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CFD Simulation of Non-Premixed Light Duty Dual Fuel (Diesel + Natural Gas) Combustion Engine and Evaluating Different Type of Pollutant Emissions

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Abstract: ***This study investigated dual-fuel operation with a light duty Diesel engine with Natural gas over a wide engine load range. Natural gas was hereby injected into the intake duct, while Diesel was injected directly into the cylinder. At low loads, high fuel shares are critical in terms of combustion stability and emissions of unburnt hydrocarbons. Dual-fuel combustion has the advantage of providing diesel-like efficiency with Natural gas as the primary fuel, providing potential increases in efficiency of 50% while reducing emissions. Typically a small liquid fuel pilot is injected into a lean mixture of air and a more volatile fuel that is less inclined to auto-ignite. Often it is difficult to simulate the separate chemical effects of the two fuels. In present study we are using non premixed type of combustion model for better mixing and penetration of fuel and air so the complete combustion is achieved and emission is reduced by a great amount as compare to premixed method. NOx emission is reduced as compare to previous base research. Fluent accurately tracks flame propagation, which is critical for dual-fuel cases where the injection and auto-ignition of the liquid pilot fuel serves to initiate the flame propagation. In Fluent the simulation can simultaneously consider both auto-ignition and flame-propagation modes of combustion progress. Fluent fluid flow allows investigations of fuel or additive composition effects, impacts on liquid pilot amount and timing, and NOx reduction techniques such as EGR, etc.***

Key words: Dual fuel, Natural gas, Non premixed combustion, Any (Fluent), CFD, Chemkin mechanism, NOx etc.

I. INTRODUCTION

Natural gas (NG) consisting of mainly methane has been recognized as a viable clean alternative fuel for its abundant resource, attractive features including producing less greenhouse gas (GHG) benefiting from the low carbon/hydrogen ratio of methane, low emissions of pollutants, especially particulate matter (PM), and high thermal efficiency. Natural gas can be burned as either the sole fuel in spark ignition (SI) engines or as supplemental fuel in compression ignition (CI) diesel engines. When burned in CI diesel engines, NG is usually fumigated into the intake mixture or directly injected into the cylinder early in the compression stroke, which forms a homogeneous NG-air mixture during the intake or early compression stroke. At the end of the compression stroke, a pilot of diesel fuel is injected into the hot NG-air-diluents mixture and serves as an ignition source. Prior to the injection of pilot diesel fuel, gaseous fuels have been well mixed with air and compressed to high temperatures, but usually not high enough to initiate the auto-ignition process of NG. After being injected into the hot bulk mixture, the pilot diesel is atomized, vaporized, mixed with the hot NG-air mixture, and ignited through compression ignition. The energy released by the pilot diesel fuel serves as an ignition source of the gaseous fuel. Detailed information about the dual fuel engine ignition and combustion process can be found in the literature. Compression ignition dual fuel engines have been recognized as an attractive combustion mode for their potential to burn gaseous fuels at a thermal efficiency comparable to diesel engines and reduced PM emissions. Numerous researchers have examined the combustion process of dual fuel engines. For example, Karim examined the heat release process derived from cylinder pressure and classified the heat release process of dual fuel combustion into three modes: (1) the ignition of the pilot fuel, which usually has higher reactivity than gaseous fuels fumigated into the intake mixture; (2) the concurrent combustion of diesel and NG presented within the diesel spray plume, (3) the combustion of a diesel free, NG-air mixture. The research conducted in the past decades has focused on the detailed experimental measurement of the impacts of engine speed, load, substitution ratio of NG, exhaust gas recirculation (EGR), the mass of NG injected into intake manifold, and the amount of diesel fuel injected in each cycle in the dual fuel engine combustion process. Recently, there has been increasing interest in examining the impact of pilot fuel injection timing

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and injection pressure on the combustion process and exhaust emissions from dual fuel engines. The combustion process of NG was controlled by the mixing processes of the pilot fuel with the premixed charge (i.e. no flame propagation or bulk ignition) and whether or not the premixed NG-air mixture is too lean to support the propagation of the turbulent flames if initiated by pilot fuel. Past research on the combustion process of NG-diesel dual fuel engines has focused on the overall heat release process of NG and pilot diesel. In comparison, to the best of our knowledge, little research on the combustion process of gaseous fuels, such as methane, in dual fuel engines has been conducted. It is technically difficult to split the heat release of dual fuel engines to that of pilot fuel and gaseous fuel, respectively. NG-diesel dual fuel engines have been criticized for their high emissions of unburned methane and carbon monoxide (CO). The methane emissions from dual fuel engines not only contribute to overall GHG emissions but also cause a waste of energy. Many researchers have investigated the methane emissions from NG-diesel dual fuel engines. decreased with the increase in engine load. With the concerns of fuel conversion efficiency in dual fuel engines, there has been interest in examining the combustion efficiency of methane fumigated into the intake mixture in NG-diesel dual fuel engines. The emissions of methane, CO, and carbon dioxide (CO2) and the flow rates of fuels and air were further processed to derive the combustion efficiency of methane with the following two assumptions: (1) the methane emitted from the dual fuel engine was that added into the intake mixture; and (2) the CO emissions above that of pure diesel operation was due to the incomplete combustion of methane while disregarding the possibility of incomplete combustion of diesel and other hydrocarbons in natural gas. The lowest combustion efficiency observed at low (10%) load operation was about 65%. The maximum combustion efficiency observed at 70% load was about 95%, similar to that of SI NG engines. It is evident from these early investigations that the improvement of methane combustion efficiency of dual fuel engines at low load is one of the key challenges for the wide application of dual fuel engines especially when low load operation is frequently involved.The contribution of unburned methane to GHG emissions and the desire to further improve the efficiency of dual fuel engines have raised researchers' interest to understand the mechanism for methane to survive the combustion process and slip through the combustion chamber without participating in combustion. Some researchers tried to investigate the combustion process of dual fuel engines using advanced combustion diagnostic technologies and managed to measure the propagation of flames through the premixed mixture of NG and air. A high-speed digital camera recorded time-resolved combustion luminosity. An intensified charge-coupled device (CCD) camera was used for single cycle OH∗ imaging. The propagation of the turbulent flame through the diesel fuel free bulk gas (premixed NG-air mixture) was observed when the NG-air mixture was richer than the lean flammability limit [24]. However, the NG-air mixture leaner than the flammability limit was not able to support the propagation of the flames initiated by the pilot diesel fuel. The combustion in different zones representing the lean premixed methane-air mixture and pilot fuel diffusion combustion was distinguished using the temporally resolved natural luminosity imaging. The impact of fuel injection strategy and equivalence ratio of the premixed NG-air mixture on the flame propagation through the premixed NG-air mixture was also examined. Combining the natural luminosity image with the heat release rate (HRR) helped to better understand the overall heat release process and the burning of pilot and gaseous fuels. The research identified the multi-pulse fuel injection strategies as a promising and effective strategy capable of enhancing the flame propagation toward the center of the combustion chamber, which was usually not burned with a single pulse injection strategy. The research on the spatial distribution of methane in-cylinder, quantification of the percentage of methane burned in each combustion stage and the mechanism for methane to survive the combustion process is of critical importance for the development of technical approaches optimizing the dual fuel engine combustion process and minimizing methane emissions. However, because of the difficulty in experimental techniques, the spatial distribution of methane within the combustion chamber and the mechanism for methane to survive the combustion process in dual fuel engines have never been experimentally identified.

II. LITERATURE

Chunhua Zhang et.al The diesel-LNG (liquefied natural gas) dual-fuel combustion mode was conducted on a high-pressure common-rail six-cylinder diesel engine to find an assistant parameter to assess the brake thermal efficiency (ge) and nitrogen oxides (NOx) emission of the diesel-LNG dual-fuel engine. The results show that the diesel injection timing has a prominent impact on the centroid angle of combustion duration (α) which is closely related to ge and NOx emission. At low and medium loads, when a is near to top dead center (TDC) and is after TDC, the ge and NOx emission are higher. Nevertheless, when α is before TDC, the result of NOx emission is opposite. Therefore, for optimal ge and NOx emission at low and medium loads, it would be the best way altering diesel injection timing to retard a to ATDC and ensuring a in 1–2 ˚CA ATDC. 2.Jeongwoo Lee et.al Reactivity controlled compression ignition (RCCI) is one of representative dual-fuel combustion concepts for low NOx, soot emissions and high thermal efficiency. Overall lean and highly premixed auto-ignition combustion make low combustion temperature and the reduction of heat transfer loss. Although premixed compression ignition (PCI) combustion using a single fuel, i.e., diesel, also shows low emissions

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and higher thermal efficiency, combustion characteristics of RCCI (dual-fuel PCI) are different from single-fuel PCI due to reactivity gradient from two different fuel characteristics as well as local equivalence ratio due to the fuel distribution. Therefore, it is necessary to know the influence of above two factors on the dual-fuel combustion characteristics for better understanding of dual-fuel combustion and its effective utilization. In this research, the characteristics of dual-fuel combustion are evaluated comparing to single-fuel combustion.

Also, dual-fuel combustion modes are classified according to the analysis of heat release rate (HRR) shapes. Major factors in the classification of dual-fuel combustion modes are the degree of fuel reactivity gradient and the local equivalence ratio in the cylinder. Thus, the diesel injection timing, diesel and port injected gasoline fuel ratios and the overall equivalence ratio were selected as the main variables to characterize each dual-fuel combustion mode. The result emphasizes that the dualfuel combustion could be classified as three types by HRR shapes, and it was mainly affected by reactivity gradient and overall equivalence ratio. 3.Carmelina Abagnale et.al the effect of different fuel ratios on the performance and emission levels of a common rail diesel engine supplied with natural gas and diesel oil. Dual fuel operation is characterized by a diesel pilot injection to start combustion in an intake port premixed NG/air mixture.

The combined numerical – experimental study of the dual fuel diesel engine that is carried out in this paper aims at the evaluation of the CFD potential to predict the main features of this particular engine operation. The experimental investigations represent a tool for validating such a potential and for highlighting, at the same time, the major problems that arise from the actual engine operation with different NG / diesel oil fuel ratios. 4.PengGeng et.al Diesel engines are the main source of rapidly-growing energy consumption worldwide. Diesel consumption is responsible for serious air pollution, which includes nitrogen oxides (NOx), hydrocarbon (HC), carbon monoxide (CO) emissions and some particulate matter (PM) discharged from the combustion chamber. In the past few decades, alternative fuels, such as alcohol, biodiesel, natural gas, and Di Methyl Ether (DME), have been used in diesel engines to reduce energy costs and environmental pollution. As a result of alternative fuels directives, an increasing number of diesel engines have adapted dual fuel blends, and an enormous amount of research is focused on new and inadequately studied combustion and emission profiles. Compared to conventional diesel fuel, the application of dual fuels would add new parameters to combustion and emission profiles for diesel vehicles worldwide.

This review aims to reveal (1) Known and anticipated combustion characteristics and emissions products from dual fuels. (2) Toxic properties and the expected influence on engine performance. (3) Identifying promising alternative fuels for emissions control in compression combustion engines.

The results presented herein will show a significant reduction of regular gas and PM emissions by the use of alcohol/diesel dual fuel, while unregulated emissions such as methanol, ethanol, acetaldehyde, formaldehyde, ketone, have increased compared to those from diesel fuel. PM emissions decreased significantly with the increase of alternative fuels, such as alcohols, natural gas, biodiesel and DME, while regular gaseous emissions varied depending on the type alternative fuel and the engine conditions.

As one new and cleaner substitute for diesel engines, DME operation has a longer injection delay, lower maximum cylinder pressure, a lower ratio of pressure rise, and shorter ignition delay in comparison with diesel operation–the opposite of alcohol/diesel and dual fuels. This review evaluates the effects of some alternative fuels (alcohol, biodiesel, natural gas and Di Methyl Ether (DME)) on combustion characteristics and emission products from diesel engines to meet future emission regulations using alternative fuel.

III. OBJECTIVE OF THE STUDY

Present study investigates the mixing of chemical species and the combustion of a dual fuel (Diesel/Natural gas). A cylindrical combustor burning (Diesel +Natural gas) in air is studied using the eddy-dissipation model in ANSYS (Fluent). Our main objective of the study is to analyze the dual fuel combustion model with non-premixed type of combustion and compared the previous research on the basic of combustion rate and emissions. In second part of our study is to evaluation of Thermal NOx and Prompt NOx due to non premixed type of combustion and reduced it as per environment norms. Current study evaluates and use following type of models:

A. Specific turbulent flow with chemical species mixing and reaction.
B. Initiate and solve the combustion simulation using the pressure-based solver.
C. Compare the results computed with constant and variable specific heat.
D. Examine the reacting flow results using graphics.
E. Predict thermal and prompt NOx production.
F. Use custom field functions to compute NO parts per million.

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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.
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.

B. Solution

1) *Solution Method* : Choose the Solution method to solve the problem i.e. First order, second order
2) *Solution Initialization:* Initialized the solution to get the initial solution for the problem.
3) *Run Solution:* Run the solution by giving no of iteration for solution to converge.
4) *Post Processing:* For viewing and interpretation of Result. The result can be viewed in various formats: graph, value, animation etc.
5) .*Step I*– CAD Model

Figure 4.1 Cad Model

6) *Step 2*

a) *Mesh file* –To be Meshed

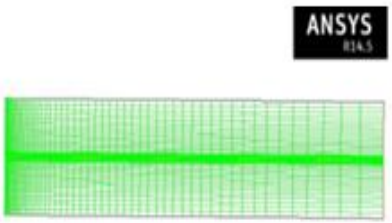

Figure 4.2 Mesh Model

7) *STEP 4 Simulation Setup*

a) *Boundary conditions*
b) *Mass Flow Air inlet:* - Mass flow rate is 0.5 kg/s,
c) *Mass flow Fuel inlet* – 0.05 kg/ s of Mixtu
d) *Outlet* – pressure based

C. MATERIAL

1) *Diesel+ Natural gas*

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2) *Fluid:* The natural gas was selected as a four-component mixture of methane (>90%), ethane, propane and n-butane, whereas diesel oil was represented by the Diesel Oil Surrogate (DOS) model, in which liquid fuel properties are the same of real diesel oil, while fuel vapour is made up of a blend of n-heptane and toluene
3) *Mixture:* Species I H_20, II-O2, III-Fuel -EG, IV-CO_2, V-N
4) Mixing law is used.
5) *Thermal conductivity:* - Define two polynomial coefficients

a) 0.0065234 (b) $8.72369*10^{-6}$

6) Polynomial coefficient for viscosity

a) 5.2348e-07 (b) 5.12365e

7) For absorption coefficient take stable domain.
8) Scattering coefficient is 1.2e-8.

D. Method

1) Coupled
2) 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 so presto can only be used with quadrilateral or Hexahedral
3) *Solution Initialisation***: -** The solution is initialized
4) *Run Calculation:-* Start the calculation for 2000 iterations.

V. RESULTS AND CONCLUSION

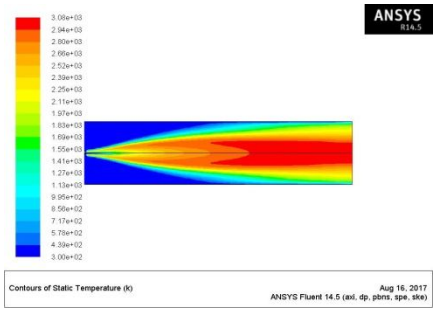

Figure 5.1 Static Temperature of flow field at constant Cp

The peak temperature, predicted using a constant heat capacity of 1000 J/KG-K is over 3000 K .This over prediction of the flame temperature can be remedied by a more realistic model for the temperature and composition dependence of the heat capacity.

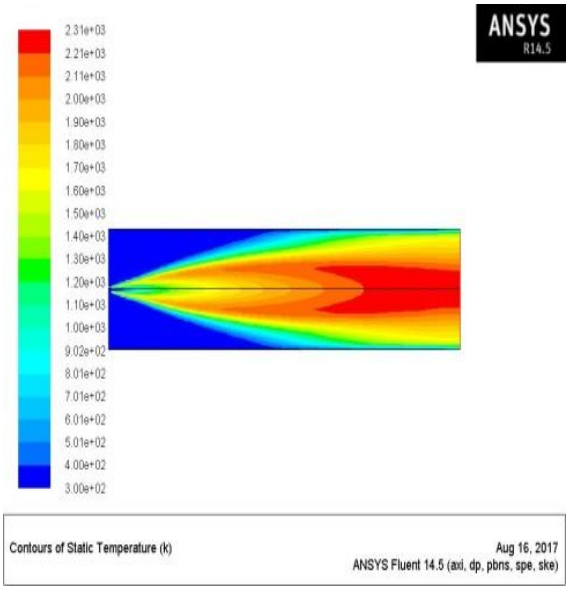

Figure 5.2 Static Temperature of flow field at variable Cp

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The peak temperature has dropped to approximately 2300 K as a result of the temperature and composition dependent specific heat.

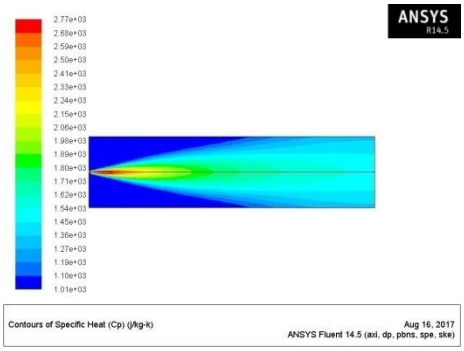

Figure 5.3 Specific heat of mixture in stream function

The mixture specific heat is largest where the fuel is concentrated, near the fuel inlet, and where the temperature and combustion product concentrations are large. The increase in heat capacity, relative to the constant value used before, substantially lowers the peak flame temperature.

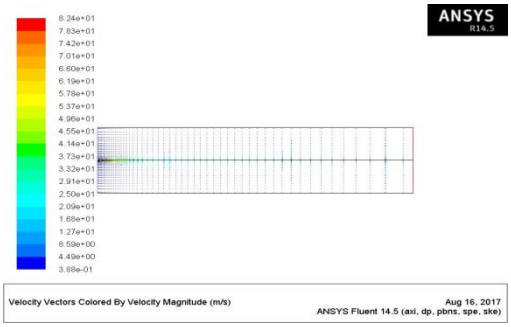

Figure 5.4 Velocity vectors

The fixed length option is useful when the vector magnitude varies dramatically. With fixed length vectors, the velocity magnitude is described only by colour instead of by both vector length and colour.

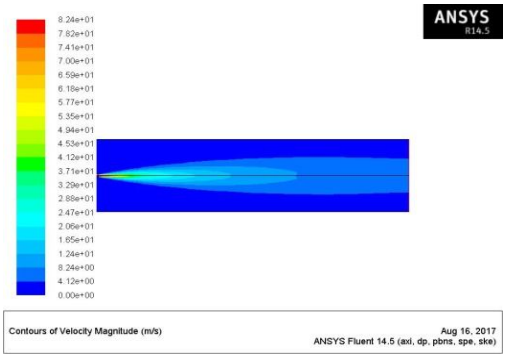

Figure 5.5 Velocity contours

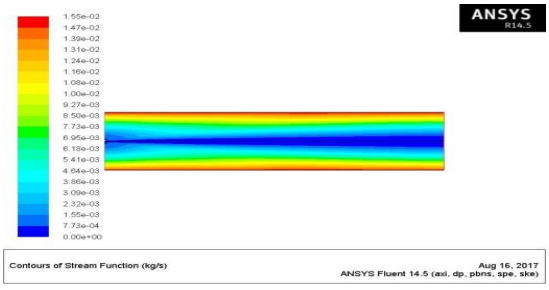

Figure 5.6 Stream function of flow field

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The entrainment of air into the high-velocity dual fuel mixture is clearly visible in the streamline display.

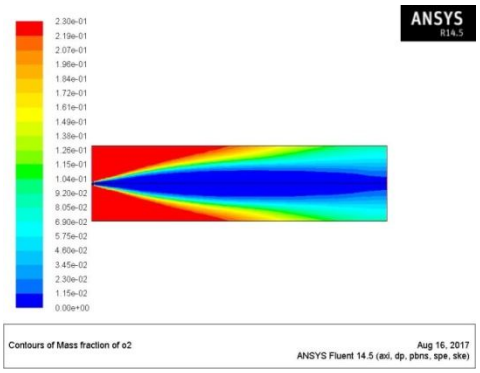

Figure 5.7 Mass fractions of 0_2

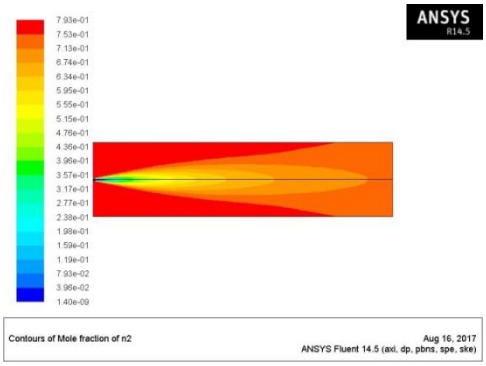

Figure 5.8 Mass fraction of N_2

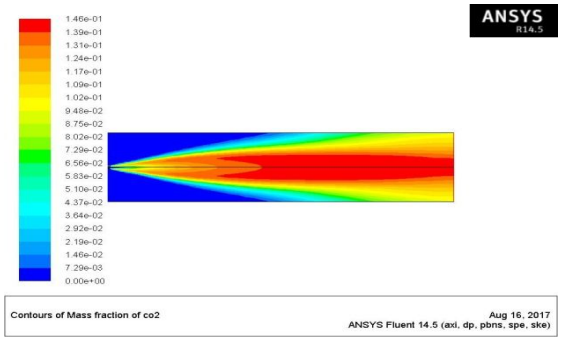

Figure 5.9 Mass fraction of CO_2

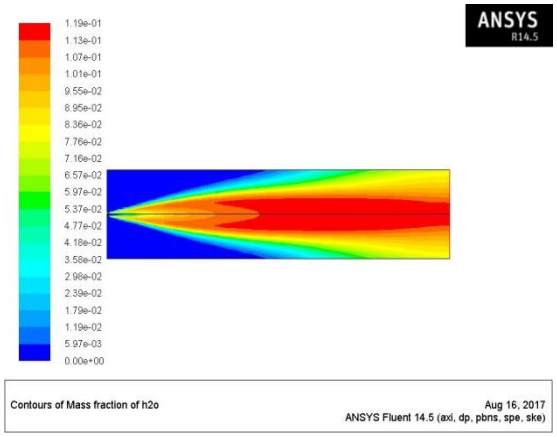

Figure 5.10 Mass fraction of H_2O

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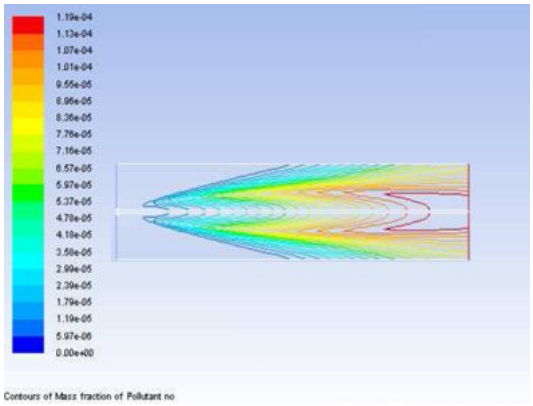

Figure 5.11 Mass fraction of NO (Prompt NOx)

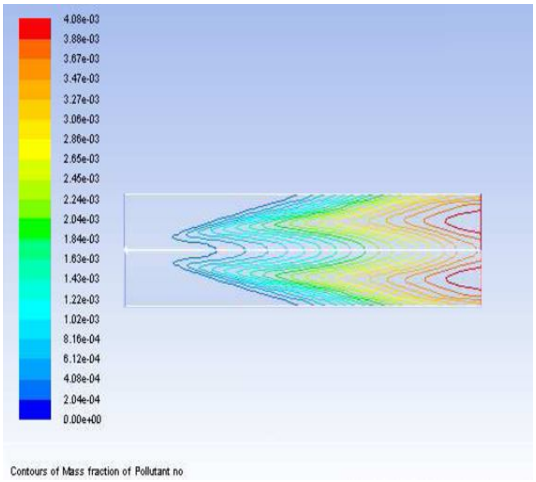

Figure 5.12 Mass fraction of NO_2 (Thermal NOx)

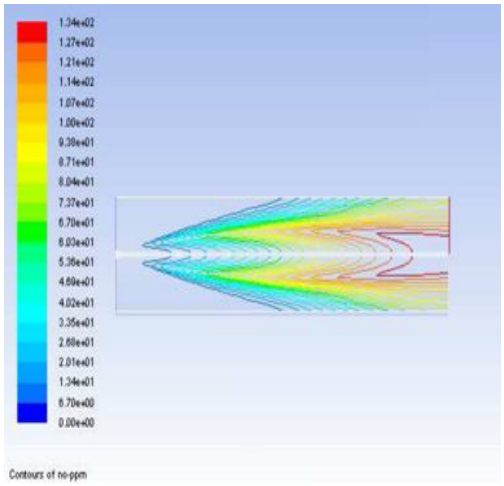

Figure 5.13 Contours of NO –PPM (Part per Million)

VI. CONCLUSION

In present study we used ANSYS (Fluent) to model the transport, mixing, and reaction of chemical species. The reaction system was defined by using and modifying a mixture-material entry in the ANSYS (Fluent 14.5) database. The procedures used here for simulation of dual fuel combustion can be applied to other reacting flow systems. This study illustrates the important role of the mixture heat capacity in the prediction of flame temperature. The combustion modelling results are summarized in the following table.

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	Peak Temp. (K)	Exit Temp. (K)	Exit Velocity (m/s)
Constant C_p	3080	2241	4.03
Variable C_p	2300	1834	3.29

The use of a constant Cp (specific heat of mixture) results in a significant over prediction of the peak temperature. The average exit temperature and velocity are also over predicted. The variable Cp solution produces dramatic improvements in the predicted results. The NOx production in this case was dominated by the thermal NO mechanism. This mechanism is very sensitive to temperature. Every effort should be made to ensure that the temperature solution is not over predicted, since this will lead to unrealistically high predicted levels of NO. Further improvements can be expected by including the effects of intermediate species and radiation, both of which will result in lower predicted combustion temperatures. In present study we are using non premixed type of combustion model for better mixing and penetration of fuel and air so the complete combustion is achieved and emission is reduced by a great amount as compare to premixed method. NOx emission is reduced as compare to previous base research.

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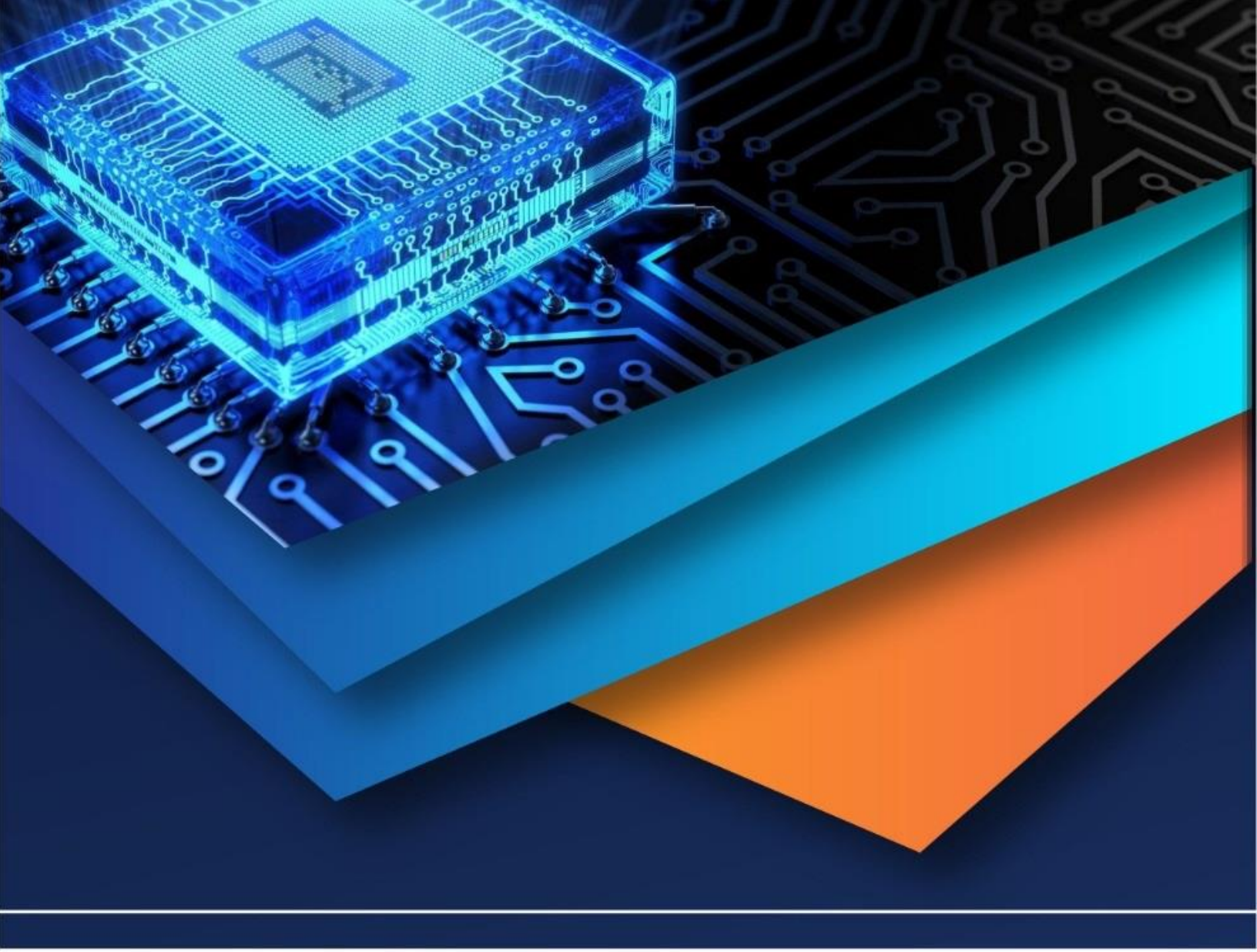

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