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Numerical Analysis of a Homogeneous Charge Compression Ignition Engine using Ethanol as a Fuel

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Abstract: ***In current field of automotive industry enhancing the economy of fuel and emission reducing are the major challenges, the different fuels and novel combustion ideas are rising to face each pollution and fuel crises. Even though it late, the conception of homogenous Charge Compression Ignition, has been receiving extended attention, thanks to its potential for at the same time reducing fuel consumption, ox and especially Emissions. Specifically in HCCI engine analysis, wherever combustion is regarded to be a chemical-reaction-governed method, the value of correct chemical kinetic mechanisms and their machine potency is emphasized. Throughout this paper examines the Ethanol (C_2H_5OH), and also investigating trends of ignition method in a variable volume reactor for finding initial pressure, initial temperature and preservative fuels. This chemical experimentation of Ethanol was formulated in CHEMKIN using 57 species and 383 reactions for understating of analysis procedure characteristics of Combustion like cylinder pressure rise, ignition delay and formation of species characteristics were studied in HCCI engine and therefore the analysis was done by using COMSOL computer software code. The analyzed results exhibit that the water temperature of the fuel air mixture could be a potential standardization parameter for ignition. A rise in pressure resulted in a rise with in the species concentrations within the fuel-air mixture, leading to the conventional enhanced ignition times.***

Keywords: homogeneous charge compression ignition engine, chemical kinetic model, combustion, oxidation of ethanol.

1. Introduction

For automotive application IC engines have become indispensible prime movers. Lightweight and rider vehicle being met with gasoline engines wherever as diesels area unit meeting lightweight, medium and serious duty applications. Thanks to standard combustion processes adopted, it's turning into difficult task to fulfill tight emissions norms with this engine. Of late, researcher's area unit operating to. Create it possible a brand new combustion process- HCCI, a hybrid of the normal spark ignition (SI) and also the compression ignition processes. The HCCI combustion method will give fuel conversion efficiencies as high as compression-ignition direct injection (CIDI) engines whereas, in contrast to CIDI engines, manufacturing ultra-low oxides of (NOx) and material (PM) emissions. HCCI engines treat the principle of getting a dilute, throughout the cylinder premixed charge that burns and reacts volumetrically, because by the piston it is compressed. Thus, in some regard, HCCI incorporates the best options of each compression ignition and spark ignition (SI) engines However, in contrast to either of those standard engines, the combustion happens at the same time throughout the amount instead of during a flame front. This vital attribute of HCCI permits combustion to occur at abundant lower temperatures, dramatically reducing engine-out emissions of Nox [1].

The idea of HCCI is predicated on self-ignition of the fuel-air combination, removing mechanical or electrical tool controlling the exact time of ignition. It includes combustion of an exceptionally diluted homogeneous mixture with collection of exothermic chemical reactions mostly managed with the aid of chemical kinetics [2]. To gain better gasoline economy and emissions discount precise combustion evaluation is wanted. A whole lot of studies paintings is going on combustion analysis in both experimental and numerical ways. Because of the stepped forward computational abilities numerical research became easier than the experimental studies, that involve several time and, value.

The mixture of elaborated hydraulics model and a close chemical mechanics model would be an ideal analyzing tool for learning engine combustion numerically [3]. Currently days a lot of attention is paid to elaborated chemical kinetic models than the hydraulics models because the combustion chemistry is changing into crucial for rising engine performance. The whole numerical simulation would need bigger procedure capability, time and value. The simplified models show nice validation with the experimental results [4].

Chemical kinetics yield information about the reaction's mechanism and transition states, as well as the construction of mathematical models that can describe the characteristics of a chemical reaction. In the present work the chemical kinetics mechanism of the Ethanol (C2H5OH), developed by Marinov [3] is adopted. A large amount of kinetic and thermodynamic data required to set up the problem is taken from the Physical and Life Sciences Directorate (PLSD) [5], and is readily made available by importing relevant files into the Reaction Engineering interface. The detailed mechanism can be used over a wide range of pressure, temperature, and

gas composition when intermediate species and reactions associated with the minor species are included. The neglect of minor species in operational models makes it difficult for them to accurately describe the production of unwanted byproducts or pollutants like NOx in combustion systems. The minor species can have a large effect on the overall reaction rates. It is observed from the literature, many researchers have done on the development and adoption of HCCI concept with conventional fuels. Due to complex chemical kinetics of conventional fuels, the rate controlled reactions could not be understood in greater detail to implement HCCI concept. The present work aims at adopting a eco-friendly fuel, ethanol, in HCCI mode enabling its wide use to mitigate pollution related problems and achieving self sustainability.

2. Salient Feature of Present Model

The detailed chemical kinetic models of practical IC engine fuels like diesel, petrol are not available, moreover it is very difficult to form homogeneous mixtures for HCCI with these conventional fuels, considers the combustion of Ethanol, as available in the PLSD, incorporating a detailed reaction mechanism of 57

A. Variable Volume Reactor

This is a predefined model in the Reaction Engineering interface and it represents the combustion cylinder with a perfectly mixed batch system of variable volume, a reactor type. Figure 1 shows a drawing of an engine cylinder, and it points out parameters relevant for calculating the instantaneous cylinder volume. Where La is the length of the crank arm, Lc gives the length of the connecting rod; D equals the cylinder diameter, and α is the crank angle [7].

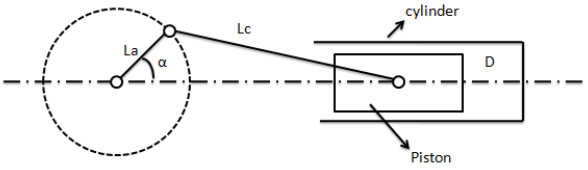

Figure 1: Schematic Diagram of Engine Cylinder.

Table 1: Engine Specifications

Engine Specification	Variable Name	Value
Crank arm length	L_a	86mm
Connecting rod length	L_c	150mm
Stroke	S	172mm
Bore diameter	D	83.1mm
Compression ratio	CR	16.5
Engine rpm	N	1500

The following parameters define the basic geometry, of a reciprocating engine [8].

1. Crank mechanism: With time the variation in the Volume

$$\frac{V}{V_c} = 1 + \frac{(CR-1)}{2}\left[R + 1 - \cos\alpha - \sqrt{R^2 - (\sin\alpha)^2}\right] \quad (1)$$

Where, V is the cylinder volume (m^3), V_c gives the clearance volume (m^3), CR equals the compression ratio, and R denotes the ratio of the connecting rod to the crank arm (L_C/L_a).

2. 'α' (rad) is the Crank angle it is lso a Function of Tim, the engine speed in rpm is N, and(t) time (s).

$$\alpha = \frac{2\pi N}{60} t \quad (2)$$

3. V_s is the Volume Swept of the Piston during a cycle is calculated using.

$$V_s = \frac{\pi D^2}{4} S \quad (3)$$

4. V_c is the Clearance Volume, , and it is calculated from:

$$V_c = \frac{V_s}{(CR-1)} \quad (4)$$

Mass and energy Balance Equations

With variable volume reactor,the balances of mass is defined as perfectly mixed

$$\frac{d(Vc_i)}{dt} = VR_i \quad (5)$$

where c_i it is denotes s the species concentration (mol/m^3), and R_i represents the species rate expression ($mol/(m^3 \cdot s)$). For an ideal gas mixture, the reactor energy balance is the

species molar heat capacity (J/(mol·K)), T is the temperature (K), and p gives the pressure (Pa). In this equation, Q is the heat due to chemical reaction (J/s)

$$Q = -V_r \sum_j H_j r_j \quad (6)$$

$$V_r \sum_i c_i C_{p,i} \frac{dT}{dt} = Q + Q_{ext} + V_r \frac{dp}{dt} \quad (7)$$

where H_j is the enthalpy of reaction (J/(mol·K)), and r_j equals the reaction rate ($mol/(m^3 \cdot s)$). Q_{ext} denotes heat added to the system (J/s). The model being described assumes adiabatic conditions, that is, $Q_{ext} = 0$.

3. Oxidation of Ethanol

In this model, Ethanol is combusted under lean conditions, that is, supplying more than the stoichiometric amount of oxidizer [9]. The stoichiometric requirement of the oxidizer (air) to combust Ethanol is found from the overall reaction

$$C_2H_5OH + 3(O_2 + 3.76N_2) = 2CO_2 + 3H_2O + 11.28N_2 \quad (8)$$

$$\Phi = \frac{(A/F)_{stoic}}{(A/F)} \quad (10)$$

Assuming that the composition of air is 21% oxygen and 79% nitrogen, the stoichiometric air-fuel ratio is

$$x_{fuel} = \frac{1}{4.76 \cdot 2/\Phi + 1} \quad (11)$$

The equivalence ratio relates the actual air-fuel ratio to the stoichiometric requirements.

This model sets the equivalence ratio to Φ = 0.5.
From Equation 9 and Equation 10 you can calculate the molar fraction of fuel in the reacting mixture as and subsequently the initial concentration is

$$c_{\text{fuel}} = \frac{x_{\text{fuel}} p_{\text{init}}}{\text{Rg} T_{\text{init}}} \qquad (12)$$

The P*init* and T*init* initial pressure and the initial temperature are variable model parameters.

By considering the parameters of the variable model are initial temperature and initial pressure.

4. Numerical Analysis of Fuels

A. Effect of super charging pressure

The present study concerned with the analysis of super charging pressure impact on load bearing capabilities of the HCCI engine [13]. An attempt is made to improve the load bearing capability of the HCCI engine which is known for their poor load bearing capability [12]. The analysis is aimed at studying the parameters like in cylinder pressures, temperatures, emissions like CO, CO_2, NO_x. In the present study emphasis is given for minimizing the NOx emissions [10].

B. In-Cylinder pressures

The change in in-cylinder pressures with super charging pressure is plotted in Fig. A. The increase in in-cylinder pressures is due to increase in super charging pressure.

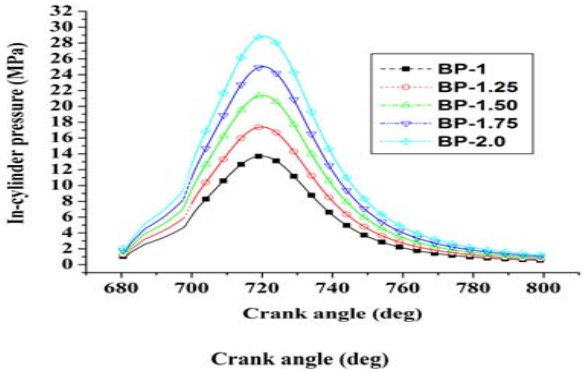

Figure A: In-cylinder pressure Vs Crank angl

A maximum in-cylinder pressure of 13.714 Bar at 719.7 CA and 28.835 Bar at 721.3 CA was obtained at a super charging pressure of 1 bar and 2 bar respectively. A total increase of 110.259% in in-cylinder pressures was obtained when the super charging pressure was increased from 1bar to 2bar.

C. In-cylinder Temperatures

Fig B shows the variation of in-cylinder temperatures with increase in super charging pressure[11]. A maximum in-cylinder temperature of 1206.478 K at 720.075 CA and 1266.534 K at 721.85 CA was obtained at 1 bar and 2 bar super charging pressures respectively. A total increase of 4.97% in in-cylinder temperatures was obtained when the super charging pressure was increased from 01 bar and 2 bar.

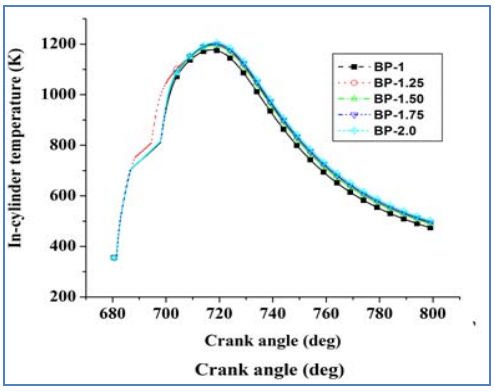

Figure B: In-cylinder temperature Vs Crank angle

5. CO and CO_2 emissions

In-cylinder temperatures play a major role in the formation of emissions [14]. Higher in-cylinder temperatures facilitate the conversion of CO to CO_2 and lower temperatures reduce the formation of NO_x.

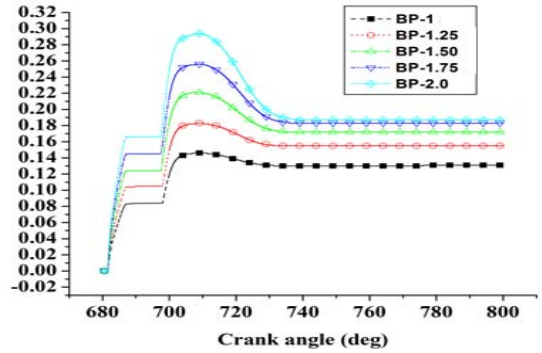

Figure C: CO emissions Vs Crank angle

Fig.C represents variation of CO emissions with super charging pressure. CO emissions of 0.131 g/kg fuel and 0.187g/kg fuel are obtained when the engine runs under super charging pressures of 1 bar and 2 bar.A total of 42.74 % increase in CO emissions was observed with increase in super charging pressure.

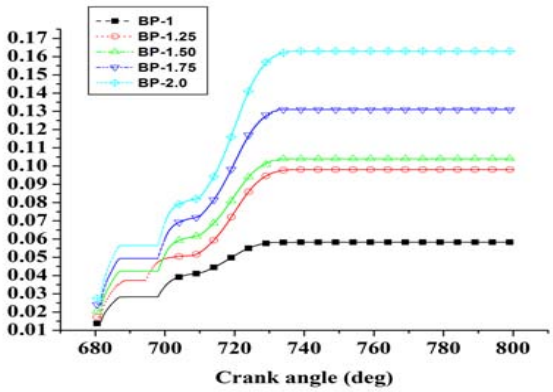

Figure D: CO_2 emissions Vs Crank angle

CO_2 emissions of 0.0583 g/kg fuel and 0.163 g/kg fuel are obtained when the super charging pressure increased from 1 bar to 2 bar. A total increase of 179.588 % was obtained when the super charging pressure is increased from 1 bar to 2 bar.

2. Nox emissions

The formation of NO_X is highly dependent on the in-cylinder temperatures, oxygen concentration and residence time for

the reaction to take place. From Fig.E with increase in super charging pressure decrease in NOx emissions can be observed. NO is temperature sensitive even below the thermal NO temperature limit.

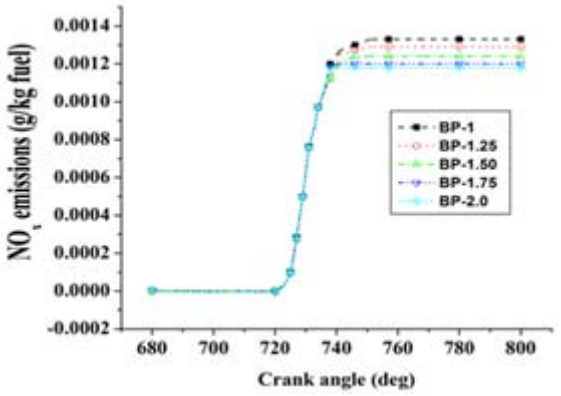

Figure E: NO_x emissions Vs Crank angle

The higher super charging pressures are favorable for low NO_x emissions. Out of the entire super charging pressures the lowest NOx emissions were obtained at 2 bar, proving it to be the optimum super charging pressure for this particular engine. Lowest NOx emissions of 0.00118g/kg fuel and 0.00133 g/kg fuel are obtained when the engine run with 1bar and 2 bar super charging pressure. Thus, a total decrease of 12.711% in NOx emissions was obtained when the super charging pressure increased from 1 bar to 2 bar.

3. Effect of Compression ratio.

The performances of a variable compression ratio HCCI engine with diesel as fuel have been studied here [14][15]. Analysis was done considering four compression ratios ranging from 18 to 21. Analysis of the effect of compression ratio on a single cylinder HCCI engine was simulated, using a COMSOL CFD model. The results are plotted and discussed below.

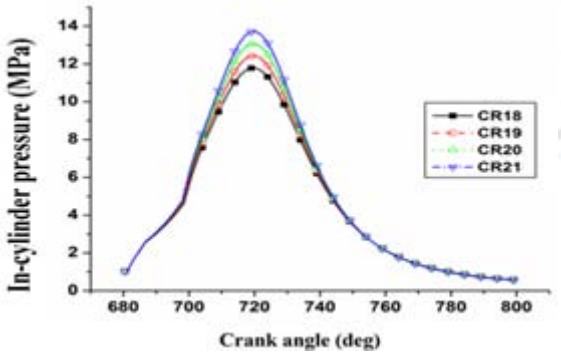

Figure F: In-cylinder pressure Vs Crank angle

a) In-cylinder pressures Vs Crank Angle

The in-cylinder pressure increases with increase in compression ratio. In Fig. F, A maximum in-cylinder pressure of 13.714 MPa at 719.775 CA and 11.787 MPa at 719.675 CA was obtained for CR 21 and CR 18 respectively. A total increase of 13.387% in in-cylinder pressures was obtained when the compression ratio was increased from CR18 to CR21.

b) In-cylinder temperatures Vs Crank Angle

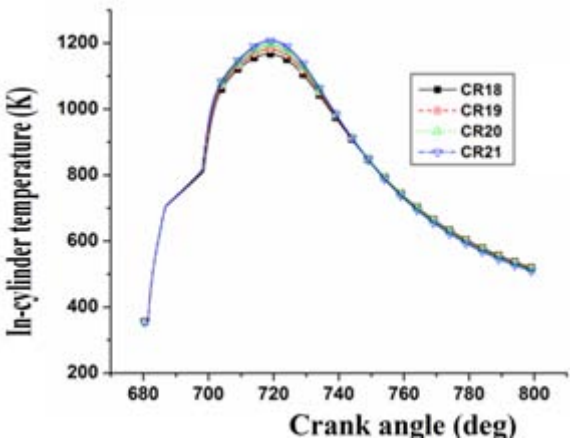

Figure G: Temperature Vs Crank angle

In Fig G. A maximum in-cylinder temperature of 1166.917 K at 718.675 CA and 1206.478K at 719.125 CA was obtained for CR 18 and CR 21 respectively. A total increase of 3.27% in in-cylinder temperatures was obtained when the CR increased from 18 to 21.

C) CO and CO_2 emissions

In-cylinder temperatures play a major role in the formation of exhaust emissions. Higher in-cylinder temperatures facilitate the conversion of CO to CO_2 and lower temperatures reduce the formation of NO_x. An increase in-cylinder temperature from 1166.917 K at718.675 CA and 1206.478K at 719.125 CA for CR 18 and CR 21 can be seen from the Fig. H With increase in CR CO emissions got decreased. Decrease in CO emissions with increase in CR can be seen in Fig.H. The reduced convective heat losses with increase in CR are responsible for the reduction in CO emissions. CO emissions of 0.147 g/kg fuel and 0.131 g/kg fuel are obtained with CR 18 and CR 21 was obtained for respectively. A total decrease of 10.88% in CO emissions was obtained when the CR was increased from 18 to 21.

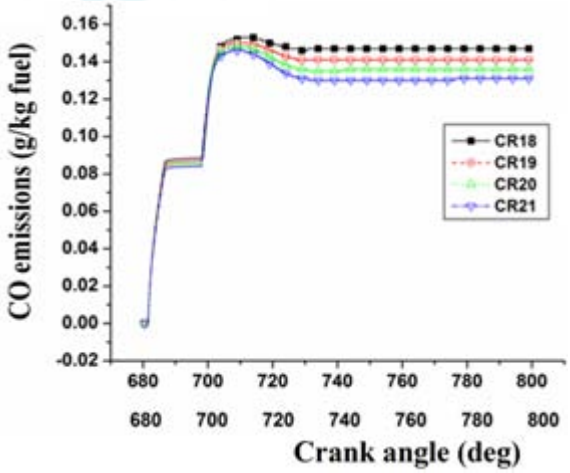

Figure H: CO emissions Vs Crank angle

The increase in CO_2 emissions with increase in CR can be seen in Fig. I. The increase in CO_2 emissions with increase in CR is because of conversion of CO into CO_2 representing complete combustion. CO_2 emissions of 0.052 g/kg fuel and 0.0583 g/kg fuel are obtained with 18 and 21 CR. A total increase of 10.80% in CO_2 emissions was obtained when the CR was increased from 18 to 21.

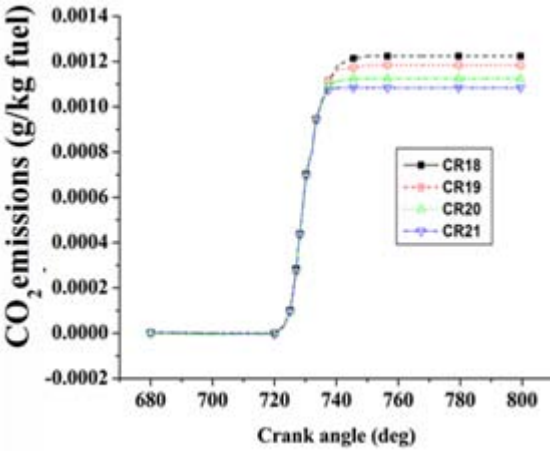

Figure I: CO_2 emissions Vs Crank angle

d) NO_x emissions

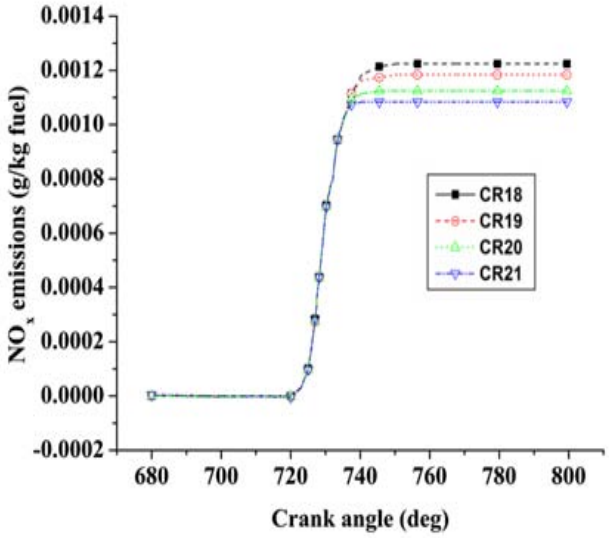

Figure J: NOx emissions Vs Crank angle

From the figure J, This concludes that higher CR are favorable for low NO_x emissions.NO_x emissions of 0.001091 g/kg fuel and 0.00123 g/kg fuel are obtained with 18 and 21 CR c was obtained. A total decrease of 11.300% in NO_x emissions was obtained when the CR was increased from 18 to 21.

6. Result Analysis

This paper gives the study about how the fuel properties could affect the HCCI engine performance and emissions. For the analysis purpose different fuels with different Cetane Numbers (CN) were considered and ran the simulations under same operating conditions[17]. The fuels considered for the analysis are Ethanol (CN-5), n-heptane (CN-53), iso-Octane (CN-63) and n-dodecane (CN-80). The results of the analysis are interesting in terms of performance and emissions. The variation of different emission and performance parameters with the fuels considered are discussed below.

a) In-cylinder pressure

The in-cylinder pressure variation when fuel with different cetane number fuels was used can be seen in Fig.K The in-cylinder peak pressure of n-dodecane was observed to be very high when compared with other fuels[16]. The high cetane number of n-dodecane responsible for the higher peak pressures when compared with the other. The iso-octane is showing the lowest peak pressure the combustion process was incomplete in its case. In case of ethanol and n-heptane the peak pressures are as per the cetane number. From Fig. K it is clear that fuel properties show a considerable effect on the performance of the engine. Initial combustion because of low temperature reactions and main combustion can be seen clearly in case of Ethanol, n-heptane and n-dodecane from Fig.K

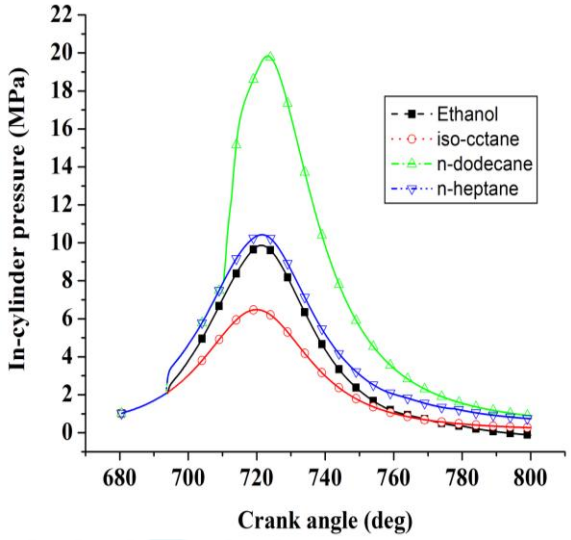

Figure K: In-cylinder pressure Vs crank angle

b) In-cylinder temperature

Higher in-cylinder temperature was observed with n-dodecane when compared with other fuels. The in-cylinder temperature analysis revealed that the higher cetane number fuels peak pressures and peak temperatures were shifted towards right showing 50% burn pint occurring near TDC which is ideal burn process in case of HCCI engines.

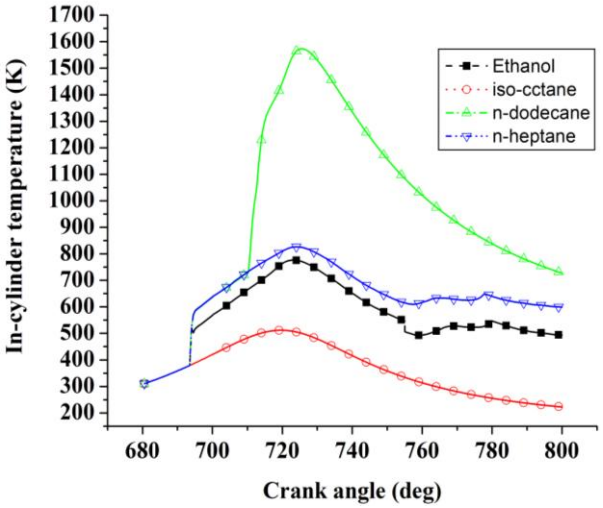

Figure L: In-cylinder temperature Vs Crank angle

C) CO and CO_2 emissions

It was observed that a sudden increase in CO emissions during combustion initiation for n-dodecane fuel and but during the later stages the CO emissions of n-dodecane decreased to minimum because of lower convective heat loss at the end of the combustion process facilitating oxidation of CO to CO_2.

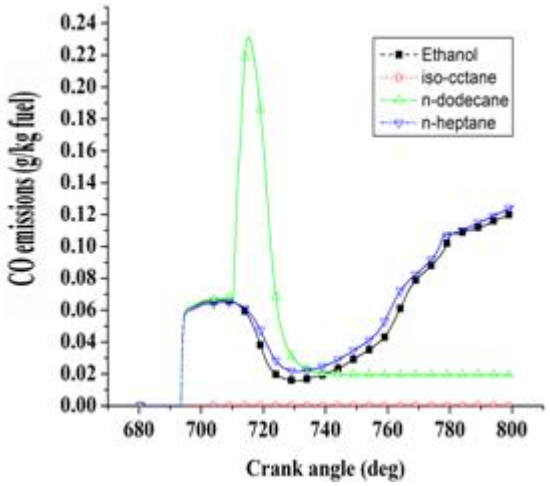

Figure M: CO emissions Vs Crank angle

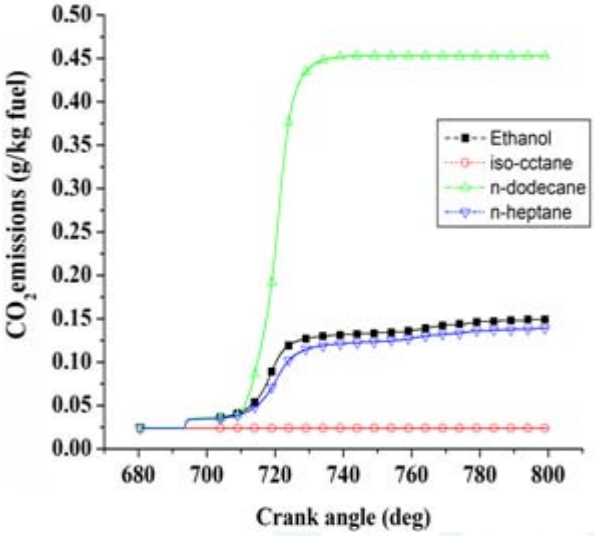

Figure N: CO_2 emissions Vs Crank angle

equivalence ratio leading to variation of CO, CO_2 .The CO emissions in case of ethanol and n-heptane were observed as low during combustion and increased at the end of combustion because of [18] lack of oxidation CO to CO_2. Iso-octane didn't show any CO emissions as the combustion process was initiated under the conditions chosen to run the engine. Fig. N shows the variation of CO_2 emissions of different fuel with crank angle. Higher CO_2 emissions can be observed in case of n-dodecane when compared with other fuels. As CO and CO_2 emissions are mutually related the higher oxidation of CO emissions in case of n-dodecane fuel was responsible for higher CO_2 emissions. The CO_2 emissions from iso-octane were observed to be not varied as it doesn't participated in combustion process. Stoichiometric requirement of fuels facilitates the availability of oxygen for CO and N_2 oxidations operated under same and N_2 emissions.

D) NOx emissions

Higher in-cylinder temperatures and availability of oxygen plays an important role in NOx emission. Fig. N shows the variation of NOx emissions of different fuels with crank angle.

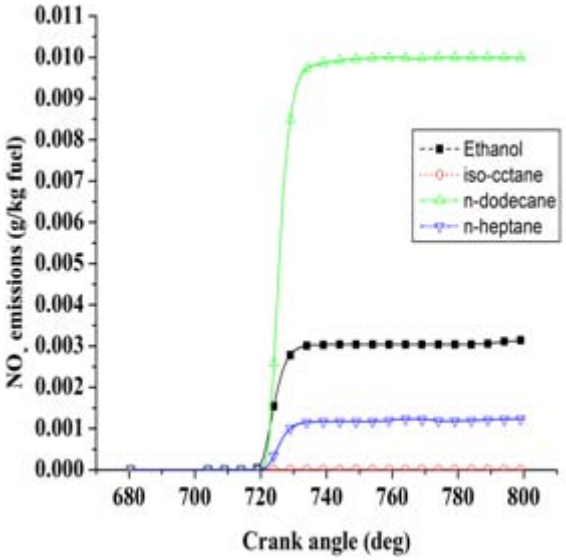

Figure O: NO_x emissions Vs Crank angle

Higher NOx emissions were observed with n-dodecane fuel because of its higher in-cylinder temperatures. Availability of oxygen and higher in-cylinder temperatures were responsible for higher NOx emissions in case of Ethanol. As no combustion occurred no variation in NOx emissions was observed in case of iso-octane.

7. Conclusion

In this paper HCCI conception has been adopted for Variable volume Batch kind Reactor that's totally machine-driven victimisation elaborate chemical mechanisms and capable of modeling unsteady operation. HCCI engine module may be a predefined module in COMSOL code package to investigate the chemical reactions and species formation throughout combustion below numerous input parameters. Vital variation in in-cylinder pressures square measure obtained on the far side a temperature of 415 K, this could be attributed to decrease in ignition delay with increasing initial temperature. The water temperature of the fuelair mixture may be a potential standardization parameter for ignition.

The overall observations among the entire scenario as fallows. The effect of compression ratio reduced the CO and NOx emissions by 10.82% and 11.475 % respectively.

COMSOL has well predicted the HCCI mode of Combustion and observed to be insensitive to engine specifications.

CFD analysis of combustion is needed to understand the HCCI concept a better way and to reduce the emissions.

Load bearing capability of HCCI engines can be improved by supercharging technique. A total of 11.12% reduction in NOx emissions and 42.59% increase in CO emissions were also obtained with increase in super charging pressure.

It was observed that fuel properties will have considerable effect on the emission of the engine. Choosing a suitable fuel ca reduce the emission of the engine.

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