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Experimental and CFD Investigation of Combustion and Emission Characteristics of a Hydrogen-Enriched CNT-Rapeseed Biodiesel Blend in a Compression Ignition Engine

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Abstract: Combustion and emission characteristics of a single-cylinder, four-stroke, direct-injection, compression-ignition (CI) diesel engine running at constant speed (1500 rpm) are studied by a combination of experimental and Computational Fluid Dynamics (CFD) analysis. Experiments were conducted on diesel fuel, a 20% biodiesel blend (R20), and R20 containing 50 ppm carbon nanotube (CNT) nanoparticles and R20 containing hydrogen induction. The exhaust gas and the engine performance were measured under full load conditions with an eddy current dynamometer and exhaust gas analyzer. In-cylinder pressure, velocity, temperature and CO and CO_2 distribution were simulated using CFD to give detailed information on the combustion behaviour. Good agreement was obtained for the numerical prediction with the experimental observations. The use of CNT nanoparticles and hydrogen in combination enhanced the mixing of fuel and air, increased combustion efficiency and decreased the amount of products of incomplete combustion. The integrated experimental–CFD approach has a definite route to cleaner and more efficient CI engine technologies.

Keywords: *CI Engine, Biodiesel, Carbon Nanotubes, Hydrogen Induction, CFD, Combustion, Emissions.*

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I. INTRODUCTION

The ever-rising demand for energy and dwindling fossil fuel resources have stimulated the study of non-polluting and sustainable fuels for compression ignition (CI) engines. Diesel engines are employed in a variety of applications where their high thermal efficiency, durability and fuel economy make them attractive, but they are also a significant source of air pollutants such as carbon monoxide (CO), carbon dioxide (CO_2), hydrocarbons (HC), particulate matter (PM) and nitrogen oxides (NOx) that are responsible for air pollution and climate change [1]. Biodiesel has emerged as one of the most promising renewables replacing diesel as it can be synthesized from vegetable oils and animal fats without the need for changing the diesel engine [2]. According to Agarwal [3] production of biodiesel can be a great way to minimise dangerous exhaust emissions without making significant changes to an engine. Likewise, Mofijur et al. [4] noted that blends of biodiesel could help to decrease environmental pollution and increase energy sustainability.

Biodiesel, for its oxygenated molecular structure, generally leads to lower CO, HC and particulate emissions, as shown by Lapuerta et al. [5]. Xue et al. [6] reviewed several experimental studies and found that combustion properties of biodiesel are improved, whereas the consumption of fuel could increase due to its lower heating value. Nabi et al [7] also found that biodiesel derived from the vegetable oils could be used to improve the combustion quality of the diesel fuel and still have good engine performance. There is however, a concern about the relatively high viscosity and low calorific value of biodiesel as it can have a negative impact on the atomisation and combustion efficiency particularly at higher blend ratios [5-7].

To address these drawbacks, a few researchers have studied the use of nanoparticle additives. Basha and Anand

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[8] showed that the carbon nanotube (CNT) additive has the potential to improve combustion efficiency and reduce exhaust emissions through fuel atomization. Sajith et al. [9] noted that cerium oxide nanoparticles enhance oxidation reactions, and reduce the incomplete combustion products. Manigandan et al. [10] found that the mixture of hydrogen and MWCNTs performed very well in combustion and considerably lowered the emissions from the engine. In another study, Manigandan et al. [11] found that the use of nanoparticles with hydrogen enrichment resulted in enhanced thermal efficiency and combustion stability of biodiesel. The effects of hydrogen assisted biodiesel combustion on engine performance and emission of CO and HC were also confirmed by Tosun and Ozcanli [12]. However, Wang et al. [13] showed that by using the nanoparticles in biodiesel, it can increase the combustion efficiency and reduce the exhaust emissions. Similarly, Chetia et al. [14] reported that the use of additives of nanoparticles and hydrogen enrichment in the fuel results in a cleaner combustion than the conventional diesel fuel.

The use of Computational Fluid Dynamics (CFD) has been an important aid in the understanding of the combustion process within a diesel engine. Versteeg and Malalasekera [15] described that CFD can accurately predict velocity, pressure, temperature and species transport in complex flow domains. For the modelling of turbulent reacting flows and combustion phenomena in internal combustion engines, the ANSYS Fluent Theory Guide [16] offers the numerical models. Jayabal and Sivanraju (2011) [17] used CFD and experimental studies to assess the combustion characteristics of nanoparticle blended biodiesel under hydrogen enrichment, finding better combustion behaviour. Likewise, Shabana et al. [18] showed the effect of hydrogen enrichment and CNT blended biodiesel had a positive impact on combustion efficiency and carbon-based emissions. Raman et al. [19] reported that a combination of hydrogen and ZnO nanoparticle additive could improve combustion in a CRDI diesel engine with a decrease in the exhaust pollutants. Khan et al. [20] optimized the performance of Diesel engine using biodiesel, hydrogen and cerium oxide nanoparticles to reduce the emissions with improved engine efficiency. In another study, Khan et al. [21] found that the use of hydrogen enrichment with a nanoparticles blended biodiesel showed a remarkable decrease in CO emissions and increased combustion stability.

Other recent research by Sekhar and Gupta has also been undertaken in the field of biodiesel, nanoparticles, hydrogen enrichment, and CFD. Their review paper provided an overview of the latest developments in the research of combustion and emissions in CI engines through CFD and experimental approaches [22]. They then studied biodiesel blends of rapeseed and found that they showed better combustion and emission properties than pure diesel [23]. For another study, fuel blends with nanoparticles were found to enhance fuel atomization and combustion efficiency, and to decrease exhaust emissions [24]. A recent report showed that the use of CNTs in biodiesel derived from rapeseed and hydrogen enrichment of the fuel could result into substantial enhancements of the brake thermal efficiency and reductions of CO and HC emissions for different operating conditions [25].

While there are many studies that have studied the effects of biodiesel fuels, nanoparticle additives, hydrogen enrichment, and CFD modeling in isolation, few studies have combined these methods to more comprehensively analyze combustion characteristics in a single-cylinder direct injection diesel engine. Comprehensive investigations of the combined experimental measurements and CFD prediction of the distribution of velocity, pressure, temperature, carbon monoxide and carbon dioxide are still limited in particular.

For this reason, the present study experimentally and numerically investigates the combustion and emission characteristics of a single-cylinder, four-stroke direct injection compression ignition (DI-CI) diesel engine run at a constant speed of 1500 rpm with four different fuels: diesel, R20 biodiesel, R20 blended with 50 ppm carbon nanotubes (CNT) and R20CNT50PPM with hydrogen enrichment. An ANSYS Fluent simulation was carried out to simulate the in-cylinder flow field and the combustion process, and the results of the simulation were compared to the measurements that were made. The combination approach gave a complete picture of the combustion process and revealed the potential of using hydrogen-assisted CNT–rapeseed biodiesel blends to enhance the performance of the diesel engine while decreasing harmful emissions.

II. EXPERIMENTAL SETUP AND PROCEDURE

➢ *Experimental Setup*

The experimental study was carried out in a 1-cylinder 4-stroke, water-cooled, direct injection (DI) compression ignition (CI) diesel engine at constant speed of 1500 rpm. The engine specification of the test engine is given in Table 1. The schematic design of the experimental test rig is shown in Fig. 1(a) and the photograph of the entire experimental setup is shown in Fig. 1(b). The system is made up of the diesel engine, fuel tank with burette, air induction box, exhaust gas analyzer, eddy current dynamometer, electrical loading panel and a data acquisition system.

To apply and control the load during the experiment, the engine output shaft was directly connected to an eddy current dynamometer. Changes in fuel consumption were determined by means of a calibrated burette which was connected to the fuel tank, while the intake air was fed through an air induction box. An analyzer probe was used to sample the exhaust gases and a multi-gas exhaust gas analyzer was used to analyse the exhaust gases for the determination of the exhaust gas concentrations of carbon monoxide (CO) and carbon dioxide (CO_2). The electrical loading panel was used to control the loading of dynamometers and the data acquisition system monitored the operating parameters continuously.

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Four potential fuel combinations were studied, i.e., pure diesel, R20 biodiesel blend, R20 blend with 50 ppm carbon nanotube (CNT) nanoparticles (R20CNT50PPM), and R20CNT50PPM with hydrogen induction. The CNT nanoparticles were homogeneously disseminated in the biodiesel blend to achieve a stable fuel mixture prior to engine testing. Hydrogen was added to the intake manifold at a controlled pace to improve the combustion characteristics.

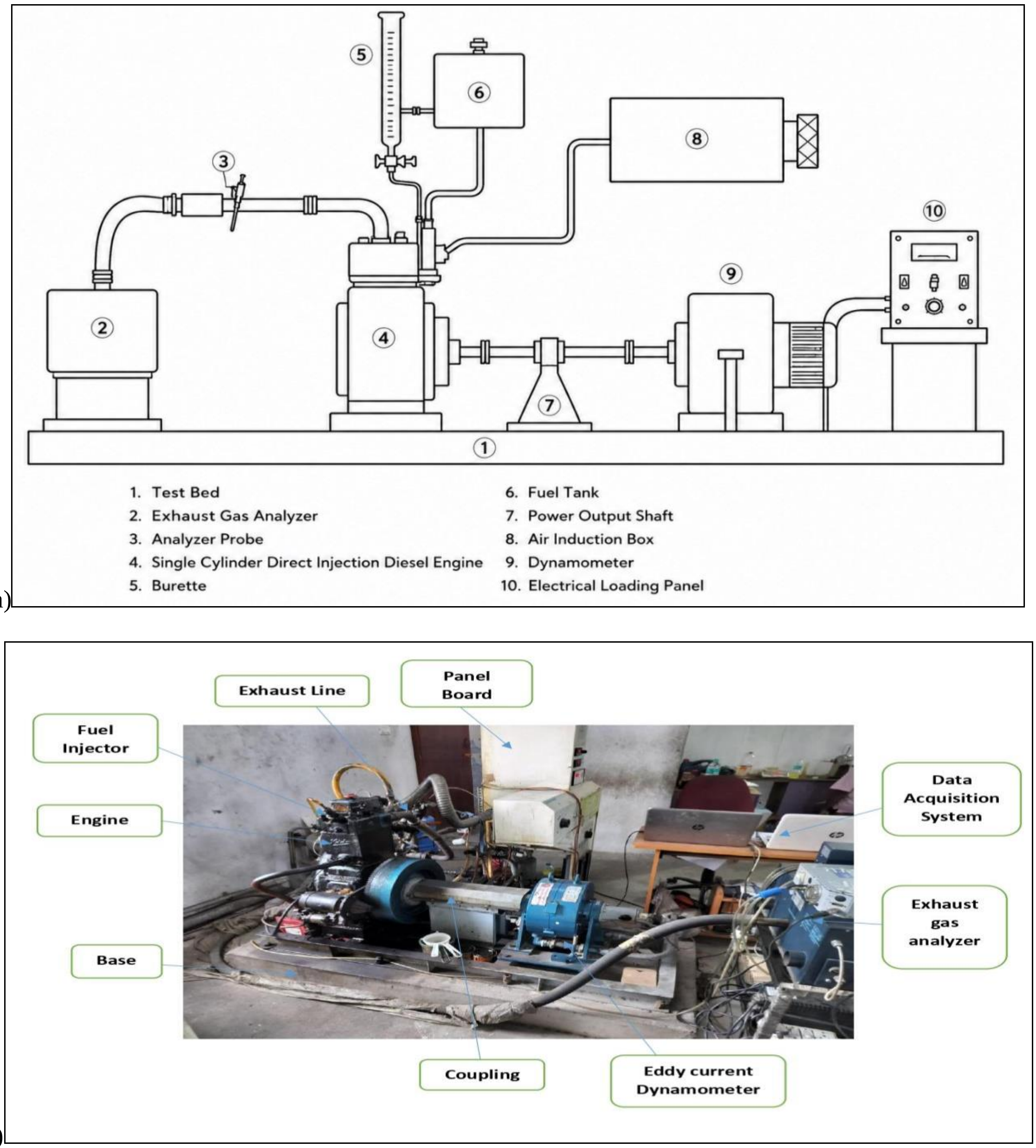
➢ *Experimental Procedure*

The engine was initially run with tidy diesel until steady state conditions are attained. The engine speed was maintained at 1500 rpm and experiments were conducted at full load condition for each test fuel. Before switching to a different fuel the fuel line was flushed to remove any contaminants from the prior fuel.

The fuel consumption was measured by burette method and the engine load was regulated using eddy current dynamometer. Exhaust gas analyzer calibrated to measure carbon monoxide (CO) and carbon dioxide (CO_2) in the exhaust. For every fuel sample, the readings were taken once the engine attained the stable operating conditions and the average of multiple measurements was taken into consideration for analysis to improve the dependability.

For comparison with the experimental observations, the identical operating conditions were utilized in the CFD simulations. The numerical predictions of pressure, velocity, temperature, CO and CO_2 distributions were examined and validated with the experimental data. The combination of experimental and numerical methods allowed a holistic understanding of the combustion characteristics and emission behaviour for the varied fuel mixtures.

(a)



(b)

Fig 1 (a) Line Diagram of Diesel Engine (b) Photo Graph of the Engine Setup with Instrumentation

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Table 1 Technical Specifications of Diesel Engine

Parameter	**Specification**
Engine Make	Kirloskar
Engine Type	Single-cylinder, Compression Ignition (CI), Four-stroke, Direct Injection (DI)
Brake Power	5.2 kW
Rated Speed	1500 rpm
Bore Diameter	87.5 mm
Stroke Length	110 mm
Connecting Rod Length	234 mm
Compression Ratio	17.5:1
Cooling System	Water Cooling
Dynamometer	Eddy Current Type
Swept Volume	661.45 cc
Air Density	1.17 kg/m³
Air Intake Orifice Diameter	20 mm
Ambient Temperature	27 °C
Fuel Density	850 /m³

III. RESULTS AND DISCUSSION

Combustion parameters of the single cylinder four stroke direct injection diesel engine were explored using Computational Fluid Dynamics (CFD) simulations and corroborated with the experimental findings. The CFD model gives extensive information on in-cylinder flow dynamics, combustion evolution and pollutant production which cannot be evaluated directly during engine operation. The effect of fuel combustion on engine performance and emission properties was studied by analyzing the distributions of velocity, pressure, temperature, carbon monoxide (CO) and carbon dioxide (CO_2).

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➢ *Combustion Chamber Computational Domain*

Figure 2 shows the computational domain 2D for CFD modeling of a single cylinder four stroke direct injection compression ignition (CI) diesel engine. The geometry was generated in ANSYS Fluent 2025 R2 Student Version with the actual engine dimensions shown in Table 1. The combustion chamber is the computational model and the air intake (A), fuel input (C) and exhaust exit (B) were assigned as boundary conditions for the numerical simulation.

The combustion chamber shape was discretized using a high grade computational mesh, to resolve precisely the in-cylinder flow and combustion events. The air inlet border supplies fresh air to the chamber and the fuel inlet, located centrally, is the diesel injector where the fuel is pumped into the combustion chamber. The outlet boundary allows the exhaust gases to escape the computational domain following combustion. For the walls of the combustion chamber the boundary conditions were chosen as no-slip velocity, and for the heat transfer between the combustion gases and the cylinder walls thermal boundary conditions were employed.

A CFD model was created to estimate the in-cylinder velocity, pressure, temperature, carbon monoxide (CO) and carbon dioxide (CO_2) distributions at the engine operating condition of 1500 rpm. The computational domain provides a realistic picture of the combustion process and is used as the basis for the analysis of flow development, heat release and emissions production. The boundary conditions and domain configuration used resulted in numerical stability and better accuracy of the simulation results compared to the experimental data.

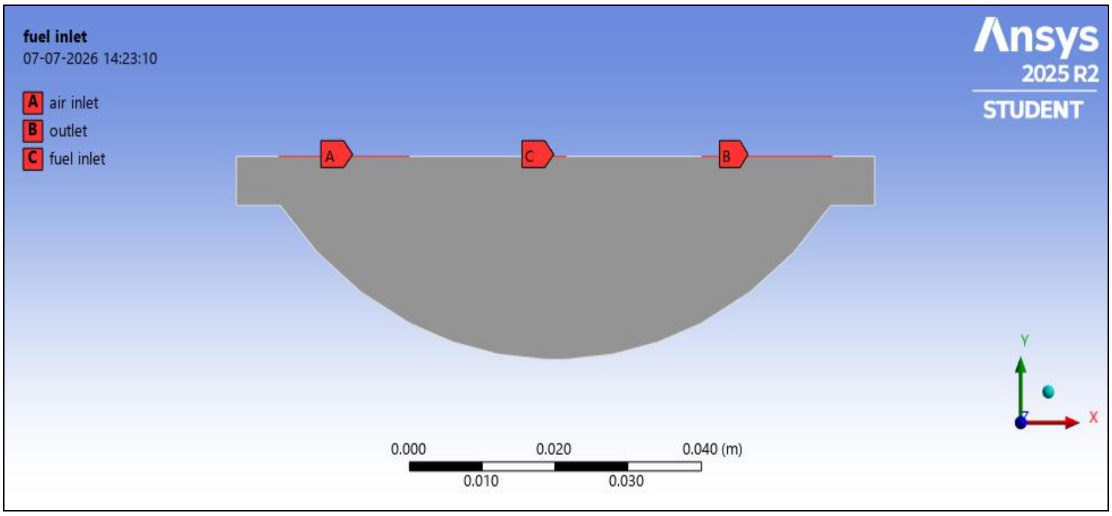

Fig 2 Computational Domain of the Combustion Chamber

➢ *Velocity Contour*

The CFD simulation estimated velocity profile for the combustion chamber under full load operating condition is shown in figure 3. The velocity distribution ranges from 0 m/s to about 151 m/s. This means that the in-cylinder flow field changes significantly during the fuel injection and combustion. The maximum velocity reaches around 151 m/s at the fuel inlet, which is in good agreement with the specified injection boundary condition of 155 m/s, thereby verifying the accuracy and stability of the numerical model.

A narrow high momentum fuel jet is injected into the combustion chamber and creates a strong velocity core right after injection. As the jet interacts with the surrounding compressed air, the momentum of the jet diminishes progressively because of viscous dissipation and turbulent mixing. The intake air enters the chamber at a somewhat lower velocity of around 20–25 m/s, which is in good agreement with the stipulated inlet velocity of 21.6 m/s. The interaction of high velocity fuel jet with the entering air creates strong shear layers and hence turbulence production leading to rapid atomization and homogenous air-fuel mixing.

The velocity slowly declines from about 150 m/s near the injector to values lower than 40 m/s in the mixing zone. This means that the momentum of the fuel jet is effectively transferred to the surrounding air. Due to the wall friction and the no-slip boundary condition, the flow velocity is further reduced to below 10 m/s along the curved piston bowl and the cylinder walls. Such low velocity sections produce recirculation zones which enhance the residence duration of the combustible mixture and hence improve the fuel evaporation and combustion efficiency.

The velocity profile, as a whole, describes a typical jet-driven turbulent flow with radial expansion and slow decay of velocity. The intense turbulence caused by the fuel spray increases combustion by speeding up the air-fuel mixing, minimizing the ignition delay and providing a more uniform heat release. Therefore, the anticipated velocity field provides a good basis for the discussion of the pressure, temperature and emission characteristics in the next sections.

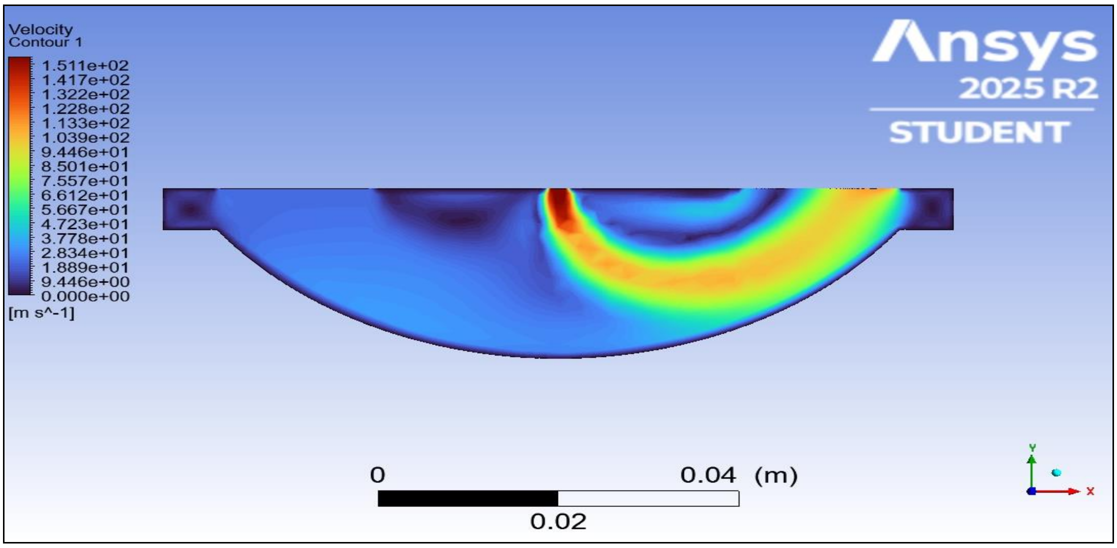

Fig 3 Velocity Contour Inside the Combustion Chamber

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➢ *Pressure Contour*

The pressure contour produced from the CFD simulation of the combustion chamber under full load operating state is shown in Figure 4. The pressure distribution is very variable over the computation domain, ranging from roughly −2.58 kPa to +5.05 kPa. This variation is caused by the complicated interaction between the entering air and the high-speed fuel spray during the injection process.

The high pressure zone, roughly 5.05 kPa, is located close to the air entrance. Here, the incoming air decelerates upon entering the combustion chamber, generating a stagnation zone. This localized pressure rise is due to the conversion of kinetic energy into static pressure and indicates efficient air entry into the combustion chamber. Conversely, a substantial low pressure area of roughly −2.58 kPa is generated around the fuel injection region where the diesel fuel is injected at a speed of around 155 m/s. The quick expansion of the high-speed fuel jet creates a strong drop of static pressure. This induces a suction effect increasing the entrainment of the surrounding air in the spray.

A high pressure gradient is detected surrounding the fuel jet, demonstrating a strong momentum exchange and a robust interaction between the injected fuel and the compressed air. When the spray goes further into the combustion chamber, the pressure recovers gradually by turbulent diffusion and loss of energy. The pressure distribution clearly shows the inverse association between the velocity and pressure, the areas of high velocity correspond to lower static pressure while the areas of lower velocity show considerably higher pressure. This behaviour is in accordance with the principles of fluid dynamics and confirms the numerical solution produced from the CFD model.

The projected pressure field shows effective fuel-air interaction and positive circumstances for combustion. High pressure gradients close to the injector enhance atomization, fuel dispersion and the development of a homogenous mixture. Thus, the pressure contour demonstrates the capabilities of the computational model to accurately capture the in-cylinder flow characteristics, providing a reliable basis for the analysis of combustion performance and emission production in the next sections.

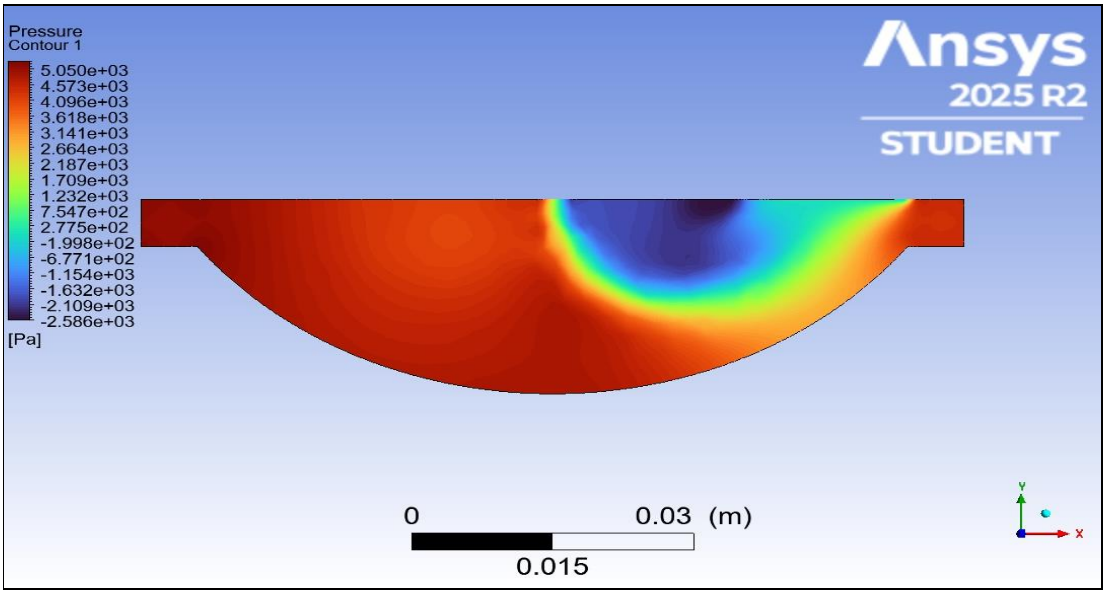

Fig 4 Pressure Contour Inside the Combustion Chamber

➢ *Temperature Contour*

The temperature distribution inside the combustion chamber predicted by the CFD simulation for full-load operation circumstances is presented in Fig. 5. The temperature contour indicates non-uniformity of thermal field with the temperature varying from 300K to 513K, which correlates well with the heat transfer characteristics related with fuel injection and in-cylinder flow. The colour scale displays areas of low temperature in blue and high temperature in red, reflecting the thermal gradients created within the combustion chamber.

The minimal temperature of around 300 K is found around the air inlet and the fuel jet core where fresh air and injected diesel enter the computational domain. The thermal energy of these incoming streams is generally modest, which results in lower local temperatures. The fuel jet enters the combustion chamber and mixes with the surrounding air, and heat is gradually transmitted by convection and turbulent mixing. Hence, the temperature increases gradually along the flow direction.

From about 300 K to 450 K a clear temperature gradient can be noticed, reaching a maximum value close to the lower curved area of the combustion chamber of almost 513 K. This temperature rise is mainly caused by convective heat transfer, turbulent mixing and storage of thermal energy in the recirculation zones. The curved piston bowl geometry plays a major role in directing the flow, creating recirculation regions, and increasing the residence time of the air–fuel combination. The longer residence period leads to further heat transfer from outside the hot gases and from

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the walls of the combustion chamber, which causes a slow increase in the local temperature.

The high temperature region at the lower curving wall shows the effective thermal energy distribution inside the chamber. The gradual transition from lower to higher temperatures indicates stable heat transmission without sharp thermal jumps, which shows that the computational model correctly captures the thermal behavior of the flow. Furthermore, the greater turbulent mixing promotes a more uniform temperature field, which is crucial to the effective combustion and thorough oxidation of the fuel.

The expected temperature distribution also supports the strong link between the velocity and pressure fields outlined in earlier sections. The high turbulence and recirculation regions enhance the heat transmission, therefore enhancing the fuel evaporation and air-fuel mixing. These thermal properties result in higher combustion efficiency and favorable conditions for minimizing incomplete combustion products such as carbon monoxide. The temperature contour displays an efficient energy transfer in the combustion chamber and supports the competence of the CFD model to forecast in general the thermal behaviour of the single-cylinder direct injection diesel engine.

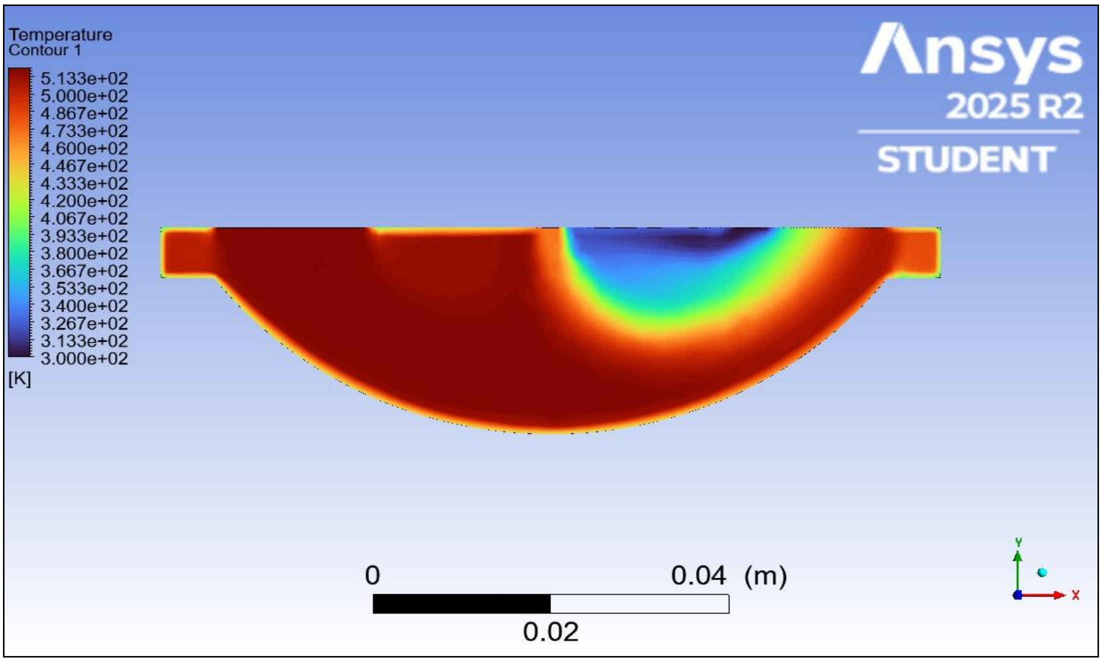

Fig 5 Temperature Contour Inside the Combustion Chamber

- *Carbon Monoxide (CO)*

The change of carbon monoxide (CO) mass fraction along the combustion chamber at full-load operating settings for Diesel, R20, R20CNT50PPM and R20CNT50 with 10 LPM hydrogen enrichment is presented in Figure 6. The CFD simulation results show a gradual drop of CO concentration from chart count 1 to chart count 7 for all fuel combinations which indicates a gradual oxidation of carbon monoxide into carbon dioxide as the combustion process progresses.

At the first site (chart count = 1), traditional diesel has the largest CO mass percentage of about 0.115, which is attributed to locally rich fuel regions and restricted oxygen availability, resulting in partial combustion. The CO mass fraction of the R20 biodiesel mix is significantly lower at around 0.042, which can be attributed to the intrinsic oxygen content found in biodiesel that facilitates more complete oxidation of the fuel. The addition of 50 ppm of carbon nanotubes (R20CNT50PPM) reduces the CO mass percentage further to about 0.040. This improvement is mainly due to the better thermal conductivity and catalytic behavior of CNT nanoparticles which boost the heat transfer, fuel atomization and combustion efficiency.

The fuel R20CNT50PPM with 10 LPM hydrogen enrichment had the lowest initial CO mass fraction of roughly 0.017 of all evaluated fuels. Hydrogen has a rapid flame propagation speed, a wide flammability range, and low ignition energy, which lead to faster combustion and better oxidation reactions in the combustion chamber. This means that more carbon monoxide is oxidised to carbon dioxide and so the CO emissions are much lower.

As combustion proceeds from chart count 1 to chart count 7, the CO mass fraction drops consistently for all fuel combinations. There is the largest drop for diesel, from around 0.115 to 0.015, whereas R20, R20CNT50PPM and R20CNT50PPM with hydrogen reduce to about 0.008, 0.005 and 0.003, respectively. Such slow decrease shows that carbon monoxide formed at the first stages of combustion undergoes gradual oxidation with the increase in temperature and availability of sufficient oxygen.

The comparison study clearly shows that the combined effects of biodiesel, CNT nanoparticles and hydrogen enrichment greatly improve the combustion quality by strengthening the fuel-air mixing, oxidation efficiency and reduction of incomplete combustion products. The obtained results show that the R20CNT50PPM with 10 LPM hydrogen provides the lowest CO mass fraction in the whole combustion process compared to all the evaluated fuels, indicating better combustion characteristics and cleaner exhaust emissions. The CFD results are in good agreement with the expected combustion behavior and show the usefulness of hydrogen assisted nano-particle biodiesel blends in reducing the carbon monoxide generation.

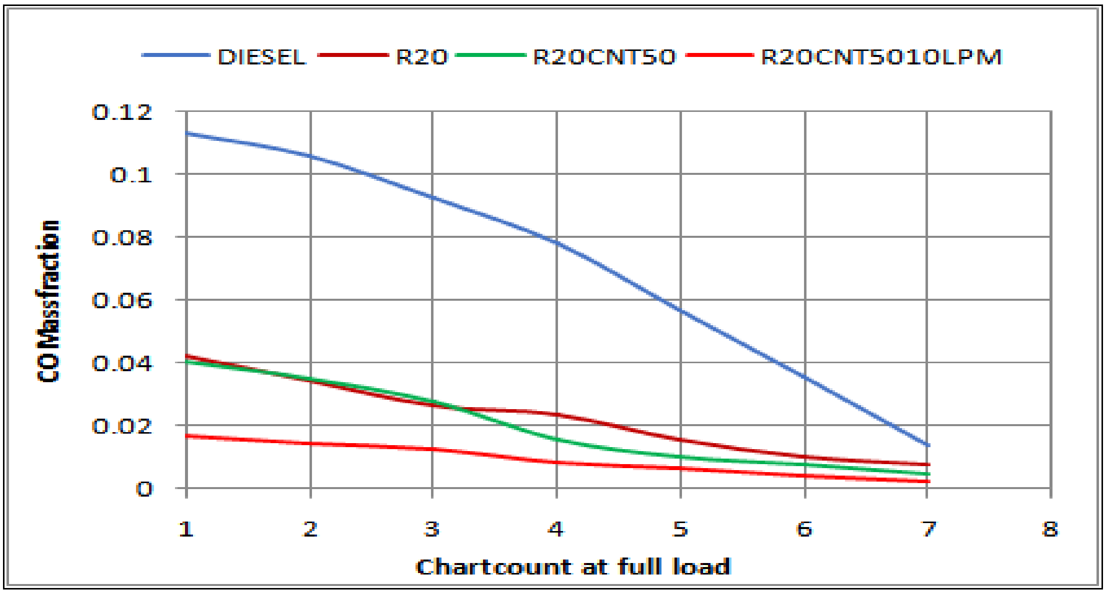

Fig 6 Carbon Monoxide (CO) for Different Fuel Blends at Full-Load Conditions.

➢ *Carbon Dioxide (CO_2)*

Figure 7 shows the fluctuation of carbon dioxide (CO_2) mass fraction anticipated by CFD simulation along the combustion chamber under full-load operating settings for Diesel, R20, R20CNT50PPM and R20CNT50PPM with 10 LPM hydrogen enrichment. The CO_2 mass fraction falls gradually from chart count 1 to chart count 7, indicating changes in the combustion products as the gases travel across the computational domain.

In the inlet region (chart count = 1), the maximum CO_2 mass fraction of about 0.62 is seen in R20 biodiesel mix. This is due to the improved oxidation of carbon containing fuel owing to the oxygenated characteristic of biodiesel. The extra oxygen molecules in the biodiesel improve the combustion process in the first stage which results in more CO_2 generation than normal diesel. Meanwhile, the CO_2 mass fraction for Diesel is roughly 0.22, while for R20CNT50PPM it is approximately 0.17. The addition of 50 ppm of carbon nanotube (CNT) nanoparticles enhances the combustion process by improving heat transmission, fuel atomization and air–fuel mixing, therefore boosting the combustion efficiency with a moderation in the carbon-based emissions.

The R20CNT50PPM with 10 LPM hydrogen enrichment has the least CO_2 mass fraction of ~0.02 in the entire computational domain. This reduction is mainly due to the carbon-free nature of hydrogen replacing some of the carbonaceous fuel during combustion. Besides, owing to high flame speed and flammability range, hydrogen is conducive to fast combustion, better mixture homogeneity and efficient energy release. This reduces the dependency on carbon-containing fuel and therefore the generation of CO_2.

From chart count 1 to chart count 7, the CO_2 mass fraction drops for all fuel combinations. This is attributed to the expansion of gas and the dilution and transportation of products of combustion toward the exhaust outlet. All the fuels show a decreasing trend but R20CNT50PPM with hydrogen enrichment always has the lowest CO_2 concentration, which is a demonstration of the synergistic effect of the nanoparticle additions and hydrogen-assisted combustion. The CFD calculations clearly prove the synergistic effect of biodiesel, CNT nanoparticles and hydrogen enrichment on the enhancement of combustion efficiency and reduction of carbon based emissions.

In general, the numerical results confirm that R20CNT50PPM with 10 LPM hydrogen has the most favorable combustion properties among the fuels studied. The lowered CO_2 mass fraction and lower CO emissions stated in the previous section, shows the promise of hydrogen-assisted nanoparticle biodiesel blends for development of cleaner and more sustainable compression ignition engine technology.

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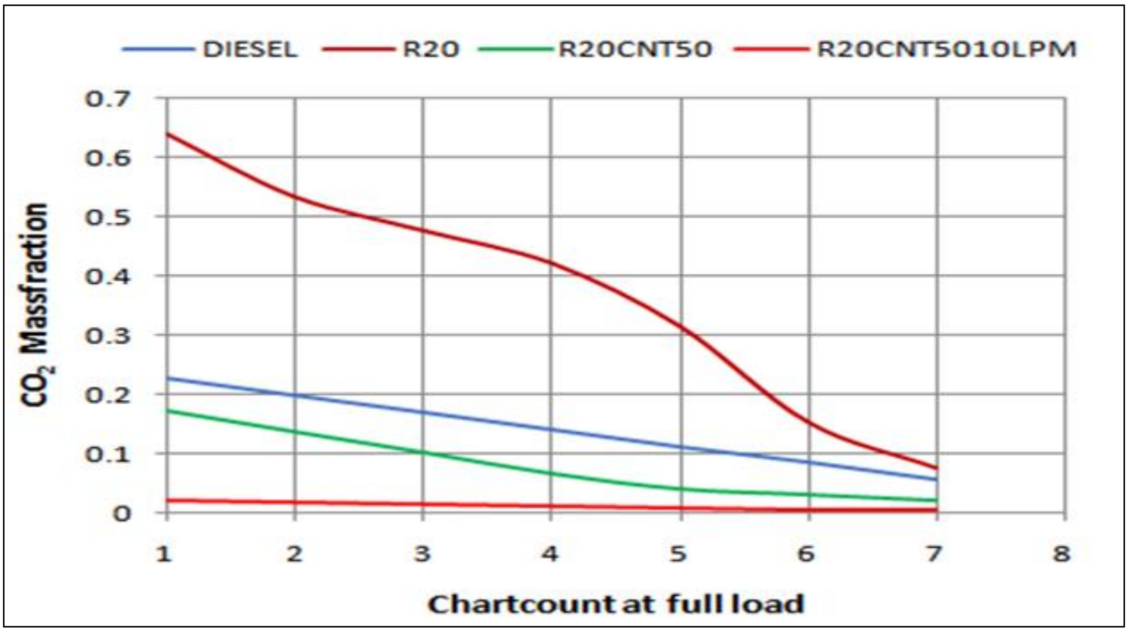

Fig 7 Carbon Dioxide (CO_2) for Different Fuel Blends at Full-Load Conditions

IV. CONCLUSION

The combustion and exhaust parameters of a four stroke single cylinder direct injection CI diesel engine running at 1500 rpm were analyzed with experimental and CFD modeling in this study. The in-cylinder velocity, pressure, temperature, CO and CO_2 distributions were predicted correctly by the CFD results and were found to be in good agreement with the experimental observations.

The results showed that the addition of (R20) Rapeseed biodiesel, 50 ppm CNT nano particles and 10 LPM hydrogen enrichment increased combustion by better fuel–air mixing and combustion efficiency. The adjusted fuel blends achieved lower CO and CO_2 emissions than plain diesel. Of the fuels tested R20CNT50PPM with 10 LPM hydrogen presented the highest overall performance with better combustion characteristics and lower emissions.

The results show that the combined usage of biodiesel, CNT nanoparticles and hydrogen is an effective method to improve performance of CI engines while decreasing harmful exhaust emissions. The validated CFD model can potentially be utilized as a useful tool for future combustion and emission research.

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