

A CFD Combustion Analysis of a Hydrogen-Biodiesel Dual Fuel System

¹Mohd. Yousuf Ali, ²M. Masood and ³S.N. Mehdi

¹Geetanjali Institute of Science and Technology, Aziz Nager (v), CB Post, Hyderabad, India

²L.I.T.S, Hyderabad-500034, India

³Professor, M.J.C.E.T, Hyd -34

Abstract: This paper describes about the project work carried out to develop a CFD simulation model to investigate the effect of the use of hydrogen-biodiesel dual fuel in a variable compression ratio diesel engine. Commercial CFD software is used in this project to study the effect of compression ratio on the performance of diesel engine. In the present study investigation is aimed at studying the effect of compression ratio on the peak pressure and temperature, turbulent KE and NO_x formation. Single cylinder variable compression ratio diesel engine is used. In this system engine is coupled to a DC dynamometer and all the experiments were carried out at a constant speed of 1500 RPM. Hydrogen is inducted along with air intake. Biodiesel is injected into the combustion chamber. The tests were carried out for the compression ratios of 17, 19, 21 and 23 and each time all the parameters were noted down. Engine exhaust emissions were also measured using an advanced AVL five-gas analyzer. CFD and experimental values are in close proximity.

Key words: *Hydrogen, Biodiesel • Compression ratio • Dual fuel engine • Emissions • Combustion • Heat release rate*

INTRODUCTION

As the world finds itself in the midst of universal energy shortage, compounded by a parallel need to reduce pollutants of all kinds, we must take an increasingly serious look at novel sources of abundant energy and methods for their best utilization. The depleting resources of fuel in the world today as well as the understanding of the need of the world environment requires the search for other types of fuel sources that may be renewed if possible [1-2].

Fuels such as natural gas, liquefied petroleum gas (LPG), are some of the alternative fuels to traditional ones that are fossil based such as diesel and gasoline. These conventional fuels have major disadvantages with regards to their exhaust emissions of nitrogen oxides (NO_x), unburned hydrocarbons (UBHC), carbon dioxides (CO₂) and particulate matter that are hazardous to humans and the environment alike [3-5]. The greenhouse effect is also one of the aftermaths from these gaseous emissions.

Biodiesel could be an excellent renewable fuel for diesel engines. It is derived from vegetable oils that are chemically converted into biodiesel. As the name implies, it is similar to diesel fuel except that it is produced from

crops like jatropha, Pongamia, soybean, sunflower, cottonseed oil and rapeseed oil. These crops are all capable of producing several gallons of fuel per acre that can power an unmodified diesel engine. Vegetable oil is converted into biodiesel through a chemical process that produces methyl or ethyl ester [6-8].

Hydrogen, with its remarkable combustion properties in the conventional internal combustion engine, appears to be proving itself as an ideal energy source for transportation systems. It has been shown that hydrogen can be economically produced in quantities great enough to power the world's automobiles for the foreseeable future [9]. Importantly, it can be used in existing internal combustion engines, yielding unprecedented efficiencies and extremely low levels of exhaust pollution [10]. Hydrogen has, for years, been recognized for its extremely high energy potential. But because of inherent difficulties in handling hydrogen in its gaseous form, technology has, over the past two decades, emphasized the utilization of hydrogen in its liquid form.

Hydrogen can be used advantageously in internal combustion engines as an additive to a hydrocarbon fuel. Hydrogen can be used in conjunction with compact liquid fuels such as gasoline, alcohol, diesel or biodiesel provided each is stored separately [11].

As with hydrogen, the drawback of lean operation with hydrocarbon fuels is a reduced power output. Lean operation of hydrocarbon engines has additional drawbacks. Lean mixtures are hard to ignite, despite the mixture being above the lowest flammability limit of the fuel. This result in misfire, which increases un-burned hydrocarbon emissions, reduces performance and wastes fuel.

Mixing hydrogen with other hydrocarbon fuels reduces all of these drawbacks. Hydrogen's low ignition energy limit and high burning speed makes the hydrogen/hydrocarbon mixture easier to ignite, reducing misfire and thereby improving emissions, performance and fuel economy. Regarding power output, hydrogen augments the mixtures energy density at lean mixtures by increasing the hydrogen-to-carbon ratio and thereby improves torque at wide-open throttle conditions.

Cfd Simulation: FLUENT is the CFD solver of choice for complex flows ranging from incompressible (low subsonic) to mildly compressible (transonic) to highly compressible (supersonic and hypersonic) flows. Providing multiple choices of solver options, combined with a convergence-enhancing multigrid method, FLUENT delivers optimum solution efficiency and accuracy for a wide range of speed regimes. The wealth of physical models in FLUENT allows you to accurately predict laminar and turbulent flows, various modes of heat transfer, chemical reactions, multiphase flows and other phenomena with complete mesh flexibility and solution-based mesh adaptation.

Fluent is a state-of-art computer program for modeling fluid flow and heat transfer in complex geometries. It Provides Complete mesh flexibility, solving flow problems with unstructured meshes that can generated about complex geometries with relative ease. Supported mesh types include 2D triangular/quadrilateral, 3D tetrahedral/hexahedral/pyramid/wedge and mixed (hybrid) meshes. FLUENT also has the capability to refine or coarsen the grid based on the flow solution.

FLUENT provides the following choices of turbulence models.

- K - ϵ models
- Standard K - ϵ model
- Renormalization-group (RNG) K - ϵ model
- Realizable K - ϵ model

The standard K - ϵ model is a semi-empirical model based on model transport equations for the turbulence kinetic energy (K) and its dissipation rate (ϵ). The model transport equation for K is derived from the exact equation, while the model transport equation for ϵ was obtained using physical reasoning and bears little resemblance to its mathematically exact counterpart. In the derivation of the K - ϵ model, it was assumed that the flow is fully turbulent and the effects of molecular viscosity are negligible. The standard K - ϵ model is therefore valid only for fully turbulent flows.

Analysis on FLUENT is being carried out using segregated, 3D solver. The model of species transport is used for defining the reacting species. The k- ϵ model is used as turbulence analysis model.

The mesh used for this model is Hex/Hybrid (Cooper). This mesh type is apt for such geometry and enables easy importing of the model into FLUENT. The model is a virtual prototype of the combustion chamber at the end of compression stroke. Diameter and height are a pre requisite for creating the cylindrical combustion chamber. Diameter of the chamber is known, which is equal to bore diameter (80 mm). The height H (i.e. distance between the piston top and cylinder head at the end of compression stroke) is calculated as shown below.

$$V_{\text{displacement}} = D/4 * d^2 * L$$

The K - ϵ Model: The transport equations for turbulent kinetic energy k and its dissipation rate ϵ are given below:

$$p \frac{DK}{Dt} = \frac{\partial K}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_i} \right] + G_k + G_b - p\epsilon - Y_m \quad (1)$$

$$p \frac{D\epsilon}{Dt} = \frac{\partial}{\partial x_i} \left[\left(\mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_i} \right] + C_{1\epsilon} \frac{\epsilon}{k} (G_k + C_{3\epsilon} G_b) - C_{2\epsilon} p \frac{\epsilon^2}{k} \quad (2)$$

$$= B g_i \frac{\mu_t}{Pr_i} \frac{\partial T}{\partial x_i} \quad (3)$$

Where:

G_k = Generation of turbulent kinetic energy due to mean velocity gradients.

$$= - \rho u'_i u'_j \frac{\partial u_j}{\partial x_i}$$

G_b = Generation of turbulent kinetic energy due to buoyancy.

For an ideal gas

Table 1: The height between the piston top and cylinder head for various compression ratios

r - compression ratio	Height H (mm)
17	6.875
19	6.111
21	5.5
23	5

Table 2: Specifications

Type	: 4-stroke, single cylinder, compression ignition engine with variable compression ratio.
Make	: Kirloskar AV-1
Rated Power	: 3.7 KW, 1500 RPM
Bore and Stroke	: 80 mm x 110 mm
Compression Ratio	: Variable from 14.3 to 25 (Approx)
Cylinder Capacity	: 552.64 cc
Dynamometer	: Electrical- AC Alternator
Cylinder Pressure	: By Piezo sensor, Range = 2000 psi
Orifice Diameter	: 15 mm
Fuel	: biodiesel and hydrogen
Hydrogen injection	: By Induction Method

$$G_b = -g_i \frac{\mu_i}{Pr_i} \frac{\partial p}{\partial x_i}$$

Pr_i = Turbulent Prandtl number for energy=0.85 (default)

$$\beta = -\frac{1}{p} \left(\frac{\partial p}{\partial T} \right) p$$

Y_M = Fluctuating dilatation in compressible turbulence to the overall dissipation rate

Boundary Conditions

Pressure Inlet Boundary Conditions: Pressure inlet boundary conditions are used to define the fluid pressure at flow inlets, along with all other scalar properties of the flow. They are suitable for both incompressible and compressible flow calculations. Pressure inlet boundary conditions can be used when the inlet pressure is known but the flow rate and/or velocity is not known. This situation may arise in many practical situations, including buoyancy-driven flows. Pressure inlet boundary conditions can also be used to define a free boundary in an external or unconfined flow.

This is applied on the nozzle and on the walls of combustion chamber.

Pressure Outlet Boundary Conditions: Pressure outlet boundary conditions require the specification of a static (gauge) pressure at the outlet boundary. The value of static pressure specified is used only while the flow is

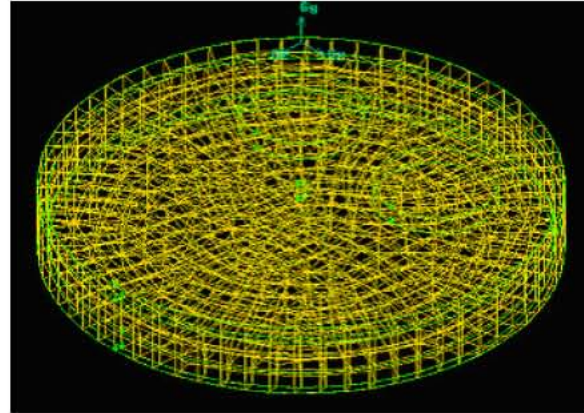


Fig. 1: Meshed Model

Boundary Conditions (Highlighted in Red)

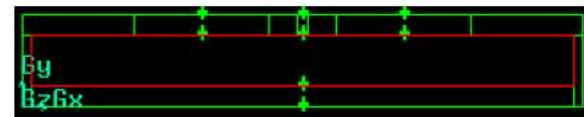


Fig. 2: Combustion Chamber



Fig. 3: Fuel Injector (Nozzle)



Fig. 4: Pressure Outlet

subsonic. Should the flow become locally supersonic, the specified pressure is no longer used. Pressure will be extrapolated from the flow in the interior. All other flow quantities are extrapolated from the interior.

A set of backflow conditions is also specified to be used if the flow reverses direction at the pressure outlet boundary during the solution process. Convergence difficulties will be minimized if you specify realistic values for the backflow quantities.

This is applied at the outlet for gases.

Experimental Setup: The engine used in the present study is a Kirloskar AV-1, single cylinder direct injection diesel engine with the specifications given below in Table 2. The engine is coupled to a DC dynamometer and all the experiments were carried out at a constant speed of 1500 rpm. The engine is modified and provision is made to vary the compression ratio from 14.3 to 25.

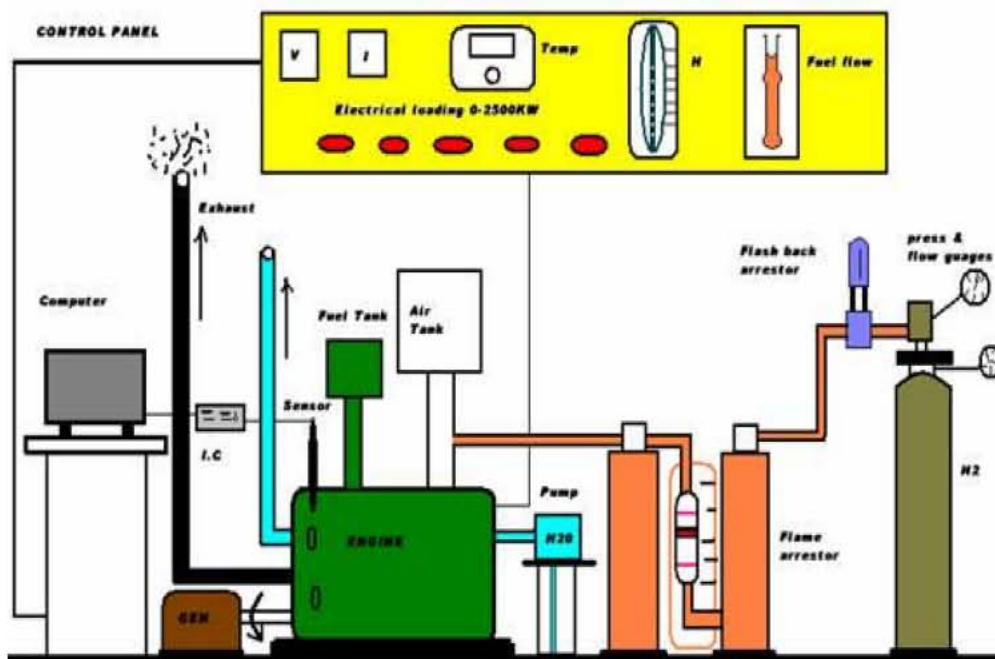


Fig. 5: The experimental set up of the engine

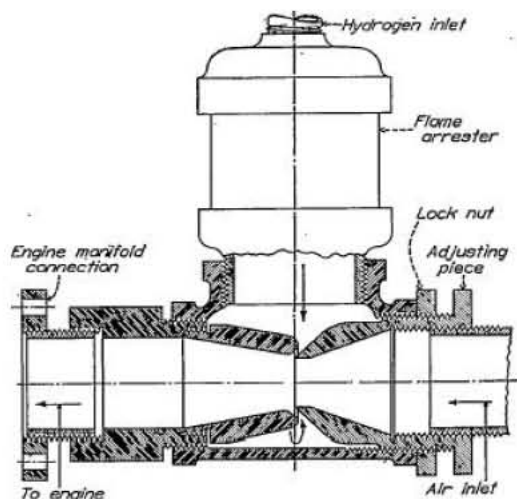


Fig. 6: Induction of Hydrogen through inlet manifold, with flame arrestor

The intake temperature and pressure were chosen to give stable and knock free engine operation. Biodiesel was injected at a pressure of 160 bar. Air and, Hydrogen were induced at atmospheric temperature and pressure.

Method of Induction: The engine is modified for the direct induction of hydrogen through the inlet manifold, as shown in the following Figure 6. The pressure of hydrogen was controlled directly by the pressure

regulator provided at the hydrogen cylinder opening. During high load application, for getting the rated speeds the flow of hydrogen was increased automatically along with the load. The biodiesel was controlled by the governor mechanism provided in the engine for the constant speed operation.

Hydrogen Flow Measurement: The hydrogen flow is measured using a specially designed hydrogen flow meter. To dampen the pressure fluctuations in the intake line, which particularly occur with large displacement single cylinder engines, a stabilizing tank is located at the inlet of the engine.

The Hydrogen gas was injected into the cylinder and a thermal mass flow controller controlled its flow rate. The maximum amount of Hydrogen supplied was limited by unstable operation at low outputs and by rough engine running due to knock at high outputs. When the hydrogen supply was increased, the biodiesel injection was automatically decreased by the governor mechanism of the engine to maintain the speed constant.

Biodiesel Flow Rate Measurement: Biodiesel flow rate is measured on volume basis using a burette and a stopwatch. The time taken for 10 cc of fuel consumption is measured using a digital stopwatch.

RESULTS AND DISCUSSIONS

Effect of Hydrogen Substitution on Peak Pressure:

Combustion pressure increases steeply with the increase in hydrogen substitution. This is because of higher flame velocities of hydrogen results in high flammability and rapid combustion. The maximum pressure obtained in case of CR 23 with 80% H₂ was 64.5 bar as seen in Figure 7 but in the case for CR 17 the maximum pressure is 48.65 bar.

As seen in Figure.8, CFD and experimental values are in close proximity. Except at CR 23 they are very close to each other. The experimental values are higher than theoretical values due to biodiesel being oxygenated fuel due to which combustion is complete and maximum pressure is obtained. The difference between the theoretical and experimental values is 17% at CR 17, it is 8% at CR19, it is 11% at CR 21 and it is 26% at CR23.

As seen in Figure 9, the CFD values of temperature are increasing with respect to percentage hydrogen substitution for all the compression ratios. Compression ratio increases the pressure and temperature of the working mixture, which reduces the initial preparation phase of combustion and hence less ignition advance is needed. High pressures and temperature also speed up the second phase combustion. Increased compression ratio reduces the clearance volume and therefore increases the density of the cylinder gases during burning. This increases the peak pressure and

temperature and the total combustion duration is reduced. Thus higher compression ratios give rise to higher flame speeds, with increasing percentage of hydrogen.

As seen in Figure 10, as the percentage hydrogen is increased, the turbulent kinetic energy has drastically increased which is a measure of rapid combustion and high rate of energy release. Higher turbulence enhances higher flame front speeds, rapid and complete combustion and higher rate of diffusion.

There are two main stages in the dual fuel mode like in biodiesel mode. The first is mainly the combustion of biodiesel and the hydrogen entrained in the biodiesel spray, while the second is mainly due to the combustion of hydrogen by flame propagation from the ignition centers formed by the biodiesel spray. The second stage is stronger than the biodiesel mode as most of heat release occurs by the combustion of hydrogen by flame propagation. The rate of heat release increases with hydrogen substitution at high outputs. As the hydrogen percentage increases, the substitution tends to richer hydrogen-air mixtures. This sets the rapid combustion rates, which tends to increase the pressure rapidly in the dual fuel mode. The flame is set with biodiesel injection in the first phase and in the second phase the combustion of hydrogen takes place by the flame propagation formed by the biodiesel spray. The rate of heat release is higher in dual fuel because of combined burning of two fuels. This is one of the reasons for higher thermal efficiency in dual fuel mode at high outputs.

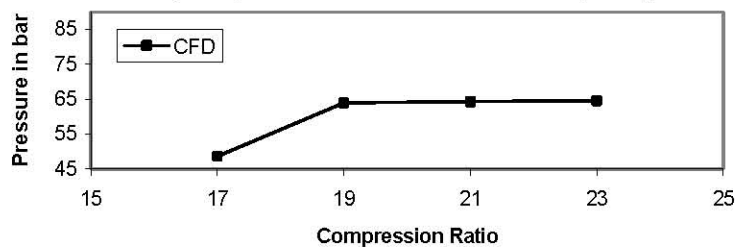


Fig. 7: Peak pressure versus compression ratio for 80% Hydrogen and 20% biodiesel at full load

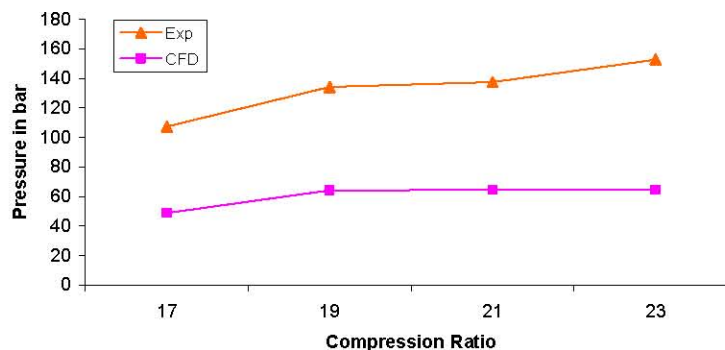


Fig. 8: Comparison of peak pressure versus compression ratio for 80% Hydrogen and 20% biodiesel at full load

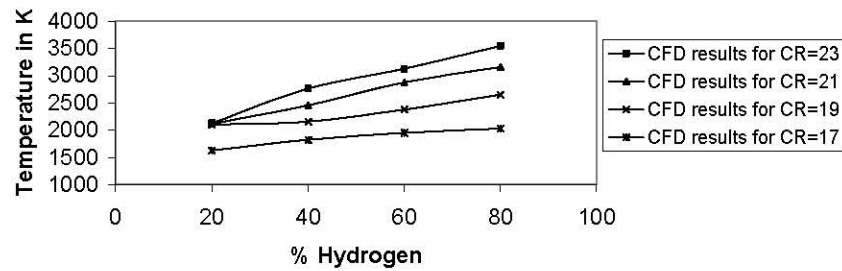


Fig. 9: CFD Results Analysis of Temperature Versus percentage Hydrogen Substitution

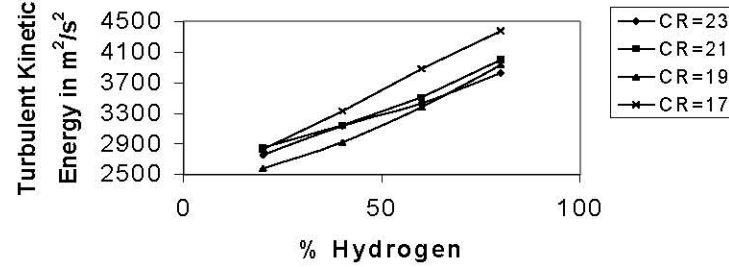


Fig. 10: CFD Result Analysis of Turbulent Energy Versus percentage Hydrogen Substitution

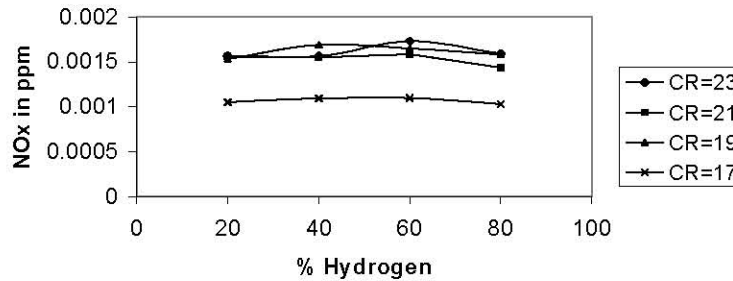


Fig. 11: CFD Result Analysis of NO_x versus percentage Hydrogen Substitution

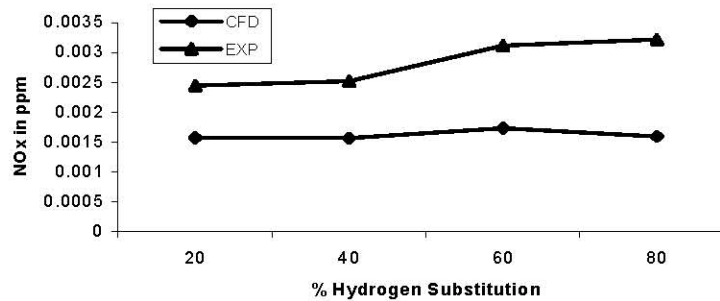


Fig. 12: Comparison of NO_x versus Percentage Hydrogen at full load

Effect of Hydrogen Substitution on Nox: As seen in the Fig. 11, there is not much change in the values of NO_x as the hydrogen is substituted at different compression ratios. It has got low values at CR 17, but as the compression ratio is increasing it is also increasing.

As seen in Figure 11, there is a good agreement between CFD and experimental values. Trend shown by CFD is decreasing, but the experimental values are showing an increasing trend. The reason could be the

CFD values take into account the moisture formation in the exhaust and correspondingly show decreasing values of NO_x, however, practically the combustion temperatures are higher and availability of oxygen in oxygenated biodiesel resulting in increasing value of NO_x. Exhaust gas recirculation is an effective method for Nox control. The exhaust gases mainly consist of inert carbon dioxide, nitrogen and possess high specific heat. When re circulated to engine inlet, it can reduce oxygen

concentration and act as a heat sink. This process reduces oxygen concentration and peak combustion temperature, which results in reduced NO_x.

CONCLUSIONS

The CFD analysis along with experimental investigations is being carried out to compare hydrogen and biodiesel dual fuel combustion and emission analysis. It has the following conclusion. At higher percentage of hydrogen substitution the model is not confirming to the experimental results. The model needs further refinement in the computational mesh. Other models in the analysis can be used to improve the quality of the work.

The following conclusions can be drawn from the present analysis.

- When the percentage substitution was varied from 10% to 80% of hydrogen, the percentage pressure rise for CR 23 was 23%. For CR 17 this difference for the same percentage substitutions was 18 %.
- The net Turbulent Kinetic energy increases as percentage hydrogen substitution increases. With the increase in Compression ratio, there is drop in the turbulent kinetic energy.
- The maximum temperature rises as the percentage hydrogen substitution increases. It is higher in the higher compression ratios. For CR17 the rise in temperature with the hydrogen substitution is 24% for 23 it is 69%.
- As the compression ratio was increased from CR 17 to CR 23, with only 10% hydrogen substitution, the value of NO_x was increased by 11.2%.
- At higher temperatures practically the combustion temperatures are higher, resulting in increasing value of NO_x.

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