# A Study on Oxy-Fuel Diesel Engine and Comparison with Conventional Air Combustion

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## Abstract

To achieve minimal carbon emissions and zero NOx emissions of a diesel combustion engine, a numerical study on novelistic Oxy-Fuel Combustion (OFC) technique (nitrogen free combustion) is carried out. Diesel engine chemical reactions mechanism indicates that the presence of nitrogen during combustion generates NOx emissions, so a nitrogen free oxidizer environment i.e. oxy-fuel combustion is investigated, analyzed and compared with the conventional air combustion engine. A 4-stroke water cooled Kirloskar type engine with Conventional Air Combustion (CAC) is experimentally tested at various load conditions, with data acquisition done on cylinder pressure, indicated brake power (IBP), indicated mean effective pressure (IMEP) and emissions. The experimental data is used to correlate and validate the 3D Computational Fluid Dynamics (CFD) simulation setup with CAC and the validated CFD model is used to study the OFC impact on in-cylinder flow, engine performance and emissions. The results indicates that NOx emissions are completely eliminated in OFC and carbon emissions are significantly reduced. Contrastingly an average drop of 45% in IBP, IMEP of OFC is noticed at all the operating conditions, which can be attributed to lean, early start of combustion and shorter combustion rates in OFC. Water injection technique is adopted to overcome the loss in engine performance with OFC, although a relative average improvement of 32% in engine performance is observed in OFC with water injection, the overall engine performance is still 10% lower compared to the conventional air combustion.

## Keywords

Oxy-fuel combustion, 3D CFD, Diesel engine, Emissions, Water injection technique

## 1. Introduction

Oxy-Fuel combustion is an unconventional combustion technology proposed by researchers to reduce the exhaust emissions (Huang et al. 2018). OFC is a nitrogen free combustion technique achieved by replacing the air by pure oxygen as an oxidizer for combustion. Absence of nitrogen in combustion eliminates the harmful NOx emissions and the exhaust contains only carbon emissions and water vapor. Equation 1 and 2 represents the combustion chemistry of CAC and OFC.

$$CxHy + O2 + N2 \rightarrow CO2 + H2O + N2 \qquad (1)$$

$$CxHy + O2 \rightarrow CO2 + H2O \qquad (2)$$

In the view of global warming & stringent emission norms industries and researchers have focused on diesel engine emission reduction techniques. The research was mainly post-combustion, in-cylinder, pre-combustion purification technologies. Concerning the in-cylinder optimization many attempts were made by varying the oxygen concentration, which resulted in reduction of carbon emissions but NOx emissions were increased due to high combustion temperatures. NOx emissions are inevitable with the presence of Nitrogen, which reacts with combustion bi-products under high in-cylinder temperatures. To zero down the NOx emissions, novelistic combustion process OFC is investigated. In OFC pure oxygen is used as an oxidizer replacing the conventional oxidizer air, which eliminates the generation of NOx during combustion and avoids the need of post-combustion purification processes (Donahue et al. 2000).

### 1.1 Objectives

The present paper focuses specifically on the application of Oxy-Fuel combustion in a diesel engine and investigates the impact of this new combustion technique on the in-cylinder flow, engine performance and emissions, in comparison with the Conventional Air Combustion. The study aims to eliminate the NOx emissions and to reduce CO, CO2, unburnt hydrocarbon emissions of the diesel engine with Oxy-Fuel Combustion and attempts to maintain the same engine performance as that of Conventional Air Combustion. The Sequence of steps followed in this study to achieve the goal are listed below

1. Experimental analysis and data acquisition on a single cylinder water cooled 4-Stroke diesel engine with Conventional Air Combustion at various load conditions.
2. Generating a CFD model of the diesel engine with Conventional Air Combustion in Ansys Forte and validating the simulation model results with experimental data.
3. Numerical investigation of diesel engine with Oxy-Fuel Combustion in Ansys Forte using the validated CFD model and comparison of in-cylinder flow, engine performance and emission parameters with Conventional Air Combustion.
4. Quantification of engine performance enhancement in Oxy-Fuel Combustion with water injection technique.

## 2. Literature Review

History of the OFC application indicates that this technology was mostly used for solid fuel combustors using pulverized coal, recent research has realized the significance and need of application of OFC towards liquid and gaseous fuels. Abraham et al. (1982) has projected the significance of OFC with coal in enhanced oil recovery (EOR) by utilizing the high concentration of carbon dioxide in exhaust gases. Researchers and scientists have applied OFC on modern internal combustion engines to achieve zero NOx and reduced carbon emissions. Stanger et al. (2015) summarized the three various types of OFC, the turbine based, oxy-pulverized coal-fired and oxy-circulating fluidized bed techniques for power production and discussed the possibilities of commercialization of OFC. Schluckner et al. (2020) used numerical CFD methods to investigate the application of OFC with natural gas and discussed the complex NOx formation due to residue nitrogen presence during combustion. Shaw et al. (1983) applied OFC on a diesel engine and named the engine as “non-air-breathing diesel engine” and indicated that this engine can achieve zero emissions with a high compatibility for Carbon Capture and Storage.

Azmi Osman et al. (2009) proved the feasibility of OFC on an internal combustion engine indicating the improvement in thermal efficiency and investigated water injection technology to control in-cylinder temperatures. Zhijun Wu et al. (2016) have studied the application of OFC into spark ignition (SI) engine by theoretical and experimental analysis indicating 56% thermal efficiency in for the proposed OFC IC engine and water injection process is proved to have great impact in system thermal efficiency improvement by waste heat recovery. Raouf et al. (2020) performed 3D CFD simulations to improve the output performance parameters of a diesel engine with OFC in HCCI combustion mode. CHEN et al. (2014) proposed a new combustion model using pure oxygen and CO2 in part of the exhaust gas to constitute the combustion environment of the internal combustion engine.

Zhong et al. (2018) compared the oxy-CO2 and oxy-H2O combustion techniques with conventional air-fired conditions using 2D, 3D direct numerical simulation (DNS). This study found the specific dilution ratios of CO2 and H2O, where the oxy-CO2 and oxy-H2O combustion temperature profiles are similar to conventional air-fired conditions. Zheng et al. (1992) conducted numerical analysis on intake compositions of nitrogen, oxygen and CO2 of an air-independent diesel engine and illustrated the influence of mass concentration on the engine performance. Hawley et al. (1994) (1998) performed experiments and simulations on a multi-cylinder diesel engine by replacing nitrogen with CO2. The study indicates a reduction in brake power and increase in Brake Specific Fuel Consumption under maximum torque conditions with preheated oxygen and 30 mol% of CO2.

The references cited above indicates the feasibility and advantages of IC engines on performance, emissions with OFC technology. The schematic representation of Oxy-Fuel Diesel engine configuration is presented in Figure 1. In the current research project a diesel engine is coupled with OFC to achieve zero NOx emissions. The research focuses in evaluating the feasibility of Oxy-Fuel Diesel engine by comparing the In-cylinder flow parameters, performance and emissions with CAC, which are computed using an experimentally validated CFD model. This study targets to achieve an equivalent performance of diesel engine with OFC as that of the CAC. Oxygen consumption being the prime cost factor in OFC, the present work also aims to improve the average equivalence ratio in OFC to enhance the engine economic performance.

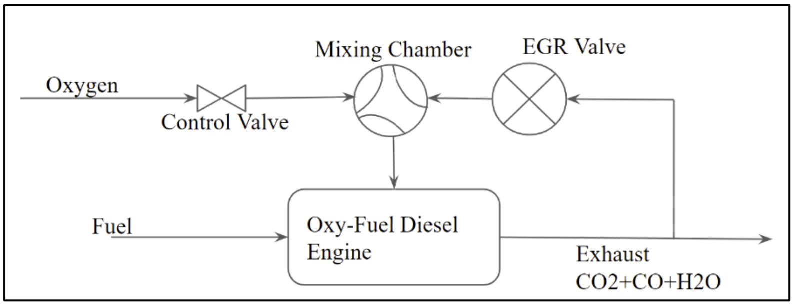

Figure 1. General schematic of Oxy-Fuel Diesel engine configuration

## 3. Methods

In this study a conventional diesel engine with CAC is evaluated experimentally under various load conditions and the experimental data is used to correlate and validate the representation of the engine in 3D CFD simulation. Figure 2 illustrates the flowchart of research roadmap. The first step of the roadmap is to validate the CAC simulation model with experimental results at four different load conditions. The validated simulation setup is further used to investigate the application of OFC to evaluate the impact on engine performance and emissions. As this study aims to achieve an equivalent OFC performance with CAC, the engine powers are compared at the final step, to deploy the power enhancement iterations, in a case the power is lower in OFC.

ANSYS Forte 19.3 is used to simulate the engine with RNG k-Ɛ model used for the turbulence and diesel is modelled as n-heptane with 35-species 74-reaction chemical kinetics scheme. Forte is a CFD tool customized to simulate internal combustion processes. Forte produces accurate results by coupling detailed chemical kinetics with liquid fuel spray and turbulent gas dynamics. The fuel injector used in experimentation was an equally spaced 8-hole injector, so to gain the computational advantage of periodicity, the diesel engine in CFD is modelled as 45° sector model (360°/8) with an assumption of symmetry in injection and combustion properties with respect to each nozzle-hole of the injector in the combustion chamber. The models used in this CFD simulation work are indicated in Table1.

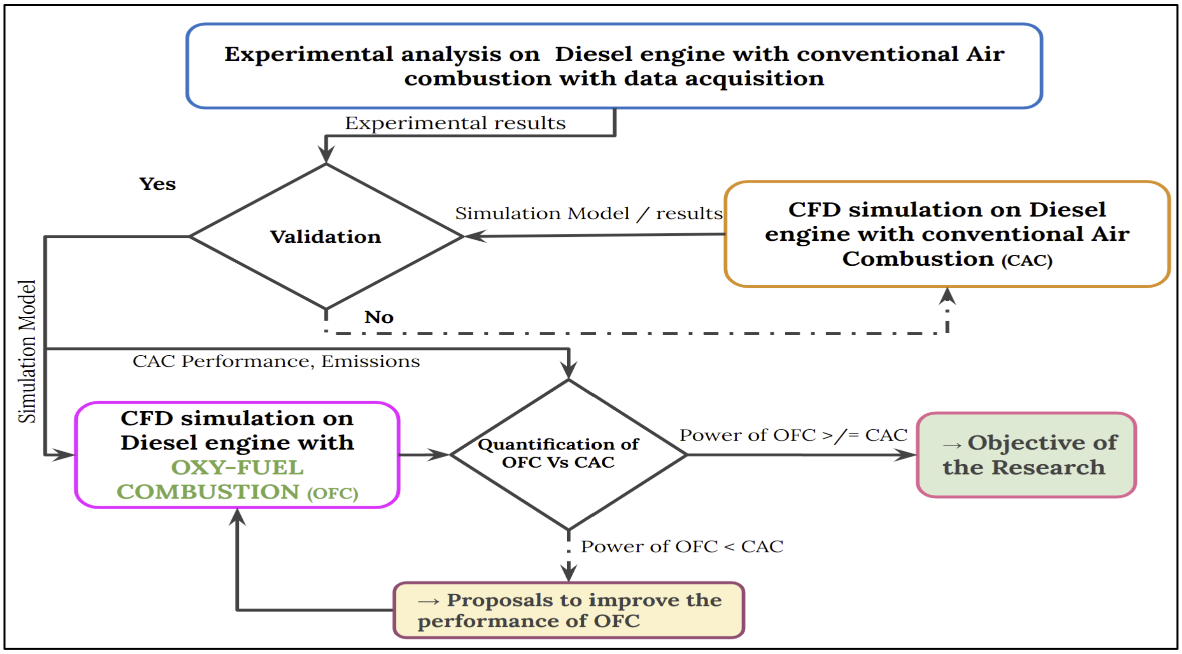

Figure 2. Flow chart of research roadmap

Table1: CFD Simulation sub-models

| Description | Value |
|---|---|
| Periodicity | 45 degree |
| Wall model | Law of the wall |
| Turbulence model | RNG k−ε model |
| Combustion model | Mixing controlled combustion (MCC) |
| Fuel chemistry model | n-heptane reduced mechanism |
| Droplet breakup model | KH-RT model |
| NOx formation mechanism | Zeldovich mechanism |
| Soot model | Two-step semi-empirical model |

## 4. Data Collection

The schematic of conventional diesel engine test setup is shown in Figure 3. The adopted engine is a 4-stroke water cooled Kirloskar type engine with compression ratio of 15.6:1 and the engine specifications are listed in Table2. The experimentation is carried out at four load conditions 25%, 50%, 75% and 100%. A pressure transducer and emission testing machine AVL DI GAS 437 gas analyzers are used to capture the in-cylinder pressure and pollutants.

### 4.1 Error analysis

The accuracy of the experimental data acquisition is subjected to the uncertainty, equipment errors and parameters considered during the test. The uncertainties are majorly influenced by calibration, use of instruments, skill of the observer in reading the data and consistency of the environmental situations. Uncertainties associated in the current experimental setup are evaluated using partial differentiation method for the instruments and the uncertainties of independent parameters are accounted by calculating the mean values of 16 repetitive readings. With these approaches the experimental absolute uncertainty is found to be 2.4%.

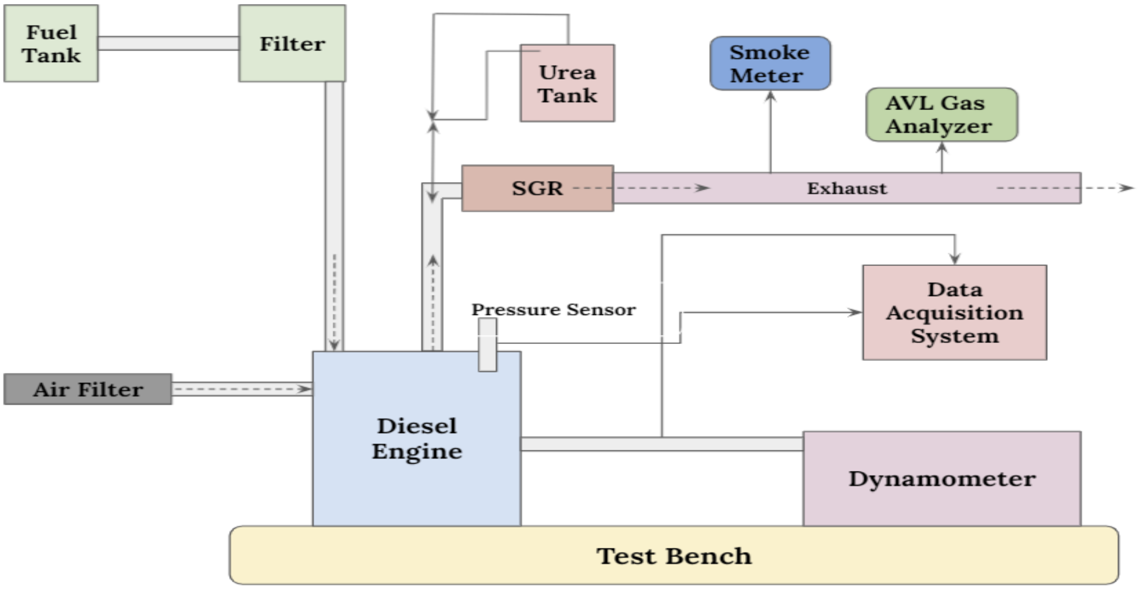

Figure. 3 Schematic of experimental setup

Table2: Engine Specifications

| Description | Value (units) |
|---|---|
| Engine | 4-Stroke Diesel engine |
| Number of Cylinders | Single cylinder water cooled |
| Bore | 87.5 (mm) |
| Stroke | 110 (mm) |
| Compression ratio | 15.6 : 1 |
| Connecting rod length | 234 (mm) |
| Engine speed | 1500 (rpm) |
| Load | Electric load |
| Orifice diameter | 29.6 (mm) |
| Coefficient of discharge | 0.6 (mm) |

## 4.2 Validation

Figure 4 represents the comparison of in-cylinder pressure simulation results with experimental data. The CFD results indicate a marginal difference in the trend of in-cylinder pressure Vs CAD, but the peak magnitude of in-cylinder pressure and the corresponding CAD is well predicted. The variation in trend is less than 5%, which can be treated as a good compatibility with experimental measurements. The minor variation in trend can be attributed to the reasonable approximation made in modelling the IC engine, the simulation is carried out only from Inlet valve closing to the exhaust valve opening in which the internal gas residuals of the last combustion cycle are not taken into account.
The quantitative results shown in Figure 5, such as in-cylinder pressure, IBP, IMEP and carbon monoxide (CO), Oxides of Nitrogen (NOx) emissions obtained from CFD simulation setup in Ansys Forte with conventional combustion are validated against the experimental data at various load conditions. The comparison shows a good correlation between the simulation results and experimental results, on both engine performance and emissions characteristics at all the load conditions, concluding the CFD setup to be considered as experimentally validated for all the engine load conditions.

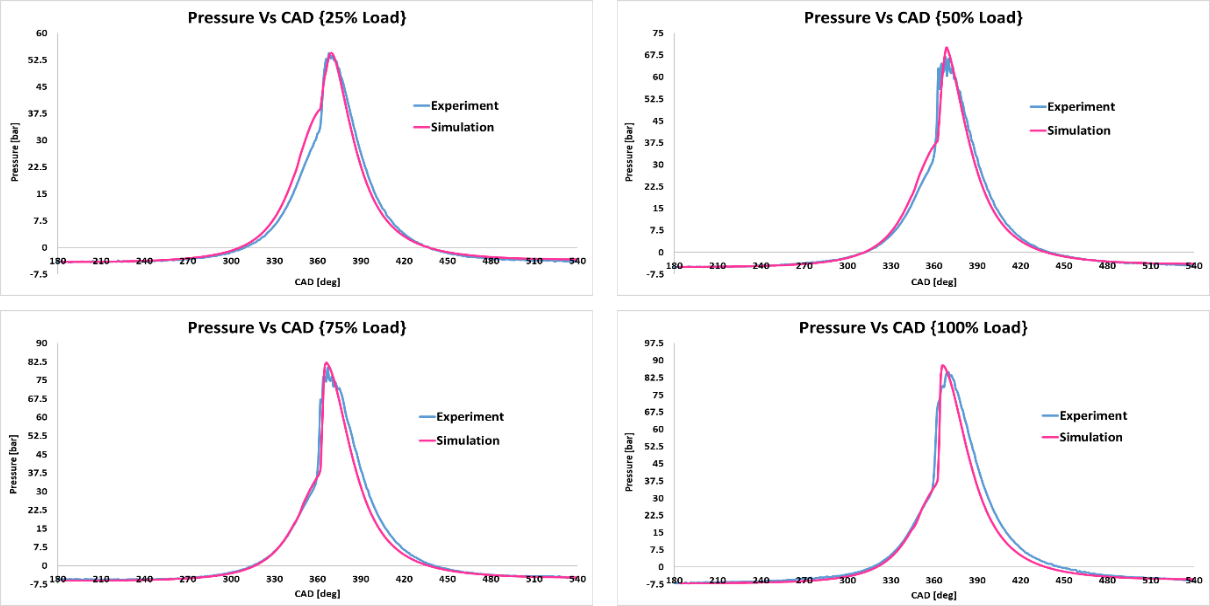

Figure 4. Comparison of simulation and experimental in-cylinder pressure of CAC engine

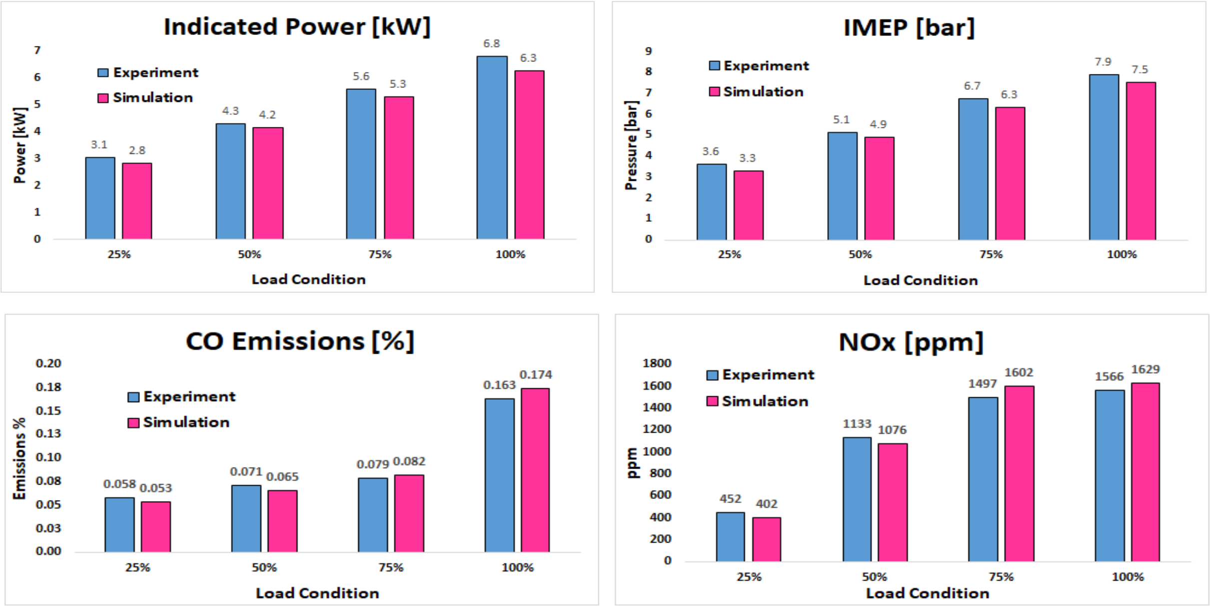

Figure 5. Comparison of simulation, experimental engine performance and emissions of CAC

## 5. Results and Discussion

### 5.1 In-cylinder pressure and temperature variation

Figure 6 and Figure 7, shows the comparison of in-cylinder pressure and temperature respectively. Oxygen being more reactive than nitrogen, accelerates the oxidation of fuel improving the rate of combustion and inducing an early start of combustion. Also, the increased volume of oxygen reduces the average equivalence ratio (AER) resulting a lean combustion in OFC. Due to the combined effect of lean and early start of combustion, the peak pressure and temperature in OFC are relatively lower than CAC. The rate of increase in pressure, temperature verses CAD is higher in OFC, indicating the higher combustion rate. The pressure envelope indicates that the piston is exposed for a higher duration of pressure in OFC than CAC.

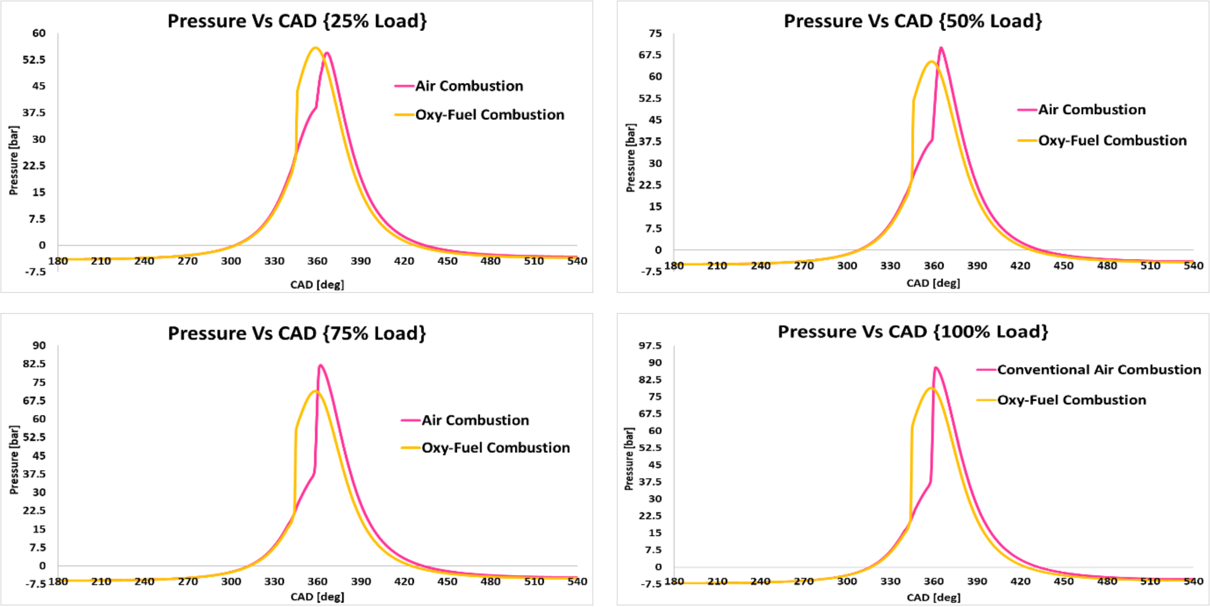

Figure 6. Comparison of in-cylinder pressure at various load conditions

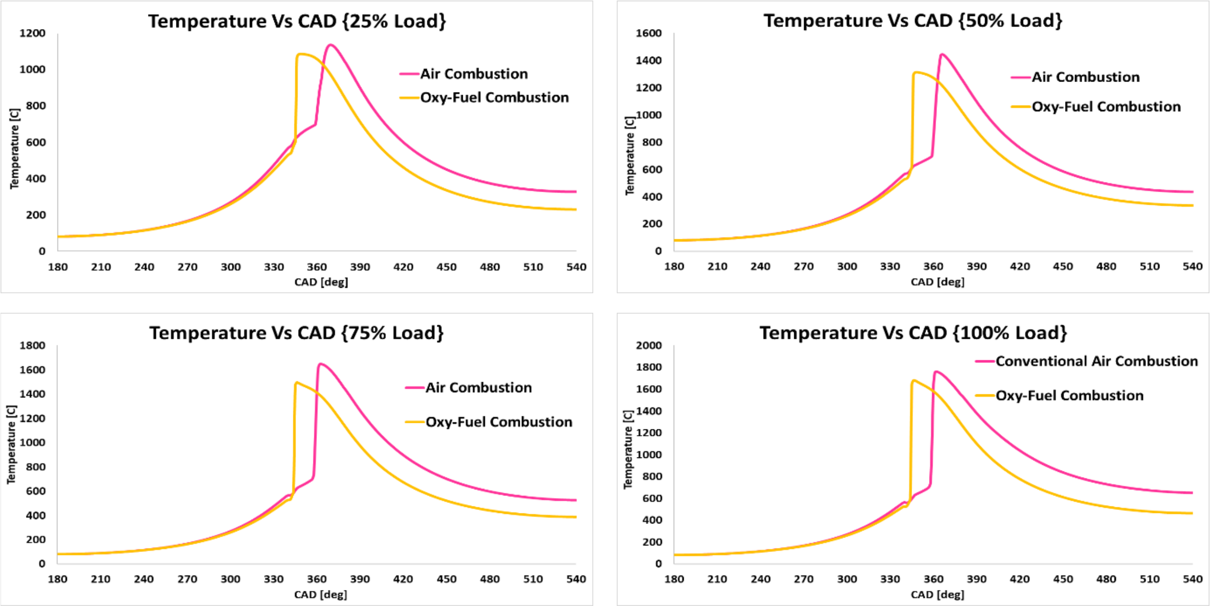

Figure 7. Comparison of in-cylinder temperature at various load conditions

## 5.2 Heat release and heat transfer

The trend of chemical heat release and apparent heat release variation with CAD is indicated in Figure 8. The ultimate chemical heat energy released is same in both CAC and OFC, representing the combustion efficiency is same in both the combustion conditions. However, the rate of chemical heat release is higher in OFC and so the ultimate chemical heat energy is achieved at an early CAD than in CAC. On the other hand, the apparent heat release, which is defined as the useful energy available for the work done is lesser in OFC, thereby the engine is under performing with OFC than CAC. The wall heat transfer represented in Figure 9, which is a measure of heat transfer loss through the cylinder walls is observed to be 2.5times higher in OFC, is most contributing factor for the drop in apparent heat release. The higher losses in OFC, can be attributed to the huge variation in effect thermal conductivity (ETC) of the working fluid.

Absence of nitrogen has a considerable impact on the chemical and physical properties of the in-cylinder working fluid, the ETC of the combustion gases is observed to be very high in OFC, as shown in Figure 10, encouraging a higher heat transfer from working fluid to the cylinder walls, yielding a lower peak and exhaust gas temperature at all the operating engine conditions.

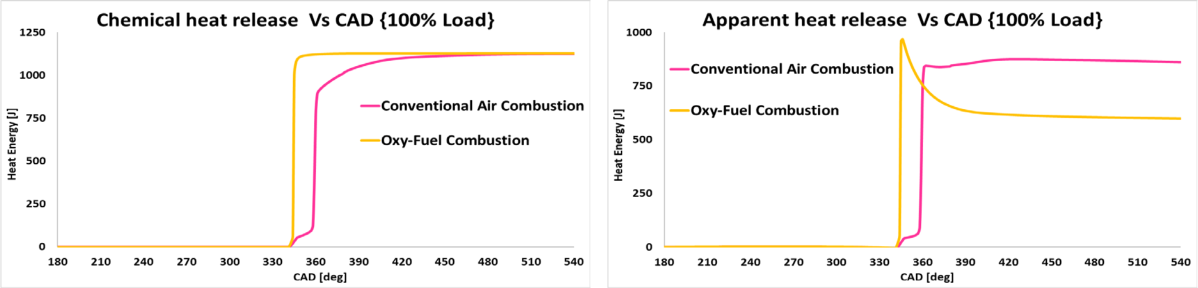

Figure 8. Variation of heat release at 100% load

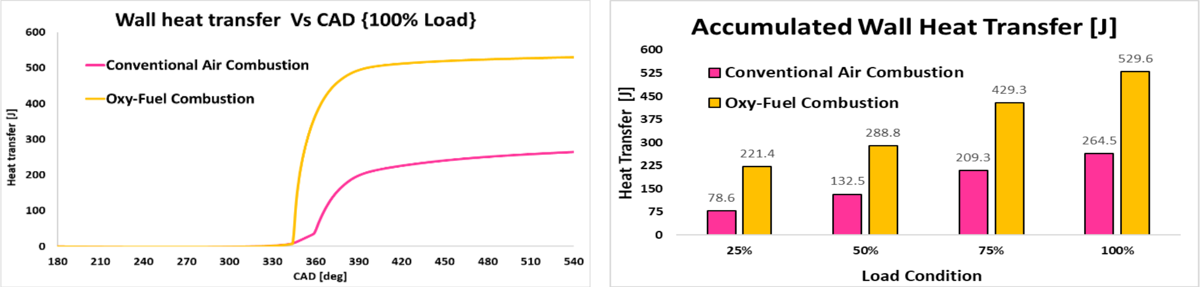

Figure 9. Variation of Wall heat transfer

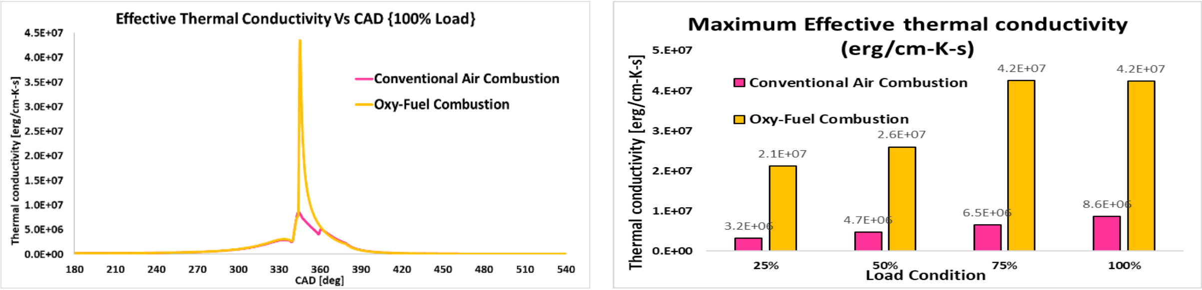

Figure 10. Variation of effective thermal conductivity

### 5.3 Comparison of engine performance parameters

From Figure 11, it is observed that in OFC the IP, IMEP are reduced by around 45%, this is due to the chemical and physical properties variation in the in-cylinder working fluid, as the complete nitrogen volume is replaced with oxygen. The thermal diffusivity of the combustion gases is higher in OFC, which improves the flame propagation, accelerates the oxidation of fuel thereby reducing the overall combustion duration, with the combined effect of above the start of combustion is shifted to an early CAD than the conventional combustion. Contrastingly this phenomenon is also responsible for reduction in IP in OFC, as the energy transformation starts before the TDC due to shorter combustion duration and early combustion. The other major factor is cylinder wall heat transfer losses, the coupled effect of thermal diffusivity and thermal conductivity is increasing the losses through cylinder walls by 2.5 times in OFC, this phenomenon has a huge impact on reduction of IP and increase in Indicated Specific Fuel Consumption (ISFC). In OFC, as the complete nitrogen volume is replaced by oxygen, the average equivalence ratio (AER) is relatively very less, quantitatively the oxy-fuel AER is ~10% as that of the conventional engine AER which results a lean combustion and thus reducing the IP at all engine load conditions.

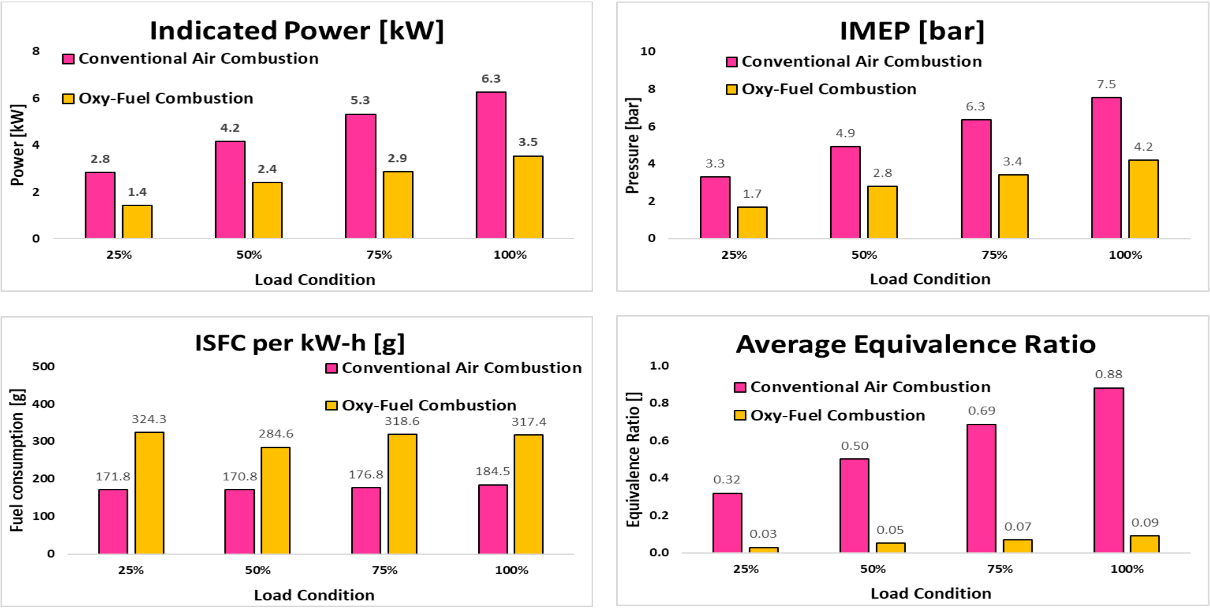

Figure 11. Comparison of engine performance parameters

### 5.4 Comparison of exhaust emissions

The quantitative comparison of exhaust emissions in shown in Figure 12, a significant reduction in emissions is observed in OFC. Despite OFC having the maximum in-cylinder temperature to be higher and being at lean burn strategy no NOx. Absence of nitrogen during combustion is having no impact on the CO2 emissions, but the CO and unburnt hydrocarbon emissions are relatively very low at all the engine load conditions in OFC, due to higher flame propagation rates and fuel oxidation in OFC than CAC.

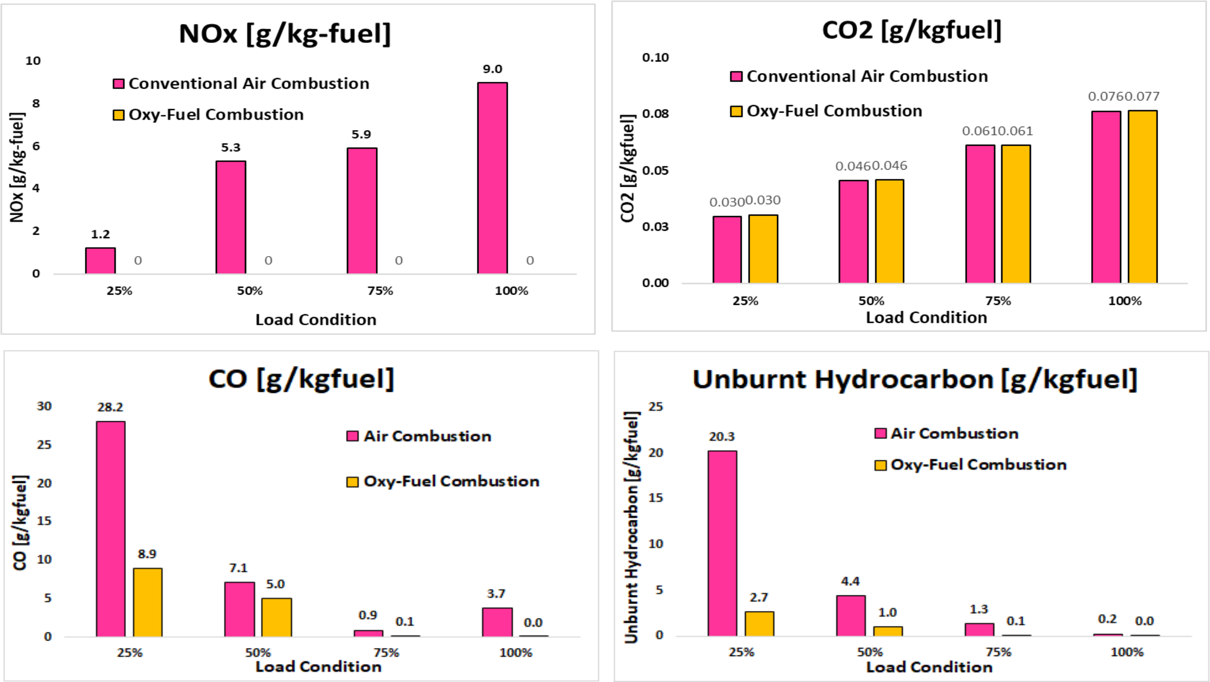

Figure 12. Comparison of exhaust emissions at various load conditions

### 5.5 Proposed Improvements

Although OFC shows a superior emissions characteristics by eliminating NOx, but the change in combustion process is arising new challenges like reduction in power output and the economic aspects associated with the residual oxygen after the combustion. To address these challenges water injection technique is adapted with OFC. Recent researches indicate that by adoption of water injection strategy in OFC controls the rate of raise of in cylinder temperature by optimizing the combustion process and relatively improves the power out of the engine. To predict the optimal mass fraction of the water to be injected into the engine, a design of experiments [DOE] is conducted with the constraints to achieve the maximum power and minimum emissions. The results of DOE indicate optimal mass fraction of water is to be at 0.7.

Figure 13 represents the impact of water injection with OFC on the rate of increase in pressure, temperature. Injection of water is delaying the combustion phasing leading a slight drop in peak cylinder pressure and temperature, also the burn rates and heat losses are controlled resulting a similar trend of variation as that of CAC. From Figure 14 it is observed that the engine performance is also enhanced by the water injection, a relative average improvement of 32% on all the performance parameters is observed at all the engine loading conditions, remarkably at 75% and 100% of engine load. On the other hand, no impact on exhaust emissions are noted with water injection.

However the extent of influence of water injection is limited, even under the maximum water mass fraction in combustion with OFC, the overall engine performance is still 10% lower compared to the conventional air combustion. Any further injection of water will interrupt the fuel atomization and also leads to a strong negative effect on in cylinder flow and heat release rate.

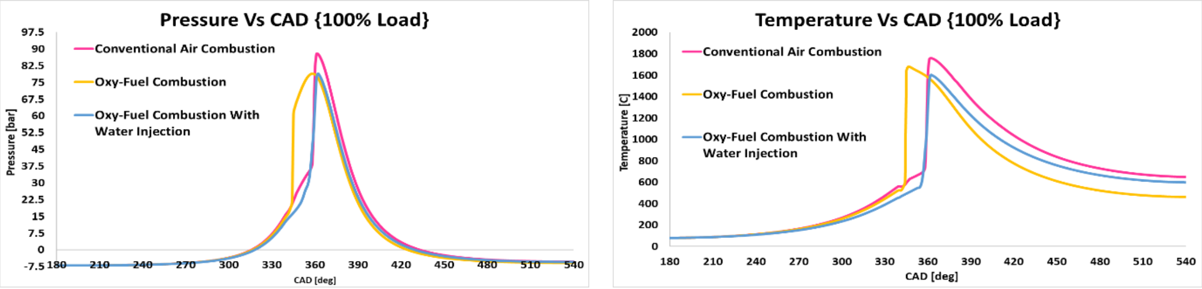

Figure 13. Comparison of in-cylinder pressure and temperature with water injection at 100% load

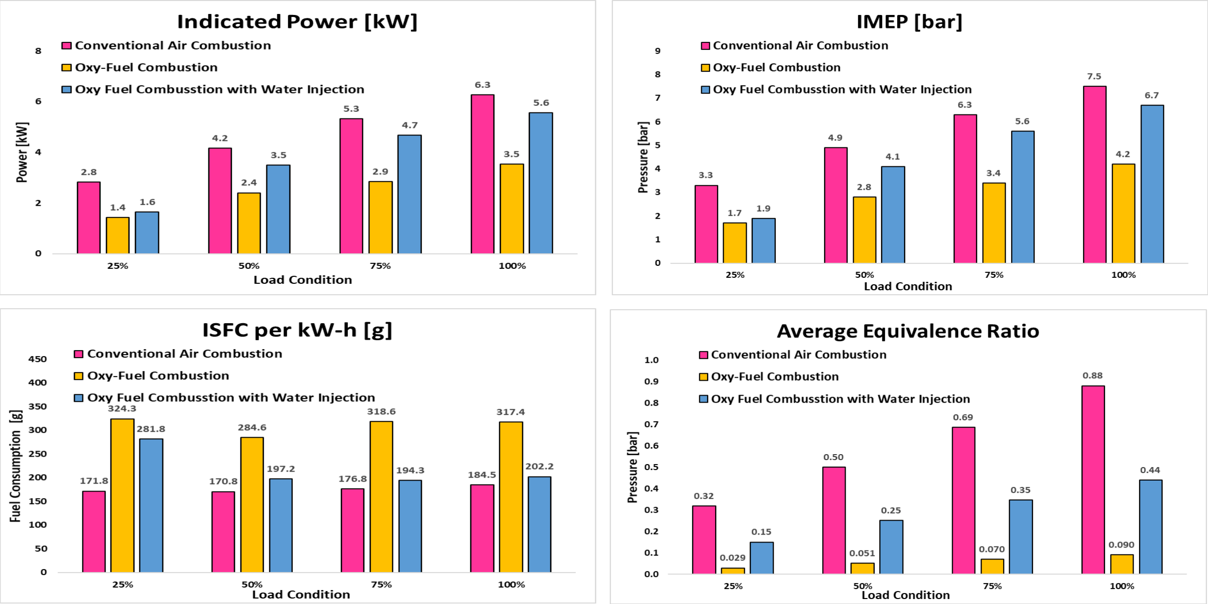

Figure 14. Comparison of engine performance parameters with water injection

## 6. Conclusion

This research is about an investigative study on converting a conventional combustion diesel engine into an OFC to evaluate the variation in in-cylinder parameters, engine performance and emissions at various engine load conditions. Below are the significant conclusions of this research

- The start of combustion in CAC is occurring at 358CAD, whereas in OFC it is at 345CAD signifying an early combustion and resulting a relatively lower peak pressure and temperature.
- The effect of increased oxygen volume during in combustion is inducing a very high effective thermal conductivity of the working fluid in OFC, thereby increasing the heat transfer loss through the cylinder walls and resulting a 45% reduction in IP, IMEP.
- In OFC, NOx is completely eliminated and a remarkable reduction in CO emissions and unburnt hydrocarbon emissions are observed.
- The loss in engine performance with OFC can be recovered by water injection technique. Water injection is controlling the early start of combustion, rate of combustion and wall heat transfer losses, yielding a relative average improvement of 32% at all the engine loading conditions with unchanged emissions.
- Though the overall engine performance in OFC with water injection is still 10% lower compared to CAC, the loss in performance is well compensated by the reduced carbon emissions and zero NOx emissions.

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