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Mathematical Modelling and Analysis of Diesel-Biodiesel-Ethanol blends and ZnO Addition effects into the Combustion and Emissions Characteristics in CI Engine

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Abstract: Increasing interest in diesel engine technology and the continuous demand of finding alternative sustainable fuels as well as reducing emissions has motivated over the years for the development of numerical models, to provide qualitatively predictive tools for the designers. Among the alternative fuels, biodiesel especially second generation biodiesel is considered as a sustainable and the most promising option for the diesel engine.

Biodiesel is a bio-fuel which has similar properties to diesel and can readily be used in a diesel engine with minimal modifications. Promising results have been determined using mixtures of biodiesel and diesel with the reduction of soot and emissions of a diesel engine. Experimental analysis of diesel engines can be expensive and therefore Computation Fluid Dynamics programs are used to analyze the combustion process. Present Study deals with the effect of zinc oxide nanoparticle addition to diesel-biodiesel-ethanol blends by using Computational Dynamics Method. In the current study, we investigate that as we increased the percentages of Bio-fuels and Ethanol the efficiency of the blended fuel is increasing and pollutant like COx and NOx are decreasing which shows solubility test as in a previous work was stable.

In a CI engine, the NOx emission is one of the major pollutants and is predominantly influenced by the amount of oxygen available and the in-cylinder temperature. The NOx emission is composed of NO, NO2, N2O, N2O5, NO3. Nitric oxide is the major constituent and NO2 is a minor constituent, while the others are negligible. At elevated temperatures (i.e.) above 1500 C, N2 can react with O2 faster and may result in more NOx emission. As CI engines have a higher compression ratio and are lean burn engines, the peak temperature is well above 1500 C; hence, there is a higher NOx formation. In present work the evaluation of the NOx (Prompt and Thermal) is also carried out we investigate from CFD Results that NOx percentages are decreasing with the addition of ZnO (225 ppm) and higher no. of BDE because as the temperature is getting higher the N-O bond will we collapsed due to this Nitrogen is released to the environment, hence NOx percentage is decreasing from lower no. of BDE to the higher no. of BDE

Key words: Biodiesel; Ethanol; Diesel-biodiesel-ethanol blends; Zinc oxide nano particles, CI engine, Ansys (Fluent).

I. INTRODUCTION

In recent times there is an extensive focus on developing sustainable energy supply options and reducing the global reliance on non-renewable fossil fuels with finite reserves, as well as reducing the effects energy production has on global warming, largely related to the burning of these fossil fuels. The transport industry relies very heavily on the use of oil, and in particular the oil derived fuel diesel, used in a large number of trucks, buses, trains and ships as well as an ever growing number of cars. It is essential that a sustainable alternative fuel source is to be developed to reduce the global dependence on oil, particularly as cheap and reliable oil supplies are reducing. Second generation biodiesel is a significant step forward in the quest to develop a sustainable alternative fuel source. It can be used in unmodified diesel engines; it has been shown to substantially reduce exhaust emissions of carbon monoxide, carbon dioxide, hydrocarbons and particulate matter, so it is good for the environment. It could have a number of economic benefits through increasing the stability of Australia’s fuel market, creating new industries and jobs in both refineries and agriculture, without impacting significantly on food supplies. The second generation biodiesels are mainly produced from non-edible oils. and sometimes produced from waste or recycled oil and animal fats . The biodiesel produced from non-edible oil has gained the attention due to the problems associated with food versus fuel, environmental and economic issues related to edible oils. Moreover, non-edible vegetable oils are considered over the edible vegetable oils due to its low feedstock cost .Unlike first generation biodiesels, this means they have minimal or no impact on food supply or food prices. The Australian BLS (Calophylluminophyllum) has a high potential for large scale second generation biodiesel production as it can tolerate harsh environmental conditions such as drought, salinity, acidity and a large range of temperature, requires little maintenance, is non-edible, has a large yield of fruit of around 3,000-10,000 seeds/tree/year and has high kernel oil of around 65%. The wild tree lives for up to 200 years, producing fruit twice a year. The BLS is estimated to be able to produce up to 4,000 litres of oil per hectare per year. Modern diesel engines can run on biodiesel and biodiesel blends with no modifications, however the performance, efficiency and emissions can all be optimized by making adjustments within the engine. There are a range of different parameters that can be adjusted to optimize the compression ignition (CI) engine running on biodiesel, including fuel injection timing, injection pressure, air-fuel ratio, crank angle and combustion chamber geometry such as piston, piston ring, cylinder head, inlet and outlet valve. Some recent studies have investigated the performance and emission characteristics of biodiesel engines at different engine speeds, loads and biodiesel ratios. These results indicated that the engine performance is sensitively affected by the ratio of biodiesel in the fuel. Nevertheless, there is no shortcut way to determine the optimal biodiesel ratio because the factors (e.g., fuel cost and amount of exhaust emissions) are opposing each other . It is the only way to determine the optimal biodiesel ratio by conducting numerous experiments on a dynamometer subject to the user's requirements. Therefore, creating a computational model for biodiesel engines may be the best solution to the above abridgement because the optimal biodiesel ratio can then be determined by applying computer-aided optimization method to the engine model. However, the main aim of this study is to develop a combustion model to maximize the combustion performance of an automobile engine fuelled with second generation biodiesel produced from BLS. The computational fluid dynamics (CFD) model for the turbulent combustion of biodiesel in an internal combustion engine will allow a range of benefits to be evaluated and be a guide for engine manufacturers, biodiesel producers, biodiesel users and policy makers. Some of these benefits include improving internal combustion engine technology, reducing harmful gas emissions, and increasing fuel efficiency, sustainability and optimum uses of second generation biodiesel as engine fuel. Biodiesel from vegetable oils is one of the renewable fuels that can be used in a diesel engine with or without some minor modifications. Using Biodiesel increases the oxygen content resulting in better combustion. Other properties of biodiesel are also similar to diesel. However, higher viscosity and density of the biodiesel lead to higher BSFC and higher smoke emissions. To minimize this limitation, one alternate method is addition of ethanol. The addition reduces the viscosity and density of the blend and becomes similar to diesel. Biodiesel-diesel-ethanol blends produce lesser emissions of smoke and NOx emissions compared to diesel, due to addition of ethanol. More and more consumption of fossil fuels evacuate the oil reserves at a rapid rate. The projections of 30 year period of 1990–2020 from a survey resulted that the demand of fossil fuel will be three times and will give a severe impact on environment. Also the author suggested that biodiesel from vegetable oils is potential source for alternate fuels to replace or reduce the consumption of diesel . Chong et al. studied the Debnathetal.investigated the effect of emulsified palm oil methyl ester. Due to emulsification, better efficiency was observed along with the reduction in BSFC. Also, NOx emissions were reduced as the water reduces the cylinder temperature. Lesnikanalyzed the influence of biodiesel on the injection characteristics advancing injection timing increases the in-cylinder pressure. There was a reduction in CO emissions and increase in NOx emissions. Also, the EGT was reduced due to lower calorific value of the fuel.\ Nagaraja et al. studied the effect of compression ratio on preheated palm oil biodiesel blends. Results showed that the brake power of palm oil biodiesel-diesel blend is higher than that of standard diesel at higher compression ratio and full load condition. There was an increase in mechanical efficiency and thermal efficiency and indicated mean effective pressure. Also, there was a reduction in CO and unburned hydrocarbon with increase in CO_2 emissions

II. LITERATURE

1. B. Prabakaran *, AnuragUdhoji- This study is to investigate the effect of zinc oxide nano particle addition to diesel biodiesel-ethanol blends. Solubility tests were done for the fuels at three different temperatures. Out of eighteen blends, six blends were stable at 5 _C, 15 _C and above 25 _C. Out of the six blends, two blends were checked for properties as per ASTM standards. One of them was chosen for testing the performance, combustion and emission characteristics in a diesel engine. In the same blend, zinc oxide was added in the amount of 250 ppm. Property testing of the blended fuel indicated that there was an increase in calorific value due to addition of nano particle. The performance tests were conducted on a single cylinder four stroke direct injection diesel engine at a constant speed of 1500 rpm. For the blend containing zinc oxide, there was an increase in BSFC, HRR and cylinder pressure. Also, there was a decrease in BTE, NOx and smoke, as compared to diesel. The addition of zinc oxide nano particles increased the BTE and decreased the BSFC as compared with the biodiesel diesel ethanol blend at full load. This study gives a direction to utilize the

renewable fuel to reduce the consumption of fossil fuel. 2.C. A. Harch, M. G. Rasul*, N. M. S. Hassan, M. M. K. Bhuiya- Increasing interest in diesel engine technology and the continuous demand of finding alternative sustainable fuels as well as reducing emissions has motivated over the years for the development of numerical models, to provide qualitatively predictive tools for the designers. Among the alternative fuels, biodiesel especially second generation biodiesel is considered as a sustainable and the most promising option for diesel engine. In this study an engine combustion model has been developed using computational fluid dynamics (CFD) software, AVL Fire, which can predict the engine performance, and emission characteristics for second generation biodiesel produced from Australian native beauty leaf seed (BLS). This model involves simulation of fuel atomization, burning velocity, combustion duration, and temperature and pressure development in a combustion chamber. The model has been developed for petroleum diesel (normal diesel used in automobiles), 5% BLS biodiesel (B5) and 10% BLS biodiesel (B10) for different injection timings and compression ratios. The simulation results revealed that overall B10 biodiesel provides better performance and efficiency, and significantly reduced engine emissions. On the other hand, the B5 blend provides slightly improved performance and efficiency, and moderately reduced emissions compared to petroleum diesel. 3. Dean Bishopa, RongSitua*, Richard brownb, Nicholas Surawskic- Biodiesel is a biofuel which has similar properties to diesel and can readily be used in a diesel engine with minimal modifications. Promising results have been determined using mixtures of biodiesel and diesel with the reduction of soot and emissions of a diesel engine. Experimental analysis of diesel engines can be expensive and therefore Computation Fluid Dynamics programs are used to analyses the combustion process. The AVL Fire ESED program is currently being employed to investigate the effects of biodiesel on the diesel engines soot, emissions and power generation from a Cummins ISBE220 engine. Investigation is performed on pre and post injection-rate shapes on the combustion process establishing the results correlate accurately with researched data. A pre injection was determined to increase maximum power, reduce combustion generated noise, increase early in cylinder temperature and reduce fuel consumption due to the increase in power. A post injection was verified to reduce soot emissions while increasing NOx emissions marginally. The investigation of the injection-rate shape established the soot- NOx trade-off which was also found in the research. The models developed were agreeable with biodiesel data with percentage error in indicated power ranging from 1.62-8.85%. The models suggested that biodiesel assists in reducing NOx and soot emissions. The soot- NOx trade-off was further investigated determining the theory that then by reducing the combustion temperature in the combustion chamber the NOx emissions can be reduced while increasing soot emissions. By increasing the temperature in the combustion chamber the opposite effect was found to occur. 4. SzuhánszkiJ.a, Black S.a, Pranzitelli A.*a, Ma L.a, Stanger P.J.a,b, InghamD.B.a, PourkashanianM.a- The utilisation of biomass in coal-fired power plants can mitigate CO2 emissions, especially when combined with carbon capture and storage (CCS) technologies, such as oxy-fuel combustion. In this paper, a commercial computational fluid dynamics software was used, with small or no modifications to the physical submodels, to predict the performance of a 500 MWe sub-critical coal fired boiler under air and oxy-fuel conditions when firing coal, biomass, and a 20% biomass blend, for the same thermal input. The results suggest that for a wet recycle retrofit, the optimum oxygen concentration lies between the simulated range of 25 and 30%, where heat transfer characteristics of the air-fired design could be matched when firing either coal or a 20% biomass blend. However, for 100% biomass firing modifications of the firing arrangement may be necessary to achieve an output closer to the original design.

III. OBJECTIVE OF THE STUDY

In previous research reference [1] various blend grade (as per ASME Standard) has been investigated at constant Peak load and different temperature stages was also checked on the basic of combustion efficiency and emission rate. In the reference work we have seen that all the cases are not stable in various temperature stages. In present work our main objective is to analyze those stable cases which are shown Stable in all Temperature phases, improved results or better efficiency and less emission rate. For Simulation we have used Ansys (Fluent14.5) as CAE tool and model is simulate using Computational fluid Dynamic Technique for Investigating the performance of Diesel-Biodiesel(Palm Oil Methyl ester)- Ethanol with additives Nano particle (ZnO) on the basic of various Parameters like Static Temperature, Energy , and emission rate of Cox and NOx. All the Dimension, Boundary condition, Material specifications, Fuel property is taken from reference [1]

IV. METHODOLOGY

A. Basic Steps to Perform CFD Analysis

1) *Pre-processing: CAD Modeling:*Creation of CAD Model by using CAD modeling tools for creating the geometry of the part/assembly of which you want to perform FEA.CAD model may be 2D or 3d.

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2) *Meshing:* meshing is a critical operation in cfd. In this operation, the cad geometry is discretized into large numbers of small element and nodes. The arrangement of nodes and element in space in a proper manner is called mesh. The analysis accuracy and duration depends on the mesh size and orientations. With the increase in mesh size (increasing no. Of element), the cfd analysis speed decrease but the accuracy increases.
3) *Type Of Solver:* choose the solver for the problem from pressure based and density based solver.
4) *Physical Model:* choose the required physical model for the problem i.e. Laminar, turbulent, energy, multi-phase, etc.
5) *Material Property:* choose the material property of flowing fluid.
6) *Boundary Condition:* Define the desired boundary condition for the problem i.e. Temperature, velocity, mass flow rate, heat flux etc.
7) *Solution*

a) *Solution Method :* choose the solution method to solve the problem i.e. First order, second order
b) *Solution Initialization:* initialized the solution to get the initial solution for the problem.
c) *Run Solution:* run the solution by giving no of iteration for solution to converge.

8) *Post Processing:* for viewing and interpretation of result. The result can be viewed in various formats: graph, value, animation etc.
9) *Cfd Method Applied :*the model was simulated and the required geometry configurations were pre-processed in ansys 14.5. This following section illustrates the method used in the cfd simulations in this particular study.

a) *Step I Geometry Or Model Formation:*the study focuses on the to calculate the cox and nox percentage and the geometry used for the simulations is therefore only a part of the whole exhaust gas system in order to save computational time. The generation of the model by using ansys shown below:-
b) *Step 3 Checks The Mesh:*Various Checks on the mesh and reports the progress in the console. Also check the minimum volume reported and make sure this is a positive number select mesh to mm.
c) *Step 4 Simulation Set Up*

10) *Boundary Conditions*

a) Mass flow inlet: - mass flow rate is 1 kg/s,
b) Outlet – pressure based, pressure outlet.
c) *material:* specification of the nano- particle (zno) is taken from reference[1]

Nano particle specifications.

Chemical formula	ZnO
Purity	99.9%
Average particle size	30 nm
Density	5.606 gm/cc
Color	White
Crystal phase	Single crystal

Table 1

Properties of fuel.

Property	Diesel	Ethanol	Palm oil biodiesel	D40 B30 E30	D40 B30 E30 + ZnO (250 ppm)
Density (kg/m^3) at 30 °C	855	821.6	866	828.5	836.3
Kinematic viscosity, cst (at 40 °C)	2.95	1.1	4.802	2.42	2.32
Flash point (°C)	60-80	13	174	10	16
Calorific value (KJ/Kg)	43,000	27,000	36,764	34,907.11	36,896.36
Oxygen content (wt%)	-	35	11.7	0.82	0.80
Cetane number	52	8	63	57	55

Table 2

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Stable proportions.						
S. No.	Diesel%	Ethanol%	POME%	>25 °C	15 °C	5 °C
A5	55	20	25	Stable	Stable	Stable
A6	50	20	30	Stable	Stable	Stable
B5	50	25	25	Stable	Stable	Stable
B6	45	25	30	Stable	Stable	Stable

Table 3

In table 3 different proportion of diesel- biodiesel-ethanol with zno (nano particle) is shown as a optimum fuel blending grade which is stable in all temperature phases as per experimental analysis in the reference[1]

Fluid:- diesel- biodiesel-ethanol with zno (nano particle – it is a very popular alternate fuels for c.i. Engine in recent days as per fuel efficiency ,less emission rate , cost effective and availability. Various stable grade are available as per asme standards and represents as bde.

In present study 5 different grade of bde is investigated by cfd method and these blend are b25d55e20 as case i, b30d50e20 as case ii, b25d50e25 as case iii, b30d45e25 as case iv and b30d40e30 as case v

Based on the piston and injector geometry parameters and mesh parameters, the piston model mesh has been created. For the initial simulation to compare the five different fuel types, the injection timing has been set at a crank angle (ca) of 11° before top dead centre (tdc). This model is capable of simulating a range of different parameters in the combustion chamber including combustion duration, burning velocity, fuel atomization and pressure development. The model could then be maximized in a number of different ways including making adjustments to the fuel injection timing, injection pressure, air-fuel ratio, crank angle and combustion chamber geometry such as piston, piston ring, cylinder head, inlet and outlet valve to increase the performance and efficiency, and reduce the emissions and operational limitations for the engine running on second generation biodiesel.

11) Step 5 solutions

a) Method

i) Coupled

ii) Presto model is used: Presto model is often used for buoyant flows where velocity vector near walls may not align with the wall due to assumption of uniform pressure in the boundary layer sopresto can only be used with quadrilateral or exhahyderal .

b) Meshes: pseudo transient is enabled

i) 0.1 time scale factor of turbulent kinetic energy and turbulent dissipation rate

ii) Time scale factor of species and energy is 10

iii) Note: - higher time scale size is used for the energy and species equation to converge the solution in less number of iterations.

iv) Solution initialisation: - the solution is initialized

v) Run calculation: - start the calculation for 1000 iterations.

V. RESULTS & DISCUSSION

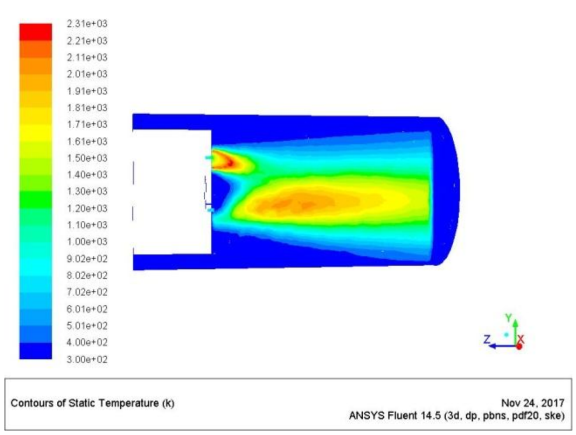

Figure 5.1: Static Temperature of Case 5 (B30D40E30)

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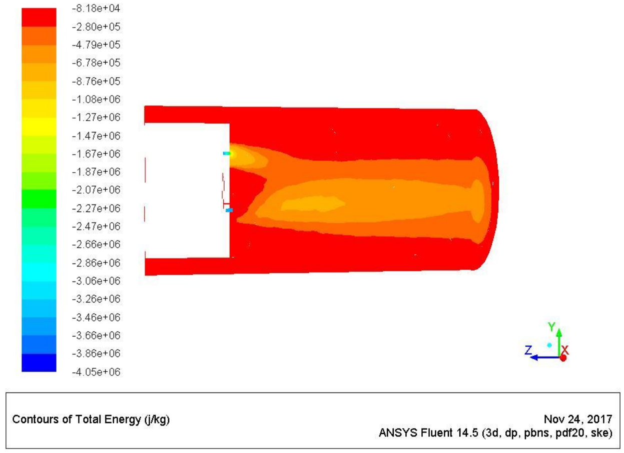

Figure 5.2: Total Energy of Case 5 (B30D40E30)

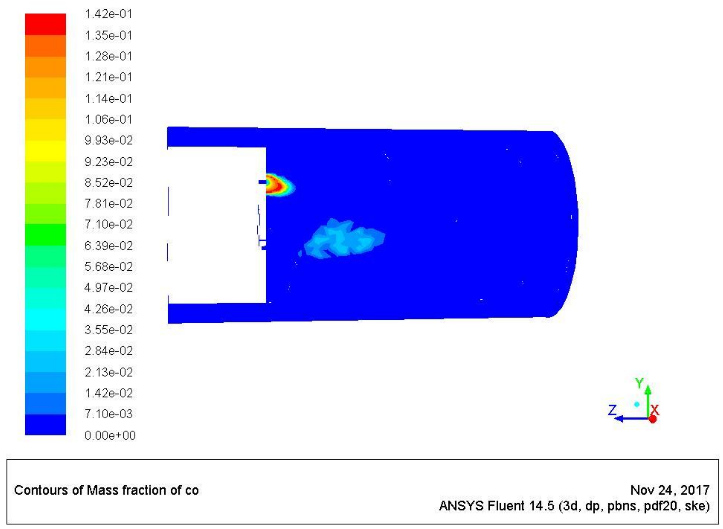

Figure 5.3 Mass fraction of CO in Case 5 (B30D40E30)

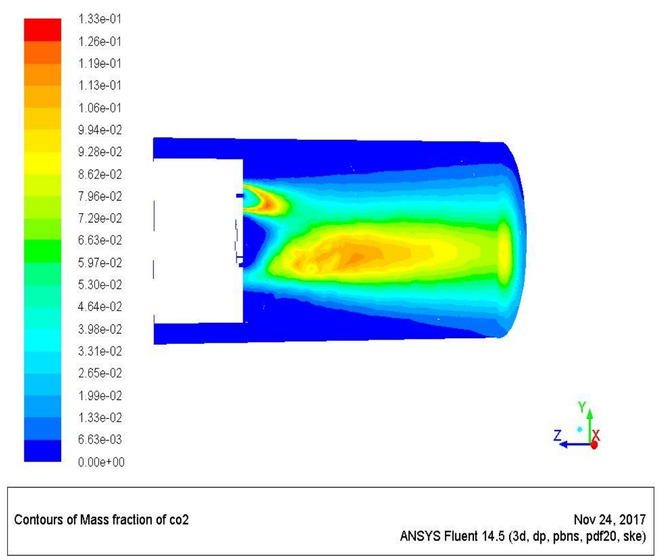

Figure 5.4 Mass fraction of CO_2 in Case 5 (B30D40E30)

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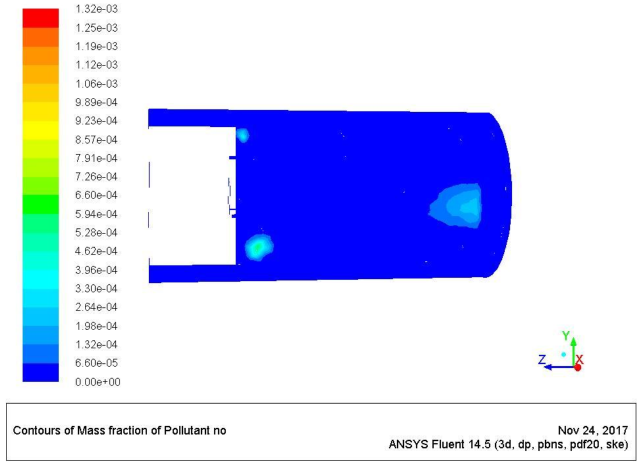

Figure 5.5 Mass fraction of NO in Case 5 (B30D40E30)

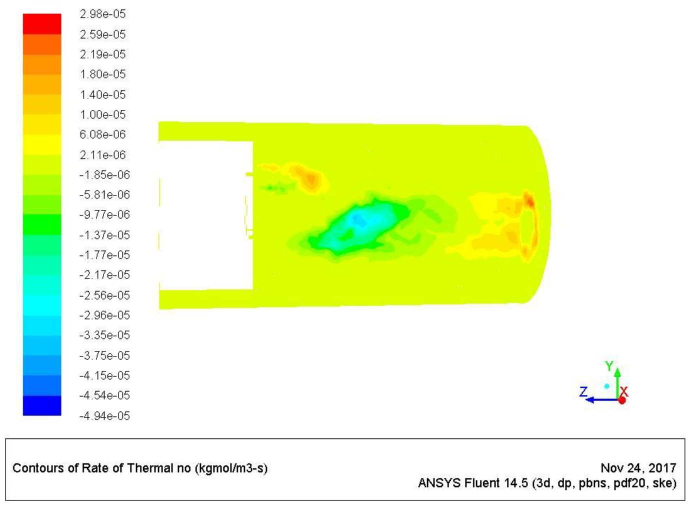

Figure 5.6 Rate of Thermal NO in Case 5 (B30D40E30)

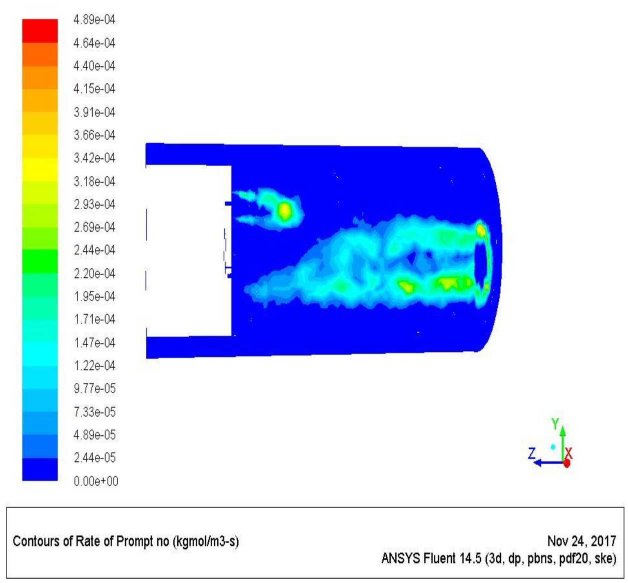

Figure 5.7 Rate of Prompt NO in Case 5 (B30D40E30)

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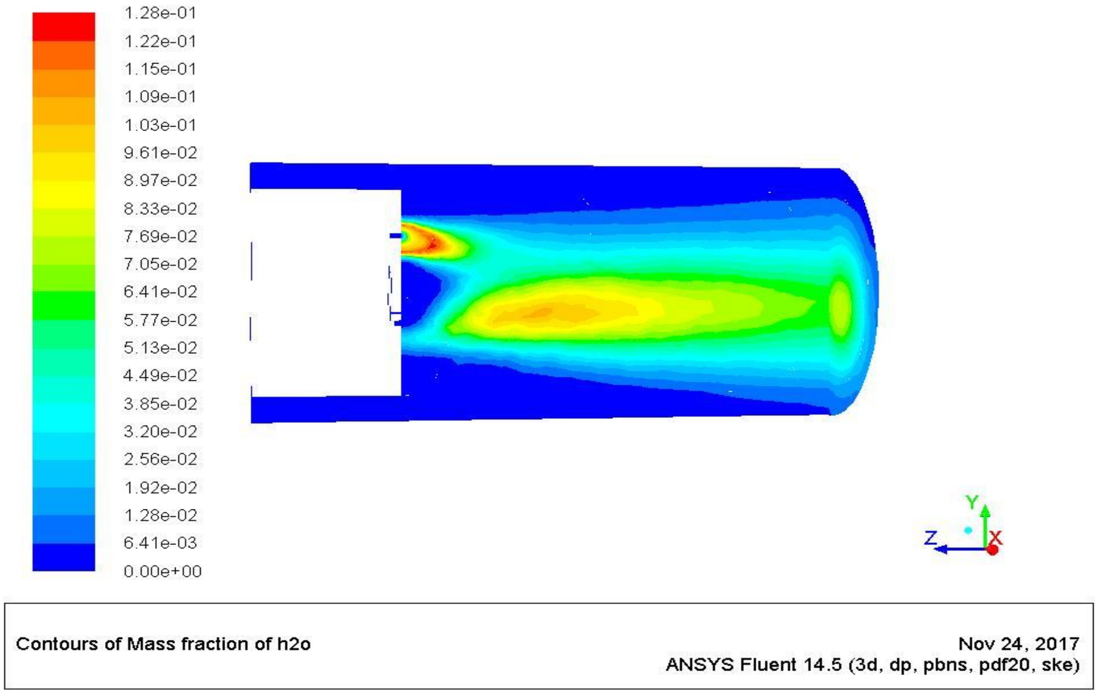

Figure 5.7 Mass fraction of H_2O in Case 5 (B30D40E30)

Results Table

CASE	FUEL GRADE	TEMPERATURE (K)	TOTAL ENERGY (J/Kg)	MASS FRACTION OF CO	MASS FRACTION OF CO_2	MASS FRACTION OF NO
1	B25D55E20	1750	2.49+03	1.15e-01	1.64e-01	8.08e-02
2	B30D50E20	1770	4.11e+04	1.15e-01	1.65e-01	2.3e-02
3	B25D50E25	2000	4.38e+04	1.26e-01	1.61e-01	1.72e-02
4	B30D45E25	2050	7.35e+04	1.30e-01	1.57e-01	5.52e-03
5	B30D40E30	2310	8.18e+04	1.42e-01	1.33e-01	1.32e-03

VI. CONCLUSION

From Results table, we can conclude that as we increase the percentages of Bio fuels and Ethanol, the temperature is increased by an efficient manner and the total energy is continuously increasing which means the combustion rate is improved while the addition of bio fuel and Ethanol. The efficiency of the blended fuel is increasing from Case 1 to case 5 because of the stable blending which already analyzed in previous research by experiments and now The Simulation results proved that all the stable grade have a great amount of energy and release less amount of pollutants. Simulation results show that as the addition of Bio fuels +Ethanol is in higher order, the intermediate carbon oxides is increasing which means combustion process is getting towards complete combustion that gives a high amount of energy and at the end release lesser amount of carbon dioxide. In present work the evaluation of the NOx (Prompt and Thermal) is also carried out we investigate from CFD Results that NOx percentages are decreasing with the addition of ZnO(225 ppm) and higher no. of BDE because as the temperature is getting higher the N-O bond will we collapsed due to this Nitrogen is released to the environment, hence NOx percentage is decreasing from lower No. of BDE to the higher No. of BDE

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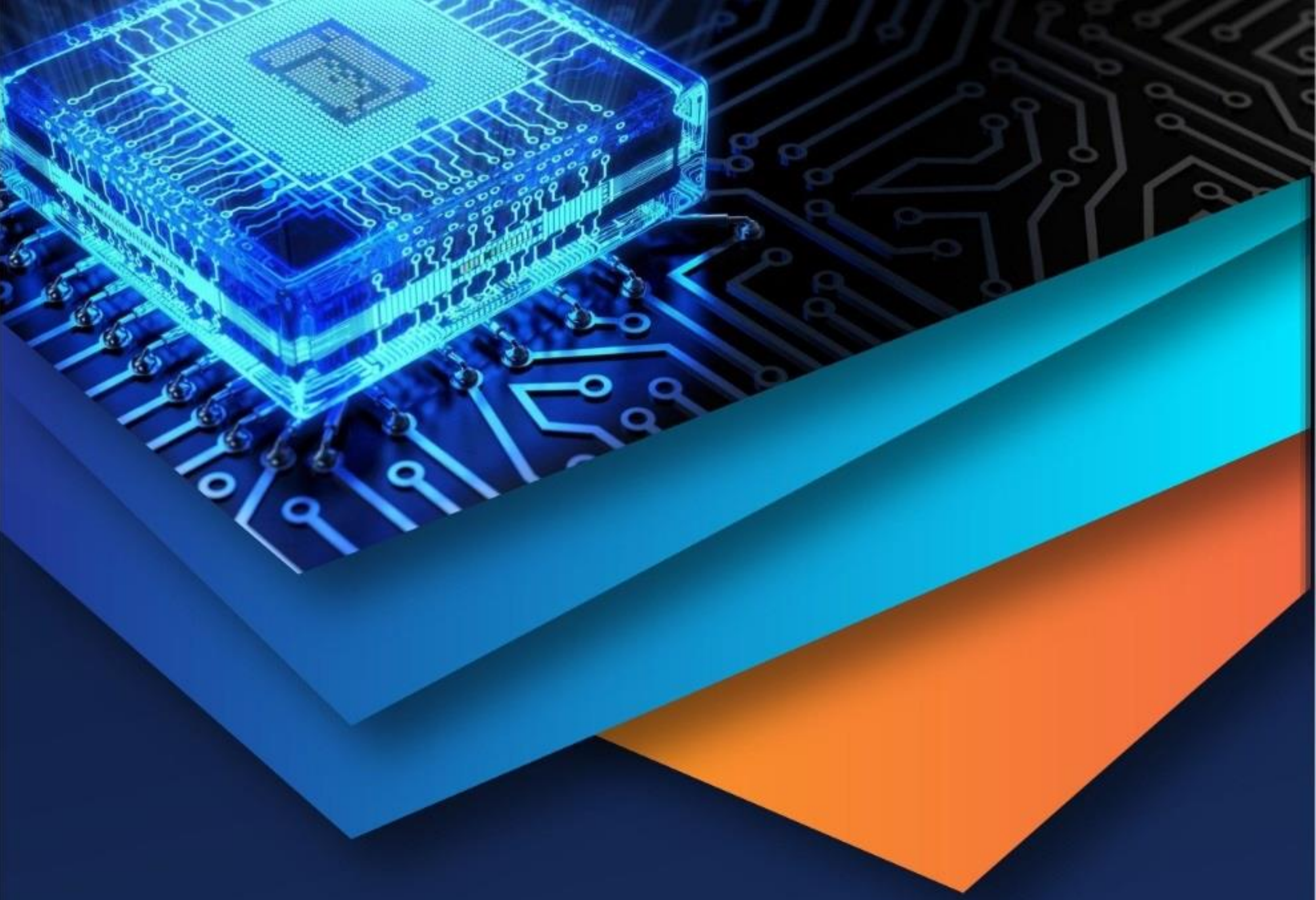

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