Modeling of Reduced N-Heptane Combustion in Compression Ignition Engine

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***Abstract*: Conventional compression ignition engines have high emission rates of Nitric oxides (NOx) and particulate matters (PM) than spark ignition engines despite being the most fuel efficient engines ever developed for transportation purposes thus the interest for research on it to make it more efficient and to meet the stringent legislation imposed by many nations' government.**

Reduced N-Heptane (29 species, 52 chemical reactions) which is a representative of Diesel fuel was utilized in the model by importing it from the relevant files into the chemical reaction interface using the relevant governing equations and solved with COMSOL 5.0 which employs the finite difference method of solution. The model was used to study the effect of compression ratio and engine speed on the performance of the engine as it relates to species concentration, peak temperature and pressure, and the derived mechanical energy.

The derived mechanical energy, peak temperature and pressure increased with increased compression ratio. The concentration of species n2, o2 and co2 also showed an increase with increase in compression ratio.

The engine speed affects the period required to complete the combustion process, the time being shortened with increased engine speed. The derived mechanical energy also decreased with increased engine speed, the value being -1370.7J at a compression ratio of 18 and engine speed of 1500rpm and -1353.6J at the same compression ratio but engine speed of 2000rpm.

***Keywords:* Compression ignition engine, Species, Comsol 5.0, Reduced N-Heptane, Compression ratio, Engine speed**

I. INTRODUCTION

Compression ignition engines are the most fuel efficient engines ever developed for transportation purposes, due largely to their high compression ratio and lack of throttling losses. However, conventional compression ignition engines have high emission rates of Nitric oxides (NOx) and particulate matters (PM) than spark ignition engines. The high emission of the toxic substances coupled with the stringent legislation imposed by many nations' government gingered the interest for research on compression ignition engines, which have significantly led to more fuel efficient engines. The concept of homogenous charged compression ignition (HCCI) engine evolved as a possible solution to some of these problems, as it posses the high efficiency values in regards to the conventional compression ignition engines and low emission of pollutants when compared to the traditional spark ignition engines, but despite the huge beneficial potential of the HCCI engines, it has not been commercially developed mainly due to its low operation range – low load, medium load and high load.

At low loads, the charge needs to be very lean, and at some points the auto-ignition of the compressed lean charge will be very difficult implying incomplete combustion and increased emission of CO and HC. At high loads, the combustion of the compressed charged can be violent due to generation of high pressures which can lead to noise and knocking of the engine.

II. LITERATURE REVIEW

According to Dec (1), advanced compression ignition engines have evolved along two fronts; the homogenous charged compression ignition (HCCI) and the low temperature combustion (LTC). He conducted research on the in-cylinder processes in compression ignition engines, along the two emerging fronts of HCCI and LTC. He reported better performance of the engine in terms of lower NOx emission and improved low load efficiency.

HCCI engine is a hybrid between spark-ignition and compression-ignition engines. HCCI combustion can be described as the oxidation of the fuel driven solely by chemical reactions governed by chain breaking mechanisms. Two temperature regimes exist for these reactions – one below 850K and the other around 1050K. HCCI can possibly be controlled through temperature stratification, while at high load a local high temperature in-homogeneity will be the driver of uniform slow propagating HCCI combustion, and at low load multiple temperature in-homogeneities can be introduced in the combustion cylinder to simultaneously ignite the charge at multiple locations. (2).

HCCI engines allow the use of fuels other than diesel and petrol, Chauhan et al (3) summarized the effect of alternative fuels for an HCCI engine combustion process. It was reported that IMEP increased with increasing premixed ratio of fuel at low and medium loads with a significant reduction in NOx and smoke for the tested combustion modes in comparison to conventional diesel engine.

A study on alternative fuels for HCCI engines and the recent developments was undertaken by Rajendra et al (4) where they concluded that despite the huge prospects for better fuel economy and emission reductions, the HCCI engines is still taken back by the effect of rapid pressure rise which is akin to experiencing “knock” as like a spark ignition engine and also the problem of combustion timing, which must be further researched on to make the technology a viable one.

Attention is now being shifted towards the development of mathematical models for simulations which are true representation of the activities going on in an engine which in some cases cannot be measured during experiments.

Anant et al, (5) carried out the mathematical modeling of the fuel engine cycle which was used to predict the value of peak cylinder gas pressure, IMEP, brake power, brake thermal efficiency and ignition delay period to an accuracy of between 0.2 to 2.5% in relation to experimental values and thus were able to develop a model that can be used for the optimization of a number of design parameters of a dual fuel engine for any application.

Developed radial basis function network (RBFN) showed closed agreement with experimental outputs, and it was concluded that artificial neural networks (ANN) could be utilized in lieu of experiment to study the performance and emission characteristics of HCCI engines. (6)

The Nox and soot emissions relationship with compression ratio of an engine were studied by Loguitton et al (7) in their quest to establish how an engine NOx emission can be reduced to meet the ‘EURO 6’ emission target. The effect of reducing the compression ratio of a single cylinder compression ignition engine from 18.4:1 to 16:1 was investigated. They reported that reducing the compression ratio of a premixed charged combustion ignition in a direct ignition compression ignition engine led to reductions in NOx and soot emission.

The performance and emission characteristics of a compression ignition engine operated on diesel, and in a dual-fuel mode with a 4-stroke single cylinder of 5.2Kw rated power at 1500rev/min shows that the NOx emission of the dual fuel mode was better but fared lesser in terms of performance where the brake thermal efficiency was reduced by between 12-14%. (8), (9), (10).

The impact of compression ratio and engine speed on the performance of a compression ignition engine operated on reduced N-Heptane was understudied by the authors. This was conducted as it relates with species concentration, combustion temperature and pressure, and species molar fraction.

III METHODOLOGY

The combustion of fuel is governed by the generalized Navier-Stokes equation.

$$\rho\frac{\partial \Theta}{\partial t} + \rho\ (\Theta.\ \Delta)\ \Theta = \Delta = \Delta.\ [-\ \rho l + \mu\ (\Delta\Theta + (\Delta u)^{T})] + F \qquad 1$$

Where Θ is a dependent variable such as momentum, energy, turbulence e.t.c

F is the source term for the Θ variable

From which the energy equation is derived as

$$\rho Cp\frac{\partial T}{\partial t} + \rho CpU.\Delta T = \Delta.(k\Delta T) + Q + Qh + Wp \qquad 2$$

The governing equations were solved numerically in 2-D axi-symmetry using Comsol 5.0 software.

Energy and mass balances that describe the combustion of N-Heptane in a variable-volume system were solved. The mass balances describing a perfectly mixed reactor with variable volume are summarized by

$$\frac{d(Vci)}{dt} = VRi \qquad 3$$

Where *ci* represents the species concentration (mol/m3), and *Ri* denotes the species rate expression (mol/ (m3·s)).

The reactor energy balance is;

$$Vr\sum_i CiCp,i\,\frac{dT}{dt} = Q + Qext + Vr\frac{dP}{dt} \qquad 4$$

Where *Cp,i* 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)

$$Q = -\ Vr\sum_j Hjrj \qquad 5$$

Where *Hj* is the enthalpy of reaction (J/(mol·K)), and *rj* equals the reaction rate (mol/ (m3·s)). *Q*ext denotes heat added to the system (J/s), and for this model it is zero as adiabatic conditions is assumed.

Reduced N-Heptane (29 species, 52 chemical reactions) which is a representative of Diesel fuel was utilized in the model by importing it from the relevant files into the chemical reaction interface.

The following assumptions were made;

- The heat energy, generated by combustion, is added uniformly over the domain.
- The convection effects in the combustion chamber are neglected.
- All the equations are solved on the original domain, and the effect of change in the cylinder volume is accounted for manually in the equations.

The current cylinder volume, *V*, is computed by subtracting the piston swept volume from the initial cylinder volume. ($V = V0-\pi*rp^2*xp$) 6

The initial cylinder volume 'V0' = $2*\pi*r$ 7

The piston displacement, *xp*, as a function of crankshaft rotation, θ, can be written as

$xp = \sqrt{(l^2 - (rcSin\Theta)^2)} - rcCos\ \Theta - (l - rc)$ 8

Where *xp*, *rc*, *l* and θ represent the piston displacement, crank radius, connecting rod length and crank angle, respectively.

IV RESULTS AND DISCUSSION

In this study, the combustion in a compression ignition engine was analyzed numerically. Computations were performed for compression ratio of 15 and 18 at RPM of 1500rev/min and equivalence ratio of 0.5, and for compression ratio of 18 at RPM 0f 2000rev/min and equivalence ration of 0.5. Cylinder bore D = 0.0875m, stroke length S = 0.11m, connecting rod length Lc = 0.2m and crank arm length La = 0.04375m. N-Heptane (C_7H_{16}) was used as fuel.

In order to observe the effect of compression ratio on engine performance as it relates to the concentration of species, combustion temperature, combustion pressure, species molar fraction with respect to time were plotted at compression ratios of 15 and 18 at the engine speed of N = 1500rpm as depicted in figs 1a to 6b. The plots at an engine speed of N = 2000rpm for compression ratio of 18 shows the effect of engine speed on the combustion period, and is depicted in figs 7 to 12.

The species concentration of n2 (Nitrogen) was shown to increase with increased compression ratio as evident in figs. 1a and 1b and this implies that for the same initial temperature and pressure, more Nitrogen molecules take part in the chemical reaction to produce NOx at compression ratio of 18 as compared to a compression ratio of 15 and this is consistent with literature.

The peak combustion temperature and pressure was also found to be dependent on the compression ratio as depicted in figs. 2a, 2b and 3a, 3b. The peak temperature at a compression ratio of 15 is about 2500k and 2600K at a compression ratio of 18.

The production of HO2 and H2O2 that in turn produce OH radicals in amounts critical to fuel ignition can also be seen to be favoured by a higher compression ratio as depicted in figs. 4a and 4b.

Figs. 5a and 5b shows the Pressure versus volume plots for a compression ratio of 15 and that of 18 respectively, while the pressure versus crank angle is as shown in figs. 6a and 6b. More energy is derived from the engine at a compression ratio of 18 when compared with that released when the compression ratio was 15; this is clearly visible from the plot, where the derived mechanical energy (ME) at a compression ratio of 15 was 1028.8J and that at a compression ratio of 18 is 1370.7J.

Figs. 7 to 12 when compared with Figs. 1b, 2b, 3b, 4b, 5b and 6b shown marked resemblance in term of the peak species concentration, temperature and pressure except that the time taken to get to the peak values are relatively shorter for engine speed N = 2000rpm when compared with that of engine speed N = 1500rpm, which explains the fact that combustion period is shortened with increase in engine speed, because the reactants (fuel and air) have little time to fully participate in the combustion process as evidenced in the reduction of the derived mechanical energy (ME) at a engine speed of N = 2000rpm (1353.6J) from that which was obtained at an engine speed of N = 1500rpm (1370.7J)

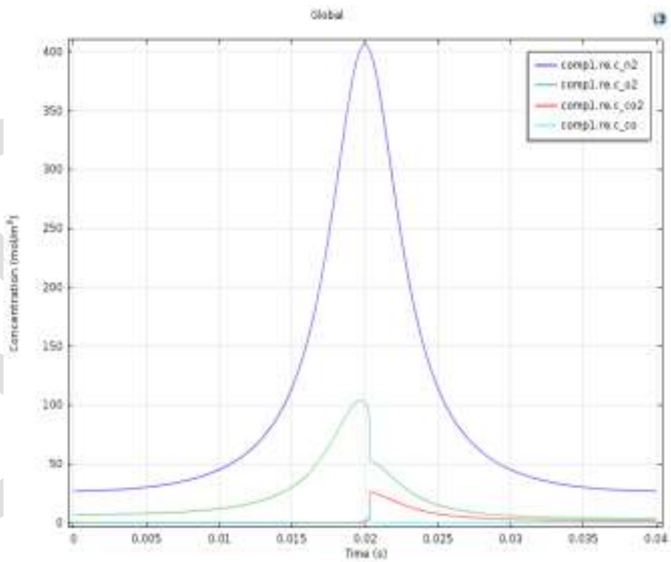

Fig. 1a Species Concentration plots (CR 15, RPM 1500, ER 0.5)

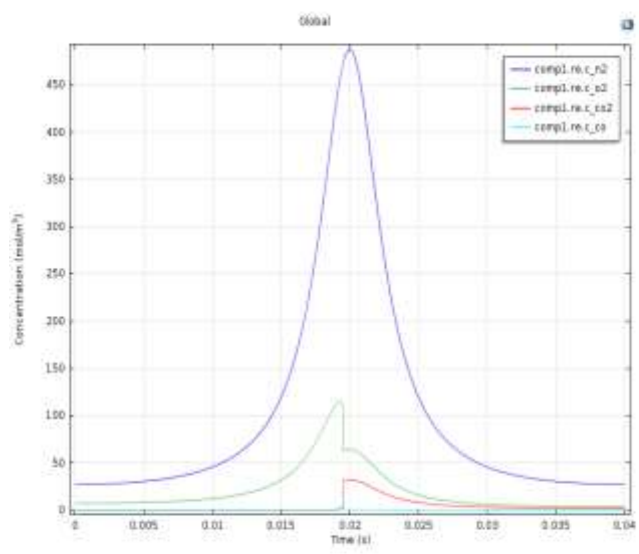

Fig. 1b Species Concentration plots (CR 18, RPM 1500, ER 0.5)

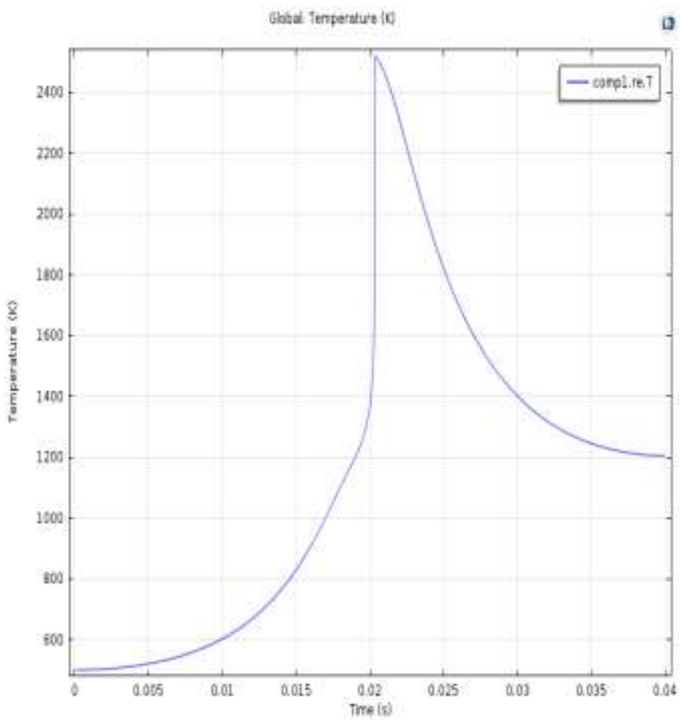

Fig. 2a Temperature plot (CR 15, RPM 1500, ER 0.5)

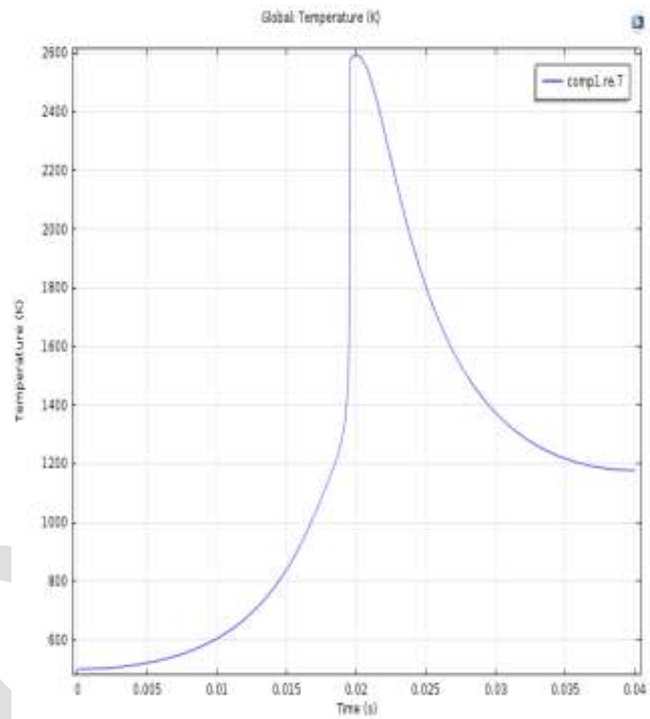

Fig. 2b Temperature plot (CR 18, RPM 1500, ER 0.5)

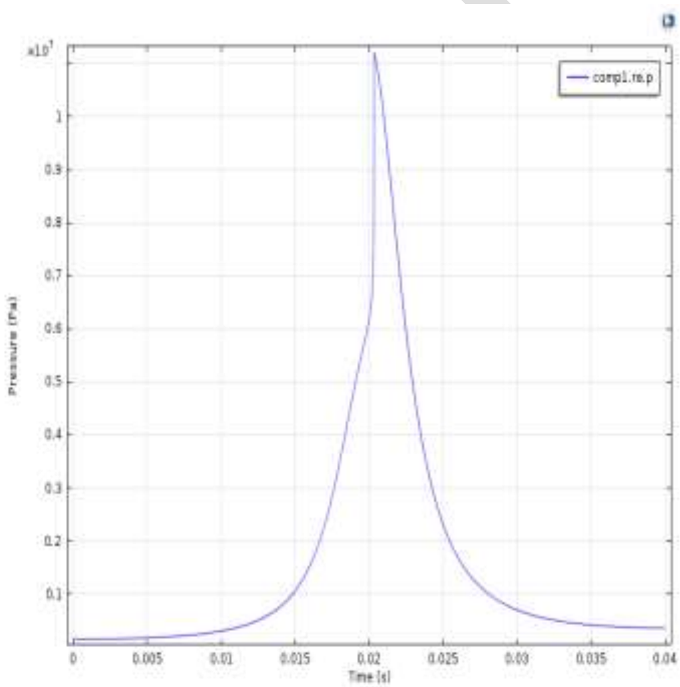

Fig. 3a Pressure plot (CR 15, RPM 1500, ER 0.5)

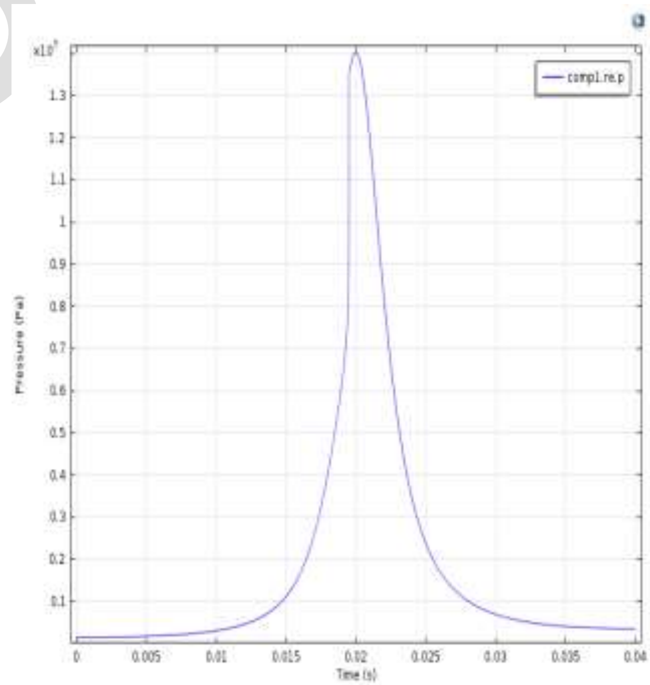

Fig. 3b Pressure plot (CR 18, RPM 1500, ER 0.5)

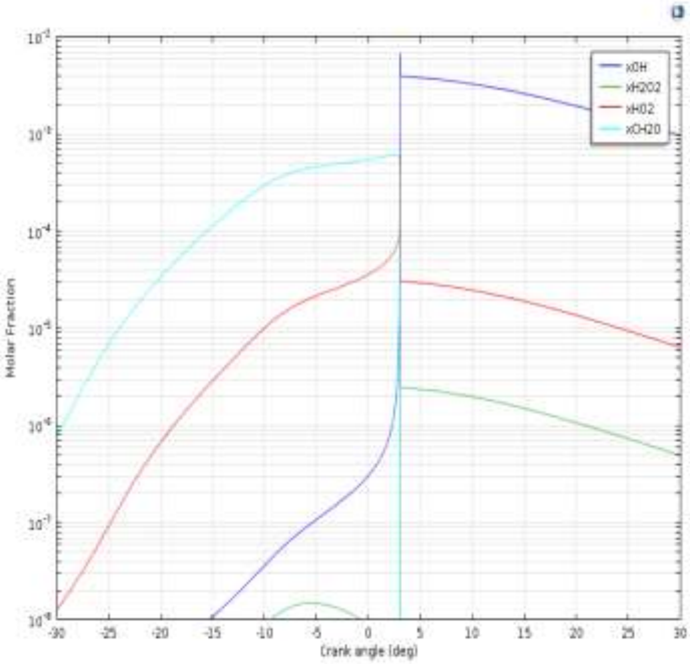

Fig. 4a Molar fraction (CR 15, RPM 1500, ER 0.5)

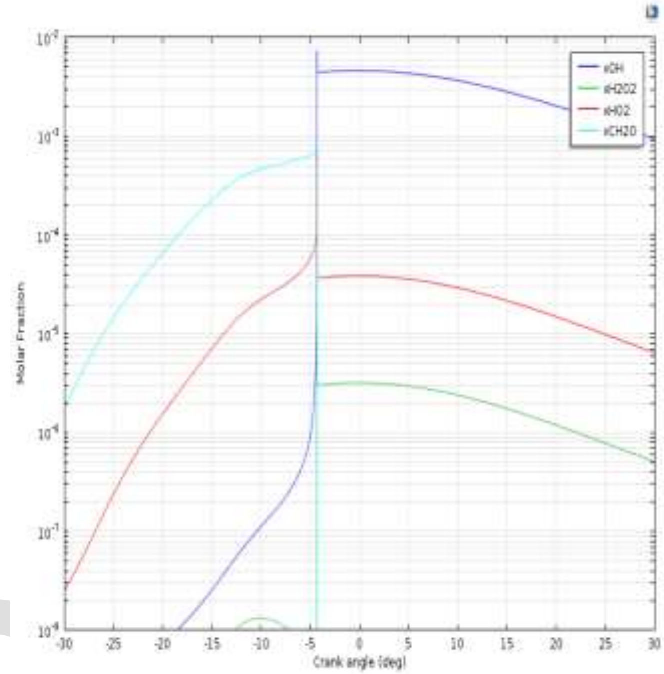

Fig. 4b Molar fraction (CR 18, RPM 1500, ER 0.5)

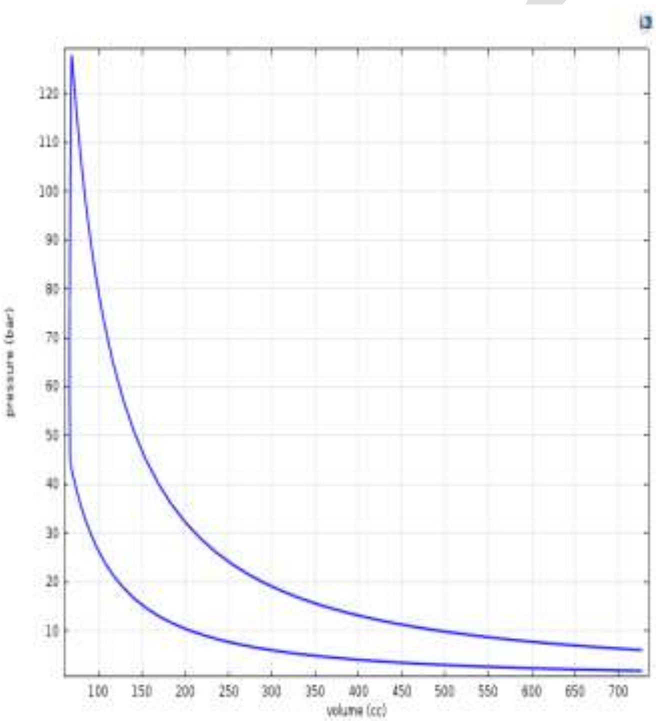

Fig. 5a Pressure-Volume plot (CR 15, RPM 1500, ER 0.5) ME = -1028.8J

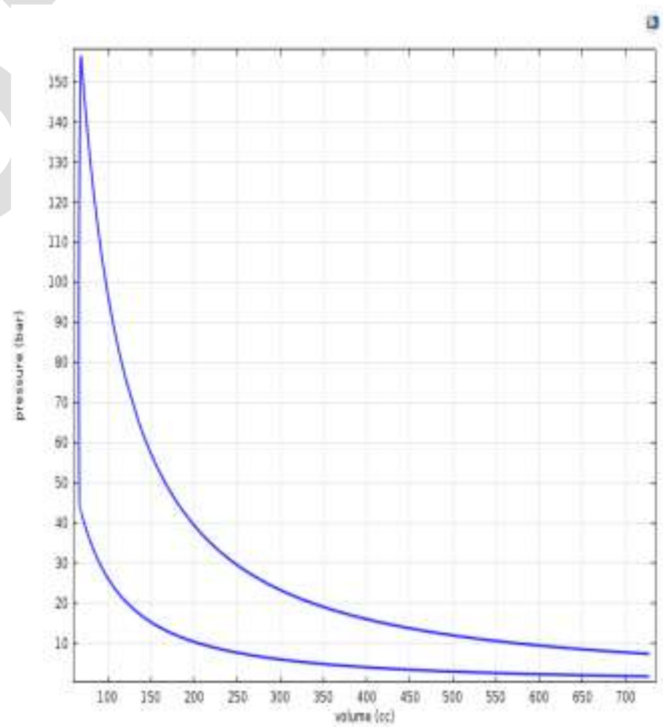

Fig. 5b Pressure-Volume plot (CR 18, RPM 1500, ER 0.5) ME = 1370.7J

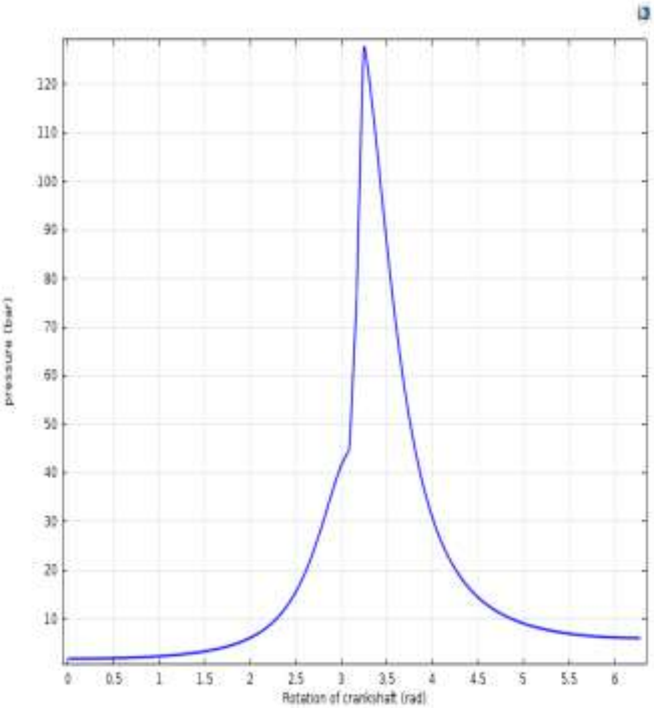

Fig. 6a Pressure-Crank angle plot (CR 15, RPM 1500, ER 0.5)

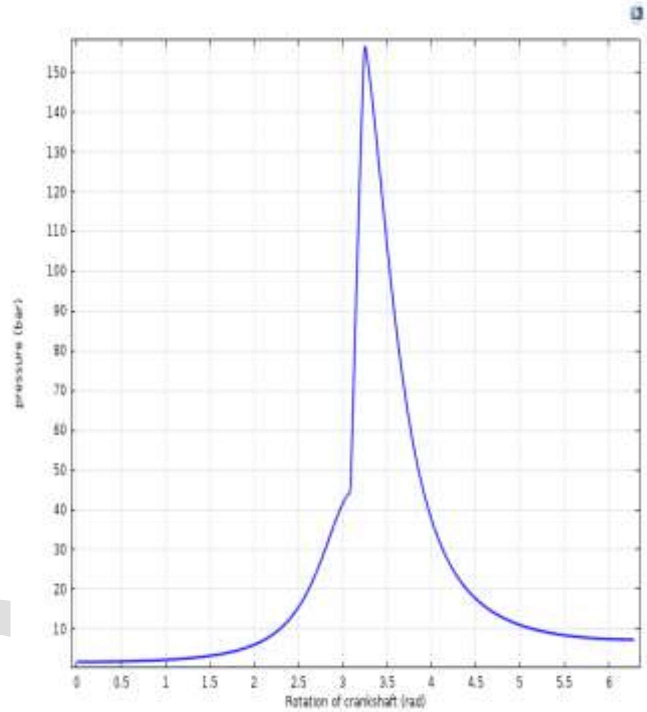

Fig. 6b Pressure-Crank angle plot (CR 18, RPM 1500, ER 0.5)

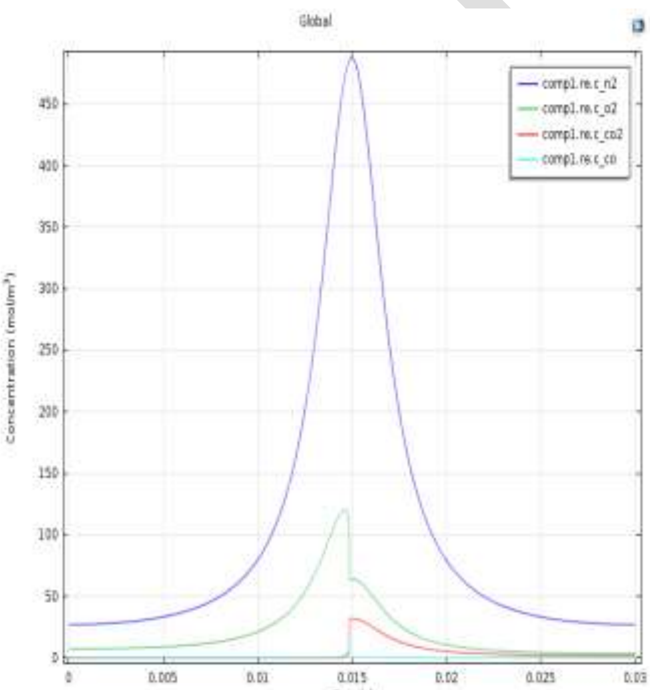

Fig. 7 Species Concentration plots (CR 18, RPM 2000, ER 0.5)

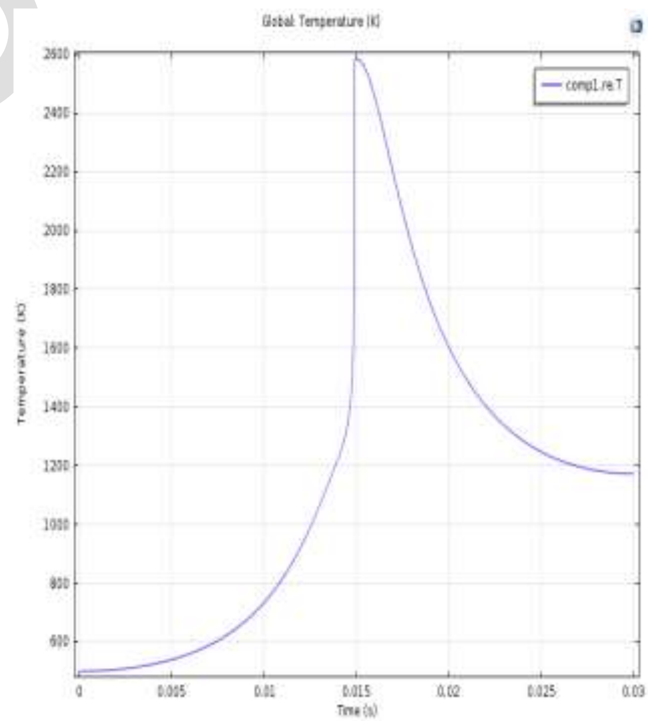

Fig. 8 Temperature plot (CR 18, RPM 2000, ER 0.5)

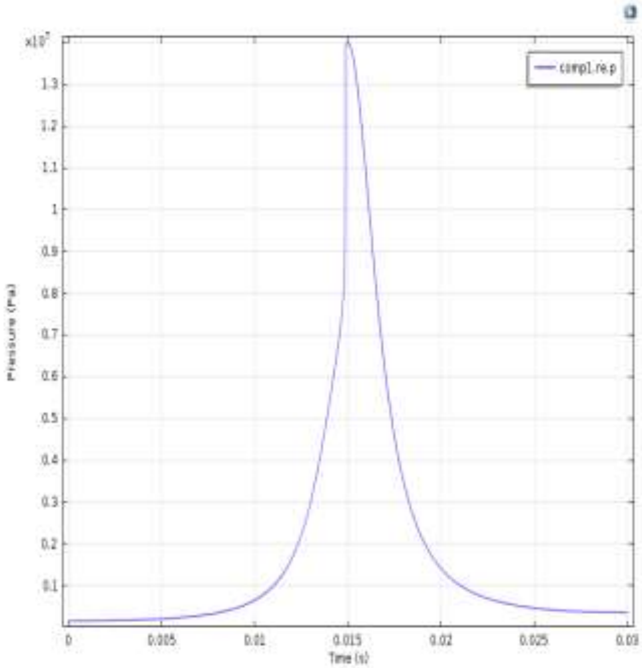

Fig. 9 Pressure plot (CR 18, RPM 2000, ER 0.5)

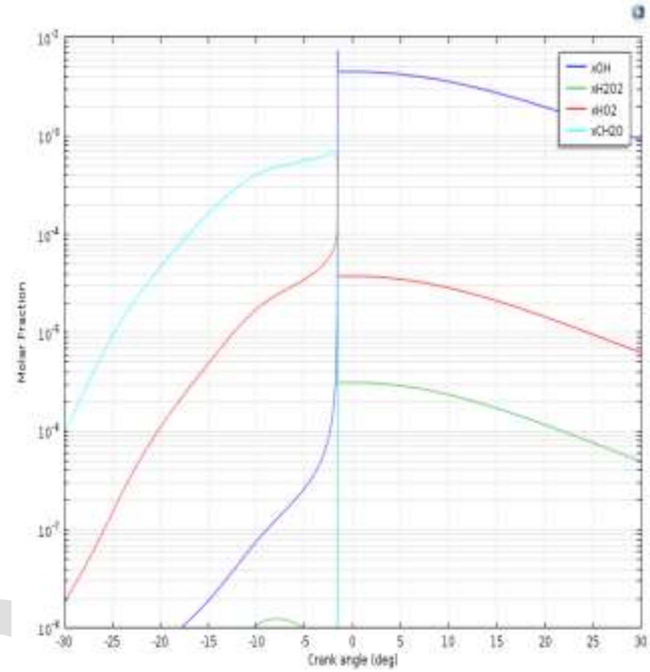

Fig. 10 Mole fraction (CR 18, RPM 2000, ER 0.5)

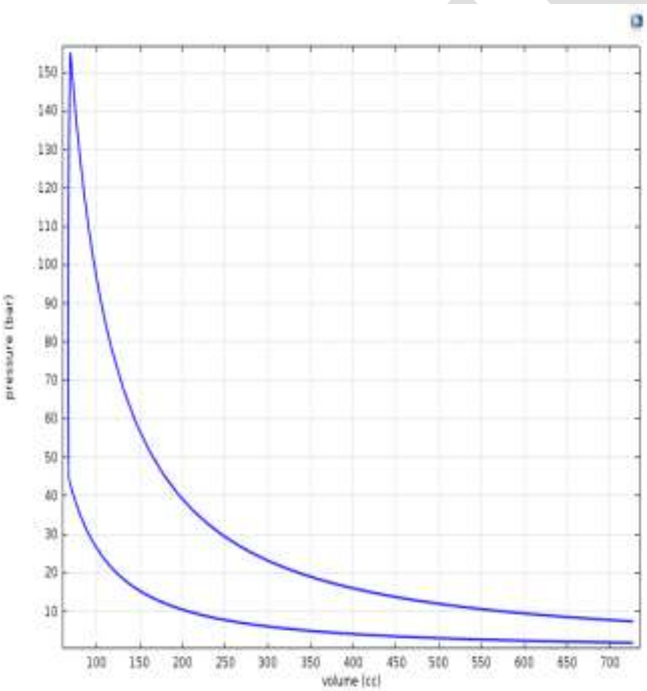

Fig. 11 Pressure-volume plot (CR 18, RPM 2000, ER 0.5) ME = -1353.6J

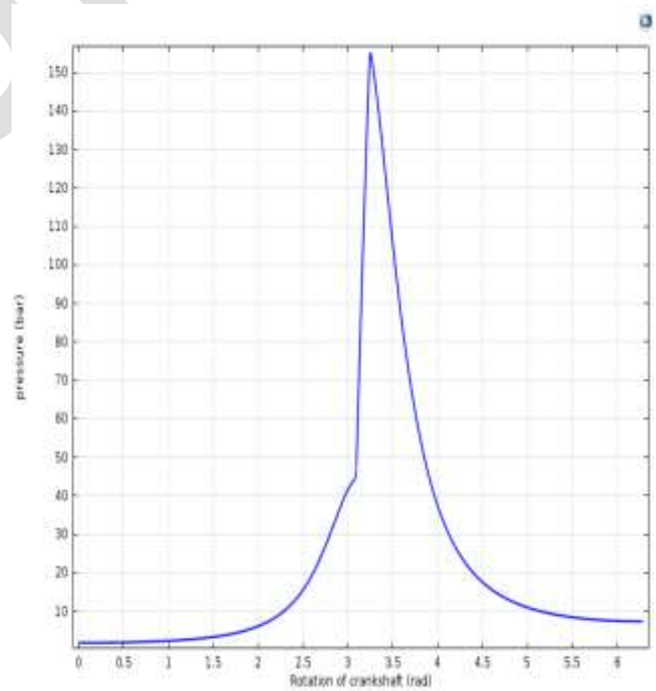

Fig. 12 Pressure-crank angle plot (CR 18, RPM 2000, ER 0.5

V. CONCLUSION

The engine characteristics was modeled by finite element method using COMSOL 5.0, while N-Heptane (29 species – 52 chemical reactions) was utilized as the fuel. The derived mechanical energy was found to be favoured by a higher value of compression ratio, although not without an attendant increase in NOx due to more amount of Nitrogen specie taking part in the chemical reaction. Both the peak temperature and pressure attained in the engine was also shown to increase with increase in the compression ratio. Increasing the engine speed leads to shortening of the time required for the combustion process.

VI. RECOMMENDATION

This study does not take the convection effect in the combustion chamber into cognizance, as it was assumed that the convection effects in the combustion chamber were neglected and the turbulence equation does not come into play. Studies are being conducted by the authors to see the effect of turbulence in the combustion chamber and thus take the convection effect in the combustion chamber into consideration to make the model closer to real life activity in a compression ignition engine.

VII. ACKNOWLEDGEMENT

Reduced N-Heptane (29 species, 52 chemical reactions) was downloaded from https://www.erc.wisc.edu/chemicalreaction.php
The engine geometry used for the modeling was from COMSOL file reciprocating_engine_2d.mphbin

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