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A Numerical Study of the effects of IEGR on the Set-off Auto-Ignition in an HCCI Engine

Paul Osei-Owusu*, Salah Ibrahim and Rui Chen

***p.osei-owusu@lboro.ac.uk**

**Department of Aeronautical and Automotive Engineering, Stewart Miller Building,
Loughborough University, Loughborough, Leicestershire, LE11 3TU, UK.**

Abstract

The shortcomings of traditional combustion techniques are being continually evaluated and alternate combustion modes are being sought. One such combustion mode that is receiving a lot of attention is Homogenous Charge Compression Ignition (HCCI). HCCI is a combustion process that has the potential to be highly efficient and produces low emissions. It can provide high, diesel-like efficiencies using gasoline, diesel, and most alternative fuels. The major drawback with HCCI is controlling the ignition timing over a wide range of load and speed. The local chemical and thermal conditions of the charge mixture, towards the end of the compression stroke, have significant influences on the set-off auto-ignition. In this paper, numerical study has been carried out to examine the effects of mixture quality on the occurrence of auto-ignition at the end of the compression stroke inside a pentroof combustion chamber. The effect of different Internal Exhaust Gas Re-circulation (IEGR) are investigated. The use of IEGR acts as an indirect control method, the rate of combustion can be slowed down; however the percentage of IEGR retained in the cylinder affects the onset of auto-ignition. The calculated results have been validated against published experimental data, so that the correlation between the two can be discussed. It is found that the inhomogeneity of the air, fuel and the IEGR mixing, presented here in terms of temperature distribution, plays an important role in initiating, and potentially further controlling the HCCI combustion. During the compression process, certain parts of the engine charge are found to reach a higher temperature which auto-ignited depending on the percentages of IEGR used.

Introduction

During much of the previous two centuries, reciprocating Internal Combustion (IC) engines have generally been thought of as being of two basic ignition types, Spark-Ignition (SI) gasoline engines and Compression-Ignition (CI) diesel engines. However, with the ever changing energy situation, widespread consumption of limited fossil-fuel reserves and the growing concern over the impact of combustion produced exhaust pollutants on the environment and health, researchers, in increasing numbers, have been re-examining engine combustion. The shortcomings of traditional combustion techniques are being continually evaluated and alternate combustion modes are being sought.

A third IC engine receiving a lot of attention is Homogeneous Charge Compression Ignition (HCCI). HCCI is currently under widespread investigation due to its potential to lower NO_x and particulate emissions while maintaining high thermal efficiency [1-6]. Called by various names, such as Active Thermo-Atmosphere Combustion (ATAC), Lean Homogeneous Combustion (LHC), Compression Ignited Homogeneous Charge Combustion (CIHC), Active Radical Combustion (AR), Homogeneous Charge Compression Ignition Diesel Combustion (HCDC), Diesel Fumigation, Multiple Staged

Diesel Combustion (MULDIC), Premixed Direct- Injection Combustion (PREDIC), and Premixed Compression Ignited Combustion PCIC). The HCCI process essentially involves a premixed fuel/air mixture that is inducted into the cylinder at equivalence ratios that can vary from lean to Stoichiometric [5]. Once within the cylinder, the homogeneous fuel/air charge is then compressed until ignition commences. Ignition leads to a very rapid combustion phase.

From a fundamental point of view it is generally accepted that HCCI combustion is dominated by local chemical-kinetic reaction rates [3], with no requirement for flame propagation. This concept has been supported by spectroscopic data indicating that the order of radical formation in HCCI combustion corresponding to self-ignition rather than flame propagation [7]. It is also considered that if a truly homogeneous mixture exists at the time of combustion, turbulence has little direct effect on HCCI combustion, but it may have an indirect effect by altering the temperature distribution and the boundary layer thickness within the cylinder. Small temperature differences inside the cylinder have a considerable effect on combustion due to the sensitivity of chemical kinetics to temperature.

In the early stages, research in the field of HCCI was heavily dominated by experimental work, however, with advances in the understanding of higher hydrocarbon chemistry and rapid increases in computational power, more researchers have begun to formulate theoretical descriptions of HCCI combustion. It is generally accepted that the HCCI process with its auto-ignition characteristic is controlled primarily by chemical kinetics. This has increased the number of researchers in the field of HCCI modelling to implement detailed reaction mechanisms in a variety of simulation codes to provide in-depth descriptions of HCCI combustion by using models of varying complexity [1, 8-10]. These models, depending on their intended use, have been developed using different descriptions of both the in-cylinder and the engine process. A literature survey on HCCI has shown that model development tends to focus on the following modelling approaches:

1. Zero-dimensional thermo-kinetic
2. Multi-dimensional approach
3. Segregated, sequential fluid mechanic - thermo-kinetic multi-zone

The basic modelling approach is the zero-dimensional thermo-kinetic approach. This assumes that the fluid mechanics have no implications on the combustion event, aside from possible heat transfer effects. Examples of this approach are the models reported by Christensen et al [11] and Dec et al [12]. In an attempt to improve the zero-dimensional modelling approach, Fiveland and Assanis [1] have reported the development of a complete, four-stroke cycle simulation that integrates complex chemical kinetic mechanisms with physical models of gas exchange and in-cylinder processes, including turbulence and heat transfer. Overall, while zero-dimensional models have shown the ability to provide satisfactory results for engine performance, they are found to under-perform when predicting the rate of heat release, combustion completeness, and emissions.

Attempts have been made to use three-dimensional Computational Fluid Dynamics (CFD) models coupled with detailed chemistry to study compression ignition under HCCI like-conditions. Agarwal and Assanis [13], reported on the coupling of a detailed

chemical kinetic mechanism for natural gas ignition, which included 22 species and 104 elementary reactions, with the multi-dimensional reacting flow code KIVA-3V [14, 15] to explore the auto-ignition of natural gas injected in a quiescent chamber under diesel-like conditions. Kong et al [16] also proposed a more practical approach to account for turbulence effects on auto-ignition by proposing a reaction rate incorporating the effects of both chemical kinetics and turbulent mixing through characteristic time scales.

In order to retain some of the resolution given by CFD models and reduce the computational cost, a segregated, sequential multi-zone modelling approach was proposed by Aceves et al [17, 18]. In the latter, a computational fluid dynamics code is run over one part of the engine cycle, typically from Bottom Dead Centre (BDC) until a transition point before Top Dead Centre (TDC), and then the fluid is divided into mass-temperature groups. Each temperature group is solved within the context of a single zone, but the groups are solved simultaneously. The model shows promising results in capturing the in-homogeneities in the temperature field, resulting from heat losses occurring near the wall and in the crevices.

From a previous experimental study [19], it was found that the potential hybrid combustion concept consists of four regions: conventional spark ignition combustion, spark ignition controlled auto-ignition, spark ignition assisted auto-ignition, and spark ignition free controlled auto-ignition. This study showed that the percentage of IEGR affected the onset of auto-ignition. Also an earlier numerical study [20] showed inhomogeneity inside the combustion chamber towards the end of the compression stroke at TDC existed. This finding indicated that the number of cells contained within the volume fraction at TDC with high temperature initiates auto-ignition, with a dominate effect on HCCI and therefore need to be identified.

It is therefore the aim of the current study to use KIVA-3V [14, 15] to investigate the influence of mixture quality at the end of the compression stroke inside a pentroof combustion chamber. The effect of IEGR on HCCI is investigated. Previously published experimental data [19] have been used to provide input data for the model, and the results are validated against experimental measurements for pressure to examine the trends. It is found that the inhomogeneity of the air, fuel and the IEGR mixing, presented here in terms of temperature distribution, plays an important role in initiating, and potentially further controlling the HCCI combustion. During the compression process, certain parts of the engine charge are found to reach a higher temperature which auto-ignited depending on the percentages of IEGR used.

Numerical Analysis

Engine Configuration

The calculations are performed using a pentroof engine geometry; Figure 1 shows an outline of the computational mesh. The engine geometry is a generic four valve pentroof combustion chamber arrangement, with two inclined intake and exhaust valves. Details of the engine used for the computational study and experimental testing are given in Tables 1 and 2 respectively. The geometric properties for the experimental study and the computational study differ slightly, however this does not pose any problems in terms of the results as they aim of this study is to show the trends that exists, and discuss the effects of IEGR on the set-off auto-ignition in an HCCI engine. Good agreement was obtained between the two calculated results, which would suggest that the presented results accurately outlines the general trends.

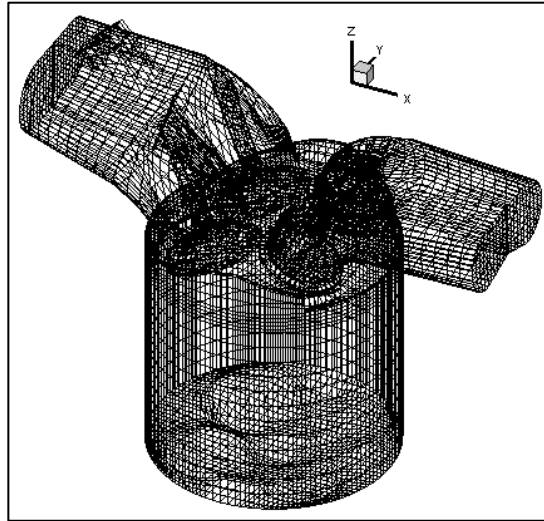


Figure 1: Outline of Computational Mesh used at BDC

Table 1: Geometric Properties of the Computational Engine

Bore	92mm
Stroke	85mm
Compression Ratio	10.1:1
Pentroof Angle	140°
Connecting Rod Length	147mm
Test Speed	2000-4500rpm
Number of Valves	4
Fuel Injection	Port Fuelled
Fuel Type	Gasoline

Calculations are carried out through the intake and compression strokes, starting at the Exhaust Valve Closure (EVC) and ending at TDC. The computational time step was one crank angle. The exhaust valves are closed for the portions of the cycle considered here. The valves are moved through a prescribed lift profile. The computational mesh shown in Figure 1 has a maximum number of grid cells of about 60,000 cells. This study considers 60,000 cells to be sufficient to show the mixing quality (to reduce CPU time) as reported by Kong et al [21].

The Numerical Model

In this work, the KIVA-3V engine code [14, 15] has been used to simulate the gas exchanges over the induction and compression phases. Initial conditions outlined in Table 3 were taken from published experimental data [19]. These initial conditions were maintained for all calculations reported here.

Table 2: Geometric Properties of the Experimental Engine

Bore	80.5mm
Stroke	88.2mm
Compression Ratio	10.5:1
Pentroof Angle	137°
Connecting Rod Length	131mm
Test Speed	2000rpm
Number of Valves	4
Fuel Injection	Port Injected
Fuel Type	Gasoline

Table 3: Initial Modelling Condition

IEGR ¹ (%)	Initial Pressure ² (bar)	Wall Temperature ³ (K)	In-Cylinder Temperature ⁴ (K)	Exhaust Temperature ⁵ (K)
36	1.84	395.80	872.20	750.55
46	1.81	397.34	838.06	714.88
59	1.53	392.85	786.85	668.15

¹ IEGR refers to the percentage of burned gases retained in the cylinder

² Initial Pressure refers to the pressure used at the start of the simulation for the six different IEGR's. This pressure was obtained from experimental study

³ Wall Temperature refers to the temperature used for the cylinder walls or liner, cylinder head and the piston face at the start of the simulation

⁴ In-Cylinder Temperature is the temperature of the burned gases at the start of the simulation

⁵ Exhaust Temperature is the temperature of the burned gases within the exhaust port

Following the usual practice, the governing equations of the in-cylinder flow problem are formulated in terms of ensemble averaged values, namely all quantities in the governing equations are to be interpreted as averages at a given crank angle position over many engine cycles. The equations, namely the momentum, mass and energy conservation equations, including the k-ε turbulence model, are solved by means of the finite volume method. Spatial differences are formed on a finite-difference mesh that subdivides the computational region into a number of small cells that are hexahedrons.

The number of species and chemical reactions that can be accounted for are arbitrary. The numerical calculation procedure is performed on a structured mesh.

The fluid induced through the intake port is a homogeneous Stoichiometric mixture (i.e. $\lambda = 1$) of iso-octane and air. The temperature and pressure of the fluid at the entrance of the intake ports are kept at 299.15 K and 1 bar, respectively. The mixture contained within the cylinder at the initial condition is assumed to be a homogeneous Stoichiometric mixture of burned products. The initial temperature and bulk pressure of fluids in the cylinder are outlined in Table 3.

All calculations were performed at a 2000rpm for the three different IEGR's reported in this paper (36%, 46% and 59%). The valve timing values were taken directly from experimental data; see Table 4 for the values used for the different IEGR's. The simulations started at Exhaust Valve Closing (EVC), with the piston and the valve assigned to their appropriate positions and speeds. The pressure and temperature were taken from experiment measurements [19], so bulk average quantities are applied. Adiabatic wall boundary conditions were assumed.

Table 4: Experimental and Simulation Valve Timing Data

IEGR (%)	IVO CA (Degrees)	IVC CA (Degrees)	EVO CA (Degrees)	EVC CA (Degrees)
36	426	575	144	295
46	437	575	144	284
59	452	575	144	269

Results and Discussions

Model Validation

Discussions in this section on the model validations are based purely on trends observed between the experimental and calculated results. A good correlation is obtained between the experimental and computed pressure traces. Both traces were taken at 2000rpm. Figures 2 shows the average experimental and calculated in-cylinder pressure against varying crank angles. At 360°CA pressure peaks at just over 15bar for 59% IEGR and 11bar for 36% IEGR. The traces presented in this Figure accounts for the exhaust compression (from EVC to 360°CA) and exhaust expansion (after 360°CA).

The Figure also shows variation of the calculated plots which starts at EVC, the starting points for each of the IEGR's are different as these were taken from experimental data. The values for these can be found on in Table 4. The experimental pressure trace, is an average of 300 consecutive cycles. For both studies it can be seen that as the IEGR amount increases, the peak cylinder pressure increases. Figures 2 show a good agreement for the trends observed for the exhaust compression and exhaust expansion. On both plots the exhaust compression angle is larger than the exhaust expansion angle, this agrees with thermodynamics theory as more time is required to compress the mixture.

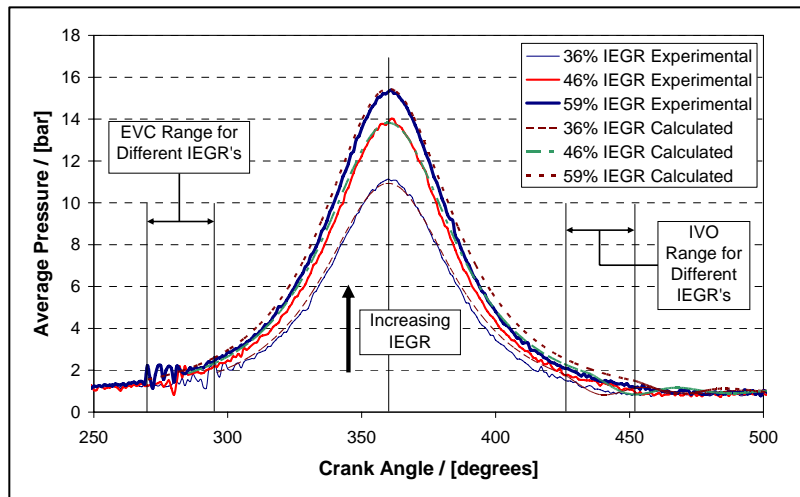


Figure 2: Comparison between Experimental and Calculated Averaged In-Cylinder Pressure at Different Crank Angles

The results for the experimental traces for the different IEGR is not smooth, there are is a noticeable points of interference at EVC. There are a number of possible causes for the interference observed. One logical explanation for this observation may be due to surges from the Active Valve Train (AVT) system operating the valves, as it occurs when the valves are being closed. Another cause could be a mechanical vibration inducing noise in the pressure transducer, however the best explanation for this observation could be the pressure oscillation from the sudden closure of the valve. The smoothness issue was most likely acquired due to the data acquisition system used.

The initial and average calculated in-cylinder temperature with varying IEGR are shown in Figure 3. It shows that as the IEGR increases the initial in-cylinder temperature decreases. This is simply due to the dilution effect caused by the burned gas which contribute almost no energy towards the heat release of the combustion event on the previous cycle, but rather absorb a large amount of heat due to its high heat capacity. However, when examining the average in-cylinder temperature at 720CA, a different story appears. When the IEGR increases, instead of reducing the engine temperature, the in-cylinder temperature is actually increased, making the engine run hotter than at lower IEGR conditions. This overall effect would indicate that the likelihood of auto-ignition occurring is higher when the amount of IEGR is increased.

To help illustrate this point, Figure 4 shows the initial conditions at the start of the calculations (from 295°CA for 36% IEGR down to 269°CA for 59% IEGR) and the conditions at the end of calculations (720°CA). It can evidently be seen that the initial temperature decreases as the IEGR increases at the start of the calculation (from 295°CA for 36% IEGR down to 269°CA for 59% IEGR), but at the end of the calculation (720°CA) the temperature increase as the IEGR increases.

The trends experienced in Figure 3 can be put down to the heat balance. Figure 3 which indicate that although the initial in-cylinder temperature decreases as IEGR increases due to the burnt gas dilution effect, the average in-cylinder temperature actually increases since more hot gas has been introduced. This explains the phenomenon that more IEGR ensures pure auto ignition while less IEGR requires spark assistance.

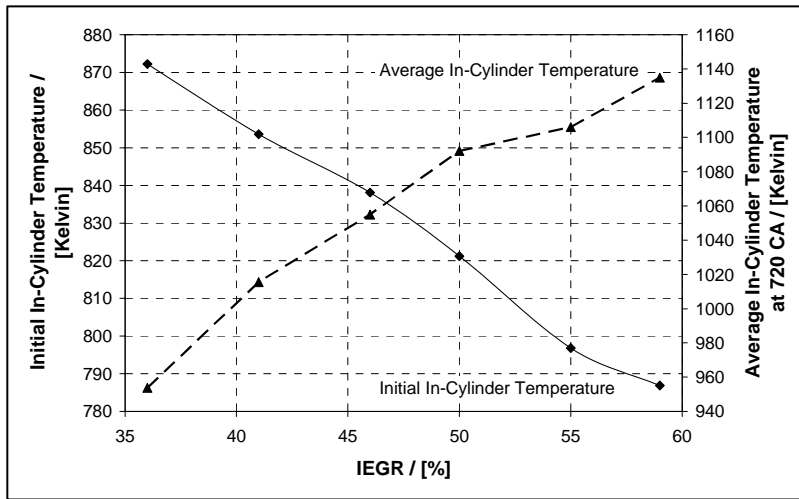


Figure 3: Calculated Initial (at EVC) and Average In-Cylinder Temperature at different IEGR

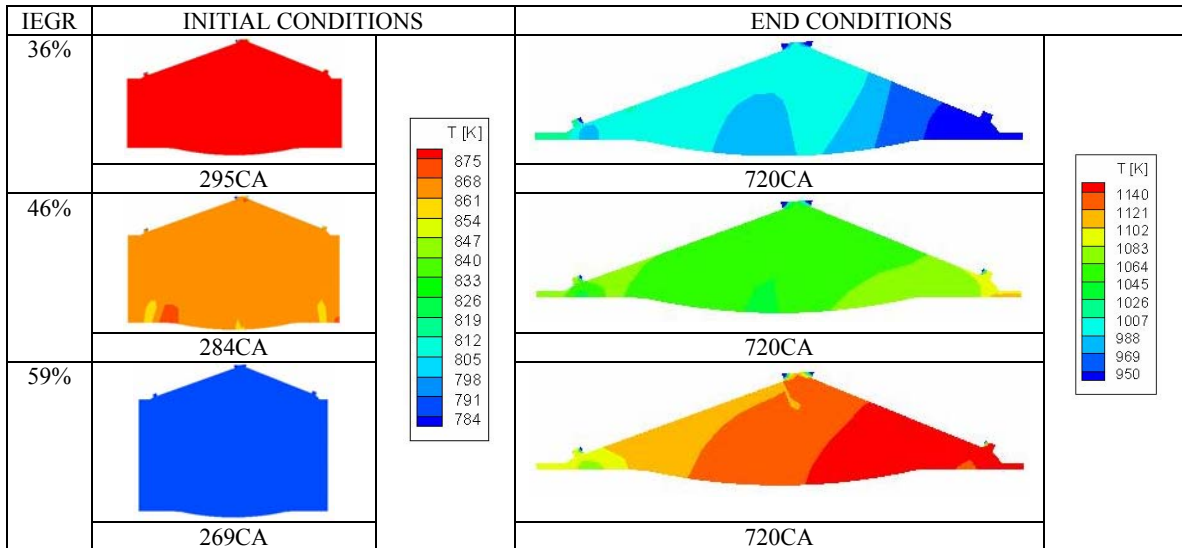


Figure 4: Calculated Temperature Field at Initial (EVC) Conditions and End Conditions

In order to provide a good assessment of the mixture quality at 720CA, all computational cells (volume) contained within the intake and exhaust ports were eliminated from the analysis once the simulation was concluded. The reason for this is that cells from the intake and exhaust ports do not contribute to the in cylinder mixing quality at 720CA. The following analysis has been performed at 720CA for the three different IEGR's at 2000rpm. From combustion theory, auto-ignition usually occurs when the temperature reaches a value of 1000-1100K [22] and over for high-octane fuels, therefore, the remaining cells within the cylinder were then analyzed at 1000K and 1100K to try and provide some fundamental understanding to the auto-ignition phenomena. The calculations have provided some interesting results which are reported below.

Effects of Varying IEGR

The experimental study conducted by Chen et al [19] concluded that the potential hybrid combustion concept consisted of three regions (parts): The first region (region I) was to vary the IEGR from 36% to 41.5%, this region was defined as spark activation controlled auto-ignition. The second region (region II) with the IEGR from 41.5% to 43.4% was defined as spark assisted auto-ignition combustion. The third and final region (region III) was found when the trapped IEGR amount was higher than 43.4%, was defined as the region of spark ignition free controlled auto-ignition. These regions identified in the experimental study will be taken into considerations when analyzing the calculated results, however new regions have also been identified to fit the calculated results.

For the purpose of clarity the word ‘zone’ is used to identify different sections of the calculated results outlined on Figure 5. From the calculated results three distinctive zones have been identified, the first zone (zone I) has IEGR varying from 36% to 41%, the second zone (zone II) has IEGR varying from 41% to 46%, and the third and final zone (zone III) is when the IEGR is above 46%.

Figure 5 shows the volume fraction above 1000K and 1100K at varying IEGR with the three different zones indicated. As shown for the volume fraction above 1000K, the volume fraction increases as the IEGR increases. This observation can also be seen in the second zone, however in the third zone the volume fraction moves above 90% when 46% IEGR is reached and remains above 90% till 59% IEGR.

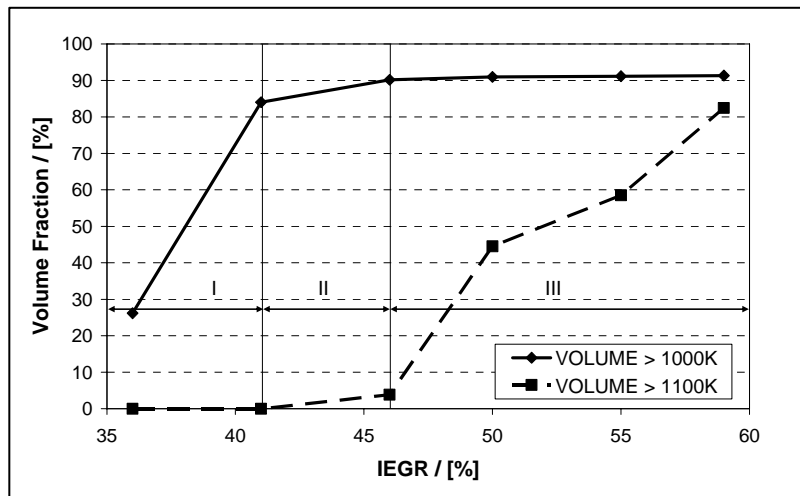


Figure 5: Calculated Volume Fraction of mixture Over 1000K and 1100K at Different IEGR

Auto-ignition usually occurs when the temperature reaches a value of 1000-1100K [22]. Consensus has been developed as to the nature of HCCI combustion. It is generally agreed that HCCI combustion is dominated by local chemical-kinetic reaction [3], with no requirement for flame propagation [7], if a truly homogeneous mixture exists at the time of combustion. It is also accepted that small temperature differences inside the cylinder have a considerable effect on auto-ignition and combustion due to the sensitivity of chemical kinetics to temperature. If this fundamental understanding of HCCI is applied to Figure 5 then, with under 46% IEGR, the likelihood of pure auto-ignition will be less

likely. The reason for this is that with auto-ignition being sensitive to temperature, under 46% IEGR, there is a wide spread in the volume fraction ranging from 20% to 90%, this would indicate that the mixture contained within this volume is not totally homogeneous, thus reducing the likelihood of auto-ignition.

The sensitivity nature of temperature on HCCI auto-ignition can be appreciated in Figure 5, when the three identified zones are analyzed in relation to the IEGR. In the first zone (IEGR ranging from 36% to 41%), the total volume fraction over 1000K ranges from 20% to 90%, this is a spread of 70%, indicating that the temperature contained within the volume will be varied, so the probability for auto-ignition occurrence in this zone will be very low, thus requiring some form of spark to initiate auto-ignition of the mixture. The second zone (IEGR ranging from 41% to 46%), the volume fraction increase with only a 30% spread, this would indicate that the probability for auto-ignition occurrence in the second zone has improved from the first zone, however in this zone again some form of spark is required to initiate auto-ignition of the mixture as the occurrence of pure auto-ignition will not be guaranteed. The third and final zone (IEGR above 46%), yields the term “critical point”. The critical point in the context of this study is the point where notable change occurs for the different IEGR's. In the third zone, the volume fraction moves above 90%, from fundamental HCCI understanding this indicates that the temperature within the volume will be close to homogenous, and with just 10% of the volume missing, auto-ignition in this range can be considered pure with no spark assistance required.

Also plotted on Figure 5 is the volume fraction above 1100K. This plot supports the findings for the volume fraction above 1000K. Although the percentage of the total volume is down from the data analyzed for volume over 1000K, it can clearly be seen that as the IEGR is increased the volume fraction increases

The critical point identified can also be used to yields the level/quality of the mixture homogeneity. Homogeneity within the context of this section is defined as the point (IEGR), where the volume fraction moves above a certain percentage and either remains at that level or increase above it. If this theory is applied to Figure 5, this would suggest that as the level of IEGR increases the homogeneity of the mixture also increases. This notion is well supported by Figure 5, as when the critical point is reached it can be seen that the total volume fraction with high temperature increases, thus increasing the level of homogeneity.

It can therefore be concluded both from Figure 5, that certain parts of the charge will reach a higher temperature which will auto-ignite with the level of mixture homogeneity not totally perfect at the point of auto-ignition. The explanation for the inhomogeneity at the point of auto-ignition is because the highest attainable volume fraction temperature over 1000K is 90%; this means that 10% of the total volume are not represented. The 10% of the total volume not represented here, will generate inhomogeneity within the total volume at 720CA (this is the point were the calculated data was analyzed), this will in turn influence the timing of auto-ignition which is sensitive to a degree of temperature.

Conclusion

A numerical study has been carried out to investigate the influence of mixture quality at the end of the compression stroke inside a pentroof HCCI combustion chamber. The

effect of a three different IEGR has been investigated. The following conclusions may be drawn from the presented results:

- It was found that for HCCI engines, as the IEGR level is increased the temperature of the mixture contained within the cylinder at the start of the calculation decreases giving a linear relationship with negative gradient. This effect is due to the dilution of the burned gas with the fresh charge. However, when the temperature within the cylinder was examined at the end of the calculation it increased as the IEGR was increased, giving again a linear relationship but this time with a positive gradient.
- From the calculated results three distinctive zones were identified, the first zone (zone I) has IEGR varying from 36% to 41%, the second zone (zone II) has IEGR varying from 41% to 46%, and the third and final zone (zone III) was when the IEGR was above 46%. It was found that under 41% IEGR auto-ignition will not occur and assistance will be required to initiate the mixture. Between 41% to 46% IEGR auto-ignition could occur, however this could be rather sporadic so some form of assistance will be required. Above 46% IEGR pure auto-ignition would be obtained with no requirement for assistance to initiate the mixture.
- By increasing the IEGR level, the homogeneity of the mixture increases, as the total volume fraction contained within the cylinder with high temperature has increased. However it should be noted that as the IEGR increases, certain parts of the charge reach a higher temperature which will auto-ignite with the level of mixture homogeneity within the cylinder is not totally perfect at the point of auto-ignition

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