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Emission Control Using Methanol, Ethanol And Butanol In Diesel Engine: A Comparison Through CFD Simulation

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***Abstract**:This present investigation is primarily focused on comparison of emission reduction in diesel engine by biofuels namely Methanol, Ethanol and Butanol when added to diesel as blends with the help of CFD simulation. The simulation is performed on a 1.9L, four-cylinder direct injection diesel engine using a commercial code AVL FIRE for a rectangular piston geometry . To perform the combustion simulation, hexahedral mesh of engine bowl shape was created using AVL FIRE ESE diesel module. Further, ECFM-3Z type of combustion model based on laminar flame let concept is applied in the present work. The three fuel Methanol (D+M), Ethanol (D+E) and Butanol (D+B) are blended to diesel in the ratio of 5% (M5, E5 and B5) and 10% (M10, E10 and B10) by volume. The effects of these blended fuels on the emission such as NO, SOOT, CO and HC are compared. The results indicated minimum value of NO while using 5% Methanol and 10% Ethanol with Diesel whereas Soot increased while using with Methanol, Ethanol and Butanol with blends compared to pure diesel fuel. Peak value of HC (Hydrocarbons) was recorded by using pure diesel fuel compared with other blends. Pure diesel fuel indicated higher CO values compared with blends while blends were same at 5% by using methanol and butanol whereas decreased for 10% blends of Ethanol, Butanol and Methanol respectively. In general, it can be concluded that 5% Methanol is suitable quantity to blend with diesel while any one can be choose as fuel with 10% blend as it reduces emissions at comparatively up to sufficient level.*

***Keywords:-** Diesel, Diesel - biodiesel blends, CFD approach*.

I. Introduction

In the wake of stringent emission norms and rapidly dwindling fossil fuel reserve, researchers around the world are keen to find alternative fuels for diesel engine so that their emission levels can be brought down further while preserving the engine performance. As a renewable and oxygenated biofuel such as Methanol, Ethanol and Butanol can be considered as prospective fuel for vehicle, which can be blended with diesel or be injected into the engine cylinder directly. There are numerous experimental studies on the application of these biofuel in diesel engine, which focus on the three aspects particularly properties of diesel - biofuel blends, techniques through which these biofuel being applied in diesel engine and their effects on the combustion and emission characteristics of diesel - biofuel blends.

As on increasing demand of biofuels, one should think about the alcohols those have similar properties like diesel fuel and tendency to reduce emissions then diesel fuel burn alone. Number of experiments with biofuels increasing year and year, and have shown good impact by using blends in terms of performance parameters and emissions reduction. Sahin et.al, 2015 [1] used Low ratio butanol - diesel blends which have been investigated experimentally under varying loads and speeds concluded that smoke was low with blend of nb4 (4% butanol + 96% diesel by volume) at 2500 rpm while NO_X reduces at 2000, 3000 and 4000 rpm with nb4 blends. Yilmaz et al, 2014 [2] used butanol as blend in biodiesel and diesel at different engine loads in which it seems to get reduction by using butanol blends in NO emissions but CO and HC were higher side compared with neat biodiesel. In case of low concentration of butanol-diesel blends (say 5% and 10%), result reported low CO and high NO but no significant change in HC. Zheng et al, 2015 [3] carried out experimental investigation at two injection pressure by using four different fuel (pure diesel and blended fuels of diesel/gasoline, diesel/n-butanol, diesel/gasoline/n-butanol) and showed that smoke emissions of blended fuels were highly dependent on post injection strategies compared to pure diesel. Choi et al, 2015 [4] employed diesel fuel blend with n - butanol (10% and 20% by volume) in turbo charged common rail direct injection diesel engine used and results were compared with neat diesel fuel. Result concluded that 20% butanol increases HC, CO and NO compared with the neat diesel fuel while 5% butanol could be a better option to reduce PM. Sharon et al,2013 [5] varied proportion of butanol with diesel and collected palm oil from different restaurants, used in a diesel engine and concluded that fuel property of blends were better than used palm oil. It also concluded that by increasing butanol content in blends, increases brake thermal efficiency and decreases CO, NO_X and smoke opacity compared with diesel fuel. Sahir et al, 2015 [6] used a ternary blend fuel (biodiesel is used as an additives in diesel alcohol blend) which have similar property as diesel fuel and significantly reduced PM (particulate matter) emissions from diesel fuel but other emissions were similar to diesel fuel and depends on operating conditions of engine. Morsy, 2015 [7] carried out an experiment by using ethanol - water mixture fumigation technique with inlet air, which had been done by different mixing ratios and result indicated that NO and exhaust gas temperature tend to decrease while CO, HC emissions and fuel consumptions tend to increase with pure ethanol / water fumigation. Herraros et al, 2015 [8] worked with high cetane number and oxygen content DGE (di ethylene glycol di ethyl ether) fuel which had tendency to reduce gaseous emissions and simultaneously reduction in both soot and NO_X. Shaafi et al,2015[9] carried out Experimental investigation by using two modified fuel blends diesel soya bean biodiesel and diesel soyabean biodiesel ethanol blends with alumina as a nano additive and result showed high NO_X at full load but reduction in CO,HC due to presence of oxygen in soyabean oil and mixing ability of nano particles. Tse et al, 2015 [10] studied comparison between DBE (diesel-biodiesel-ethanol) and ULSD (ultra-low sulfur diesel), and concluded that DBE has tendency to reduce PM and NO_X emissions. Sarjovaara et al,2015[11] used ethanol/gasoline blend (E85) which was injected at low pressure in to intake manifold and ignited with diesel at high/low load condition. Results concluded that E85 increases CO and HC emissions while reduce NO and soot emissions at all loads. Motlagh 2014[12] carried out a numerical investigation by using gasoline with ethanol by considering a jet stirred reactor and revealed that the emission of CO_2 and CO can be reduced by ethanol blending where as H_2O concentration increases with decreasing C/H ratio by ethanol addition. Qi et al, 2010[13], carried out experiment by using methanol as an additive with 5% and 10% by volume in biodiesel diesel mixture (BD50% = 50% biodiesel and 50% diesel in vol). The results indicated reduction in power, torque, smoke and CO emissions while HC and NO_X emissions of BDM5 and BDM10 were similar to those for BD50 at full engine load. An et al, 2015 [14] had an numerical simulation which concluded reduction in CO and soot emissions with 5% methanol at all load conditions while methanol was used with 5% and 10% volume, under loads of 10%, 50% and 100% with fixed engine speed of 2400 rpm. Liu et al, 2015[15] analyzed dual fuel operation in which Methanol used with air to form air/methanol lean mixture and then ignite with diesel in engine which revealed reduction in NO_X and soot at low injection pressure while soot, CO, HC were decreased and NO, CO_2 increased with high injection pressure as compare to diesel alone. Sayin et al ,2009 [16] used methanol blended diesel fuel from 0% -15% with increment of 5% were used at different injection timings and loads. Study concluded that Brake specific fuel consumption, NO_x and CO_2 emissions were increased while Brake thermal efficiency, soot ,CO and HC emissions were decreased with increasing percent of methanol in the fuel mixture. Wu yu et al, 2011[17] used a cetane number improver (0.3% and 0.6%) with Biodiesel -Methanol blend (30% methanol) in an experiment and result showed reduction in CO and HC emissions where as NO and Soot increased slightly.

Above literature survey concluded that Methanol, Ethanol and Butanol has tendancy to reduce level of emissions compared to neat diesel when engine works with diesel alone. Some researchers used them as an additives to work with diesel - biofuel blends because they are capable to affect the engine combustion characteristics, performance and emissions of a direct injection diesel engine under variable operating conditions. Fumigation techniques are showing good impact on emissions while some of these blends were fumigated with inlet air via intake manifold.

This numerical study shows combined effect of Methanol, Ethanol and Butanol on a same engine geometry which was meshed by AVL FIRE CFD code. Two different blends of biofuels by volume basis has been numerically investigated and simulation can suggest the better one out of these three biofuels. The aim of this simulation to investigate the effects of 5% and 10% blends of biofuels (Methanol, Ethanol and Butanol) with diesel in hexahedral meshed rectangular piston geometry on emission characteristics under same operating conditions. As all three biofuels used frequently in to the engine, so it is necessary to use simulation first rather than experiments to predict better fuel.

II. Validation

Validation is carried out by using a GM diesel engine model Table 1. The results of the simulation are compared with experimental results; which was conducted on the same engine at Argonne National Laboratory [18]. Following fig 1, show good agreement between experimental and simulated results in terms of in cylinder pressure and temperature at 1500 rpm.

Table 1. Engine data

Bore	82 mm
Stroke	90.4 mm
Connecting rod length	145.4 mm
Engine speed	1500 rpm
Compression ratio	16.8
Fuel	C_7H_{16}
Spray cone angle	9°
Mass of fuel	1.2495e-06 kg
Injection duration	8.5°

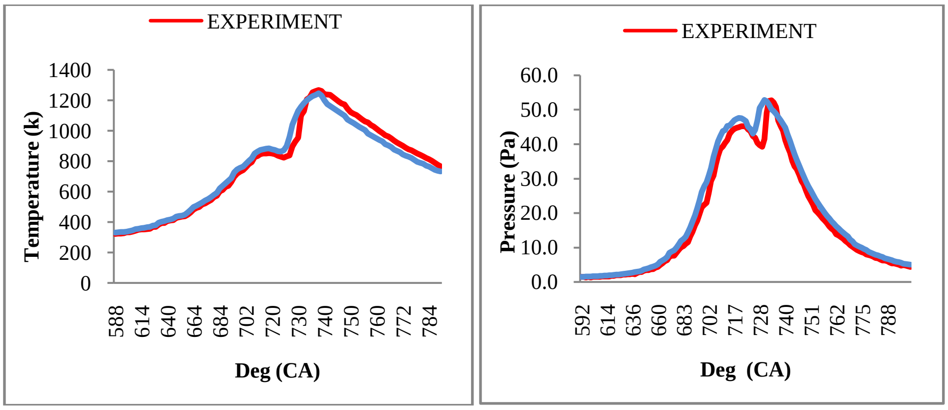

***Figure 1.** Comparison of cylinder pressure (Pa) and temperature (K)*

III. Description of the CFD models

A 4.1 L, 4 cylinder, DI diesel engine has been modeled with rectangular piston geometry shown in Fig 2. The specifications of the engine are given in Table 2. In order to perform the combustion simulation with less time consuming cell size , hexahedral mesh of rectangular bowl geometry with 35976 cell size is created using AVL FIRE ESE diesel module shown in Fig 3. Grid independency test was conducted for three different cell sizes 35976, 58452 and 78332 of the same geometry and the cylinder pressure is depicted in Fig 4 for the three meshes; the variation in pressure is found to be ±1%.Thus, the simulation was carried out with cell size of 35976 to reduce the process time. Models used in the simulation are listed in Table 3.

Present work uses a three zone coherent flam let combustion model ECFM-3Z shown in Fig 5. It is a type of combustion model based on laminar flame let concept and used to solve the problems regarding chemistry and turbulence inside combustion chamber. The flame let models assume that reaction takes place in a relatively thin layer separating unburned gases from the burned gases[19 -20]. ECFM-3Z model is applicable for auto ignition cases. This model has capability to handle both ignition procedure i.e. auto ignition and spark ignition. A non linear and extended eddy viscosity turbulence model, K-zeta-f model has been used in the simulation instead of standard K-ε model due to its reliability.

***Table 2:** Engine specifications*

Bore	0.105 m
Stroke	0.120 m
No. of cylinders	4
Displacement volume	4.1 L
Connecting rod length	0.200 m
Compression ratio	16.00
Swirl ratio	1.6
Engine speed	1800 rpm
Fluid mass	1.7286e-05 Kg

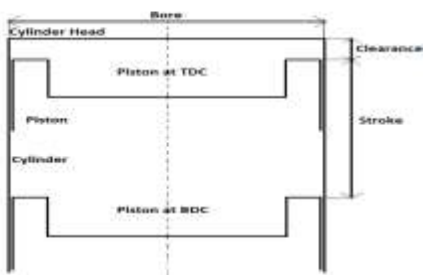

***Figure 2**. Geometry of piston having rectangular cavity.*

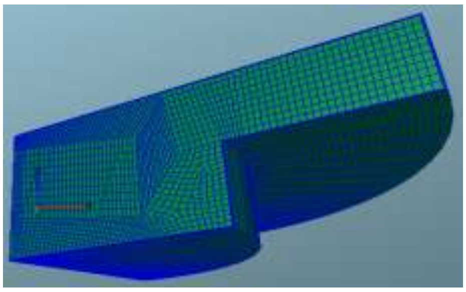

Figure 3. *Computational grid at TDC*

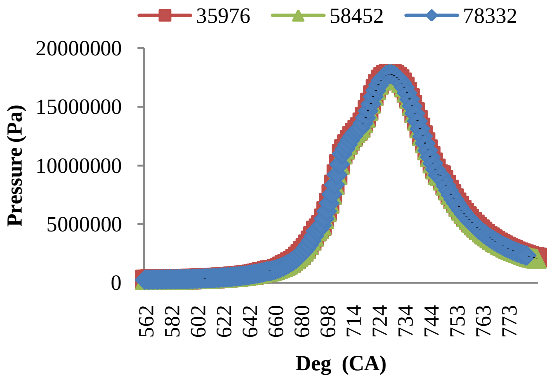

Figure 4*. Grid independency test.*

Table 3*: Models used.*

Model	Use
ECFM-3Z	Combustion
K-ZETA-f	Eddy viscosity Turbulence
Kinetic Soot Model	Soot formation and Oxidation
Dukowicz model	Droplet evaporation
Wave model	Droplet break up
Zeldovich mechanism	NO emission model

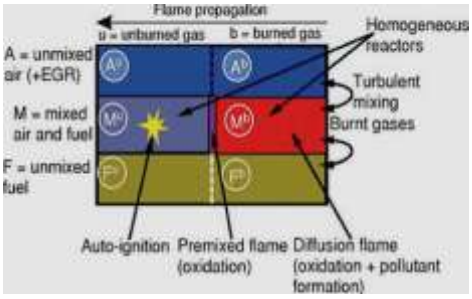

Figure 5*. ECFM-3Z Model computational cell*

Kinetic soot model is based on chemical kinetics which has been applied for the calculation of soot formation and oxidation of present simulation. This model has ability to solve behavior of soot formation and oxidation for different fuel classes [20]. Dukowicz model [21], wave model [19] and Zeldovich mechanism is applied for droplet evaporation, droplet breakup and NO emission formation respectively in present simulation. For the simulation of compression and power strokes, the volume of gases has been considered enclosed between three wall boundaries namely piston, cylinder head and liner. In order to close the system of equations, boundary conditions needs to be prescribed at these boundaries; the temperatures of cylinder head and piston are 570.15 K and that for the liner is 470.15 K.

IV. Result and discussion

Numerical study is carried out by using three biodiesel with diesel fuel at two blends of 5% and 10% by volume basis and result has been summarized by following figures.

Table 4: Comparison of fuel properties [22]

Properties	**Methanol**	**Ethanol**	**Butanol**
Chemical formula	CH_3OH	C_2H_5OH	C_4H_9OH
Molecular weight	32.04	46.07	74.12
Oxygen content, wt%	49.93	34.73	21.59
Carbon content, wt%	37.5	52.2	64.8
Hydrogen content, wt%	12.5	13.1	13.5
Stoichiometric AFR	6.43	8.94	11.12
Lower heating value, Mj/kg	20	27	33
Heat of evaporation, Kj/kg	1178	840	578.4
Research octane number	112	111	113
Motor octane number	91	92	
Vapor pressure (psi at 37.7)	4.6	2	0.33

V. NO Emissions

It can be seen from Fig 6. that NO emission can be control by using biodiesel as part of fuel. Results reported reduction in NO emission when biodiesel used with diesel than diesel alone. M5 takes heat from combustion chamber to burn itself which causes reduction in cylinder temperature inside combustion chamber. Reduction of temperature reduces formation of NO too [22-24] , however some studies show other face of NO emissions. Researches indicates high NO formation due to high oxygen content in methanol fuel [25]. Similarly presented study is also showing high NO when volume of blend is move from 5% to 10%. It has been seen that the effect of temperature is dominating over oxygen content effect because of 5% blend but in case of higher side i.e. 10% blend oxygen content effect is dominating over temperature. Result clearly indicating towards use of 10% ethanol is better than other fuel while using same blend ratio with methanol and butanol. E10 is choose as a appropriate fuel because it has high miscibility (mixability) with diesel in all proportion of blends and high cooling effect at high blends. This proper mixing results to further reduction in temperature as well as NO emissions.

VI. Soot Emissions

Soots are defined as unburned carbon particles. Increasing ratio of blends from 5% to 10% results to decrease in cylinder temperature than diesel alone. Reduction of temperature results in high number of unburned carbon particles inside combustion chamber those incorporated with soot at the exhaust. As shown in Fig 7, increasing blend ratio of methanol from M5 to M10 results in high soot formation. Same trend of high soot formation is recorded with E5, E10, B5 and B10 as well.

VII. HC Emissions

HC emissions are present in exhaust due to incomplete combustion of the fuel. Methanol, Ethanol and Butanol are high oxygenated fuel and responsible to increase the amount of oxygen inside combustion chamber. It can be seen from Fig 8, that HC emissions are decreased while diesel used with biodiesel at 5% and 10% blends by volume. Results are not showing any major difference of HC emissions as diesel used with Methanol, Ethanol and Butanol because all three fuels are oxygenated which results to proper mixing of fuel with air and provide sufficient amount of oxygen for complete combustion of the mixture.

VIII. CO Emissions

CO emissions found in exhaust gases because of partial oxidation of fuel rich zone inside combustion chamber. It can be seen from Fig 9 that M5 and M10 blends decreases CO emissions when compared with pure diesel. As discussed above that Methanol is one of the high oxygenated fuel and permits proper mixing inside chamber, thus it prevents the formation of fuel rich zones inside chamber reduce partial oxidation as well. Addition of more oxygen take place while blend of Methanol moved from M5 to M10, leads to complete combustion of fuel rich zones which results to reduction in CO emissions. It is also important to see that methanol is high oxygen content fuel (49.93 %) compared with Ethanol (34.73 %) and Butanol (21.59 %), So Methanol can be used as good CO emission reducer than Ethanol and Butanol as shown in Fig 9.

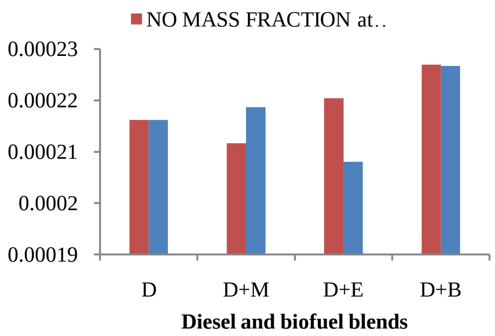

Figure 6. NO Emissions

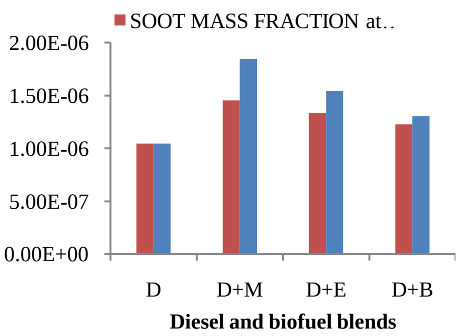

Figure 7. SOOT Emissions

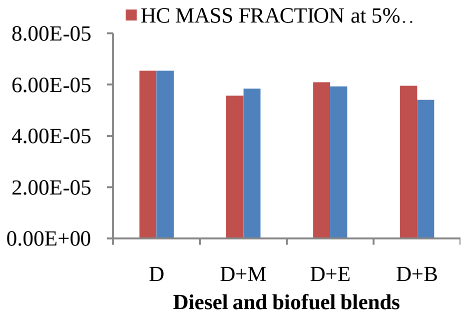

Figure 8. HC Emissions

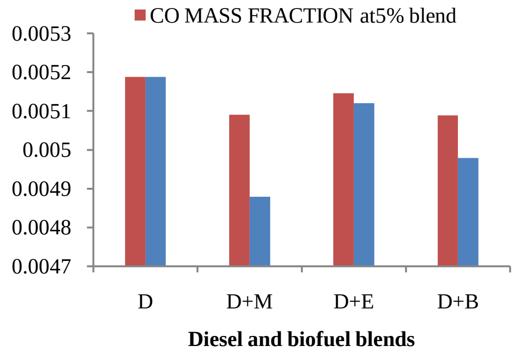

Figure 9. CO Emissions

IX. Conclusions

Present study predicts the emissions characteristics of three biofuels under same operating condition and at two diesel - biofuels blends. There is change in every parameter of emission which have been discussed above while amount of blend increased from 5% 10%. Conclusion can be done by following two ways-

1. ***Emission specified conclusion:-***

In case of NO emissions, E10 is showing promising results over other blends while working with 5% blend ,M5 will be a good option. Soot is showing just reverse effect of NO emission because both are temperature dependent but in opposite manner. Butanol is reducing much soot formation comparison other fuels in both blends of B5 and B10. As discussed earlier, HC is same for all fuels at all blends so any one blend can be use appropriately when reduction of HC emissions is prime motive. It is obvious to use Methanol to reduce CO emissions from exhaust compared with other fuels but M10 is looking better than M5.

2. ***Blend specific conclusion***

If engine has to run with only one blend at a time to reduce emissions than one should use M5 blend as it reduces NO, HC and CO up to some extent comparison to other fuels at same percentage of blend. As it can be seen from results that it is very difficult to choose a single fuel when engine has to run with 10% blend as Ethanol is effective with NO, Butanol seems good with soot and Methanol is showing considerable reduction in CO with compare to other fuels of 10% blend. So any fuel can be used with blend of 10% in a diesel engine.

Finally it can be concluded from above study that M5 is best option for 5% blend while at 10% blend, choice is depends up on aim to reduce specific content emission from exhaust gas of the engine.

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