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# COMPUTER SIMULATION STUDIES ON A FOUR STROKE CYCLE SPARK IGNITION ENGINE USING GASOLINE AND HYDROGEN AS ALTERNATIVE FUELS

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#### **ABSTRACT**

This paper describes the results of computational studies on a single cylinder four stroke cycle spark ignition engine using Hydrogen as an alternative fuel to petrol. The simulation is done in the professional engine simulation software from AVL Austria named as BOOST. The modeling methodology involves the use of first law of thermodynamics for 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 data was used as per petrol engine needs, and results for engine performance and emissions characteristics were generated. 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. It was observed that the power output was decreased with hydrogen as an alternative fuel due to lower volumetric efficiency, the brake specific fuel consumption was comparable in both cases due to higher calorific value of hydrogen. The emissions were also reduced with hydrogen as fuel because of no carbon atoms as compared to petrol fuel. No CO emission was produced with hydrogen, there was reduction in NOx emission and also there was drastic reduction in hydrocarbon emissions with hydrogen as fuel. It is proposed that hydrogen can be successfully used in petrol engine as an alternative future fuel.

Keywords: Engine, Petrol, Propane, Alternate fuels, Simulation, Performance, Emissions

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#### **INTRODUCTION**

Computer simulation studies helps to predict the behavior of the engine in the petrol and Hydrogen fuel modes. We prepare the models for Petrol and Hydrogenfuel modes for the engine systems and feed the actual data corresponding to the design and operating conditions of the system. It helps to simulate the results without actually performing experiments. Thus a lot of money and time is saved. Moreover we can simulate and compute those results which are very difficult to be measured experimentally. Favorable computed results pave the way for further experimental investigations.

The objectives are to investigate the feasibility of Hydrogenas alternative fuel in petrol engines. It is also intended to choose Hydrogen as fuel because it has no carbon atoms as compared to petrol and therefore will produce minimal pollution. Table 1 at the end gives physico-chemical properties of Hydrogen and petrol which help us to investigate the feasibility of using Hydrogen as an alternative fuel to petrol.

#### **THEORETICAL BASIS**

The theoretical background including the basic equations for all elements used in the present model is summarized below to give a better understanding of the program.

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:

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

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

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

$$\frac{dm_{BB}}{d\alpha}$$
 = 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.

Eq.1 is valid for engines with internal and external mixture preparation. However the terms which take into account the change of gas composition due to combustion, are treated differently for internal and external mixture preparation.

For internal mixture preparation it is assumed that

- The fuel added to the cylinder charge is immediately burnt.
- The combustion products mix instantaneously with the rest of cylinder charge and thus form a uniform mixture.
- As a consequence, the Air-Fuel ratio of the charge diminishes continuously from a high value at the start of combustion to the final value at the end of combustion.

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

$$p_c = \frac{1}{V} . m_c . R_o . T_c$$
 -----(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:

$$L_{st} = 137.85 \cdot (\frac{c}{12.01} + \frac{h}{4.032} + \frac{s}{32.06} - \frac{o}{32.0})$$
 [kg Air/kg Fuel] -----(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:

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

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.**

The vibe function is used to approximate the actual heat release characteristics of an engine:

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

$$dx = \frac{dQ}{Q}$$
 (Eq.6)  
$$y = \alpha - \frac{\alpha_0}{\Delta \alpha_c}$$
 (Eq.7)

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

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

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

#### Gas Exchange Process, Basic Equation

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

$$\frac{d(m_{c.u})}{d\alpha} = -\frac{p_{c.d}V}{d\alpha} - \sum \frac{dQ_w}{d\alpha} + \sum \frac{dm_i}{d\alpha.h_i} - \sum \frac{dm_e}{d\alpha.h_e} - \dots - (Eq.9)$$

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

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

#### **Piston Motion**

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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  $\alpha$  can be written as:

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

$$\psi = \arcsin(\frac{e}{r+l})$$
 -----(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:

$$Q_{wi} = Ai . \alpha_w . (T_c - T_{wi})$$
 ------(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:

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

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

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:

$$\alpha_{w} = 130.D^{-0.2}.p_{c}^{0.8}.T_{c}^{-0.53}.\left[C_{1.c_{m}} + C_{2.}\frac{V_{D.T_{c,1}}}{p_{c,1}.V_{c,1}}.(p_{c} - p_{c,o})\right]^{0.8}$$
-----(Eq.16)

C1 = 2.28 + 0.308.cu/cm

C2 = 0.00324 for DI engines

C2 = 0.00622 for IDI engines

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

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

$$C_3 = 6.18 {+} 0.417.c_u \! / c_m$$

#### **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. In addition, the amount of fuel specified is fed into the air flow.

In the case of carburetor model, the fuel flow is set to a specified percentage of the instantaneous mass flow.

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.

The fuel is added in gaseous form to the pipe flow. No evaporation is considered.

#### **Pipe Flow**

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

the equation for the conservation of momentum

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

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  $\lambda_f$ :

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

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:

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

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

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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

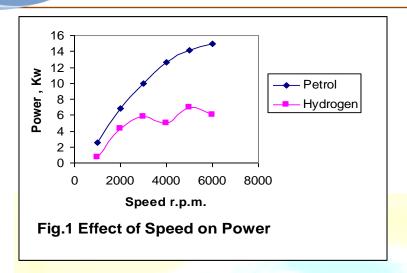
#### **RESULTS AND DISCUSSION**

## **Effect of Speed on Power**

The Fig.1 below shows the effect of speed on power. It is seen as the speed increases the power also increases due to more number of power cycles per unit time. Further it is seen that the power developed by petrol as fuel is higher than hydrogen due to higher volumetric efficiency with petrol.

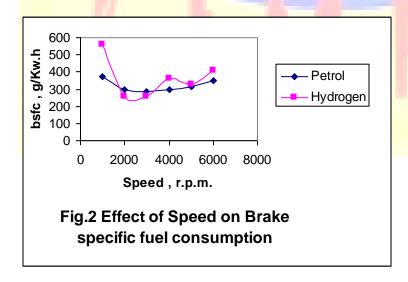


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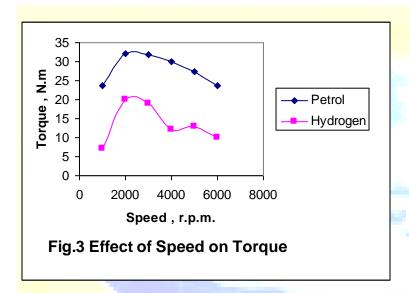
#### **Effect of Speed on Brake Specific fuel Consumption. (bsfc)**

Fig.2 below shows the effect of speed on brake specific fuel consumption (fuel consumed per unit power output). It is seen that the operation of hydrogen engine is approximately as economical as the petrol fuel. From the physical and chemical properties of petrol and hydrogen it is seen that hydrogen has higher heating value but at same time its volumetric efficiency is lesser.



#### Effect of Speed on Torque.

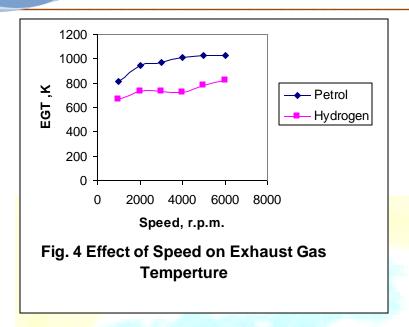
Fig.3 below shows the effect of speed on torque. It is seen that in each case the maximum torque is produced at 2000 r.p.m.. This is because the combustion characteristics and in-cylinder pressure development is best at this speed. Petrol produces better torque due to its higher volumetric efficiency as compared to hydrogen.



#### Effect of Speed on Exhaust Gas Temperature.

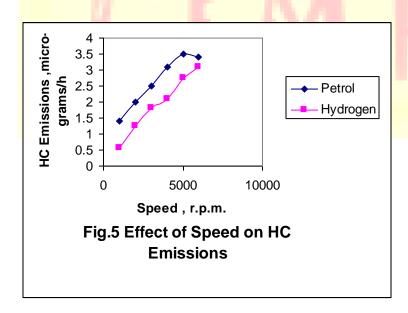
Fig.4 below shows the effect of speed on exhaust gas temperature. It is seen from the graph that the exhaust gas temperatures in case of petrol is higher. This is also a clear indication that petrol produces higher temperatures due to overall better combustion characteristics.





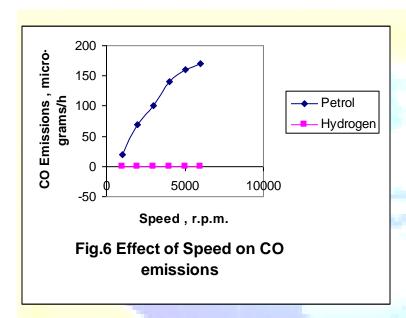
## **Effect of Speed on HC Emissions**

Fig.5 below shows the effect of speed on hydrocarbon emissions. The HC emissions are much less with hydrogen fuel. The contribution of HC emissions with hydrogen fuel is mainly due to crank case lubrication which circulates the hydrocarbon based lubricating oil into cylinder for piston cylinder lubrication.



## Effect of Speed on CO Emissions.

Fig.6 below shows the effect of speed on carbon monoxide emissions. CO emissions with petrol are significant due to many carbon atoms in petrol. No CO emissions are 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 at higher speed.

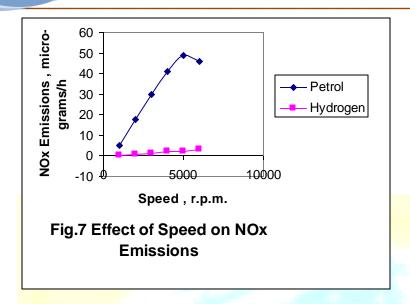


#### Effect of Speed on NO<sub>X</sub> Emissions

Fig.7 below shows the effect of speed on NOx emissions. The NOx emissions with petrol fuel are higher as higher temperatures are produced with petrol as compared to hydrogen. For the formation of NOx emissions presence of oxygen and nitrogen from air at higher temperatures for long time is desirable and favourable condition.



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#### **CONCLUSIONS**

- 1. Hydrogen can safely be used in petrol engines as an alternative fuel to conventional petrol.
- 2. Pollution formation from engines using Hydrogen as fuel will be much less.
- 3. Lesser power is produced by Hydrogen fuel as compared to petrol.
- 4. The Hydrogen engine operation is as economical as petrol approximately.

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#### REFERENCES

- [1] AVL LIST GmbH, Examples, AVL BOOST Version 2009.1
- [2] Richard L. Bechtold, Alternative Fuels Handbook, SAE Publication.



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#### APPENDIX-A

#### **NOMENCLATURE**

a = speed of sound

A = pipe cross-section

 $A_{eff}$  = effective flow area

A<sub>i</sub> = 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<sub>v</sub> = 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

C2 = 0.00622 for IDI engines

Cm = mean piston speed

Cu = circumferential velocity

 $c_u$  = circumferential velocity

D = cylinder bore

D = pipe diameter

dm<sub>i</sub> = mass element flowing into the cylinder

dm<sub>e</sub> = mass element flowing out of the cylinder

d<sub>vi</sub> = 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  $(=\rho. cv.T + \frac{1}{2}.\rho.u^2)$ 

f = fraction of evaporation heat from the cylinder charge

 $F_R$  = wall friction force

h = mass fraction of hydrogen in the fuel

 $h_{BB} \quad = \quad \quad enthalpy \ of \ blow-by$ 

 $h_i \qquad = \qquad \text{enthalpy of in-flowing mass}$ 

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	$h_{e}$	=	enthalpy of the mass leaving the cylinder
	$H_{\boldsymbol{u}}$	=	lower heating value
	k	=	ratio of specific heats
	1	=	con-rod length
	m	=	shape factor
	m .	=	mass flow rate
	$m_c$	=	mass in the cylinder
	m <sub>ev</sub>	=	evaporating fuel
	$m_{pl}$	=	mass in the plenum
	n	=	mass fraction of nitrogen in the fuel
	0	=	mass fraction of oxygen in the fuel
	p	=	static pressure
	P <sub>01</sub>		upstream stagnation pressure
	Pc,o	- )	cylinder pressure of the motored engine[bar]
	Pc,1	- [	pressure in the cylinder at IVC[bar]
	p <sub>pl</sub>	=	pressure in the plenum
	p <sub>c</sub>	=	cylinder pressure
	$p_2$	= ``	downstream static pressure
	q <sub>ev</sub>	=	evaporation heat of the fuel
	$q_{\rm w}$	=	wall heat flow
	Q	=	total fuel heat input
	Q <sub>F</sub>	=	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)		temperature in the cylinder at intake valve closing (IVC)	
	$T_{c}$	=	gas temperature in the cylinder
	$T_{wi} \\$	=	wall temperature ( cylinder head, piston, liner)

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$T_L$	=	liner temperature
T L,TD	oc =	liner temperature at TDC position

 $T_{L,BDC}$  = liner temperature at BDC position

 $T_{\rm w}$  = 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

 $\alpha$  = crank angle

 $\alpha_{\rm o}$  = start of combustion

 $\Delta \alpha_{\rm c}$  = combustion duration

 $\alpha_{\rm w}$  = heat transfer coefficient

 $\rho$  = density

 $\mu\sigma$  = flow coefficient of the port

crank angle between vertical crank position and piston TDC position

 $\lambda f$  = wall friction coefficient

 $\Delta t = time step$ 

 $\Delta x = \text{cell length}$ 

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Petrol Engine Specifications					
Bore	84 mm				
Stroke	90 mm				
Compression Ratio	9				
Number of Cylinders	1				

# **APPENDIX-C**

Table 1: Physico-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,	34.3	14.7
weight		
Octane number	130	80-98