**COMPUTATIONAL INVESTIGATIONS WITH HYDROGEN AND PETROL FUELS ON A SINGLE CYLINDER PETROL ENGINE AT CONSTANT SPEED AND VARIABLE LOAD CONDITIONS.**

**M.Marouf Wani**
**Mechanical Engineering Department, National institute of Technology, Srinagar India.**

**ABSTRACT**

*The computational investigations carried out on a single cylinder four stroke cycle petrol engine with hydrogen as an alternative fuel are presented in this paper. The results have been simulated in the professional internal combustion engine simulation software from AVL Austria named as BOOST. The modeling of the entire engine system is done by selecting and joining the elements available in the software. For calculating various thermodynamic properties the first law of thermodynamics is applied to the engine as an open system when valves are open and engine as a closed system when valves are closed. To include the effect of gas exchange in the intake and exhaust manifolds when the valves are open, the modeling is done using Navier -Stokes equations for manifolds. The design parameters are fixed by engine geometry. A matrix was prepared for the operating variables to carry out the simulation. First the mapping of the input and output characteristics of the baseline engine was done by using conventional petrol as fuel. The operation was revised with data for proposed hydrogen engine and its performance and emissions characteristics were studied. The software gave successful results in both the cases.*
*In comparison with the conventional petrol fuel it was observed that the power output of the engine was decreased with hydrogen. However the brake specific fuel consumption was lower with hydrogen fuel.The CO and HC emissions were reduced with hydrogen while as there was increase in NOx emissions. It is proposed that hydrogen can be successfully used in petrol engine as an alternative future fuel.*

*Keywords : Engine , Petrol , Hydrogen , Alternate fuels , Simulation , Performance , Emissions*

**INTRODUCTION**

The constant speed and variable Load engines are used in Power generation. The concept of constant speed and variable load for power generating units is based on the fundamental principle of maintaining the frequency of the alternating current being generated constant. Normally a governing mechanism is used to maintain the speed and frequency constant .The variations in frequency is harmful for the electronic equipments designed and used throughout the world as per national and international standards. Keeping this practical concept of frequency of the AC in mind the computational investigation at constant speed has been carried out on a single cylinder petrol engine. First the mapping was done by carrying out the investigations with conventional petrol. The investigations for performance and emission analysis were repeated with hydrogen as an alternative fuel for power generation in future. The investigations were carried out for 40, 60, 80 and 100 percent load.

Table 1 at the end gives physical and chemical properties of Hydrogen and Petrol which help us to investigate the feasibility of using Hydrogen as an alternative fuel to diesel for power generation.

**THEORETICAL BASIS**

**THE CYLINDER , HIGH PRESSURE CYCLE, BASIC EQUATION.**

The calculation of the high pressure cycle of an internal combustion engine is based on the first law of thermodynamics:

$$\frac{d(m_c.u)}{d\alpha} = -\frac{p_c.dV}{d\alpha} + \frac{dQ_F}{d\alpha} - \sum \frac{dQ_w}{d\alpha} - \frac{h_{BB}.dm_{BB}}{d\alpha} \quad \text{------------------------------------------------(Eq.1)}$$

where

$\frac{d(m_c.u)}{d\alpha}$ = change of the internal energy in the cylinder.

$-\frac{p_c.dV}{d\alpha}$ = piston work.

$\frac{dQ_F}{d\alpha}$ = fuel heat input.

$\sum \frac{dQ_w}{d\alpha}$ = wall heat losses

$\frac{h_{BB}.dm_{BB}}{d\alpha}$ = enthalpy flow due to blow-by

$\frac{dm_{BB}}{d\alpha}$ = blow-by mass flow

The first law of thermodynamics for high pressure cycle states that the change of internal energy in the cylinder is equal to the sum of piston work, fuel heat input, wall heat losses and the enthalpy flow due to blow-by.

In order to solve this equation, models for the combustion process and the wall heat transfer, as well as the gas properties as a function of pressure, temperature, and gas composition are required.

Together with the gas equation

$$p_c = \frac{1}{V} .m_c.R_o.T_c \quad \text{------------------------------------------------------------(Eq.2)}$$

Establishing the relation between pressure, temperature and density, Eq. 2 for in-cylinder temperature can be solved using a Runge-Kutta method. Once the cylinder gas temperature is known, the cylinder gas pressure can be obtained from the gas equation.

**COMBUSTION MODEL**

The following equation for the stoichiometric air requirement specifies how much air is required for a complete combustion of 1 kg fuel:

$$L_{st} = 137.85 \,.(\frac{c}{12.01} + \frac{h}{4.032} + \frac{s}{32.06} - \frac{o}{32.0}) \quad \text{[kg Air/kg Fuel]} \text{------------(Eq.3)}$$

For lean combustion, the total heat supplied during the cycle can be calculated from the amount of fuel in the cylinder and the lower heating value of the fuel. The lower heating value is a fuel property and can be calculated from the following formula:

$H_u = 34835 \,.\, c + 93870 \,.\, h + 6280 \,.\, n + 10465 \,.\, s - 10800 \,.\, o - 2440 \,.\, w$ [kj/kg] -------(Eq.4)

In rich air fuel mixture combustion, the total heat supplied during the cycle is limited by the amount of air in the cylinder. The fuel is totally converted to combustion products even if the amount of air available is less than the amount of stoichiometric air.

**HEAT RELEASE APPROACH**.

**VIBE TWO ZONE**

The rate of heat release and mass fraction burned is specified by the Vibe function given by equation No.5 below.

The first law of thermodynamics is applied separately to the burned and unburned mixture while assuming that the temperatures of these two mixtures is different.

$$\frac{dx}{d\alpha} = \frac{a}{\Delta\alpha_c} \,.\, (m+1) \,.\, y^m \,.\, e^{-a.y(m+1)} \text{-------------------------------------(Eq.5)}$$

$$dx = \frac{dQ}{Q} \text{-------------------------------------------------------------------(Eq.6)}$$

$$y = \alpha - \frac{\alpha_0}{\Delta\alpha_c} \text{-----------------------------------------------------------------(Eq.7)}$$

The integral of the vibe function gives the fraction of the fuel mass which was burned since the start of combustion:

$$x = \int (\frac{dx}{d\alpha} . d\alpha) = 1 - e^{-a.y(m+1)} \text{----------------------------------------------(Eq.8)}$$

**GAS EXCHANGE PROCESS , BASIC EQUATION**

The equation for the simulation of the gas exchange process is also the first law of thermodynamics:

$$\frac{d(m_c.u)}{d\alpha} = -\frac{p_c.dV}{d\alpha} - \sum \frac{dQ_w}{d\alpha} + \sum \frac{dm_i}{d\alpha.h_i} - \sum \frac{dm_e}{d\alpha.h_e} \text{-----------------------(Eq.9)}$$

The variation of the mass in the cylinder can be calculated from the sum of the in-flowing and out-flowing masses:

$$\frac{dm_c}{d\alpha} = \sum \frac{dm_i}{d\alpha} - \sum \frac{dm_e}{d\alpha} \text{---------------------------------------------------------(Eq.10)}$$

**Piston Motion**

Piston motion applies to both the high pressure cycle and the gas exchange process.

For a standard crank train the piston motion as a function of the crank angle α can be written as:

$$s= (r+l).\cos\psi-r.\cos(\psi+\alpha)-l.\sqrt{1-\{\frac{r}{l}.\sin(\psi+\alpha)-\frac{e}{l}\}^2} \text{ ----------------------------(Eq.11)}$$

$$\psi = \arcsin(\frac{e}{r+l}) \text{ ------------------------------------------------(Eq.12)}$$

**HEAT TRANSFER**

The heat transfer to the walls of the combustion chamber, i.e. the cylinder head, the piston, and the cylinder liner, is calculated from:

$$Q_{wi} = A_i .\alpha_w . (T_c-T_{wi}) \text{ ----------------------------------------------------(Eq.13)}$$

In the case of the liner wall temperature, the axial temperature variation between the piston TDC and BDC position is taken into account:

$$T_L = T_{L,TDC} . \frac{1-e^{-cx}}{x.c} \text{ ---------------------------------------------(Eq.14)}$$

$$c = \ln\{\frac{T_{L,TDC}}{T_{L,BDC}}\} \text{ -------------------------------------------------(Eq.15)}$$

For the calculation of the heat transfer coefficient, the Woschni 1978 heat transfer model is used.

**Woschni Model**

The woschni model published in 1978 for the high pressure cycle is summarized as follows:

$$\alpha_w = 130.D^{-0.2}.p_c{}^{0.8}.T_c{}^{-0.53}.\left[C_1.c_m + C_2.\frac{V_D.T_{c,1}}{p_{c,1}.V_{c,1}}.(p_c-p_{c,o})\right]^{0.8} \text{ ------------------(Eq.16)}$$

C1 = 2.28+0.308.cu/cm

C2 = 0.00324 for DI engines

For the gas exchange process, the heat transfer coefficient is given by following equation:

$$\alpha_w = 130.D^{-0.2}.p_c{}^{0.8}.T_c{}^{-0.53}.(C_3.c_m)^{0.8} \text{ -------------------------------------(Eq.17)}$$

$C_3 = 6.18+0.417.c_u/c_m$

**FUEL INJECTOR**

The fuel injector model is based on the calculation algorithm of the flow restriction. This means that the air flow rate in the fuel injector depends on the pressure difference across the injector and is calculated using the specified flow coefficients.

For the injector model, a measuring point must be specified at the location of the air flow meter. In this case the mean air flow at the air flow meter location during the last complete cycle is used to determine the amount of fuel. As is the case for continuous fuel injection, the fuelling rate is constant over crank angle.

**PIPE FLOW**

The one dimensional gas dynamics in a pipe are described by the continuity equation

$$\frac{\partial \rho}{\partial t} = -\frac{\partial(\rho.u)}{\partial x} - \rho.u.\frac{1}{A}.\frac{dA}{dx},$$ ------------------------------------------------(Eq.18)

the equation for the conservation of momentum

$$\frac{\partial(\rho.u)}{\partial t} = -\frac{\partial(\rho.u^2 + p)}{\partial x} - \rho.u^2.\frac{1}{A}.\frac{\partial A}{\partial x} - \frac{F_R}{V},$$ ---------------------------------(Eq.19)

and by the energy equation

$$\frac{\partial E}{\partial t} = -\frac{\partial[u.(E+p)]}{\partial x} - u.(E+p).\frac{1}{A}.\frac{dA}{dx} + \frac{q_w}{V}.$$ ------------------------------(Eq.20)

The wall friction force can be determined from the wall friction factor $\lambda_f$ :

$$\frac{FR}{V} = \frac{\lambda f}{2.D}.\rho.u.|u|$$ ----------------------------------------------------------------(Eq.21)

Using the Reynold's analogy, the wall heat flow in the pipe can be calculated from the friction force and the difference between wall temperature and gas temperature:

$$\frac{q_w}{V} = \frac{\lambda_f}{2.D}.\rho.|u|.c_p.(Tw - T)$$ -------------------------------------------------------(Eq.22)

During the course of numerical integration of the conservation laws defined in the Eq.20, Eq.21 and Eq.22, special attention should be focused on the control of the time step. In order to achieve a stable solution, the CFL criterion (stability criterion defined by Courant, Friedrichs and Lewy ) must be met:

$$\Delta t \le \frac{\Delta x}{u + a}$$ -------------------------------------------------------------------------(Eq.23)

This means that a certain relation between the time step and the lengths of the cells must be met. The time step to cell size relation is determined at the beginning of the calculation on the basis of the specified initial conditions in the pipes. However, the CFL criterion is checked every time step during the calculation. If the criterion is not met because of significantly changed flow conditions in the pipes, the time step is reduced automatically.

An ENO scheme is used for the solution of the set of non-linear differential equations discussed above. The ENO scheme is based on a finite volume approach. This means that the solution at the end of the time step is obtained from the value at the beginning of the time step and from the fluxes over the cell borders.

## RESULTS AND DISCUSSION

### EFFECT OF LOAD ON POWER

The Fig.1 below shows the effect of load on power. It is seen as the load increases the power output also increases due to additional amount of fuel supplied by governing mechanism to maintain the speed constant at a particular air-fuel ratio.

Further it is seen that the power developed by petrol as fuel is higher than hydrogen due to higher volumetric efficiency with petrol as a liquid fuel than hydrogen as a gaseous fuel. Also since the chemically correct air fuel ratio of hydrogen is 34.5 as compared to 14.6 of petrol, it also restricts the additional amount of hydrogen fuel which could be supplied to the cylinder for each cycle. Further due to the fundamental differences in the physical and chemical properties of petrol and hydrogen, the peak heat release rate of petrol is 53 J/deg as compared to 41.5 J/deg of hydrogen fuel. This results in drastic change in the rate of pressure rise in cylinder as a result of which the area enclosed under the pressure-crank angle diagram for each cycle for petrol is higher than hydrogen fuel. Since the work done by engine and also the power developed depends on the area enclosed under the pressure-crank angle for each cycle, higher power is developed by engine run by petrol fuel as compared to hydrogen.

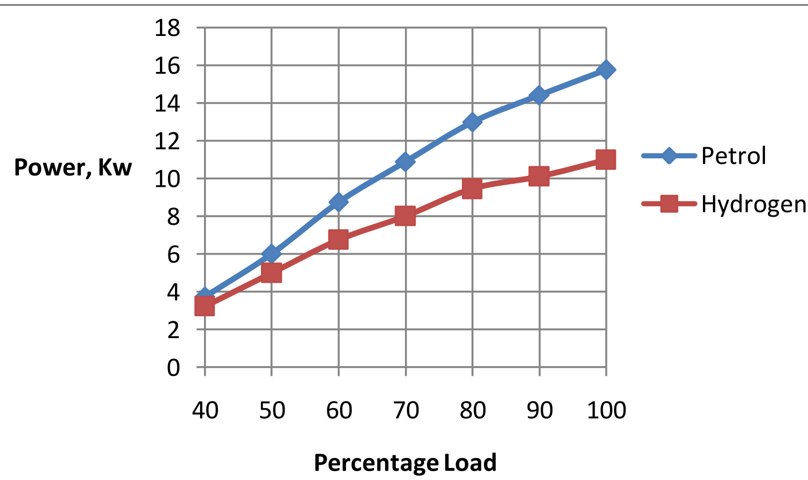


**Fig.1 Effect of Load on Power**

### EFFECT OF LOAD ON BRAKE SPECIFIC FUEL CONSUMPTION.

Fig.2 below shows the effect of load on brake specific fuel consumption which is defined as fuel consumed per unit power output. The BSFC decreases with increase in load as the increase in power output with load remains a dominant factor as compared to increase in fuel supplied with respect to increase in load.

Although the power output with petrol fuel is on higher side the BSFC is lower for the engine run by hydrogen fuel. This is because comparatively quite lesser amount of hydrogen fuel goes to engine of same displacement volume under chemically correct air to fuel ratio for both fuels.

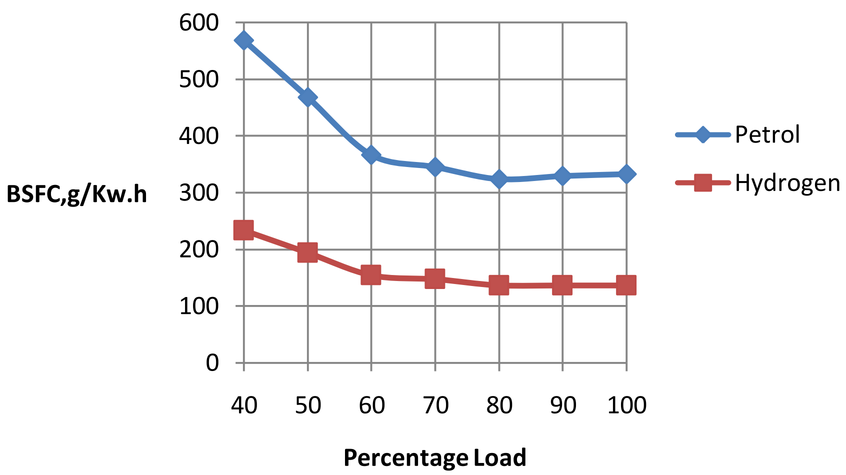


**Fig.2: Effect of Load on Brake Specific Fuel Consumption.**

**EFFECT OF LOAD ON TORQUE.**

Fig.3 below shows the effect of load on torque. It is seen as the load increases the torque developed by engine also increases due to additional amount of fuel supplied by governing mechanism to overcome the additional increase in load in order to maintain the speed constant at a particular air-fuel ratio.
Further it is seen that the torque produced by petrol as fuel is higher than hydrogen due to higher pressures developed in petrol mode.

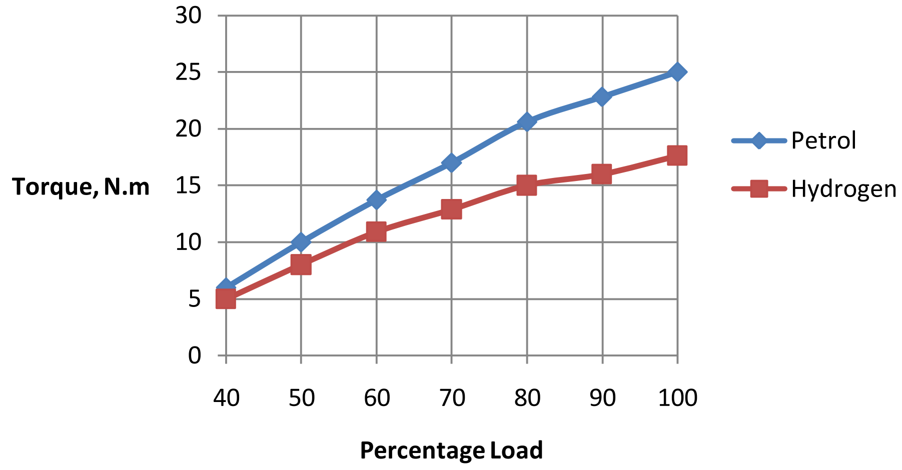


**Fig.3: Effect of Load on Torque**

**EFFECT OF LOAD ON EXHAUST GAS TEMPERATURE.**

Fig.4 below shows the effect of load on exhaust gas temperature. It is seen from the graph that the exhaust gas temperatures increases with increase in load as more amount of fuel is burned at higher loads.

Higher temperatures are developed by hydrogen fuel as compared to petrol due to higher calorific value of petrol.

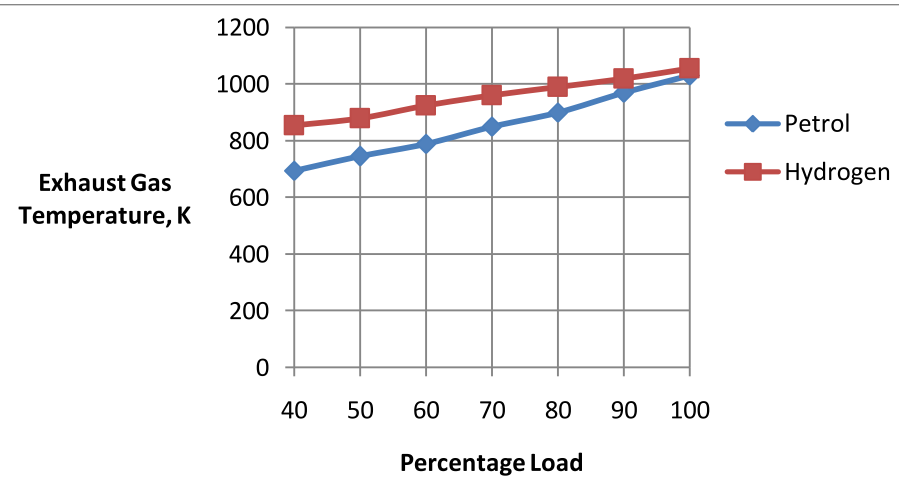


**Fig.4: Effect of Load on Exhaust Gas Temperature**

**EFFECT OF LOAD ON CO EMISSIONS.**

Fig.5 below shows the effect of load on carbon monoxide emissions.

CO emissions increase with increase in load as more amount of fuel is supplied to the engine at higher loads. The increase in CO emissions is lower till 80% load. Beyond 80% load there is higher rise in CO emissions due to the higher amount of fuel is supplied to cylinder. Since the speed is maintained constant the amount of air going to engine cylinder decreases as the volumetric efficiency decreases at higher loads. This results in sharp rise in CO emissions.

CO emissions are not produced with hydrogen fuel as there is no carbon atom in hydrogen. The CO emissions with petrol are higher at higher speeds as there are more number of power cycles per unit time at higher speed.

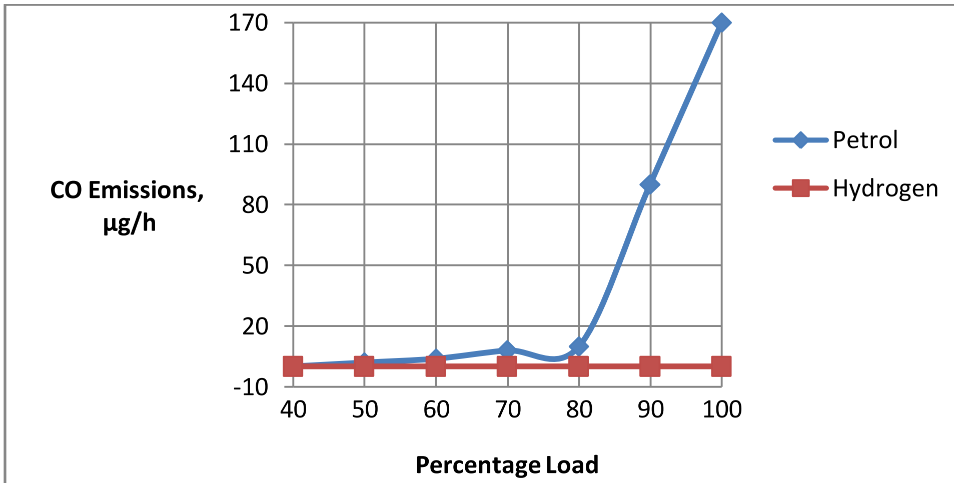


**Fig.5: Effect of Load on Carbon monoxide Emissions**

**EFFECT OF LOAD ON $NO_X$ EMISSIONS**

Fig.6 below shows the effect of load on NOx emissions. There is marginal increase in NOx emissions upto 60% load. There is sharp increase in NOx emissions beyond 60% load the higher temperature of the gases developed in the cylinder is favourable for NOx formation.

Higher NOx emissions are produced with hydrogen fuel as compared to petrol because of higher temperatures developed in hydrogen mode. Also as the chemically correct air to fuel ratio for hydrogen much higher than petrol, more amount of air is available for NOx formation with hydrogen fuel.

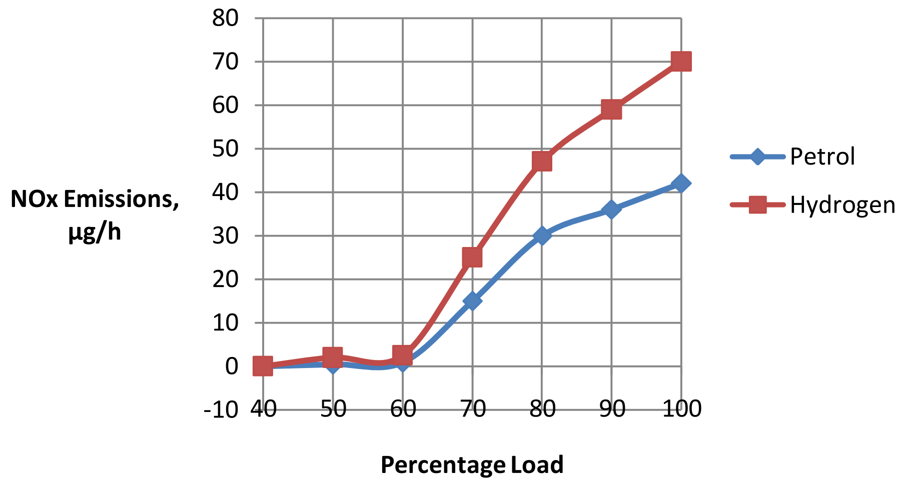


**Fig.6: Effect of Load on NOx Emissions**

**EFFECT OF LOAD ON HC EMISSIONS**

Fig.7 below shows the effect of load on hydrocarbon emissions.

HC emissions are lower and fairly constant till 80% load. Beyond 80% load there is sharp rise in HC emissions due to the higher amount of fuel being supplied to cylinder. Also since the speed is maintained constant the amount of air going to engine cylinder decreases as the volumetric efficiency decreases at higher loads which results steep hike in HC emissions.

Higher HC emissions are produced in petrol mode as comparatively more amount of petrol goes to cylinder for each cycle due to lower chemically correct air to fuel ratio for petrol as compared to hydrogen. Also as the flame speed and other combustion characteristics are better for hydrogen, it results in lower HC formation in hydrogen mode.

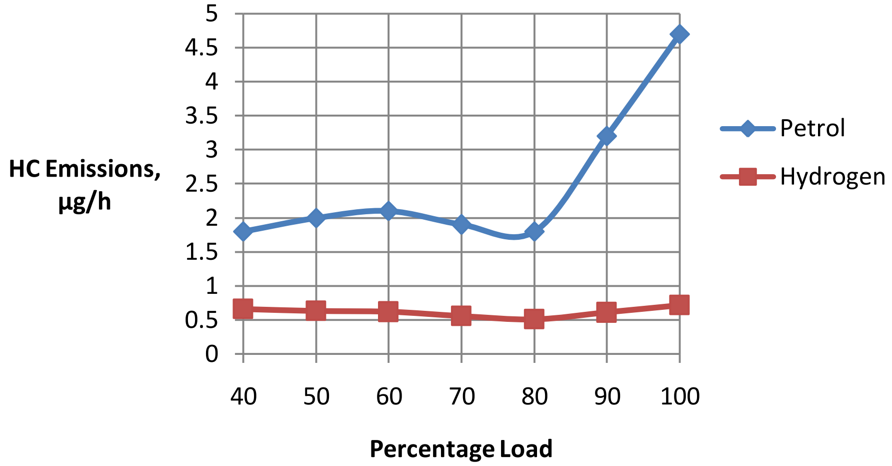


**Fig.7: Effect of Load on Hydrocarbon Emissions**

**CONCLUSIONS**

1. Hydrogen can be used as an alternative fuel in S.I .engines for power generation although the power produced in hydrogen mode is on lower side.
2. The hydrogen engine runs more economically as compared to petrol engine.
3. Less HC emissions are produced by hydrogen fuel as compared to petrol.
4. No CO emissions are produced in hydrogen mode.
5. The NOx emissions produced by the engine run by hydrogen fuel are on higher side as compared to petrol. This can be brought down by using a suitable reduction type of catalytic convertor in the exhaust manifold.

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**APPENDIX-A**

**NOMENCLATURE**

| | | |
|---|---|---|
| a | = | speed of sound |
| A | = | pipe cross-section |
| $A_{eff}$ | = | effective flow area |
| $A_i$ | = | surface area (cylinder head, piston, liner) |
| $AF_{CP}$ | = | air fuel ratio of combustion products |
| $A_{geo}$ | = | geometrical flow area |
| c | = | mass fraction of carbon in the fuel |
| $c_V$ | = | specific heat at constant volume |
| $c_p$ | = | specific heat at constant pressure |
| C1 | = | 2.28+0.308.cu/cm |
| C2 | = | 0.00324 for DI engines |

| | | |
|---|---|---|
| Cm | = | mean piston speed |
| Cu | = | circumferential velocity |
| $c_u$ | = | circumferential velocity |
| D | = | cylinder bore |
| D | = | pipe diameter |
| $dm_i$ | = | mass element flowing into the cylinder |
| $dm_e$ | = | mass element flowing out of the cylinder |
| $d_{vi}$ | = | inner valve seat diameter (reference diameter) |
| $\frac{dm_{BB}}{d\alpha}$ | = | blow-by mass flow |
| e | = | piston pin offset |
| E | = | energy content of the gas (=ρ. $\bar{c}_V.T + \frac{1}{2}.\rho.u^2$) |
| f | = | fraction of evaporation heat from the cylinder charge |
| $F_R$ | = | wall friction force |
| h | = | mass fraction of hydrogen in the fuel |
| $h_{BB}$ | = | enthalpy of blow-by |
| $h_i$ | = | enthalpy of in-flowing mass |
| $h_e$ | = | enthalpy of the mass leaving the cylinder |
| $H_u$ | = | lower heating value |
| k | = | ratio of specific heats |
| l | = | con-rod length |
| m | = | shape factor |
| $\dot{m}$ | = | mass flow rate |
| $m_c$ | = | mass in the cylinder |
| $m_{ev}$ | = | evaporating fuel |
| $m_{pl}$ | = | mass in the plenum |
| n | = | mass fraction of nitrogen in the fuel |
| o | = | mass fraction of oxygen in the fuel |
| p | = | static pressure |
| $P_{01}$ | = | upstream stagnation pressure |
| Pc,o | = | cylinder pressure of the motored engine[bar] |
| Pc,1 | = | pressure in the cylinder at IVC[bar] |
| $p_{pl}$ | = | pressure in the plenum |
| $p_c$ | = | cylinder pressure |
| $p_2$ | = | downstream static pressure |
| $q_{ev}$ | = | evaporation heat of the fuel |
| $q_w$ | = | wall heat flow |
| Q | = | total fuel heat input |
| $Q_F$ | = | fuel energy |

$Q_{wi}$ = wall heat flow (cylinder head, piston, liner)
r = crank radius
$R_0$ = gas constant
s = piston distance from TDC
t = time
T = temperature
Tc,1 = temperature in the cylinder at intake valve closing (IVC)
$T_c$ = gas temperature in the cylinder
$T_{wi}$ = wall temperature ( cylinder head, piston, liner)
$T_L$ = liner temperature
$T_{L,TDC}$ = liner temperature at TDC position
$T_{L,BDC}$ = liner temperature at BDC position
$T_w$ = pipe wall temperature
$T_{01}$ = upstream stagnation temperature
u = specific internal energy
u = flow velocity
V = cylinder volume
V = cell volume (A.dx)
VD = displacement per cylinder
w = mass fraction of water in the fuel
x = relative stroke (actual piston position related to full stroke)
x = coordinate along the pipe axis
α = crank angle
$\alpha_o$ = start of combustion
$\Delta\alpha_c$ = combustion duration
$\alpha_w$ = heat transfer coefficient
ρ = density
μσ = flow coefficient of the port
ψ = crank angle between vertical crank position and piston TDC position
λf = wall friction coefficient
Δt = time step
Δx = cell length

**APPENDIX-B**

| **PETROL ENGINE SPECIFICATIONS** | |
|---|---|
| Bore | 84 mm |
| Stroke | 90 mm |
| Compression Ratio | 9 |
| Number of Cylinders | 1 |
| Operating Speed | 6000 rpm |

**APPENDIX-C**

Table 1: **PHYSICAL AND CHEMICAL PROPERTIES OF PETROL AND HYDROGEN (2)**

| Fuel Property | Hydrogen | Petrol |
|---|---|---|
| Formula | H2 | C4 TO C12 |
| Molecular weight | 2.02 | 100-105 |
| Lower heating value, MJ/Kg | 121 | 42.5 |
| Stoichiometric air-fuel ratio, weight | 34.3 | 14.6 |
| Octane No. | 130 | 80-98 |

**REFERENCES**

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