# Investigation of Auto Ignition, Combustion and Emission in a Premixed Charge Compression Ignition Engine for Different Mixture Equivalence Ratios

V. Venkatesan<sup>1</sup> and E.James Gunasekaran<sup>2</sup>

**Abstract**— This paper presents the results of the investigations carried out on a single cylinder gasoline engine for different premixed mixture qualities. Computational fluid dynamic analyses have been conducted for predicting the onset of combustion and propagation and formation of pollutants. To reduce the computational time the investigations have been conducted for the closed phase of the valves and the cylinder is initialized with premixed mixtures of different equivalence ratios. The premixed mixture equivalence ratios varied from 0.6 to 2. The Extended Coherent Flame Model is used to predict the ignition and combustion characteristics. The results reveal that the mixture with equivalence ratio 1.2 produce highest in-cylinder pressure and temperature, while the mixtures with lowest strength (0.6) and richest mixture (2.0) produce lower in-cylinder pressure. The mixture with slightly lean mixture (0.8) produces highest emission of NO<sub>x</sub> whereas the CO emissions are highest from the ultra-rich mixture (2.0). The earliest onset of auto ignition is reported for the mixture with strength 1.0. From the studies it can be concluded that dilution of charge has a more profound effect on combustion and emission.

**Index Terms**— *GDI* - *Gasoline Direct Injection, PCCI* - *Premixed Charge Compression Ignition, HCCI- Homogenous Charge Compression Ignition, CFD- Computational Fluid Dynamic*, LTO – Low Temperature Oxidation, HTO - High Temperature Oxidation.

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# **1** INTRODUCTION

The tremendous growth in personal transportation and increased reliance on internal combustion engines as the main power plant on most of the vehicles has put enormous pressure on environment. The recent climatic conference on Euro has emphasized the need for reducing greenhouse emission as well. In this context the need for replacing the existing internal combustion engines with less polluting alternate technologies such as gasoline direct injection (GDI), Premixed Charge Compression Ignition (PCCI) engine has gained prominence. They are called with different names such as PCCI or HCCI engines. The premixed charge combustion engine tries to mimic the Otto cycle with constant volume combustion. HCCI engines have high thermal efficiency, low NO<sub>x</sub> and soot emissions. [1-3]. Diesel, gasoline, natural gas and many other fuel can be used in this type of engine. These type of engines are fuel flexible. The main problem with this HCCI or PCCI engines are the precise control of onset of combustion (ignition) for varying load ranges the engine operates. In the PCCI engine, spontaneous ignition occurs at unspecified points as it does in diesel engines. The flame then develops rapidly throughout the combustion chamber [4]. Some of the previous researches have attempted to incorporate two stage combustion strategy [5]. One portion was fully premixed with air to achieve homogeneous conditions in the cylinder at the beginning of the compression process, and the second portion of fuel was injected directly into the combustion chamber near Top Dead Centre (TDC). The combustion is initiated by chemical kinetics rather than either by injection or spark ignition timing. Apart from experimental studies many theoretical studies have been conducted to understand the auto ignition phenomena. Multizone models have been applied in many of the theoretical studies for the approximation of the combustion regime. Hence there is a greater uncertainties on the exact start point of combustion for different loads. Even for the same load the onset of combustion is complicated by the local ambient conditions of air such as humidity, altitude, temperature and pressure of the local environment. Different strategies like control of fuel injection timing, amount of exhaust gas recirculation controlling the intake air temperature and controlling the valve lift and valve lift duration are adopted for the initiation of combustion in these engines. With the advent of high speed electronics and control system the interest towards the implementation of these engines has gained prominence. Computational Fluid Dynamic (CFD) tools have matured enough that they can now be confidently used in predicting many of the sub physical process happening inside the engine. The two equation turbulence models such as RNG kepsilon models can be used with engine applications for predicting the flow and turbulence. The Extended coherent flame model is used to predict the combustion and pollutant formation.

## **2 NUMERICAL SIMULATION FOR VALIDATION**

For the present investigation the details of the engine and results from the literature ([13] Payri et al.) has been taken. The engine under consideration is a 4-cylinder in-line engine. In order to simplify the computational setup and reduce the computer resource and time only one cylinder is considered for the investigation. The piston type is bowl in piston type. The analytical results from the literature ([13] payri et al.) are used to estimate the appropriateness of the computational International Journal of Scientific & Engineering Research, Volume 7, Issue 5, May-2016 ISSN 2229-5518

model and also give a good guess for the subsequent experimental work. The engine parameters and input conditions are listed in Table – 1.

Table 1.	Engine	Specificat	ion and Or	perating	Conditions

PARAMETER	VALUE			
ENGINE TYPE	4 – stroke			
Speed	1000 RPM			
COMPRESSION RATIO	15			
Bore	130.0 мм			
Stroke	150.0 мм			
CONNECTING ROD LENGTH	275 мм			
DISPLACEMENT VOLUME	1991 cc			
FUEL	ISO-OCTANE			
START OF CALCULATION	-20° вТDС (340°)			
Equivalence Ratio of Premixed Mixture in Cylinder	0.6, 0.8, 1.0, 1.2, 1.4 and 2.0			
Intake Charge Temperature	303° K			
INTAKE CHARGE Pressure	1.013 bar			
VALVES / CYLINDER	4 – VALVES			

Pressure boundary condition is used on both the intake and exhaust ports. The CAD model of the domain is modelled using "CATIA" and exported to prosurf for the surface mesh generation and separation of different regions of cylinder. This is then exported to es-ice the expert tool used in the engine analysis for volume mesh and event generation. Turbulence is modelled with RNG k- $\mathcal{E}$  model [14]. The discretized engine model consists of 0.5 million cells mainly of hexagonal cells and prismatic cells at the boundary. The discretized engine geometry is shown in Fig. 1. The monotone advection and reconstruction scheme is used to discretize species scalars. NO<sub>x</sub> is modelled by Mauss soot model. The initial values of pressure and temperature are considered as homogeneous in the whole domain. The initial turbulent intensity is set at 10% of the mean flow, and the integral length scale is set at 0.1 m.

# **3 VALIDATION**

To check whether the created model is valid with the engine used in the experimental engine, validation of velocity and fluctuating velocities during the suction and compression process are done for the present investigation, the model of engine where experimental LDV measurements of flow field are available is chosen. The experimental data are available in literature where the experiments were carried out and LDV measurements are taken along the various points as shown in

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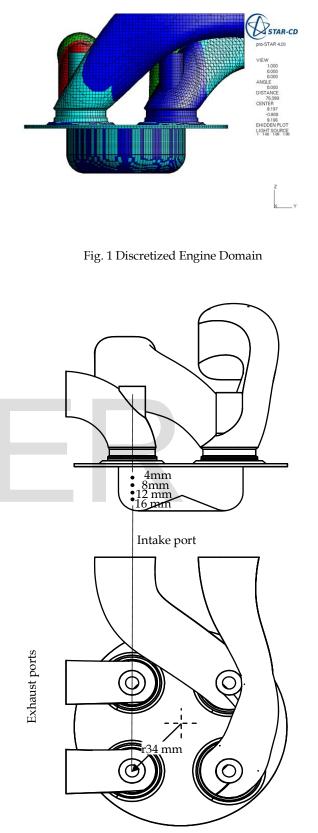
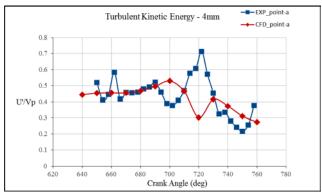
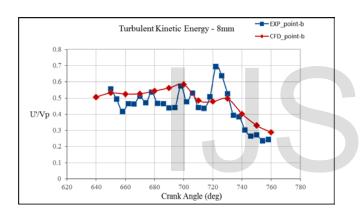


Fig.2 Location of Measurement Points inside the Cylinder for Validation.

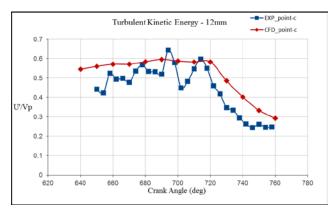
the Fig.2.The simulations are also conducted at 1000 rpm to validate the computational model against the experimental data (13 Payri et al). Fig.3 shows the validation of the CFD model against experimental data.



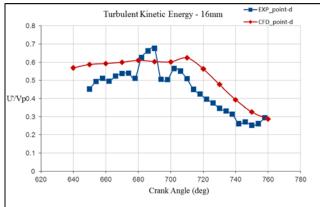
(a) TKE at 4mm location.



(b) TKE at 8mm location



(c) TKE at 12mm location



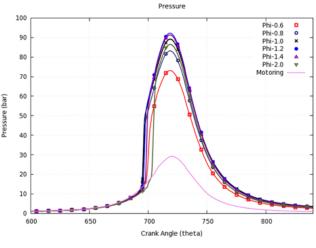
(d) TKE at 16mm location

Fig.3 Validation of Turbulent Kinetic Energy Normalized with Mean Piston Speed

It can be observed from Fig.3 that CFD slightly over predicts the turbulence at different crank angles. It can also be observed that compared to the location 4 mm, which is closer to the cylinder hear the 12 and 16 mm locations which are slightly farther from the piston head, show a better kinetic energy pattern. Nevertheless the validation is reasonably in good agreement with experimental data. Hence further analysis can be carried out.

# 4 RESULTS AND DISCUSSION

The computation starts from the closure of intake valve 55° after BDC (595°) and ends at the opening of exhaust valve 55° bBDC (845° aTDC). The cylinder is initialized with different equivalence ratios beginning from 0.6, 0.8, 1.0. 1.2, 1.4 and 2.0. Fig.4 compares the pressure and temperature inside the cylinder at various equivalence ratios.



(a) Pressure

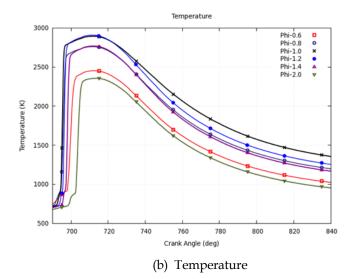


Fig.4 Comparison of Pressure and Temperature variation for Different Equivalence Ratios with respect to Crank angle

The lowest peak pressure is recorded by mixture of strength 0.6 while the mixture with equivalence ratio 1.2 recorded the highest peak pressure. The other mixtures lie in between them. The increase in peak cylinder pressure is significant with a value of 72 bars at 0.6 mixture strength to a peak pressure value of 92 bars at a mixture strength of 1.2. This is an increase of 28% value. Mixture strength beyond 1.2 results in reduced peak pressure values and peak temperature, with the mixture with strength 2.0 producing lower peak pressure and temperature values. This may be due to insufficient oxygen resulting in slower combustion eventually resulting in lower peak pressure and peak temperature. Figure 5 compares the temporal variation of equivalence ratio inside the engine cylinder for the cases mentioned above. Mixture strength of 0 means all the fuel has been burnt up. It can be observed that the case with mixture 1.0 has the quickest consumption of fuel, followed by mixtures of strength 0.8 and 1.2. Hence these cases have combustion duration of 3, 4 and 4.5 deg crank angles respectively. The mixture with strength 2 has the longest combustion duration and also it has the late start of combustion which occur at 699° CA and ends at 707° CA. This may be due to the lesser oxygen available for the case with 2.0 and also it requires higher activation energy for the start of combustion.

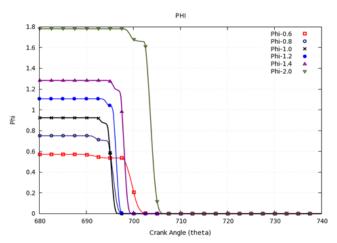
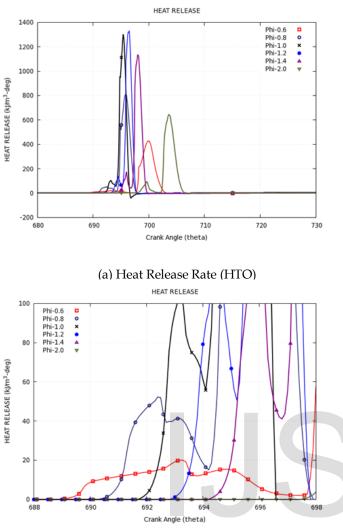


Fig.5 Comparison of fuel consumption for different mixture strength

Fig.6a compares the heat release rate for different cases. It can be observed that mixture equivalence ratios 1.0 and 1.2 have highest heat release values around 1200 kJ/m<sup>3</sup>-deg. Also the onset of combustion is earliest for these cases with mixture values 1.0 and 1.2. Mixtures with strength 1.4, 0.6 and 2.0 have lower peak pressure and also they have late start of ignition. Fig.6 (b) compares the low temperature oxidation phase of the combustion process. The beginning of combustion process is dominated by low temperature oxidation process (LTO), where initial longer chain breaking and propagation and realignment reaction occur at low speed. This energy released by the LTO process is further used to break the shorter chain which are relatively difficult and require the energy generated by the LTO process. This creates radical. Hence due to the absorption of heat for breaking the shorter chain bonds the temperature curve slightly show a downward trend. This radicals are the main components that participate in main high temperature oxidation (HTO) process. For the equivalence ratio 0.6 the LTO duration is 9° CA (689° to 698° CA), for the mixture with equivalence ratio 0.8 the LTO duration is 4 deg (690° to 694°), for mixture with strength 1.0 it is 3° (691 to 694), for mixture with equivalence ratio 1.2 it is 3 deg (693 to 696 deg CA), for mixture with equivalence ratio 1.4 it is 3 degrees (694° to 697° CA) and for mixture strength 2.0 it is 5 degrees (698° to 703° CA). One interesting feature that can be observed here is that oxygen plays an important role in the initial low temperature oxidation process. Once the strength of the mixture beyond 1.0 is increased, literally it means in-sufficient oxygen for the combustion process. Hence the beginning of LTO process is delayed for all the cases beginning with equivalence ratio 0.6 which is the most advance case which starts at 689 to the very late case with equivalence ratio where the LTO process begins only at 698° CA.



(b) Enlarged View of Heat Release (LTO)

# Fig.6 Comparison of Heat Release Rate for different Mixture Strength

Compared to mixture 1.0 the case with equivalence ratio 0.6 has an ignition delay of 5 degrees, whereas the case with mixture strength 2.0 has an ignition delay of 11 degrees. This makes it clear that increasing the mixture strength to rich side or reducing the mixture strength to lower side have adverse effects on the start of combustion. Hence changing the mixture strength from stoichiometric value either to lean side or to rich actually increases the onset of auto ignition and also the maximum heat release value decreases. The effect of this is also reflected in temperature values, where the mixture with 1.0 produces highest peak temperature followed by mixture with strength 1.2. Figure 7 compares the NO emission of the premixed fuel.

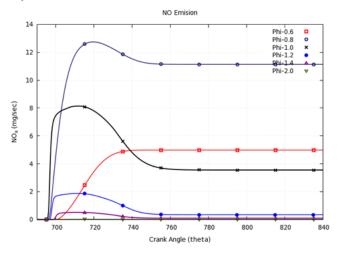


Fig. 7 Comparison of NO emission for mixture of different strength

It can be observed that NO emission by mixture 0.8 is the maximum, but the mixture with equivalence ratio produces far less amount of NO in spite of higher maximum temperature than all other cases. This may be due to lower oxygen available compared to the lean mixture case of 0.8. The still lower mixture with strength 0.6 produces lower amount of NO compared to the case with mixture 0.8 but higher than case phi 1.0. The cases with mixture 1.2, 1.4 and 2.0 have considerably lower levels of NO emission compared to the mixture case 1.0. Hence this graph confirms that for generation of NO emission a lean fuel environment is required. The Emission of CO<sub>2</sub> and CO will also give a good account of the combustion and emission formation. Fig. 8 compares the CO<sub>2</sub> emission level for different cases. Here the trend is reversed with the maximum CO<sub>2</sub> emission produced by mixture strength case 1.0 followed by mixture strength 0.8 and 1.2. This reflects on the earlier heat release and pressure curves with these cases producing better combustion and producing peak temperatures with decreasing order from 1.0, followed by 1.2 and 0.8 mixture strengths. The riches mixture with equivalence ratio 2.0 produces a lowest amount of CO<sub>2</sub>. This should be reflected in the CO emission characteristics, which would have the mixture equivalence ratio case 2.0 producing a highest amount of CO emission. Hence Fig.9 is plotted. It can be observed that the mixtures with equivalence ratios 0.6, 0.8 and 1.0 produce almost zero emission of CO compared to other cases. But the mixture with 1.2, 1.4 and 2.0 produce increasing order of CO emissions. This conforms to the fact a good combustion would result in higher quantity of CO2 and lower quantity of CO.

International Journal of Scientific & Engineering Research, Volume 7, Issue 5, May-2016 ISS: CO<sub>2</sub> Emision

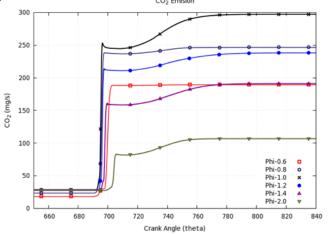


Fig. 8 Comparison of CO<sub>2</sub> emission for mixture of different strength

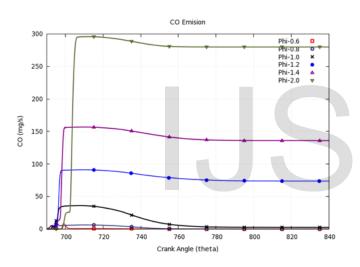


Fig. 9 Comparison of CO emission for mixture of different strength

It can be observed that the case with 0.6 equivalence ratio produce lowest peak temperature and the highest temperature is observed in case with equivalence ration 1.2. In all the cases the main combustion occur in the centre of the bowl. Relatively the wall region show a lower temperature compared to the central region of the combustion chamber. Hence the rich mixtures beyond 1.2 like 1.4 and 2.0 actually reduced maximum temperature as seen in fig 10 and also they have higher CO emission.

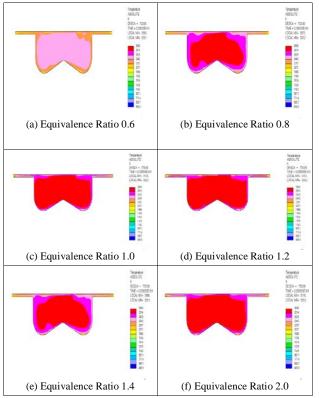


Fig. 10 Comparison of Temperature Contours on the Mid Sec-

tional Plane at TDC

## 5 CONCLUSION

Numerical analysis has been conducted on a single cylinder engine working on premixed compression ignition mode with gasoline as fuel. The results indicate that increasing the fuel concentration beyond equivalence ratio beyond 1.2 has adverse effect on the combustion and emission, while it is true that the stoichiometric mixture produce maximum in cylinder temperature, it has lower NO emission levels. Hence the NO emission caused due to the amount of oxygen available and temperature. CFD predicts the experimental values reasonably well.

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**Venkatesan V** completed his B.E (Mechanical Engineering, 1996) and M.E (Energy Engineering, 2007) from Annamalai University, Annamalai nagar – 608002. He currently pusuing his doctoral degree and has one international jounal for his credit. His area of interst includes IC engines, Power Plant and CFD.

James Gunasekaran E completed his B.E (Mechanical, 1992, Annamalai University), M.E (Energy Engineering, 1997, Guindy Engineering College) and obtained his Doctral Degree from IIT, Madras in year of 2009. He has published eleven international journals, five international conferences, two national journals and three national conferences to his credit. His current research includes emission reduction in engines, CFD application for internal combustion engines with open FOAM and Python CFD.

