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Numerical Simulation of HCCI Combustion Fuelled with Gasoline + Methyl Tert-Butyl Ether Blend

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Abstract

Background: Homogeneously charged compression ignition (HCCI) engines are generally popular for low production of NO_x and Soot formation, also consuming lower fuel as compared with conventional gasoline and diesel engine. **Objectives:** In this study, the compression ignition engine (CI) was simulated in HCCI mode fuelled with Gasoline and Methyl tert-butyl ether (MTBE) blends, and the analysis was carried out in similar operating conditions as experimentation carried out. **Methods:** The chamber pressure was maintained at 2 bar, and the air-fuel ratio was maintained at 2.75. The optimal blend for MTBE was fixed as 15 vol % (MTBE 15), and the measured properties of the blends were used in the simulation. ICE simulation module in ANSYS WORKBENCH was used for this current simulation. Both cold flow and combustion simulations were carried out and the results indicate velocity inside the cylinder, cylinder pressure, and temperature distributions for two cases such as gasoline and gasoline with MTBE15. **Findings:** The average velocity was found high with the MTBE blend, whereas in-cylinder pressure was found low with MTBE blend than with gasoline. The temperature inside the cylinder pressure was found higher with gasoline than MTBE blend. The deviation between the experimentation and simulation was found low. **Novelty:** The simulation provides a better understanding of the combustion phenomena when gasoline is mixed with MTBE and utilized in a diesel engine at HCCI mode.

Keywords: CFD; MTBE; Gasoline; HCCI; Emission reduction

1 Introduction

Every country is started to implement stringent emission regulations to reduce pollutants and greenhouse gas emissions. On the other hand, researchers keep finding alternative sources for petroleum products to fill the future demand. Many alternative fuels were kept found and tested on engines, from the testing. Also, it was noted that many fuels are suitable for the engine, but they need some modifications in either engine parts or in operational parameters. In this concern, the Homogeneous charge

compression ignition (HCCI) mode of combustion was adapted to improve the brake thermal efficiency and reduce the emission when gasoline and MTBE blends are used in a diesel engine. The HCCI combustion is a promising technology where hybrid combustion occurred between conventional spark ignition and compression ignition concepts. Though the HCCI concept is old technology, still it is recommended which fuel produces higher emissions. The HCCI mode combustion will produce high thermal efficiency and lower NO_x and soot⁽¹⁾. Though HCCI engines have more potential, HCCI mode combustion was not suitable for some fuels. The limitations were no control on the ignition, low specific output, low operation ranges, more hydrocarbon (HC) and carbon monoxide (CO) emission etc. Comparably, low soot emission from HCCI engine is noted than SI and CI engine; this is because of lower combustion temperature and good volumetric efficiency. Also, lower specific fuel consumption is another attractive benefit of the HCCI engine. Through, visualizing the combustion process of conventional SI engines and HCCI engines, it was found that flame propagation was easily seen in SI engine combustion whereas not able to see in HCCI engines⁽²⁾. Thus, proving that better volumetric combustion has occurred during HCCI combustion. The numerical investigation for the effect of Exhaust Gas Recirculation (EGR) rate on HCCI combustion in order to reduce the pressure rise by CHEMKIN and SENKIN codes. It indicated that reducing the rate of EGR will reduce the cylinder temperature and pressure rise significantly. Whereas, an increase in the EGR rate causes the extending the start of thermal ignition was observed⁽³⁾. Introducing the swirl motion in the inlet will help to enhance better homogeneous mixture formation, and it tends to reduce the NO_x formation. The lower NO_x was attained by improving the better heat transfer caused by better swirling motion⁽⁴⁾.

Spray formation analysis was carried out in a diesel engine using ANSYS ICE simulation module. The simulation was carried out with a $k-\epsilon$ turbulence model and 2400 rpm of speed. The results provide a better understanding of combustion behavior, and it will be used for extensive research on similar engines⁽⁵⁾. A light-duty single-cylinder diesel engine was simulated in CONVERGE codes. The analysis focused on the prediction of ignition timing using Reynolds Averaged Navier Stokes (RANS) approach with the spray breakup model. The results showed good agreement with ignition timing prediction along with fuel variability⁽⁶⁾. The CFD simulation was carried out in ANSYS FLUENT for diesel engines fuelled with waste plastic oil blends. The NO_x was found higher with stage 1 distilled waste plastic oil (D1WPO30) than in diesel fuel simulation. Also, soot was found high about 17% than diesel fuel values. The minimal deviation was found between experimentation and computational fluid dynamics (CFD) simulation due to the absence of inlet and exhaust port and not considering the crevice flow effect⁽⁷⁾. But, it was found an effective approach to predict the waste plastic oil combustion in order to different operating parameters. Optimization of the process of an internal combustion engine using CFD is an effective way, which can provide a better understanding of the particular fuel combustion. It may also help to extensive research on particular topics. To the author's knowledge, no work was carried out to predict the spray formation and combustion behavior of diesel engines in CFD when it operated with gasoline and MTBE blends in HCCI mode combustion.

Since the HCCI combustion has great potential, it is not recommended for gasoline-like fuel. Due to higher HC and CO emissions, no control on combustion and low specific outputs. To overcome the limitation, the MTBE is added to the gasoline in optimal proportion. Because the MTBE has a tendency to increase the octane and oxygen level to control the emissions. The article is focused to analyze the diesel engine at HCCI mode by CFD simulation, fuelled with gasoline and MTBE blend. The ANSYS Workbench- ICE combustion code was used for this simulation. A similar engine where experimentation is carried out was modelled and simulated along with RANS turbulence model. The results indicate the velocity, pressure and temperature distribution inside the cylinder. Also, the results depict the NO_x and HC, CO formation from engine combustion. The validation between CFD simulation and experimentation also be carried out for a better understanding of combustion.

2 Methodology

The TV1 Kirloskar diesel engine was selected, and it was modified to operate in HCCI mode by MTBE blended gasoline shown in Figure 1 and Figure 2. The MTBE is blended in the optimal proportion of 15vol%. Also, the Gasoline was purchased from the Indian Oil fuel Station, India. The MTBE was purchased from Validyn Engineering Solution Pvt Ltd, Namakkal, India. The thermal properties of various samples are measured and listed in Table 1. The fuel density does not vary in a noticeable amount, but the flashpoint, fire point and calorific value have been found to significant hike as comparable with commercial gasoline. This is due to reducing the aromatic compound volume by adding the MTBE. The engine and gas analyzer specifications are given in Table 2 and the diesel mode combustion was changed to HCCI mode by imparting the Port fuel injection system fitted and electronic control was used to control the fuel flow automatically based on engine running conditions.

2.1 Computational Fluid Dynamics

The HCCI mode of combustion is modelled in CFD by finite volume approach, because it engages conservation law, the integral form of Navier stokes equations and flexibility of application of structured and unstructured mesh⁽⁸⁾. First, the physical space



Fig 1. Photograph of HCCI engine experimental set-up

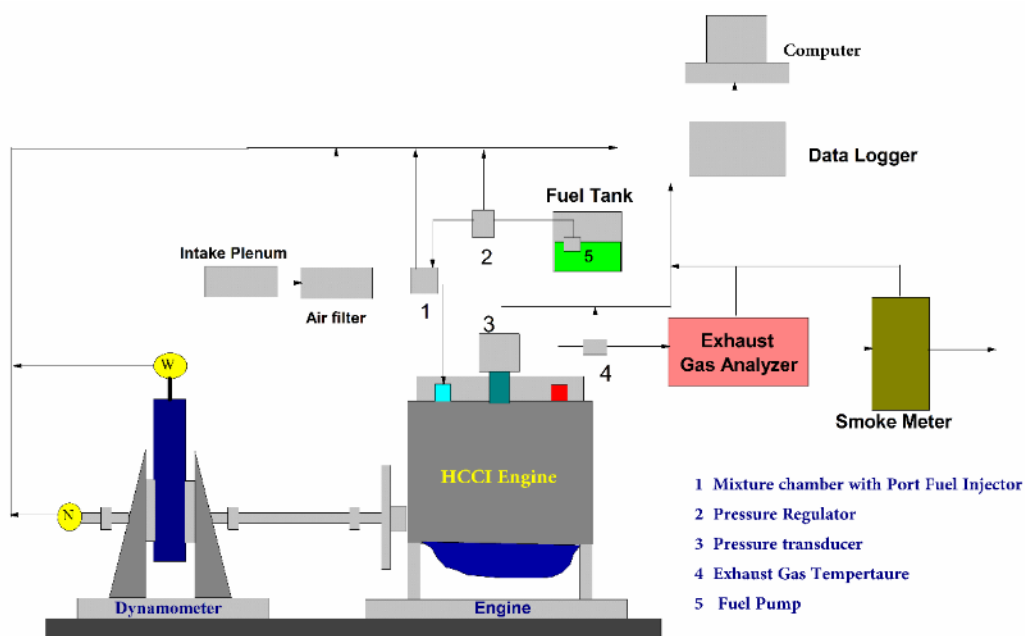


Fig 2. CCI engine Experimental set-up layout

Table 1. Property of fuel blends

| Properties | Gasoline | MTBE 5 | MTBE 10 | MTBE 15 |
|-------------------------------------|----------|--------|---------|---------|
| Density @15° C (kg/m ³) | 745 | 743 | 741 | 735 |
| Flash Point (°C) | -43 | -43 | -44 | -46 |
| Fire Point (°C) | -38 | -39 | -40 | -41 |
| Kinematic Viscosity @40° C in cSt | 0.63 | 0.6 | 0.58 | 0.56 |
| Gross Calorific Value (MJ/kg) | 47.16 | 43.56 | 43.12 | 43.83 |
| RON | 87 | 92 | 96 | 99 |

Table 2. Specification of engine and exhaust measuring equipment's

| Details | Kirloskar, single-cylinder, 4 strokes, water-cooled and CI engine with 661 cc |
|------------------------------|---|
| Cylinder bore in mm | 87.5 |
| Stroke length in mm | 110 |
| Rated Power output in kW | 5.2 with 1500 rpm |
| Dynamometer arm length in mm | 185 mm arm length, eddy current, water-cooled. |
| Lube oil sump capacity | 3.7 l |
| AVL DI Gas Analyzer | AVL 444N, 11-22 V DC, 750 - 1100 bar, 5 °C - 45 °C range |
| Smoke Meter | AVL 437C, 0 – 100%, ± 1% full scale accuracy, 0.1% resolution. |

region is separated into a finite number of control volumes. Then, the physical space is completely covered by the grid and no free space is given between cells and overlapping of cells is prevented.

Control volumes are developed to evaluate the integrals of viscous, convective and source fluxes, general conservative equation has been rewritten as⁽⁹⁾.

$$\frac{\partial \vec{U}}{\partial t} = -\frac{1}{\Omega} \left[\int_{\partial\Omega} (\vec{F}_c - \vec{F}_v) ds - \int_{\Omega} \vec{Q} d\Omega \right] \quad (1)$$

Whereas

\vec{U} - Conservative variables

\vec{F}_c - Conservative variables

\vec{F}_v - Viscous/ diffusive vector

\vec{Q} - Source vector

$$\vec{U} = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho w \\ \rho E \end{bmatrix}, \quad \vec{F}_c = \begin{bmatrix} \rho V \\ \rho uV + n_x p \\ \rho vV + n_y p \\ \rho wV + n_z p \\ \rho H V \end{bmatrix}, \quad \vec{F}_v = \begin{bmatrix} 0 \\ n_x \tau_{xx} + n_y \tau_{xy} + n_z \tau_{xz} \\ n_x \tau_{xy} + n_y \tau_{yy} + n_z \tau_{yz} \\ n_x \tau_{xz} + n_y \tau_{yz} + n_z \tau_{zz} \\ n_x \Theta_x + n_y \Theta_y + n_z \Theta_z \end{bmatrix} \quad (2)$$

$$\vec{Q} = \begin{bmatrix} 0 \\ \rho f_{e,x} \\ \rho f_{e,y} \\ \rho f_{e,z} \\ \rho \vec{f}_e \cdot \vec{v} + \dot{q}_h \end{bmatrix} \quad (3)$$

The right-hand side of the above equation (1) has two integrals, one is the sum of approximated fluxes across the control volume and the other is the source term of the integral. For solving the above equation, the following strategies are followed in finite volume schemes⁽¹⁰⁾. Cell- Central scheme where all flow variables are stored in the cell centre Cell vertex scheme with median dual control volume, where the flow variables are stored in mesh vertices or nodes. Here the variables are categorized as conservative variables and dependent variables (pressure, temperature, specific heat, etc.) Another approach is for the evaluation of diffusive and convective fluxes. Here two interpolation methods are used which are named as Central discretization method-central arithmetic averaging Upwind discretization method – a technique which contains the character of the flow. The better method for viscous flux calculation is a central discretization scheme with a structured Cartesian mesh. For unstructured mesh, viscous flux can be approximated by Galerkin finite element method and finite volume method. The convective term also can be approximated through a central scheme, but this method might lead to odd-even decoupling. Due to this, upwind discretization is more appropriate for finding convective variables both in structured and unstructured mesh schemes.

The RANS equation turbulence model was engaged with the governing equation, along with the discrete droplet phase spray model was used. The model was considered in continuum approach by solving of Navier stokes equation. The dispersed phase is denoted by a number of particles during mass, momentum and energy exchange. Every considered droplet must represent its temperature, velocity, position, density etc⁽¹¹⁾.

The initial conditions of the above-mentioned parameters of each particle must be known. Here, fluid phase and particle phase equations are coupled and denoted by gas displacement by volume occupied and other was momentum exchange between the particles and gas phase.

2.2 Model Preparation and Problem Set-Up

CFD analysis using ANSYS FLUENT was carried out to analyze the diesel engine operations in HCCI Mode. As a primary requirement, an in-cylinder model was created in Solid Works and it was exported to ANSYS Fluent. The dimension and details for the geometry have been taken from the engine which is used for experimentation and is shown in Table 2.

The Computational Domain was created for all four strokes. The combustion chemistry was evaluated by the ICE simulation model in ANSYS Workbench Software. The simulation was initiated at the intake valve opening at 4.5° before TDC (IVC) with an initial pressure of 3.45 bar, Temperature of 404 K. And Inlet valve closes at 35.5° after BDC, and the exhaust valve opened and closed at 35.5° before BDC and 4.5° after Top Dead Centre (TDC). Fuel (C 6.8 H 16.5) was used as a surrogate for MTBE blended Gasoline and was injected 23 degrees before TDC. Engine rpm was kept constant at about 1500 rpm and its effect on unburned fuel was examined. Atomization of the fuel into small droplets is done and it penetrates the combustion chamber. The atomized fuel absorbs heat from the surrounding heated compressed air, vaporizes, and mixes with the surrounding high-temperature high-pressure air. The Injector was placed 12° inclined to the vertical axis, therefore the complete 3-Dimensional model was used for simulation instead axisymmetric model.

Following experimentations, the stepped piston model was used for this simulation as shown in Figure 3. Also, it shows the different states of moving mesh at a particular crank angle with valve operation. Totally, the domain consists of 212345 elements. The grid independent study was carried out for three various mesh counts, and the combustion chamber pressure was simulated and compared with experimental results. Finally, the above-mentioned 212345 elements case was produced a peak pressure of 62.3 bar which was had good agreement with experimentation of about 60.1 bar as shown in Figure 6.

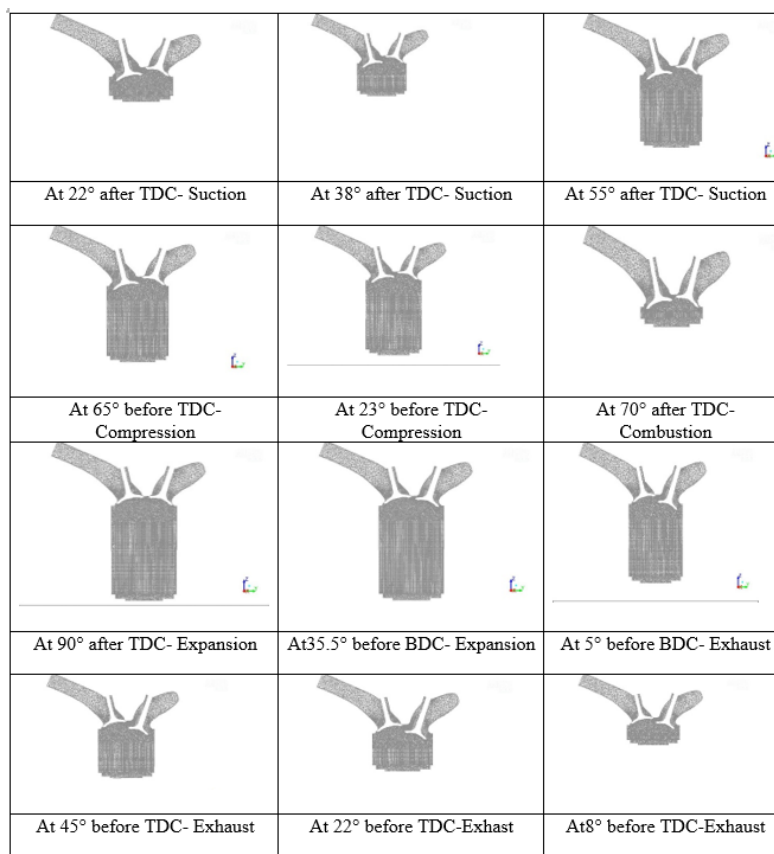


Fig 3. Mesh in different crank angles

3 Results and Discussion

This present numerical investigation focused on the effects on the combustion process of diesel engines at HCCI mode operated using MTBE15. The three-dimensional computational simulations were carried out using commercial Ansys fluent software.

The computational fluid dynamic simulation was carried out for the gasoline and IC engine-in cylinder model was followed for the simulation. The velocity, pressure and temperature contours were simulated for different crank angles.

Velocity Distributions inside the cylinder

Figure 4 shows the velocity distribution in the cylinder combustion chamber at different angles. The fresh mixture enters the chamber with a velocity between 50.5 m/s to 67.8 m/s during the inlet stroke. Also, the picture at 10° after TDC, At 22° after TDC- Suction and at 38° after TDC- Suction clearly indicated how the mixture entered and occupied the chamber. During Combustion and Expansion strokes, the velocity inside the cylinder dropped to below 20.5 m/s. Also, small perturbations were found at the end of the expansion stroke which is indicated at 65° before TDC in Figure 4. Compared with gasoline simulation, the MTBE blend circulated with little high velocity during expansion and exhaust stroke. During intake, both were found similar but after combustion, the velocity of the MTBE blend was identified as high as compared with gasoline. It is because of the density difference between gasoline and MTBE when it gets combusted.

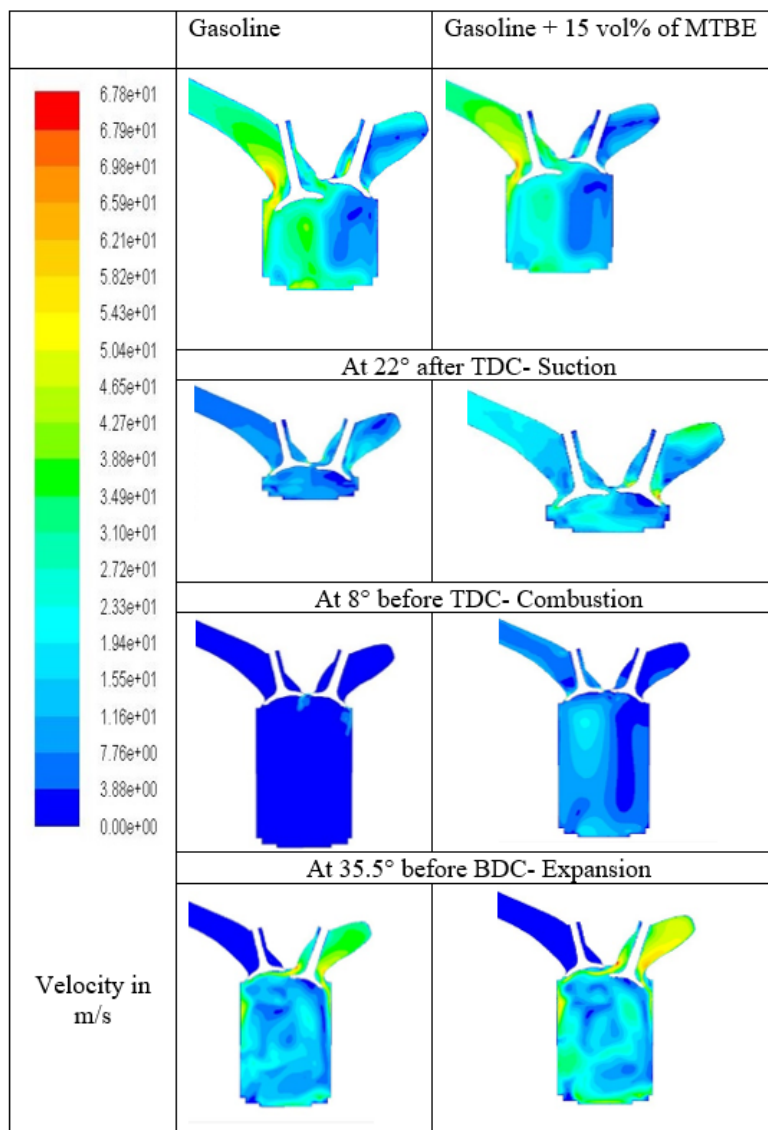


Fig 4. Velocity Contours at different crank angles

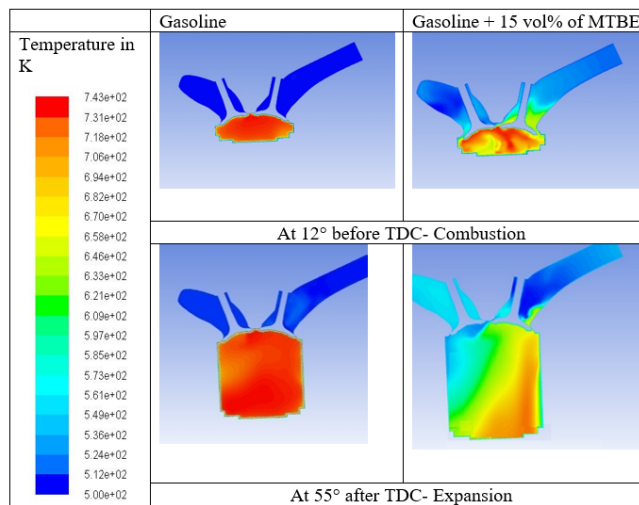


Fig 5. Temperature Distributions at Crank Angle

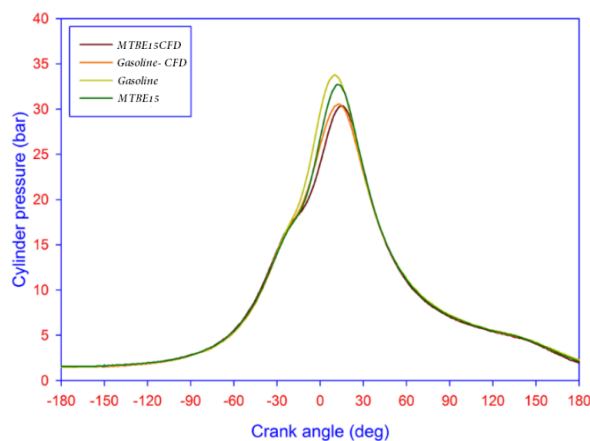


Fig 6. Cylinder pressure

3.2 Pressure distribution inside the cylinder

The in-cylinder pressure in CFD simulation for MTBE 15 is shown in figure 6 and it is compared with experimental results. Comparing both values, the pressure from CFD simulation was found high than experimental values. The reason for this deviation is unaccounted losses occurred in experimentation. The peak pressure with CFD simulation in Gasoline was about 35.4 bar whereas 30.5 bar in experimentations. But, both the peaks occurred between 365°CA and 367°CA . The peak cylinder pressure with the MTBE blend was noted as low than the gasoline simulation. The difference between CFD and experimentation for MTBE is 34.5 bar and 29.98 bar in 366°CA and 368°CA . The reason for early combustion in MTBE blend is low flash and fire points temperatures.

3.3 Temperature Distribution

Figure 5 shows the temperature distribution inside the cylinder, the maximum temperature found with the whole combustion is 743 K. From Figure 5, it is seen that the temperature inside the cylinder is sufficiently enough to vaporize the fuel droplets and ignite them when they entered the chamber. Also, the figure explains the temperature distribution at different crank angles such as during fresh mixture entering, compression, expansion and exhaust strokes. It is noted that the combustion chamber temperature was found high than gasoline combustion. The maximum temperature was between 732 K and 743 K. But, the

distribution of temperature was uniform with gasoline around 743K, but it was scattered for the MTBE blend. This is also because of the heterogeneous mixture of fuels.

3.4 NO_x Formations

Figure 7 indicates the NO_x formations from CFD simulations and it has been compared with experimental values with 50% loading conditions. The NO_x values from experimentations are found high than that of CFD simulation. But, both experimentation and simulated results confirm the low NO_x production with MTBE blends. This is because of the lower heat release rate from the MTBE blended combustion. The deviation between experimentation and simulation is not considering the unaccounted losses and cannot define the complete chemical structure of both fuels. The lowering of the NO_x is because of lowering the heating value of MTBE, which reduces the heating energy during combustion. This reduces the cylinder temperature thus reducing the NO_x formation.

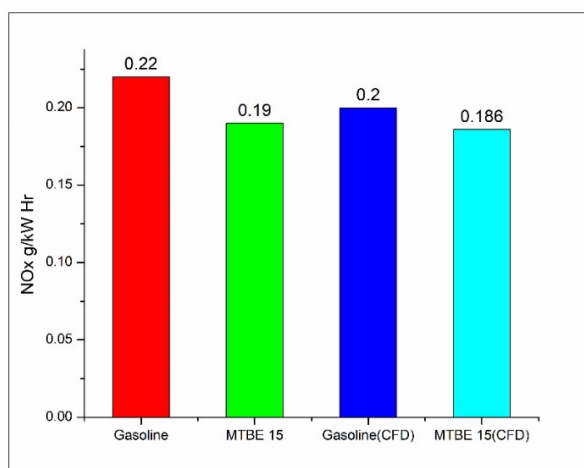


Fig 7. NO_x formation

3.5 CO Formation

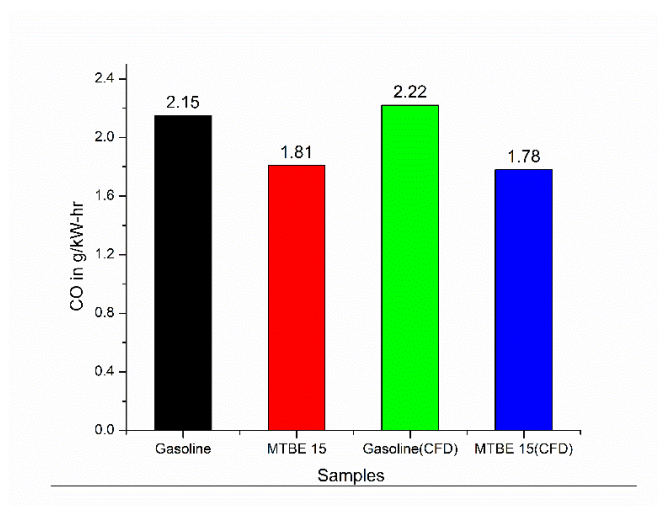


Fig 8. CO formation

The effect of MTBE on CO emission has shown in figure 8. The CO is found to be reduced when MTBE added to the gasoline. The maximum reduction was found up to 0.33 g/kW-hr in experimentation whereas 0.45 g/kW-hr in simulation. The deviation between the experimentation and simulation is to not define the complete chemical composition of MTBE in CFD codes. The MTBE could improve the fuel-borne oxygen leans the fuel-air mixture and enhances the better combustion thus reducing the CO emission.

3.6 HC Formation

The unburned hydrocarbon from HCCI combustion using both gasoline and MTBE15 were shown in Figure 9. Similar to CO, the HC was dropped when gasoline is mixed with MTBE. The maximum reduction was noted up to 2.5 g/kW-hr with experimentation and 2 g/kW-hr with CFD simulation. Normally, the HCCI combustion has a tendency to produce high CO and HC components in the exhaust due to a shortage of oxygen. But, it can be resolved by adding the MTBE with gasoline, because MTBE is oxygen-rich fuel for the gasoline engine. MTBE does not contain lead, so it will not produce any porous deposits. Also, MTBE molecules are polar, so it has not absorbed by un-polar molecules.

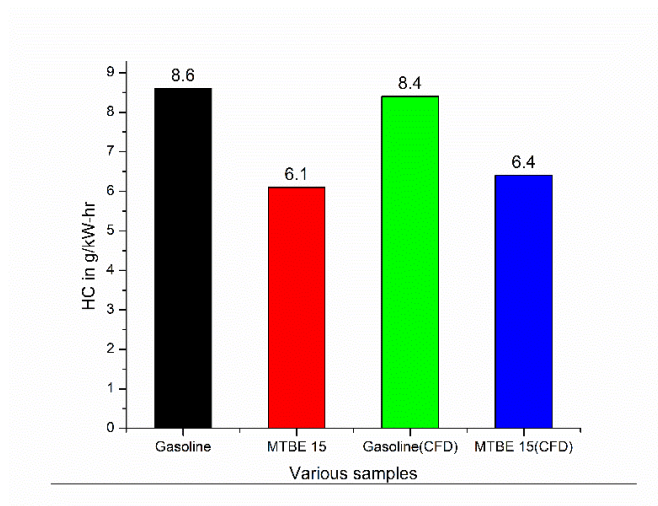


Fig 9. HC formation

3.7 Comparative analysis

Table 3. Comparative analysis of emission

| S.No | Samples | NOx in g/kW hr | CO in g/kW-hr | HC in g/kW-hr | Ref |
|------|---------------------------------------|----------------|---------------|---------------|---------|
| 1 | MTBE15 | 0.19 | 1.8 | 6.1 | Current |
| 2 | MTBE15(CFD) | 0.186 | 1.78 | 6.4 | Study |
| 3 | Ethanol+ Gasoline | 0.21 | 1.98 | 7.9 | (12) |
| 4 | Acetone-n butanol- Ethanol + Gasoline | 0.195 | 1.87 | 6.4 | (10) |

Table 3 indicates the comparative view of emissions from HCCI engines operated with gasoline and other blends. Normal ethanol and gasoline blends produced higher emissions compared with other blends as given in Table 3. Acetone-n butanol - ethanol + gasoline blends were identified very close to our MTBE blends. Generally, MTBE has good nature to mix with gasoline in order to combustion. From above table 3, it is clearly known that MTBE is a good supplement for the HCCI type combustion along with gasoline.

4 Conclusion

MTBE along with gasoline in HCCI mode combustion is a modest try for improving the performance and controlling the emission. This article is focused to analyse the numerical study for the diesel engine which has operated by an optimal gasoline-

MTBE blend. The deviation between the simulated values and experimental values is minimal. It may be occurred due to unaccounted losses, uncertainties, and limitations in experimentations. Also, the addition of MTBE along with gasoline in HCCI combustion produced better performance and controlled emission than other alternatives. The specific conclusion are follows:

- The velocity distribution was found uniform with gasoline fuel whereas scattered with MTBE blend, this is mainly due to density variation of the mixture. The average velocity was found high with the MTBE blends.
- Similarly, the cylinder pressure was found high with gasoline whereas low up to 4.5 bar to 5 bar with MTBE blend.
- The maximum combustion chamber temperature was found with Gasoline than MTBE mixture, this is due to the heterogenous nature of the MTBE blend. The average temperature inside the cylinder with gasoline about 743K. But, it is 695K for MTBE15.
- NO_x was found low up to 0.014 g/kW hr with MTBE blend simulation than gasoline simulation, this was mainly due to lower heat release rate from combustion.
- CO emission was found high with gasoline up to 0.44 g/kW-hr than MTBE 15. And HC emission was also found high with Gasoline up to 2 g/kW-hr than MTBE 15. This is mainly due to providing the oxygen-rich MTBE to better combustion.

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