effect than all the individual gases on cylinder temperature after combustion initiation. This is due to its serious effect on ignition delays. Although the main component of the simulated EGR is N_2, the small percentage of CO_2 and H_2O contained has a high impact on ignition delay due to their high thermal capacity. On the other hand, the dilution effect of the dominant species, N_2, results in large cylinder temperature reductions. Furthermore, since the combustion ignition is delayed well after TDC, the engine expansion further reduces the cylinder temperature. Overall, a much higher reduction in cylinder temperature has been observed when the simulated EGR is introduced.

Figs. 16–20 shows the calculated heat release rate with varying quantity of added gases.

Fig. 21 shows the reduction of heat release rates due to the addition of different added gases in comparison with that from of the combustion with air/fuel mixture only.

N_2 has the highest impact on combustion heat release rate among all the individual gases. Again, this is due to its dilution effect. O_2 has the least effect. This is mainly because of that O_2 advances the ignition timing. Since

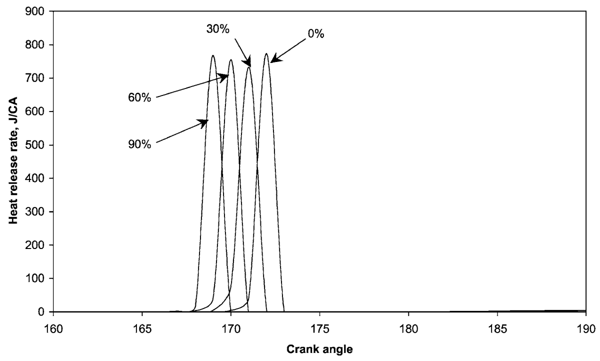

Fig. 19. Calculated heat release rate with varying quantity of O_2.

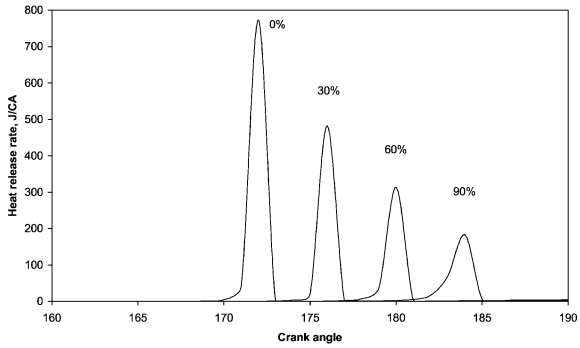

Fig. 20. Calculated heat release rate with varying quantity of EGR.

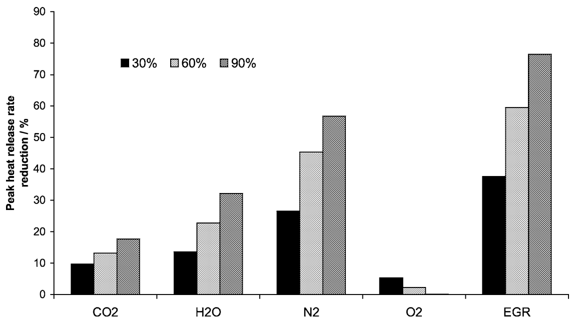

Fig. 21. Effect of added gases on heat release rate reduction.

the ignition starts well before TDC, the contribution from engine compression improves the cylinder temperature as well. The simulated EGR has the highest effect on reducing combustion heat release rates. Again, such high impact is mainly due to the fact that the ignition starts well after engine TDC, and the majority component in the simulated EGR is N_2.

In conclusion, trapped hot internal EGR appears to have two different effects towards the ignition of HCCI combustion, the high temperature advances the ignition timing, while the various chemical species inside the EGR dilute the combustible air/fuel mixture and influence both combustion ignition delays and heat release rates.

4. Conclusion

The effect of trapped hot EGR observed from some experimental studies has been simulated and analysed in this investigation. SENKIN combustion simulation software package was utilised. It was found that the trapped hot EGR has two aspects of contribution towards HCCI combustion. These can be categorised as thermal effect and chemical effect.

The thermal effect of the trapped EGR is due to its high temperature. After mixing with cool air/fuel mixture, the hot EGR improves the temperature of the entire engine inlet charge, therefore, increases the cylinder temperature uprising during compression process. Similar to the technique to generate HCCI combustion by increasing inlet temperature, hot EGR can initiate HCCI combustion and advances ignition timing if more EGR is introduced. An assumed EGR at a fixed temperature of 800 K was used to calculate its thermal effect. The trend of the calculated results agrees with experimental results.

The chemical effect of the EGR on HCCI combustion is investigated by calculating the effect of major gaseous species contained in the EGR. It was found that N_2 has little effect on ignition timing but high impact on combustion heat release rate. O_2 advances the ignition timing but has little effect on heat release rate. Both CO_2 and H_2O significantly delay the ignition timing and reduce heat release, but their effects on heat release rate are less than that from N_2 mainly due to the fact that their high heat capacities smooth cylinder temperature drop after combustion initiation. When all these gases were mixed at a ratio close to that of EGR, it was found that the N_2 contained in such simulated EGR has a dominant effect on combustion heat release rate, while the low concentration of CO_2 and H_2O significantly delay the ignition timing.

The effect of the trapped hot EGR on HCCI combustion is a combined result of its thermal and chemical effects. The thermal effect is related to the high temperature of the EGR. It increases the temperature of entire inlet charge, helps the charge to overcome its activation energy and therefore advances the ignition timing. The chemical effect comes from the chemically active species that the EGR contained. The active species decrease the activation energy level of the entire charge, and makes the ignition easier. When the temperature of the entire engine inlet charge remains constant, the more chemically active species the EGR contained, the earlier the ignition occurs. On the other hand, when quality and quantity of the EGR is fixed, higher inlet temperature results in earlier combustion ignition.

It is important to point out that varying the amounts of individual species in the exhaust is not a practical option in a real engine. The relevance of current kinetics study on HCCI combustion observed in a practical IC engine is limited. A more sophisticated IC engine simulation model should therefore be introduced if HCCI combustion in an IC engine needs to be simulated in greater details. However, the current computational studies and results formed an aid for understanding fundamental influences of certain chemical species on ignition behaviours. It has been proved theoretically that different chemical species has different influences towards combustion ignition and heat release rate. The chemical effect of EGR on HCCI combustion is a combined effect of these individual species. Potentially, such results indicate that varying the chemical composition of engine inlet charge, such as industrial air, may also be used as practical control methods for HCCI combustion.

The EGR analysed in this computation study is consisted of major burned gases only. Further investigation on the effect of other chemical components contained in the trapped hot EGR should be considered in the future work.

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