Investigation of emission parameters on HCCI Engine using chemical kinetics

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Abstract - *Homogeneous Charge Compression Ignition makes the utilization of the resources for complete combustion and is similar to that of hot bulb technology. In these, the main point is to supply the exact mixture of fuel and oxidizer to the combustion chamber to attain auto ignition. The characteristics of these technology resemble the combination of both spark and compression ignition Engine. The Engine which result in these combination provide higher efficiencies better than the conventional Engines. Diesel as the fuel and performing computation results by using CHEMKIN 17.0 with HCCI Engine parameters that are previously done on the experimental scale provides the liability for further investigation on different compositions to find reduced emission rates by performing auto ignition. Spectroscopy methods provides the necessary species that provides auto ignition. The species responsible for these condition are HO2, CH2O and O. Formation of these species can be visualized in the fuel combustion kinetics provided by CHEMKIN 17.0. Emission rates on diesel are compared by varying fuel grades and equivalence ratio.*

Keywords: Engine, HCCI, Auto ignition, Emission, Chemical kinetics.

1. INTRODUCTION

Compression ignition Engine with its thermodynamic efficiency and lower pumping loses add an advantage to continue the usage in the commercial sector for a long time. While spark ignition Engine, due to its low emissions at exhaust gives additional benefit for environmental issues because of homogeneous mixture fuel and air. In these new technology which combines these two types is called as Homogeneous Charge Compression Ignition as the name indicates, in this HCCI Engine technology has SI Engine characteristics at inlet and compression strokes and has CI Engine characteristics at combustion and exhaust strokes. This technology results us in getting higher fuel efficiency and low emissions. HCCI Engine can be accepted over conventional Engines because of its performance, durable, sustainable and economical. Homogeneous Charge Compression Ignition reduce throttling losses. It meets the standards that are to be followed for emissions. Any alternate fuels and the conventional fuels can be used for the operation. As expansion ratio is increased using HCCI Engine results in increased thermodynamic efficiency than the conventional Engine. Emission can be controlled without the application of EGR system. In HCCI at normal compression ratio only the auto-ignition occurs and load limit can be extended which reduce the residuals in the fuel mixture to achieve the starting temperature of compression, mode of combustion as they are to be maintained in limits.

HCCI Engine combustion should be started after the auto ignition where the ignition timing can't be controlled in practical because there will be variations in speed and power range. This leads to increase in emissions of HC and CO but reduction in NOx and SOx emissions. Pre-heating is done in order to provide additional energy to attain required auto ignition temperature to the in-cylinder load. Negative valve overlap is used for pre-heating but it is limited to low, medium loads only. Higher exhaust re-circulated will allow higher thermal loads because there will be increase in in-cylinder temperature. Pure auto-ignition occurs there will be fast heat release which results in increase of thermal efficiency. Supercharging allows the increase of permitted loads on Engine if there is any insufficient intake air while the Engine is working. Based on the above important points to be considered, for smooth performance of HCCI Engine certain parameters to be taken care and they are timing of ignition, cold start temperature of Engine, rate of release of heat, multi-cylinder effects, operation in transient mode, fueling systems and sensors. Fueling system has great effect on HCCI combustion, it should be taken at most care. Parameters are controlled and operated by components and auxiliaries of Engine and are kept in particular limit to provide smooth functioning of HCCI Engine. In experimental analysis can be carried out on certain controlling parameters like compression ratio, injection temperature, actuation of valves, valve timing with crank angle, amount of emissions liberated and exhaust gas temperature.

2. EXPERIMENTAL SETUP

Chemical kinetics deals with the chemical reactions with respect to their reaction rates and the re-arrangement of species which effects the experimental variables. Rate of change of proportions during the reaction phase is determined as chemical reaction rates. Chemical kinetics allows to study the breaking of bonds, further reactions and exchange of ions. Temperature has its own impact on chemical reactions. Higher the temperature higher the chemical reactions.in kinetics there will be change in phase while reactions occurs. Analyzing the reaction rates for the fuel change should be done for accurate resulting of emission characteristics.

Simulation of chemical reactions which are very complex and which can't be analyzed with mathematical theoretical calculations, a simulation software called CHEMKIN is used. It evolved into today's commercially approved quality based software provided by ANSYS. CHEMKIN enables more chemistry to reactions and simulations involved in fluid-flow. Robustness and accurate in solutions, speed optimization is achieved due to advanced analytical algorithms makes it for power users who want accurate and fast chemistry analysis. CHEMKIN –PRO can be used for strain rate calculations and to find stability in combustion.

In CHEMKIN, the feature named particle tracking and is an innovative feature which allows to track or follow the growth, aggregation, particle inspection and oxidation of the particle. Analyzing the multi zone models of Engine simplifies and optimizes the combustion analyses which includes the ignition and emissions for homogeneous charge compression ignition Engine technology. Automation and accuracy of fuels for reduction mechanism, an extended GUI is utilized as reaction workbench.

Diesel contains of various species in its composition. The mole fractions of these species decides the grade of the diesel fuel. Diesel contains saturated hydrocarbons in large number than aromatic hydrocarbons. The variation in the species percentage in saturated hydrocarbons makes variation in the grades of diesel. Primary species are considered in the analysis are CH_4, nC_7H_{16}, C_2H_4, C_3H_6 and $C_7K(C_2H_5)_{12}$.

Analyzing the intermediate species formation is the crucial step for providing better fuel for the reduction of the emissions without compromising on performance and this can be done by using spectroscopy in experimental work. Spectroscopy methods that are investigated on the working Engines provides the species required prior before the auto ignition inside the combustion chamber of IC Engine are HO_2, CH_2O and O.

3. PROCEDURE

Experimental work done on the HCCI Engine compared with conventional diesel Engine is taken as the reference for the further simulation. The chemistry set involved in the diesel are considered and compared with the experimental parameters. Results obtained are reliable for the use of chemistry set for further analysis.

Closed 0D (zero dimensional) homogeneous analysis for the IC Engine parameters can be done using CHEMKIN 17.0. Analysis for the 0D (zero dimensional) single-zone with detailed chemistry is the lowest computational cost for HCCI model. A predefined icon is setup for the closed IC Engine homogenous simulation. By incorporating the model into the diagrammatic view project can be updated for the further analysis based on the specific Engine and fuel parameters.

Pre-processing for the analysis of HCCI simulation requires chemistry set which include fuel reactions in gas phase and thermodynamic properties of individual species. Both these are incorporated into the pre-processing model and a new chemistry set is created in the working directory. Running the module can give the detailed information of the species.

Various basic Engine parameters are to be provided for the effective analysis of the HCCI conditions. Staring crank angle to 142oC before the top dead center indicates the closure of the intake value and provides the rise in the pressure inside the cylinder. Time of simulation and crank angle are linearly linked based on the Engine speed of operation. Crank angle to time with one degree span are noted from the start of simulation.

Engine physical parameters are considered from the experimental set that is previously done on the Kirloskar Engine. Considering connecting rod to crank radius ratio (R) to 3.5, bore to 80mm and stroke to 110mm. Compression ratio (C) can be modified from 11 to 22 according to the increase the load sustaining parameters such as misfire and knocking. In the present scenario it is considered as C as 14.5 and Engine speed (N) to 1500 rpm. Swept volume of the Engine is 553cc. Clearance volume (Vc) can be computed from the compression ratio and swept volume as 41cc.

Volume to time profile is the prominent in these analysis as define the volume of the Engine cylinder at the respective time of the simulation. The relation can be established from combining volume to crank angle and crank angle to time profiles. Equations for volume to crank angle as $V(\theta)/Vc=1+(C+1)/2\ (R+1-\cos\theta-\sqrt{R^2-\sin^2\theta})$ and crank angle to time profile as $T(\theta)=\theta/6N$.

HCCI simulation can be done in two ways as by considering the loss of heat from the cylinder and adiabatic condition. Loss of heat from the Engine is considered for more reliable solution. Heat transfer through cylinder calculate with in the software by providing the generalized heat transfer correlation. Retaining the same values incorporated in the previous experiments proceeding Prandtl Number from gas conductivity, mean piston speed and gas viscosity as 0.7.

Mole fraction rates of the input reactant species plays prominent role in the HCCI simulation. Equivalence ratio of fuel mixture and oxidizer normalized to 0.5 to 1. Considering the fuel species to their mole fraction is shown in table.

Table -1: Mole fractions of chemical components

	Chemical Species	Fuel Grade-1 (Mole Fraction)	Fuel Grade-2 (Mole Fraction)	Fuel Grade-3 (Mole Fraction)
Fuel	CH_4	0.33	0.38	0.394321766
	nC_7H_{16}	0.20	0.15	0.11829653
	C_2H_4	0.1	0.12	0.160883281
	C_3H_6	0.12	0.1	0.087066246
	$C_7K(C_2H_5)_{12}$	0.25	0.25	0.239432177
Oxidizer	N_2	0.79	0.79	0.79
	O_2	0.21	0.21	0.21

4. OBSERVATIONS

Auto ignition timings fuel grade-1 are predicted as 64.26°, 63.59°, 62.92°, 62.27°, 61.32° and 59.79° before top dead center based on the change in equivalence ratio from 0.3, 0.4, 0.5, 0.6, 0.75 and 1 respectively. Auto ignition timings fuel grade-2 are predicted as 64.27°, 63.60°, 62.95°, 62.30°, 61.36° and 59.84° before top dead center based on the change in equivalence ratio from 0.3, 0.4, 0.5, 0.6, 0.75 and 1 respectively. Auto ignition timings fuel grade-3 are predicted as 64.31°, 63.65°, 63.01°, 62.38°, 61.45° and 59.96° before top dead center based on the change in equivalence ratio from 0.3, 0.4, 0.5, 0.6, 0.75 and 1 respectively.

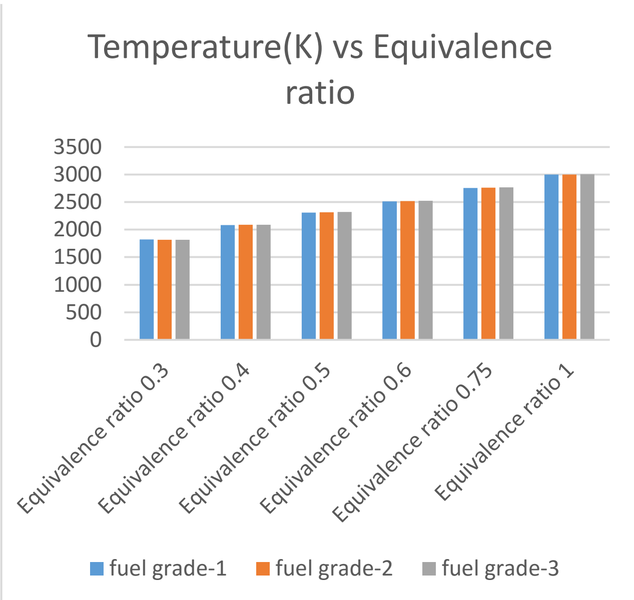

Chart -1: comparison of different fuels of different equivalent
ratios to their temperatures

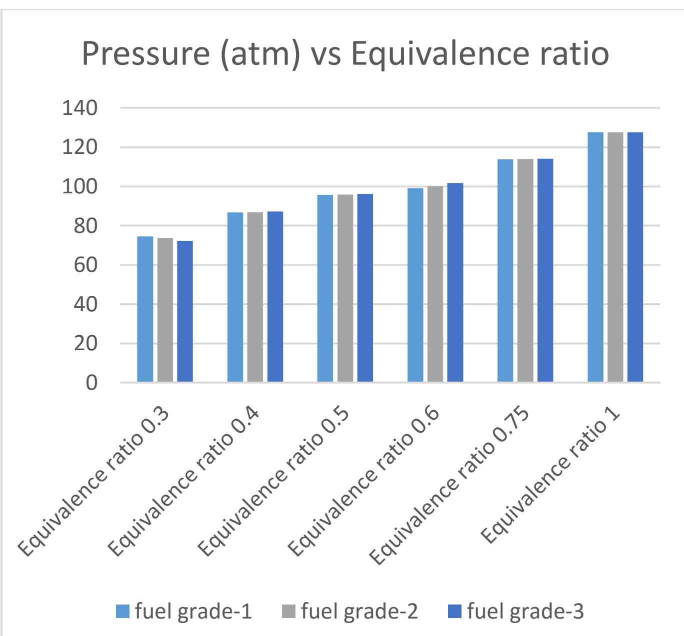

Chart -2: comparison of different fuels of different equivalent
ratios to their pressures (atm)

Species formed in the intermediate reactions that are responsible for the auto ignition can be visualized from the reaction path diagram. Reaction path diagram at start of ignition is captured for fuel-1. It is observed that the formation of the CH2O causes the auto ignition of the fuel in the chamber and provides the rise in temperature and pressure.

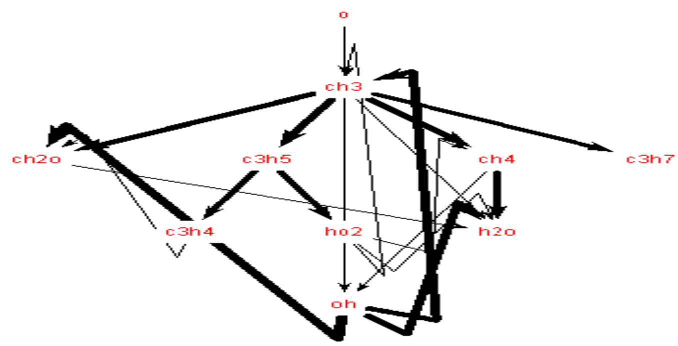

Fig-1: Reaction path diagram showing chemical species at the
start of auto ignition

Temperature and peak pressure variation with respect to crank angle for different fuels is similar to that of conventional Engines. The graph plotted between crank angle vs temperature and crank angle vs pressure for fuel-1 with different equivalence ratio are shown in below figures.

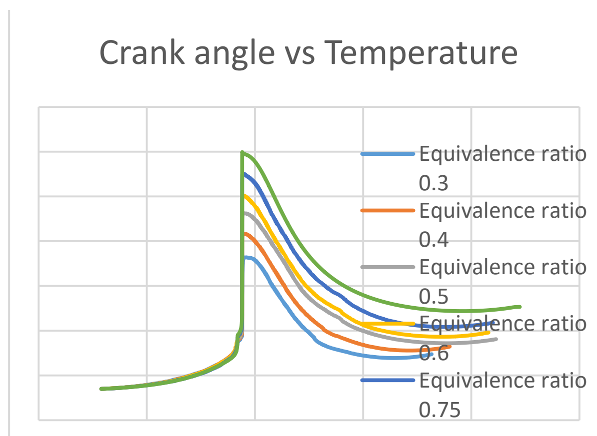

Chart -3: Typical variation of temperature (K) for different equivalence ratio to crank angle (θ)

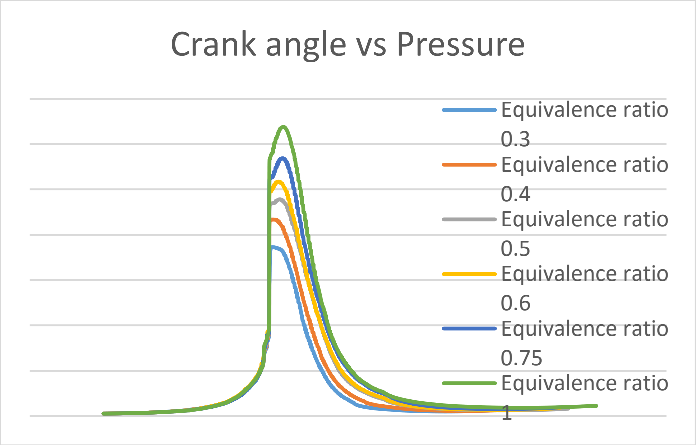

Chart -4: Typical variation of pressure (atm) for different equivalence ratio to crank angle (θ)

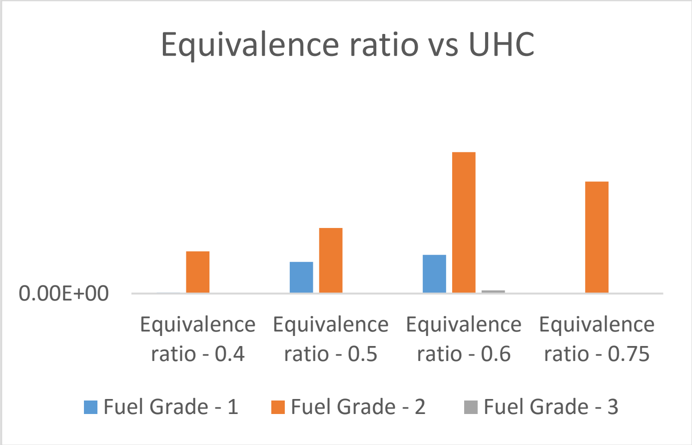

Chart -5: comparison of UHC with different fuel grades and equivalence ratios

5. RESULTS

Results obtained from the 0D (zero dimensional) simulation of internal combustion Engine provides amount of NOx emissions and unburned hydrocarbons at the end of the simulation. Different grades of the fuel are used in the simulation and capturing results according to the air fuel ratio provided in the simulation parameters. Data obtained are represented as bar charts as shown in the figures.

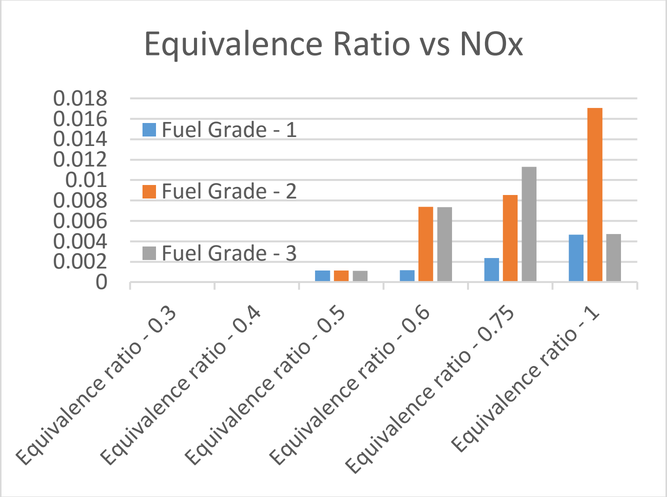

Chart -4: comparison of NOx emission with different fuel grades and equivalence ratios fuel

6. CONCLUSION

Over a keen investigation on the diesel species, it has been found that auto ignition occurs at 62° before top dead center on an average, temperature and pressure increases with the increase of equivalence ratio as the performance characteristics of HCCI Engine. Species formation in the intermediate at the ignition process is been visualized through reaction path diagram. The comparison between the grades to their emission characters are plotted in the results. Hence from the above results, it is also been found that the emission characteristics of the HCCI Engine which majorly concentrated on NOx and unburned hydrocarbons follows different patterns. Lower equivalence ratio reduces the NOx but there is a huge emissions of unburned hydrocarbons and at higher equivalence ratio both NOx and unburned hydrocarbon emissions are more when compared with lean mixtures. Grades of fuel effect shows the less effect on the NOx emission but there is significant change in the unburned hydrocarbon emissions.

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