Project Report

Performance Evaluation in an Internal Combustion Engine by Enrichment of Oxygen in the Inlet by Thermodynamics and CFD modelling

Engineering Mechanics Unit

Jawaharlal Nehru Centre for Advanced Scientific Research

IAS-INSA-NASI Summer Research Fellowship Programme

Duration:

May 2022 to July 2022

Submitted to: Prof. Santosh Ansumali

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ACKNOWLEDGEMENT

The knowledge and experience acquired through this project work is priceless. I am highly indebted to Prof. Santosh Ansumali for the guidance and wisdom imparted, throughout the project.

I am grateful to Prof. S V Diwakar, and Dr. Abhijit Dhamanekar, for their continuous support and help in providing new insights and nurturing a better approach and thinking, throughout the project.

It is a great opportunity to work as a Summer Research Fellow under the guidance of Prof. Santosh Ansumali, JNCASR. I profusely thank Indian Academy of Sciences (IAS), Indian National Science Academy (INSA), and The National Academy of Sciences, India (NASI), for providing me this opportunity and my parents, and friends for their encouragement and inspiration.

Sincerely,

Abhiram Kalluri

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ABSTRACT

There have been many automobile transmission technologies coming up in view of the increasing demand of fossil fuels, such as electric vehicles, hydrogen fuel cell transmission, biodiesel, etc. However, these transmission technologies are still new, expensive and limited to light weight drivetrains, making the conventional Internal Combustion engines driven by Diesel, Gasoline or Natural gas, still the most economical and powerful transmission models for especially heavy vehicles. However, the efficiency of the IC engines has been a matter of concern for a long time. The energy losses in IC engine limit its efficiency to around 25-30%. One of the reasons for reduced performance and efficiency of IC engines is due to incomplete combustion of fuel due to limited availability of oxygen. Also, the incomplete combustion of fuel leads to the production of hydrocarbons along with other toxic gases such as Carbon Monoxide in the exhaust posing a serious environmental concern, as well as leading to wastage of fuel due to incomplete combustion.

Hence, the project aims at computing the increase in the performance of Internal combustion engines by enriching the air with oxygen by artificially pumping oxygen along with atmospheric air in order to increase its proportion in the supply air, leading to increased availability of oxygen for combustion.

INTRODUCTION

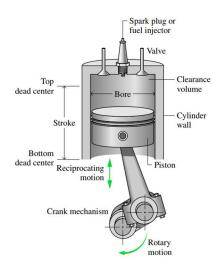
The internal combustion engines produce mechanical power from the chemical energy contained in the fuel. In internal combustion engines, as distinct from external combustion engines, this energy is released by burning or oxidizing the fuel inside the engine. The work transfers that provide the desired power output occur directly between these working fluids and the mechanical components of the engine. Otto or Gasoline engines and Diesel Engines are two most commonly used Internal Combustion engines. Because of their simplicity, ruggedness, high power to weight ratio, and low cost, these two types of engines have found wide application in transportation (land, sea, and air) and power generation.

According to PIB, Ministry of Petroleum & Natural Gas, Govt. of India, in the year 2012-13, almost 96.6% of petrol and 70% of diesel imported/ extracted in India was consumed by the Transport sector in the country, which includes both domestic as well as commercial transport vehicles.

In the month of January, 2022, 2.5 Mega Metric Tonnes of petrol consumption was reported by Petroleum Planning and Analysis cell, Govt. of India. Hence, saving the fuel even by 1% in estimate could save 25000 tonnes of petrol being burnt per month, eventually leading to a large reduction in potential emissions through combustion of gasoline.

1 Main components of IC engine

- a. **Cylinder:** It is the main part of the engine inside which piston reciprocates in a periodic to-fro motion. It is made in such a way that it withstands high temperature and pressure.
- b. Cylinder head: The top end of the cylinder is covered by cylinder head over which inlet and exhaust valve; spark plug or injectors are mounted.
 A gasket is provided between the engine cylinder and cylinder head to make an air tight joint.
- c. **Piston:** Transmit the force exerted by the burning of charge to the connecting rod. Usually made of aluminium alloy which has good heat conducting property and greater strength at higher temperature.
- d. **Piston rings:** These are housed in the circumferential grooves provided on the outer surface of the piston and made of steel alloys which retain elastic properties even at high temperature. There are 2 types of rings, namely compression and oil rings. Compression ring is upper ring of the piston which provides air tight seal to prevent leakage of the burnt gases into the lower portion. Oil ring is lower ring which provides effective seal to prevent leakage of the oil into the engine cylinder.
- e. Connecting rod: It converts reciprocating motion of the piston into circular motion of the crank shaft, in the working stroke. The smaller end of the connecting rod is connected with the piston by gudgeon pin and bigger end of the connecting rod is connected with the crank with crank pin. The special steel alloys or aluminium alloys are used for the manufacture of connecting rod.



2. Terminology used in IC Engine

- **a. Stroke:** The distance the piston moves in one direction.
- **b.** Top Dead Centre (TDC): The piston is said to be at top dead centre when it has moved to a position where the cylinder volume is a minimum. This minimum volume is known as the clearance volume.
- **c. Bottom Dead Centre (BDC):** When the piston has moved to the position of maximum cylinder volume, the piston is at bottom dead centre.
- **d. Displacement Volume:** The volume swept out by the piston as it moves from the top dead centre to the bottom dead centre position is called the displacement volume.

3. Two Stroke Engine

Smaller engines operate on two-stroke cycles. In two-stroke engines, the intake, compression, expansion, and exhaust operations are accomplished in one revolution of the crankshaft.

4. Four Stroke Engine

In a four-stroke internal combustion engine, the piston executes four distinct strokes within the cylinder for every two revolutions of the crankshaft.

- a. Intake stroke: With Suction valve open and exhaust valve closed, a charge consisting of air-fuel mixture is drawn by the movement of piston from TDC to BDC.
- b. Compression stroke: With both valves closed, the piston undergoes a
 compression stroke, raising the temperature and pressure of the charge.
 This requires work input from the piston to the cylinder contents. A
 combustion process is then initiated, resulting in a high-pressure, hightemperature gas mixture.
- c. Power stroke: A power stroke follows the compression stroke, during which the gas mixture expands and work is done on the piston as it returns to bottom dead centre.
- d. Exhaust Stroke: The piston then executes an exhaust stroke in which the burned gases are purged from the cylinder through the open exhaust valve.

POWER AND PROPULSION CYCLES

A detailed study of the performance of a reciprocating internal combustion engine would take into account many features such as combustion in the cylinder, and effects of irreversibility associated with friction and with pressure and temperature gradients etc. Owing to these complexities, to conduct elementary thermodynamic analysis of IC engine, considerable simplification is required. One procedure is to employ an Air standard analysis, having the following elements:

- a. A fixed amount of air modelled as an ideal gas is the working fluid.
- b. The combustion process is replaced by a heat transfer from an external source.
- c. There are no exhaust and intake processes as in an actual engine. The cycle is completed by a constant-volume heat transfer process taking place while the piston is at the bottom dead centre position.
- d. All processes are internally reversible.

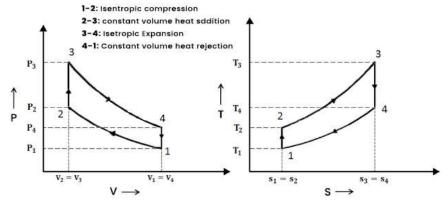
1. Air - Standard Otto Cycle

The air standard Otto cycle represents the thermodynamic cycle involved in a Gasoline engine or Spark Ignition (SI) engine, where the combustion takes place by spark ignition and heat addition takes place at constant volume.

The air-standard Otto cycle is an ideal cycle that assumes the heat addition occurs instantaneously while the piston is at top dead centre. The cycle consists of four internally reversible processes in series:

a. Process 1–2 is an isentropic compression of the air as the piston moves from bottom dead centre to top dead centre.

- b. Process 2–3 is a constant-volume heat transfer to the air from an external source while the piston is at top dead centre. This process is intended to represent the ignition of the fuel–air mixture and the subsequent rapid burning.
- c. Process 3–4 is an isentropic expansion (power stroke).
- d. Process 4–1 completes the cycle by a constant-volume process in which heat is rejected from the air while the piston is at bottom dead centre.



P-V and T-S Diagram of Otto Cycle

Since the air-standard Otto cycle is composed of internally reversible processes, areas on the T–s and p–v diagrams can be interpreted as heat and work, respectively. On the T–s diagram, area 2–3–a–b–2 represents the heat added per unit of mass and area 1–4–a–b–1 the heat rejected per unit of mass. On the p–v diagram, area 1–2–a–b–1 represents the work input per unit of mass during the compression process and area 3–4–b–a–3 is the work done per unit of mass in the expansion process.

The air-standard Otto cycle consists of two processes in which there is work but no heat transfer, Processes 1–2 and 3–4, and two processes in which there is heat transfer but no work, Processes 2–3 and 4–1.

1.1 Efficiency of Ideal Otto cycle:

The starting point is the general expression for the thermal efficiency of a cycle:

$$\eta = \frac{\text{work}}{\text{heat input}} = \frac{Q_{2-3} + Q_{4-1}}{Q_{2-3}}$$

$$Q_{2-3} = C_V(T_3 - T_2)$$

$$Q_{4-1} = C_V(T_1 - T_4)$$

$$\eta = 1 - \frac{T_4 - T_1}{T_3 - T_2}$$

We can simplify the above expression using the fact that the processes from 1 to 2 and from 3 to 4 are isentropic.

$$T_4 V_1^{\gamma - 1} = T_3 V_2^{\gamma - 1}$$

$$T_1 V_1^{\gamma - 1} = T_1 V_2^{\gamma - 1}$$

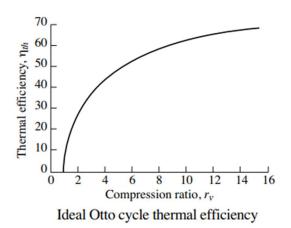
$$(T_4 - T_1) V_1^{\gamma - 1} = (T_3 - T_2) V_2^{\gamma - 1}$$

$$\frac{T_4-T_1}{T_3-T_2}=(\frac{V_2}{V_1})^{\gamma-1}$$

 $\frac{V_1}{V_2}$ = r is known as the compression ratio. In terms of the compression ratio, the efficiency of an ideal Otto cycle is given by:

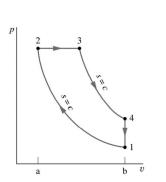
$$\eta = 1 - \frac{1}{(\frac{V_1}{V_2})^{\gamma - 1}} = 1 - \frac{1}{r^{\gamma - 1}}$$

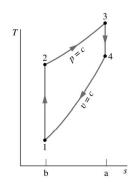
From the graph below, as the compression ratio, r, increases, η increases, but so does T_2 . If T_2 is too high, the mixture will ignite without a spark (at the wrong location in the cycle) which might lead to a condition known as engine knocking.



2. Air-Standard Diesel Cycle

The air-standard Diesel cycle is an ideal cycle that assumes the heat addition occurs during a constant-pressure process that starts with the piston at top dead centre. The cycle consists of four internally reversible processes in series. The first process from state 1 to state 2 is the same as in the Otto cycle: an isentropic compression. Heat is not transferred to the working fluid at constant volume as in the Otto cycle, however. In the Diesel cycle, heat is transferred to the working fluid at constant pressure. Process 2–3 also makes up the first part of the power stroke. The isentropic expansion from state 3 to state 4 is the remainder of the power stroke. As in the Otto cycle, the cycle is completed by constant-volume Process 4–1 in which heat is rejected from the air while the piston is at bottom dead centre. This process replaces the exhaust and intake processes of the actual engine.





Since the air-standard Diesel cycle is composed of internally reversible processes, areas on the T-s and p-v diagrams can be interpreted as heat and work, respectively. On the T-s diagram, area 2-3-a-b-2 represents the heat added per unit of mass and area 1-4-a-b-1 is the heat rejected per unit of mass. On the p-v diagram, area 1-2-a-b-1 is the work input per unit of mass during the compression process. Area 2-3-4-b-a-2 is the work done per unit of mass as the piston moves from top dead center to bottom dead center. The enclosed area of each figure is the net work output, which equals the net heat added.

2.1 Ideal Diesel cycle efficiency

$$\eta = \frac{\text{work}}{\text{heat input}} = 1 + \frac{Q_{4-1}}{Q_{2-3}} = 1 - \frac{C_v(T_1 - T_4)}{C_p(T_3 - T_2)}$$

This cycle can operate with a higher compression ratio than Otto cycle because only air is compressed and there is no risk of auto-ignition of the fuel. Although for a given compression ratio the Otto cycle has higher efficiency, because the Diesel engine can be operated to higher compression ratio, the engine can actually have higher efficiency than an Otto cycle when both are operated at compression ratios that might be achieved in practice.

PROJECT OBJECTIVE

The current Internal Combustion engines use atomization of fuel at high pressure through injectors in order to form small droplets of fuel that mix with the air entering the cylinder and undergo combustion on spark leading to production of large amount of heat leading to expansion of gases that eventually push the piston away from the Top dead centre to the Bottom dead centre, leading to production of torque, which rotates the shaft.

However, not all the fuel inside the cylinder is burnt, and most engines burn only 73-85% of the fuel injected, leading to loss of unburnt fuel, as well as leading to environmental pollution due to atmospheric release of these unburnt hydrocarbons.

The various factors that are responsible for the incomplete combustion of fuel include poor air-fuel mixing, that is generally due to large droplets of fuel injected, which sometimes leave the cylinder in liquid state without being burnt. Another factor responsible is due to limited availability of oxygen in the air entering the cylinder, leading to some parts of fuel being left unburnt. The above two stated factors are the matter of concern for the current project, however, there are various other factors such as combustion kinetics, fuel purity, presence of carbon dioxide which hinders combustion etc.

1. Importance of oxygen enrichment

Incomplete combustion of fuel is one of the reasons for increased exhaust gas emissions from the engine, as well as reduced engine performance. The production of CO, Oxides of Nitrogen, unburnt fuel particles, formation of sticky gunk leading to increased friction in the engine moving parts in the long run, etc. are a few outcomes of incomplete fuel combustion. By

enriching the incoming air with oxygen, the amount of oxygen available for the fuel will increase, leading to increased performance, reduced soot and CO release, increasing its performance, fuel efficiency as well as reducing the emissions.

Also, increased oxygen concentration means more proportion of fuel being burnt in the cylinder at a time, which means more amount of heat would be produce. This would lead to increased torque and performance of the engine. However, the increase in the temperature could lead to increase in the production of thermal NOx which could be dealt with the help of other separation mechanisms.

Although various efforts have been made lately to improve fuel efficiency by introducing hybrid engines or turbochargers or superchargers, the cost effectiveness of these drivetrains make them less accessible and feasible. Direct injection of oxygen along with atmospheric oxygen leading to increase in oxygen concentration could be a potentially cheaper and more efficient option that could potentially improve performance as well as reducing fuel consumption and harmful emissions.

The overall objective of the project is to study the performance and fuel consumption of Internal combustion engines when operated at different concentrations of supply oxygen and to study the mixing effectiveness of the air-fuel mixture inside the cylinder through CFD simulations.

CALCULATING THE HEAT PRODUCED

In this project, the study of performance improvement through oxygen enrichment will be carried out through mathematical calculations and computer simulations. For the same, a gasoline test engine will be taken into consideration. Since gasoline is a petroleum derived product comprising of a mixture of an array of organic compounds, such as octane, methane, paraffins, aromatics, organic compounds containing nitrogen etc. it is practically complex to draw out reaction mechanism for each component and calculating the heat of reaction. Therefore, the component with highest concentration i.e., octane in gasoline will be considered as a fuel for the heat of reaction calculation.

$$C_8H_{18} + 12.5 O_2 + x N_2 \rightarrow 8 CO_2 + 9 H_2O + x N_2$$

Here, *x* is the number of moles of nitrogen that would enter the cylinder depending on the proportion of oxygen and nitrogen in the incoming air.

At 298K, the heats of formation of different compounds are given by:

$$C_8 H_{18} : \overline{h}_{fC_8 H_{18}}^0 = -208447.0 \text{ J/mol}$$

$$CO_2$$
: $\overline{h}_{fCO_2}^0 = -393533.0 \text{ J/mol}$

$$H_2O: \overline{h}_{fH_2O}^0 = -241827.0 \text{ J/mol}$$

Heat of combustion of Octane = $9h_{fH_2O}^0 + 8h_{fCO_2}^0 - h_{fC_8H_{18}}^0 = -5470 \text{kJ/mol} = \overline{h_f^0}$ at 298K

$$\Delta \overline{h} = \int_{T_0}^T \overline{C}_p dT$$

$$\overline{h}=\overline{h}_{f}^{0}+\Delta\overline{h}$$

Since, the flame temperature of gasoline is 220°C, we take the temperature of the reaction to be at 220°C.

At 220°C, the heat capacities of different compounds are given by:

$$C_{pC_8H_{18}} = 228 J/mol. K$$

$$C_{pCO_2} = 37.1 \, J/mol. \, K$$

$$C_{pH_2O} = 27.6 \, J/mol. \, K$$

$$C_{p N_2} = 29.11 J/mol. K$$

$$C_{p \mid O_2} = 29.11 \, J/mol. \, K$$

Now, the heat of combustion of gasoline is given by:

$$\overline{h} = \overline{h}_f^0 - \{ (xC_{pN_2} + 8C_{pCO_2} + 9C_{pH_2O} + (\text{other components})) (T - T_0) \}$$

Other components include unburnt fuel, or excessive O_2 that has not reacted.

$$T = 493K$$
 and $T_0 = 298K$.

PERFORMANCE CALCULATION FOR IC ENGINES

The performance improvement for 4 stroke Spark Ignition engine upon enrichment of Oxygen has been calculated on the basis of a test engine with the following specifications:

Type : 4-Stroke, DOHC, 2-Valve, 1-Cylinder

Cooling System : Air Cooled

Bore and Stroke : 74mm By 57.3mm

Displacement Volume : 246 cc

Compression Ratio : 9:1

Fuel System : Modified for fuel Injection

Lubrication : Forced pressure, wet sump, SAE 10W-40

Valve Timing

Inlet : Open 8° BTDC

: Close 35° ABDC

Exhaust : Open 50° BTDC

: Close 40° ATDC

In the above engine, the displacement volume is given to be 246 cc. This means 246 cm³ of air is taken in to the cylinder for one combustion cycle comprising of 4 strokes.

Air fuel ratio for an engine is defined as the mass of air available for 1kg of fuel in the air-fuel mixture in the IC engine. In general, the air fuel ratio of 14.5:1 is maintained in Gasoline engines.

Hence, for 246 cm³ of air:

Average density of air = 0.001225 g/cm^3

Mass of air = $0.001225 \times 246 (g) = 0.30135g$

For air-fuel ratio of 14.5:1, the fuel that is required = $mass\ of\ air/14.5 = 0.30135 / 14.5 \approx 0.021\ g\ or\ 0.0001823\ mol\ fuel.$

From the reaction stoichiometry, 1 mol of fuel is completely burnt by 12.5 mol of Oxygen. Hence, to completely burn 0.0001823 mol of fuel, 12.5×0.0001823 = 0.00227881 mol of Oxygen is required.

However, the number of moles of oxygen that enters the cylinder is a constraint to the oxygen available for combustion.

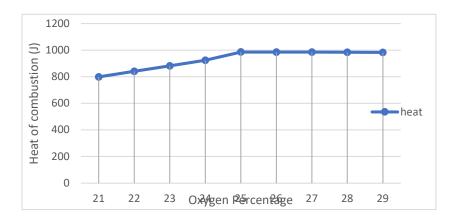
For x % of Oxygen in air, the number of moles of oxygen = $\frac{x \times 246 \times 0.001225}{32}$ where, '32' is the molar mass of Oxygen.

1. Calculating the heat produced

Assuming total combustion of fuel, if the number of moles of Oxygen entering the cylinder is more than or equal to the number of moles required for complete combustion of the fuel that is injected, there would be an excess of oxygen left and all of the fuel injected will be burnt. However, if the number of moles of oxygen is less, then there would be some amount of fuel that would be left unburnt. This is governed by the "x%" of oxygen that is entering the system.

The number of moles of fuel that would be actually burnt inside the Cylinder will in turn effect the number of moles of CO_2 or water being produced as well as the amount of heat obtained through combustion. The following tabular data shows the amount of heat produced for different concentrations of oxygen, "assuming total combustion of fuel and perfect mixing of air and fuel".

Oxygen	Nitrogen	O2 moles	N2 moles	02	Leftover fuel	Heat
				deficit/excess		Released
21	79	0.001977609	0.008502375	0.000301201	2.40962E-05	799.2474361
22	78	0.002071781	0.00839475	0.000207029	1.65624E-05	840.6019839
23	77	0.002165953	0.008287125	0.000112857	9.02865E-06	881.9565318
24	76	0.002260125	0.0081795	1.8685E-05	1.4949E-06	923.3110796
25	75	0.002354297	0.008071875	-7.54869E-05	0	986.2876102



Since this heat is for 1 cycle comprising of 4 strokes, this energy can be used to calculate the power being supplied to the engine based on the rotation speed of the crankshaft (in rpm).

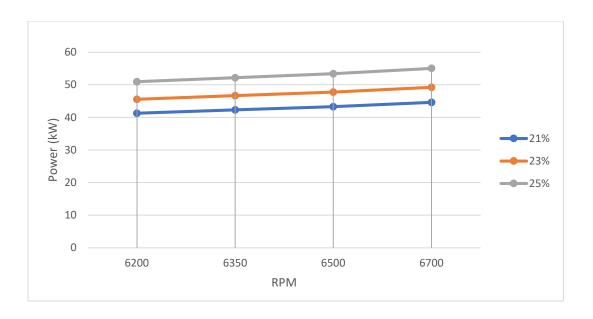
2. Calculation of Power supplied

For 1 engine cycle, the crankshaft is rotated by 720° i.e., two complete rotations. Hence, the power supplied to the engine will be given by:

Power (P) =
$$\frac{\text{RPM} \times \text{Heat in each cycle}}{2 \times 60}$$
 J/sec or Watt.

The power supplied to the engine for different RPMs at different Oxygen concentrations is given in the following table:

RPM	Power at 21% (kW)	Power at 23% (kW)	Power at 25% (kW)
6200	41.29445086	45.56775414	50.9581932
6350	42.29351016	46.67019981	52.19105271
6500	43.29256945	47.77264547	53.42391222
6700	44.62464851	49.24257302	55.06772491



3. Fuel consumption

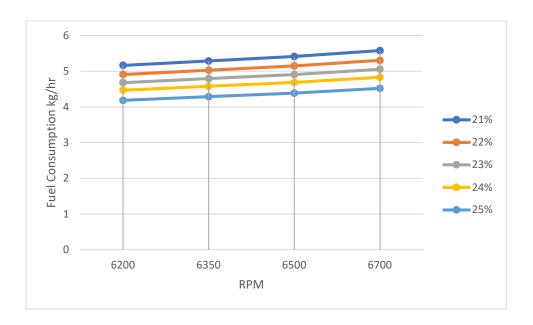
In the previous section, the amount of power produced for different Oxygen compositions has been calculated. However, for the same amount of power produced, it is obvious that the amount of fuel required will be less for higher oxygen concentration, therefore consuming lesser fuel.

The fuel injected in each cycle for 21% Oxygen = 0.021 g

Hence, for a specified rpm of crankshaft, fuel required at $21\% = \frac{rpm \times 0.021 \times 60}{2 \times 1000} kg/hr$.

The fuel consumption for x% is given by = $\frac{power\ at\ 21\%\times fuel\ required\ at\ 21\%}{power\ at\ x\%\ for\ same\ amount\ of\ fuel}\ kg/hr$

RPM	Energy at	Fuel at 21%	Fuel at 22%	Fuel at 23%	Fuel at 24%	Fuel at 25%
	21% (kW)					
6200	41.29442833	5.161694618	4.907755415	4.677632955	4.46812459	4.182825515
6350	42.29348708	5.286574327	5.026491433	4.790801494	4.576224378	4.284022907
6500	43.29254583	5.411454035	5.145227451	4.903970033	4.684324166	4.385220298
6700	44.62462417	5.577960313	5.303542142	5.054861419	4.828457218	4.520150153



4. Computing the flow rate of oxygen

For engine displacement volume of $246\,\mathrm{cm}^3$:

For 1 cycle of 4 strokes, 246 cm³ of air is taken in. Hence, for a specified engine rpm, volume of air intake

$$v = \frac{\text{rpm} \times \text{air volume}}{2}$$
 litre/min

For supplying pure Oxygen for enrichment, let x be the flow rate of (90%) pure oxygen, and y be the flow rate of air.

For p% of final oxygen concentration:

$$x + y = v$$
; $0.90x + 0.21y = \left(\frac{p}{100} \times v\right)$

On solving the above two equations, the flow rate of oxygen required to enrich the air to p% can be computed.

22%	total	air	оху	24%	total	air	оху
	flowrate	flowrate	flowrate		flowrate	flowrate	flowrate
6200	762.6	751.5478	11.05217	6200	762.6	729.4435	33.15652
6350	781.05	769.7304	11.31957	6350	781.05	747.0913	33.9587
6500	799.5	787.913	11.58696	6500	799.5	764.7391	34.76087
6700	824.1	812.1565	11.94348	6700	824.1	788.2696	35.83043
23%	total	air	оху	25%	total	air	оху
	flowrate	flowrate	flowrate		flowrate	flowrate	flowrate
6200	762.6	740.4957	22.10435	6200	762.6	718.3913	44.2087
6350	781.05	758.4109	22.63913	6350	781.05	735.7717	45.27826
6500	799.5	776.3261	23.17391	6500	799.5	753.1522	46.34783
6700	824.1	800.213	23.88696	6700	824.1	776.3261	47.77391

CORRELATING ANALYTICAL AND EXPERIMENTAL DATA

All the data above has been calculated analytically based on the following assumptions:

- 1. Perfect air-fuel mixing
- 2. Complete combustion of fuel
- 3. Nitrogen as an inert component
- 4. The air-fuel ratio is constant at all engine speeds, i.e., 14.5:1

However, in real cases, the following assumptions do not hold true. Hence, by correlating the experimental data, drawn from the published literature is used.

The efficiency of engine varies with the change the crankshaft speed. Hence, by calculating the output power on the basis of the published efficiency data, would provide the expected output power for the analytical calculation.

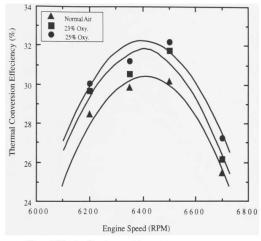


Figure 6.9 Engine Speed versus Thermal Conversion Efficiency for Gasoline

Source: Maxwell, Timothy T.; Setty, Varadaraja; Jones, Jesse C.;
Narayan, Raghu (1993). SAE Technical Paper Series [SAE
International International Fuels & Lubricants Meeting & Exposition (OCT. 18, 1993)] SAE Technical Paper Series - The Effect of Oxygen
Enriched Air on the Performance and Emissions of an Internal
Combustion Engines., 1(), -. doi:10.4271/932804

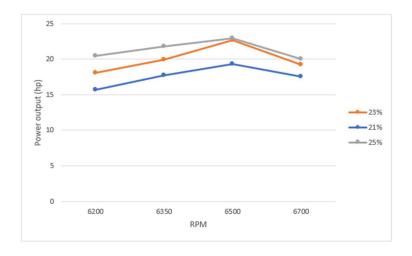
Thermal efficiency	21% Oxygen	23% Oxygen	25% Oxygen
from Literature			
6200	28.42373	29.6302	30.00462
6350	29.78374	30.46225	31.14176
6500	30.12943	31.69645	32.12635
6700	25.41448	26.10786	27.245

Power output from Literature	21%	23%	25%
(in Horsepower)			
6200	15.15633	16.45013	17.72237
6350	16.45013	17.43126	18.95148
6500	17.54986	18.99461	19.95421
6700	15.92183	16.70889	17.49595

Analytically calculated	21%	23%	25%
power output			
6200	15.73381128	18.09894998	20.49572685
6350	17.75919576	19.95095444	21.77114201
6500	19.29440453	22.69903971	22.97310345
6700	17.56240566	19.25796574	20.0672055

Analytically calculated power output =

Calculated power supply × Thermal efficiency from literature



2. Comparing the effect of Hydrocarbon (HC) and CO emissions on fuel consumption and emissions:

The literature survey indicated a reduction of CO and HC emissions by an average of 25.7% and 29.46% respectively, for an enrichment of oxygen by 2%.

The heat supplied due to enrichment of oxygen indicated in Chapter 5 was the output of the consideration that all the oxygen supplied reacts only with the fuel. However, the production of CO indicates 0.5 moles of Oxygen consumption for each mole of CO produced, and HC emissions indicate the actual amount of fuel left unburnt adding up with the fuel unburnt due to insufficient oxygen supply.

Assuming a steady state flow process, at any instant, the flow rate of incoming fresh air to the engine will be equal to the flow rate of exhaust gases out of the engine.

For engine displacement volume of 246 cm³:

- 1. For 1 cycle of 4 strokes, 246 cm³ of fresh air is taken in.
- 2. For a given rpm: $\frac{\text{rpm} \times \text{air volume}}{2}$ cm³/min of incoming air flow rate is required.

The HC and CO data, taken from the literature indicate the following:

HC emission vs	Total exhaust	HC for 25%	23% O2	21% O2 (g/min)
rpm	flow rate	O2 (g/min)	(g/min)	
	(lit/min)			
6200	762.6	0.117686	0.132807	0.187095
6350	781.05	0.113816	0.130982	0.186584
6500	799.5	0.10982	0.128919	0.180678
6700	824.1	0.117727	0.135052	0.192734

RPM	Exhaust gas	CO for 21%O2	23%(g/min)	25%(g/min)
	flow rate	(g/min)		
6200	762.6	14.75631	10.91967	10.23104
6350	781.05	14.3072739	10.75061	9.773279
6500	799.5	13.407615	9.797873	9.075924
6700	824.1	14.3517015	10.75846	10.09935

Considering the above values, the amount of heat produced reduces to:

Oxygen	Nitrogen	O2	N2	O2	Leftover	Heat
		moles	moles	deficit	fuel	Released
						(J)
21	79	0.001978	0.008502	0.00038	3.07E-05	763.0315
23	77	0.002166	0.008287	0.000171	1.39E-05	855.0963
25	75	0.002354	0.008072	-2.1E-05	4.51E-06	906.5021

ANALYSIS FOR A CI ENGINE

A Compression Ignition engine is powered by the combustion of Diesel as fuel. The engine burs fuel by ignition through temperature increase of the air-fuel mixture, due to high compression. Ideally a CI engine follows the diesel cycle (detailed explanation in Chapter 2).

Engine	Specifications
Type	Kirloskar TAF 1
Number of cylinders	1
Cubic capacity	0.662 Liters
Bore \times Stroke	87.5 × 110 mm
Compression ratio	17.5:1
Rated power	4.33 kW
Rated speed	1500 rpm
Fuel injection	Direct injection
Injection timing	21 degree btdc
Injection pressure	230 bar

Combustion of diesel in a CI engine happens through compression ignition, unlike in the gasoline engines. Hence, the temperature rise during the compression stroke is relatively higher in a diesel engine.

$$4C_{12}H_{23} + 71 O_2 + x N_2 \rightarrow 48 CO_2 + 46 H_2O + x N_2$$

Here, *x* is the number of moles of nitrogen that would enter the cylinder depending on the proportion of oxygen and nitrogen in the incoming air.

At 298K, the heats of formation of different compounds are given by:

$$C_{12}H_{23}$$
: $\overline{h}_{fC_{12}H_{23}}^0 = -6700.0 \text{ kJ/mol}$

$$CO_2$$
: $\overline{h}_{fCO_2}^0 = -393533.0 \text{ J/mol}$

$$H_2O: \overline{h}_{fH_2O}^0 = -241827.0 \text{ J/mol}$$

Heat of combustion of Diesel = -7348 kJ/mol= \overline{h}_f^0 at 298K

$$\overline{h} = \overline{h}_f^0 - \{ (xC_{pN_2} + 12C_{pCO_2} + 11.5C_{pH_2O} + (\text{other components})) (T - T_0) \}$$

Oxygen	Nitrogen	O2 moles	N2 moles	O2 deficit	Leftover fuel	Heat
						Released (J)
21	79	0.005321859	0.022880375	0.018457201	0.000260044	504.9454143
21.5	78.5	0.00544857	0.022735563	0.01833049	0.00025826	518.0328287
22	78	0.005575281	0.02259075	0.018203779	0.000256475	531.120243
22.5	77.5	0.005701992	0.022445938	0.018077068	0.00025469	544.2076573
23	77	0.005828703	0.022301125	0.017950357	0.000252906	557.2950716

The above calculations indicate the heat released for stoichiometric combustion of fuel. However, the enrichment of 0.5% has indicated an increase in heat supplied by approximately 2.7%.

The literature survey has indicated a reduction of HC emissions by 10% for 2% enrichment and by 40% for 6% enrichment of Oxygen. On the other hand, the CO emissions have reduced by 33% by 2% enrichment.

However, due to increased heat output for the same amount of fuel supplied, the increased temperatures have increased the NOx production by approximately 40% for 2% of oxygen enrichment. However, since due to enrichment, the same amount of power output can be obtained at a lower amount of fuel, the net formation of NOx has been observed to increase by 31% for 2% enrichment, which can be further possibly reduced by the help of various engine cooling mechanisms.

Source for the engine specifications CO, HC and NOx production data: P.Baskar, A. Senthilkumar, Effects of oxygen enriched combustion on pollution and performance characteristics of a diesel engine, Engineering Science and Technology, an International Journal, Volume 19, Issue 1, 2016

CFD MODELLING OF SI ENGINE

The Spark Ignition engine's 2-D combustion modelling yields the variation of Pressure, Temperature, CO production, NO production, Soot generation, etc. for different cases of enrichment of oxygen.

To maintain an air-fuel ratio of 14.5:1, the mass fraction of fuel must be approx. 0.06.

1. Computing the final pressure:

For an ideal gas, during isentropic compression (reversible adiabatic compression, considering the ideal Otto cycle), the following relation holds:

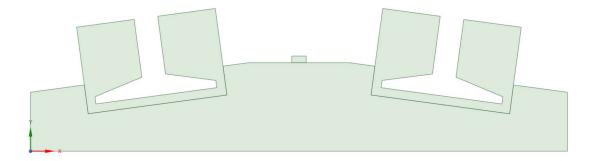
$$PV^{\gamma} = Constant$$

For a compression ratio of 9:1, the final volume is equal to $1/9^{th}$ of the total displacement volume. Hence, the pressure at the end of compression process would be equal to 9^{γ} . Here, for air, $\gamma = 1.4$. Hence, the final Pressure before the ignition stroke, would be approx. 20.65 times the initial pressure. If the intake stroke is at 1 atm pressure, then the pressure inside the cylinder at the end of compression stroke will be **20.65 atm**.

2. Computing the fuel flow velocity at inlet:

- Average fuel atomization velocities = 100m/s
- For 6200 rpm, 1 stroke takes 0.0048 sec
- Area of orifice = $\frac{\pi}{4} \times 0.002^2 = 3.14e 6 \text{ m}^2$
- Flowrate of fuel = 0.2335 kg/sec
- For injecting 0.021g fuel: 0.09 millisecond, or from crank angle 0 to crank angle 4.

3. Geometry:



• Bore: 74 mm

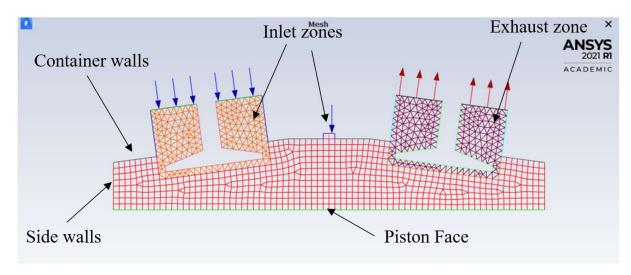
• Stroke: 57.3 mm

• Displacement volume: 246 cc

• Compression ratio: 9:1

• Air fuel ratio: 14.5

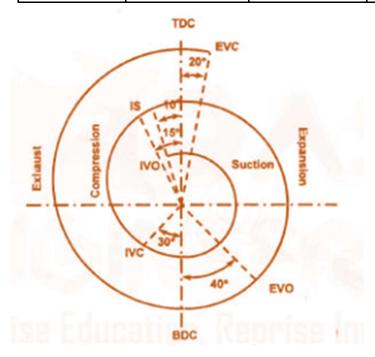
4. Meshing:



- Domain Extents:
 - x-coordinate: min (m) = 0.000000e+00, max (m) = 7.400000e-02
 - y-coordinate: min (m) = -4.531044e-18, max (m) = 1.961328e-02
- Volume statistics:
 - minimum volume (m3): 1.860227e-07
 - maximum volume (m3): 1.206090e-06
 - total volume (m3): 9.657778e-04

- Face area statistics:
 - minimum face area (m2): 6.521974e-04
 - maximum face area (m2): 1.554310e-03
- Mesh Size: 4 cell zones, 30 face zones

Level	Cells	Faces	Nodes	Partitions
0	1371	2573	1206	1



5. Dynamic mesh zones:

- Piston face: Rigid wall, moving along the Y-direction periodically, representing the piston motion.
- Side walls: Deforming walls, representing the piston side walls (they do not deform in the real case, but to represent the changing volume of the piston-cylinder arrangement).
- Alternatively activating the inlet and exhaust cell zones, representing the opening and closing valves, following the engine valve timing diagram.

6. Models and Assumptions:

- Fuel and Air from separate inlets (non-premixed)
- Spark ignition: Spark at 350-degree crank angle
- Equation of state: Ideal Gas
- Computing the mass fraction of fuel: for air-fuel ratio of 14.5:1, the mass fraction of fuel is approx. 0.06 (to be achieved by injection)
- Computing the final pressure: In isentropic compression of the piston, the final pressure would be equivalent to 9^{γ} times the initial pressure, where γ is the heat capacity ratio of gas inside the system (air in this case, $\gamma=1.4$), i.e., 20.65 atm.

• Assumptions:

- a. Non-premixed combustion, Species Transport model, Spark Ignition at 350-degree crank angle.
- b. Mixture of fuel adopted from PDF mixture containing 20 species along with n-octane (Primary Fuel), N2 and O2.
- c. NOx model: Thermal NOx and Prompt NOx.

7. NOx Model

The thermal NOx formation is determined by the temperature dependant chemical kinetics mechanism, known as the extended Zeldovich Mechanism.

$$0 + N_2 \leftrightarrow N + N0....(1)$$

$$N + O_2 \leftrightarrow NO + O \dots (2)$$

For rich fuel mixture, a third equation comes into play, for the Prompt NOx:

$$N + OH \leftrightarrow NO + H....(3)$$

The forward reaction rate constants are given by:

$$k_{f,1} = 1.8 \times 10^8 e^{-383}$$
 /T

$$k_{f,2} = 1.8 \times 10^4 Te^{-4680/T}$$

$$k_{f,3} = 7.1 \times 10^7 e^{-450/T}$$

The backward reaction rate constants are given by:

$$k_{r,1} = 3.8 \times 10^7 e^{-425/T}$$

 $k_{r,2} = 3.81 \times 10^3 T e^{-2082}$

$$k_{r,3} = 1.7 \times 10^8 e^{-24560/T}$$

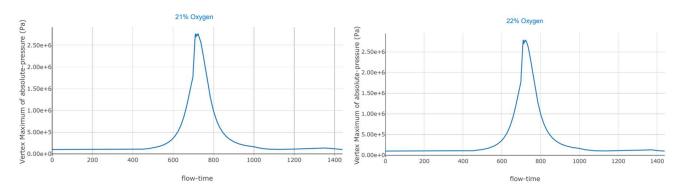
Rate of formation of NO will be given by:

$$\begin{split} \frac{d[NO]}{dt} &= k_{f,1} \left[O\right][N_2] + k_{f,2} \left[N\right][O_2] + k_{f,3} \left[N\right][OH] - k_{r,1} \left[NO\right][N] \\ &- k_{r,2} \left[NO\right][O] - k_{r,3} \left[NO\right][H] \end{split}$$

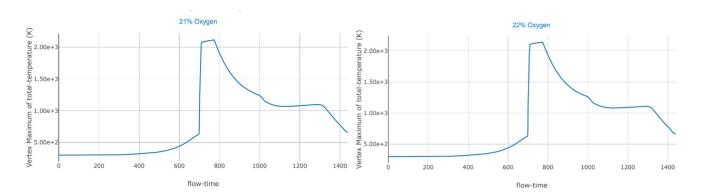
8. Plots and inferences:

The change in temperature by the enrichment of oxygen for lean mixtures has been observed to be less or close to unchanged as compared to the change in the temperature for a rich air-fuel mixture.

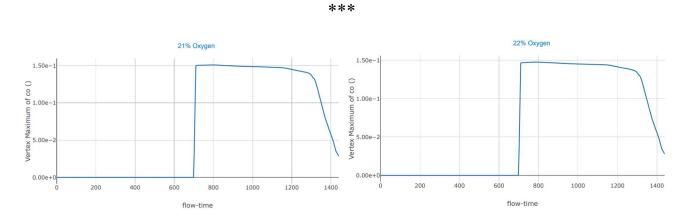
• Plots for a Rich mixture (10:1 air-fuel ratio)



Pressure plots indicate an increase in pressure by 1.42% in a 10:1 air fuel mixture.

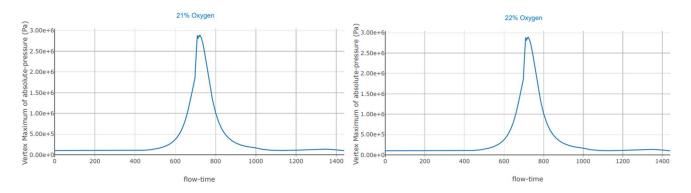


Temperature plots above, for a rich air fuel mixture indicate 1.1% increase in the temperature for 1% enrichment of oxygen

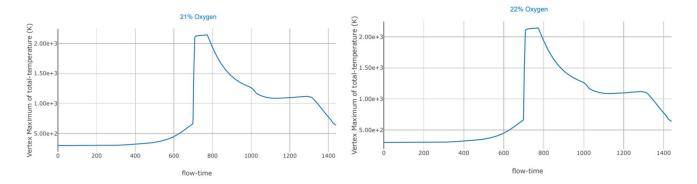


Plots for CO mass fraction for a rich air-fuel mixture indicate 2.72% decrement in CO for 1% oxygen enrichment

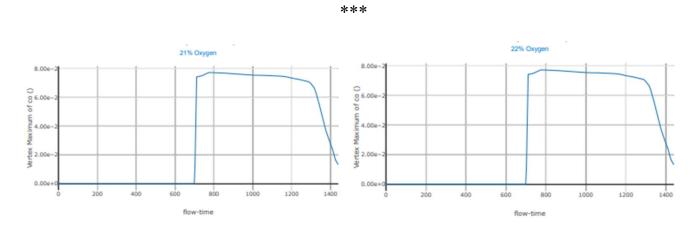
• Plots for a Lean Mixture:



Pressure plots for a lean mixture indicate 0.7% increase in pressure for 1% enrichment in oxygen.



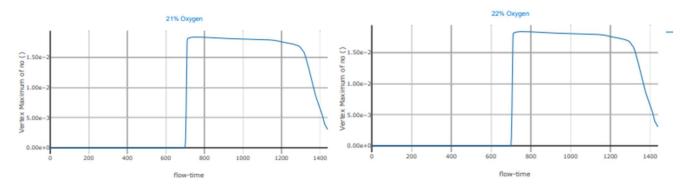
Temperature plots for lean mixture indicate 0.3% increase in temperature for 1% enrichment of oxygen



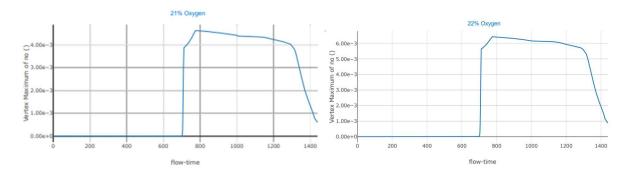
3.4% decrement in CO mass fraction in a lean mixture for 1% enrichment of oxygen

• Plots for NOx formation in rich and lean mixture

For **lean mixture**, since the temperature increase is very small, the impact on prompt NOx and thermal NOx formation for increase in Oxygen percentage is small. Plots below, indicate 15.2% increase in NOx formation by 1% enrichment of oxygen in lean mixtures (14.5:1 air-fuel ratio in this case).



For **Rich mixtures**, (10:1 air-fuel ratio in this case, the thermal as well as prompt NOx are affected due to increase in temperature as well as the fuel mixture being rich. The plots below indicate an increase of NOx by 39.2%.



9. Summary of the recorded data:

Lean Mixture (14.5:1 air-fuel ratio)

	Max Temperature	Max	CO Mass	Exhaust NO Mass
	(K)	Pressure(MPa)	Fraction in	Fraction
			Exhaust	
0.21	2136	2.87	0.07993	0.01597
0.22	2142	2.89	0.0773	0.0184
	0.3% (↑)	0.7% (†)	3.4% (↓)	15.2% (↑)

Rich Mixture (10:1 Air-fuel Ratio)

	Max Temperature	Max	CO Mass	Exhaust NO Mass
	(K)	Pressure(MPa)	Fraction in	Fraction
			Exhaust	
0.21	2114	2.76	0.1509	0.004619
0.22	2139	2.792	0.1476	0.006433
	1.42% (↑)	1.1% (↑)	2.72% (\psi)	39.2% (↑)

RESULTS AND DISCUSSION

Clearly the analytical calculations have showed a significant increase in potential performance with the enrichment of oxygen. However, the literature study indicated probable increase in exhaust gas temperatures and therefore an increase in the thermal NOx formation, however, the Hydrocarbons and CO formation has reduced on the other hand, along with a reduction in fuel consumption of the engine to produce the same amount of power.

Both CI and SI engines have indicated an increase in performance due to the enrichment of oxygen, similarly, the NOx production in both the engines has increased phenomenally, which would eventually reduce in practical situations due to a lowered consumption of fuel and could further be reduced by adopting cooling methods. The increase in thermal NOx has also been a challenge in the turbocharging mechanism, which increases the air temperature due to increased compression, which in current practice has been rectified by the use of Intercoolers.

The CFD modelling has primarily indicated an increase in cylinder pressure (and hence in the torque on the crankshaft) and internal temperature. The benefit of Oxygen enrichment on the performance of engine is small for lean air-fuel mixtures as compared to the rich air-fuel mixtures.

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