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# A Numerical Study of Combustion Variability in Hydrogen Fuelled Multicylinder Engine

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***ABSTRACT** - Importance of I.C.Engine, one of the oldest mechanical invention in today's world need hardly to be stressed. The detailed study is more even more necessary due to exhausting natural resources and to find out alternative fuel. Simulation is the process of designing a model of a real system and conduction experiment with it, for the purpose of understanding the behavior of the design. Computer modeling has gained a greater importance these days because of the availability of fast digital computers. Computer modeling is the process of formulating a model a physical system representing actual process and analyzing the same. Usually the model is a mathematical one representing the actual processes and the analysis made using a computer. The present paper deals with the insight of combustion Process in the Engine using Ideal & Real Gas Equations. The accurate analysis f the Engine is such a complex Problem that simplifying assumption have been introduced to convert physical situation to mathematical model. The total combustion period is of 24 degree of crank rotation out of which it is further divided in to 3 parts. Initially for 4 degree of crank rotation we assumed that only 5% of fuel is used in combustion process. In second part we assumed that the 85% of fuel is used and also this process is assume to be exponential. The Period will last for 16degree of crank rotation. The Last period will last for 4 degree of crank rotation in which last 10% if fuel is burnt.*
***KEYWORDS:** Computer simulation, Mathematical model, Combustion Process, Delayed Entry Technique, Hydrogen Fuel*

## INTRODUCTION

Internal Combustion Engines are those engines in which combustion of fuels takes place inside the engine and hence the chemical energy is converted in to thermal energy, which is further converted into mechanical work. The present acute shortage of conventional fuels has necessitated the need for alternate fuel research. Hydrogen, which can be produced from natural gas or water, is proved to be a practical and potential alternate fuel for the I.C. Engine. The replacement of hydrocarbons by Hydrogen in automotive vehicles is expected to results in a considerable reduction in environmental pollution, since the harmful emission of unburned hydrocarbons and oxides of nitrogen are either avoided or minimized. With Hydrogen as a fuel, the engine exhaust is free from carbon monoxide and hydrocarbon emission, except very small quantities, which may be due to the combustion of lubricating oil. Further it does not contain sulfur, lead compounds or smoke and is virtually odorless. When Hydrogen-air combustion takes place in an I.C. engine cylinder, the only product of combustion are water vapour and oxides of nitrogen and the engine will be pollution free.It has been proved that the higher thermal efficiency of Hydrogen engine can offset the higher production cost. With only minor modifications, the conventional diesel cycle engine can be operated efficiently using Hydrogen as fuel with atmospheric air supplying the necessary oxygen.

## PROPERTIES OF HYDROGEN

Table 1. Shows that main combustion properties of Hydrogen provide its use as an IC engine fuel. A low fuel conversion rate is problem with gaseous-fueled engines run with high amounts of excess air. The low quenching distance of Hydrogen offers improvement in this matter. Hydrogen flames can easily penetrate into difficult chamber zones and reach the unburnt mixtures than that of fossil fuels. Optimized Hydrogen engines can be run at higher compression ratio than that with unleaded gasoline. It makes Hydrogen powered engines 15-25 % more efficient than gasoline engines.

**Table 1: Properties of Hydrogen**

| Description | Hydrogen |
|---|---|
| Laminar flame speed | 1.96 m/sec |
| Theoretical flame Temperature | 2140 $^{o}$C |
| Minimum ignition energy | 0.02 MJ |
| Quenching distance | 0.6 mm |
| Normalized flame emmisivity | 1 |
| Normal Boiling Point | 20.27 K |
| Auto ignition temperature | 858 K |
| Burning velocity | 265 to 325 cm/sec |

 

## COMBUSTION OF HYDROGEN

•Hydrogen burns in oxygen or air to form water.
$2 H_2 + O_2 \Longrightarrow 2 H_2O$
•Oxygen will also burn in hydrogen.
•Hydrogen does not itself support combustion, as may be shown by passing a lighted taper into an inverted jar of hydrogen, when the taper is extinguished. A mixture of hydrogen with oxygen or air explodes violently when kindled, provided either gas is not present in too large excess.

## REACTION WITH NON-METALS

Hydrogen readily combines with fluorine and chlorine, less readily with bromine, iodine, sulphur, phosphorous, nitrogen, and carbon.
$H_2 + F_2 \Longrightarrow 2 HF$
Hydrogen burns in chlorine gas and a mixture of hydrogen and chlorine explodes violently when kindled or exposed to bright sunlight.
$H_2 + Cl_2 \Longrightarrow 2 Hcl$
Hydrogen combines with nitrogen on sparking or in presence of a catalyst, forming ammonia.
$N_2 + 3 H_2 \Longrightarrow 2 NH_3$

## HYDRIDE FORMATION

Hydrogen forms hydrides, (e.g. NaH) with a number of metals, including lithium, sodium and calcium.
$H_2 + 2 Na \Longrightarrow 2 NaH$
These hydrides when pure are white salt-like compounds rapidly decomposed by water.
$NaH + H_2O \Longrightarrow NaOH + H_2$
The hydrogen atom in these hydrides behaves to some extent like a halogen or electronegative element. For example, on the electrolysis of fused lithium hydride, the hydrogen is liberated at the positive electrode (i.e. a negatively charged hydrogen ion is discharged), and not the negative electrode as is the case when water is electrolyzed.
Hydrogen is also evolved at the anode in the electrolysis of a solution of calcium hydride, in fused mixture of potassium chloride and lithium chloride. This indicates that the ionic structure of the lithium hydride is Li(+)H(-).

## REDUCING PROPERTIES

When hydrogen is passed over many heated metallic oxides (e.g. copper oxide, iron oxide, or lead oxide), they are reduced to the metals. $CuO + H_2 \Longrightarrow Cu + H_2O$
Hydrogen at ordinary temperature and pressure is a light gases with a density only $1/14^{th}$ that of natural gas under the same conditions. By cooling to the extremely low temperature of $253^{o}$ C at atmospheric pressure the gas is condensed to a liquid with a specific gravity of 0.07, roughly $1/10^{th}$ that of gasoline.
The standard heating value of Hydrogen gas is 12.1 MJ/cu m compared with and average of 38.3 MJ/cu m for natural gas. The heating value of liquid Hydrogen is 120 MJ/kg or 8400 MJ/cu m ; the corresponding value of gasoline is 44 MJ/kg or 32000 MJ/cu m. Hence for producing a specific amount of energy , liquid Hydrogen is superior to gasoline on a weight basis but inferior on a volume basis. The flame speed of Hydrogen burning in the air is much greater than for natural gas, and the energy required initiating combustion is less. One subsequence of the low ignition energy is that flame less combustion on a catalytic surface is possible with Hydrogen at much lower temperature than flame burning. Mixture of Hydrogen and sir are combustible over than an exceptionally wide range for compositions: thus, the flammability limits at ordinary temperatures extend from 4 to 74 percent by volume of Hydrogen air. (Detonation can occur between 18 to 59 percent) This wide range has an important bearing on the use of Hydrogen fuel in internal combustion engines. The engine will operate, although not necessarily with the same efficiency, from very rich to very less mixtures. The adjustment of air-to-fuel Raito is thus much less critical than in a gasoline engine.

## PROPERTIES OF HYDROGEN AT VARIOUS EQUIVALENCE RATIOS

The various properties of hydrogen (specific heat, thermal conductivity, kinematic viscosity, density, prandtl no.) have been calculated at various equivalence ratios at different temperatures. Graphs of these properties have been plotted.

 

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**STOICHIOMETRIC EQUATION**

**Hydrogen**: for ($\varnothing = 1$)

2kg + ½(32+3.76×28)kg →

$H_2O$ +3.76/2 ($N_2$) .76/2)×28

Total mass of reactants = 70.64 kg

Total mass of products = 70.64 kg

**FOR REACTANTS:**

Mass fraction of $H_2$ ,$X_{H2}$ =0.02831

Mass fraction of $O_2$ , $X_{O2}$ =0.2265

Mass fraction of $N_2$ , $X_{N2}$ =0.7452

∴For reactants,

$C_p = (X_{H2}\times C_{pH2} + X_{O2}\times C_{pO2} + X_{N2}\times C_{pN2})/( X_{H2}+ X_{O2}+ X_{N2} )$

$C_p$ =(0. 02831× $C_{pH2}$ + 0.2265× $C_{pO2}$ + 0.7452× $C_{pN2}$)/1

Now by putting the values of $C_p$ we get the $C_p$ of reactants

**FOR PRODUCTS :**

Mass fraction of $H_2O$ = $X_{H2O}$ =0.2548

Mass fraction of $N_2$ = $X_{N2}$ = 0.7452

For products $C_p$ = 0.2548($C_p$) $H_2O$ + 0.7452($C_p$) $N_2$

**THERMAL CONDUCTIVITY (K)(W/M-K)**

**For reactants** , $(k)_R = X_{H2}\times k_{H2} + X_{O2}\times k_{O2} + X_{N2}\times k_{N2} = 0.02831\times k_{H2} + 0.2265\times k_{02} + 0.7452\times k_{N2}$

**For products** , $(k)_P = X_{H2O}\times k_{H2O} + X_{N2}\times k_{N2} = 0.2548\times k_{H2O} + 0.7452\times k_N$

**DENSITY:(ρ)(KG/M$^3$)**

**For reactants**,

$\rho = (X_{H2}\times \rho_{H2} + X_{O2}\times \rho_{O2} + X_{N2}\times \rho_{N2})/( X_{H2}+ X_{O2}+ X_{N2} )$

$\rho = (0.02831\times\rho_{H2} + 0.2265\times \rho_{O2} + 0.7452\times \rho_{N2})/(1)$

**For products**,

$\rho = (X_{H2O}\times \rho_{H2O} + X_{N2}\times \rho_{N2})/( X_{H2O}+ X_{N2} )$

$\rho = (0.2548\times \rho_{H2O} + 0.7452\times \rho_{N2})/( 1 )$

**MOLECULAR WEIGHT OF REACTANTS**

$M_{eq}$ = mass fraction of $H_2$ × $M_{H2}$+ mass fraction of $O_2$ × $M_{O2}$ + mass fraction of $N_2$ × $M_{N2}$

=0.02831× 2 + 0.2265×32 + 0.7452 × 28

$M_{eq}$ = 28.17022 kg/kg of mole

$R_{eq} = R / M_{eq} = 8.3143\times10^3/28.17022$

$R_{eq}$ =295.145 J/kg-K

For products,

$M_{eq}$ = 0.2548×18 + 0.7452 × 28 = 25.452 kg/kg-mole

$R_{eq} = R / M_{eq}$ = 326.66588 J/kg-K

 

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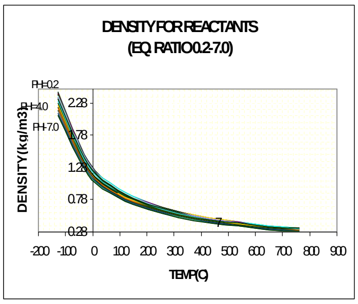
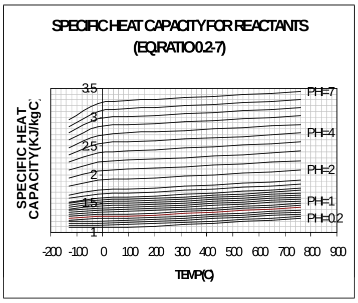
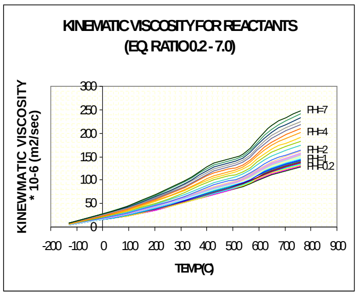
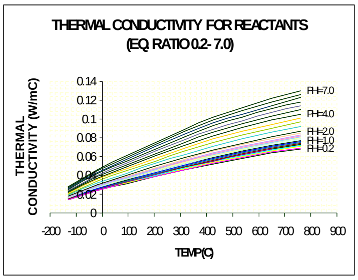
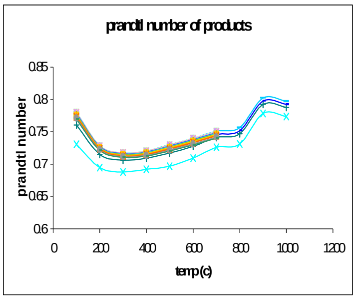
**PROPERTIES OF REACTANTS:**

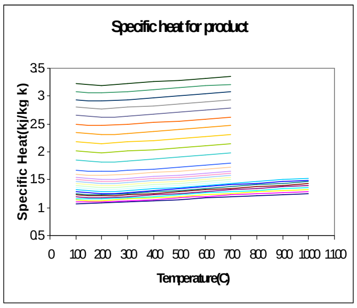


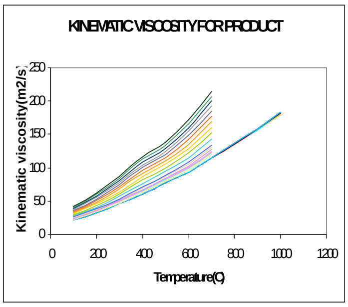



## PROPERTIES OF PRODUCT




## LITERATURE SHOWCASE

Beauties of Hydrogen were recognized as early as in 1820. In 1820, W.Cecil [1] read a paper before Cambridge philosophical society on "The Application of Hydrogen gas to produce a motive power in Machinery". Then after an elapse of century,. Ricardo [1] published in the "Report of the Empire Motor Fuel Committee" a very instructive paper on experiments carried out with Hydrogen and air used as a promoter with Petrol and Kerosene. He noticed that with a rich mixture pained by backfire, Ennen [2] in Germany, in 1933 dealt successfully with the backfire problem by injecting Hydrogen directly in to the cylinder, but the knocking persisted. King[3] made valuable contribution on the subject of pre-ignition and combustion knock in Hydrogen engine. He found that any particulate matter provides hot spot for pre-ignition and the combustion knock is an inherent property of near stoichiometric Hydrogen-air mixture due to the extremely high flame velocity.
The major conclusions derived from the available literature are as follows:

(i). Any existing engine can be converted to Hydrogen fuelled engine with minor modifications.
(ii). The part load & thermal efficiencies of $H_2$ fuelled engine are higher than gasoline air engine.
(iii). Hydrogen induction technique is easier to adopt as compared to Hydrogen injection technique.
(iv). Emission levels of $H_2$ - air engine are far less than that of gasoline – air engine if equivalence ratio is not exceeded 0.6 in $H_2$ - air engine (i.e. Lean operation)
(v). Equivalence ratio more than 0.6 results in back fire problems. If $H_2$ – air engine has to be operated in the range of 0.6 to 1.0-equivalence ratio, we have to go for EGR or water induction or delay entry technique to achieve backfire free operation and lower NOx emission.
(vi). The reported optimum spark advance for $H_2$ – air engine lies in between $7^o$ to $12^o$ BDC.
(vii). The optimum compression ratio lies in between 8 to 12 for $H_2$ – air engine.

## AIM OF THE PRESENT WORK

The aim of the present work is to model suction and Compression Processes in Hydrogen fueled Engine and by that improve fuel economy and govern power capacity of the engine. And also to describe the safe and backfire free $H_2$ fuelled engine using Delayed Entry Technique.

## DEVELOPMENT OF MATHAMATICAL MODEL

Internal combustion engines are the main power plants of the transportation systems and are responsible for a substantial fraction of fuel consumption. The scarcity of oil resources and the ever increasing standards on air pollution and emissions have dictated a need for improved, more efficient and less polluting internal combustion engine. Improvements on engine design have been achieved by traditional methods based on extensive experience. The advent of computers and the possibilities of performing numerical experiments may provide a new way of designing I.C. Engines. In fact, a stronger interaction between engine modelers, Designers and experimenters may result in improved engine designs in the not-to-distant future.The modeling of reciprocating or rotary engine is a multidisciplinary subject that involves chemical thermodynamics, fluid mechanics, turbulence, heat transfer, combustion and numerical methods. Today, millions of people depend on the automobile as their main source of transportation. Automobiles are the most efficient and convenient way to travel compared to walking or running. Unfortunately, most of the automobiles use fossil fuels such as oil. After the internal combustion engine consumes the gasoline, it releases carbon monoxide, nitrogen oxides, hydrogen carbons, and carbon dioxide. These chemicals cause air pollution, acid rain, and the buildup of greenhouse gases in the atmosphere. This results in the destruction of our precious ozone layer. In addition to these disastrous effects to the environment, gasoline is a finite energy source. Therefore, another efficient and cheap energy source needs to be found quickly. Ideally, this energy source should be unlimited in its supply and friendly to the environment The rapidly increasing world wide demand for energy and the progressive depletion of fossil fuels has led to an intensive research for alternative fuels which can be produced on a renewable basis. Hydrogen in the form of energy will almost certainly be one of the most important energy components of the early next century. Hydrogen is a clean burning and easily transportable fuel. Most of the pollution problems posed by fossil fuels at present would practically disappear with Hydrogen since steam is the main product of its combustion.

## COMBUSTION PROCESS IN HYDROGEN FUELLED ENGINE

Combustion is chemical reaction in which $H_2$ combines with oxygen liberating heat energy and causing an increase in temperature of gases. Conditions necessary for combustion are, presence of combustible mixture and source of initiating the process. In spark ignition engine proper amount of fuel and air is mixed in carburetor, which enters the cylinder during suction stroke. Later it is compressed to high pressure and temperature (**below self ignition temperature**). Spark is introduced to ignite the air-fuel mixture. Actually spark is advanced by 10-15 degree before TDC so that ignition lag is compensated.

## SIMULATION OF COMBUSTION PROCESS

At the conclusion of the compression stroke, combustion takes place, initiated by an electric spark from the spark plug. During the combustion process the chemical energy of the fuel is released in the form of heat energy, producing a temperature rise to few thousand degrees Celsius and pressure soars to many tens of atmospheres. A two zone combustion model is adopted in this simulation. A differential expression of the Vibe function is used to represent the fuel burning rate from the unburnt zone to the burnt zone. We may consider the combustion process as a extension of the compression process. we discussed earlier that in compression process the term dQ involves only the heat losses from the wall, but in the combustion process due to the burning of fuel the heat will be generated. Thus the dQ term will be summation of heat generation and heat loss from the wall. Now many authors have suggested not considering the heat losses from the wall during the combustion process. In the gasoline fueled engine the combustion process will continue about 40 to 45 degree. The equation suggested by Blair of mass burn ratio is given below with constants suitable for gasoline engines only.

$$B_\theta = 1 - e^{-a\left[\frac{\theta-\theta_s}{\Delta\theta}\right]^{m+1}}$$

But the flame speed is very high in case of hydrogen. it will take about 6 to 12 degree of crank rotation only. Thus the suggested approach is not suitable for us. We have taken very unique approach of flame speed. The mass fraction burnt ration or say the mass burn gradient is a function of both burnt and unburnt masses. it is expressed as below,

$$dMb = \left(\frac{Me - Mb}{\tau}\right)$$

Where ‘T’ is the specific time of burning. It is defined as below,

$$\tau = Li / Sl\_\varphi$$

Where Li is the specific length of turbulent eddy and S.l. is the flame speed at elevated temperature at equivalence ratio.

The flame speed of the hydrogen is 2.2 m/s at atmospheric condition. The flame speed at the elevated temperature is given below,

$$Sl = Sl_{atm}\left(\frac{T}{T_{atm}}\right)^{2.18}\left(\frac{P}{P_{atm}}\right)^{-0.16}$$

This flame speed is at equivalence ration 1 only. At equivalence ratio other than 1 Sl can be found from the equation given below,

$$Sl\_\varphi = Sl\left(1 - 1.03 \times \left(\frac{Mbt}{Mb}\right)^{0.77}\right)$$

Thus we are able to calculate the mass burnt ration w.r.t. time. So in the time of rotation of 2 degree we will find the mass burnt. From this mass burnt we will find the heat generated. Thus we know the dQ term in the first law of thermodynamics. Now the second term is dU i.e. the internal energy difference. Now as it is mentioned earlier, the internal energy is the function of temperature only.

Now the last term is the work done term expressed as below.

$$dW = \left(\frac{P2 + P1}{2}\right)(V2 - V1)$$

Now as we all know that the pressure is the function of temperature and volume. we know the volume of the cylinder at the each degree of crank rotations. Thus the only unknown variable is the temperature. Thus the all term in the first law of thermodynamic can be expressed in the two basic variable i.e. temperature and volume. And as we know the volume at each degree of the crank rotation, we left with the only variable and that is temperature.

Now to find the temperature from the modified equation it is almost impossible to express in single side variable. Thus to find the temperature we used bisection method to find the root of the equation.Now we have to consider real gas equation. There are many real gas equations but one which fits in our temperature range is Redlich Kwong real gas equation. This is given by,

$$P = \frac{RT}{V_m - b} - \frac{a}{\sqrt{T}V_m(V_m + b)}$$

But as we have to consider the differential approach, the differential form of the same equation is,

$$\frac{1}{p}\frac{dp}{d\theta} = \frac{1}{m}\frac{dm}{d\theta}(C1) - \frac{1}{V}\frac{dV}{d\theta}(C1) + \frac{1}{2T}\frac{dT}{d\theta}(C2)$$

$$C1 = \frac{\left(\bar{R}T^{3/2}V^2M^2(VM+mb)^2\right) - am\left((VM-mb)^2(2VM+mb)\right)}{m\left(\bar{R}T^{3/2}VM(VM+mb) - ma(VM+mb)\right)(V^2M^2 - m^2b^2)}$$

$$C2 = \left(\frac{2\bar{R}T^{3/2}VM(VM-mb)(VM+mb)^2 + m^2a(VM+mb)(VM-mb)^2}{\left(\left(m\bar{R}T^{3/2}VM(VM+mb) - m^2a(VM-mb)\right)(V^2M^2 - m^2b^2)\right)}\right)$$

Thus we are able to find pressure and temperature. These values will be again put in to the starting of the loop and after the iterative method we will get the pressure and temperature. The whole loop is to work over whole cycle.

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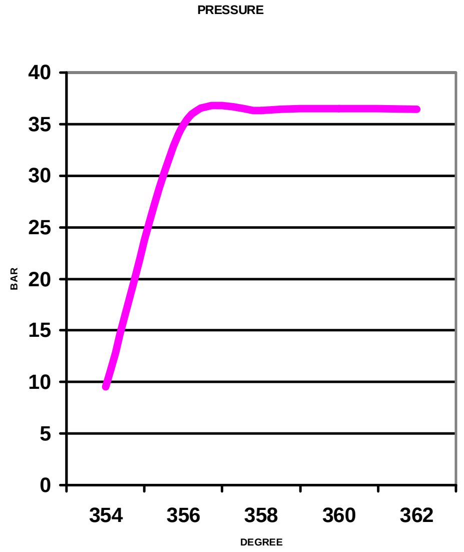
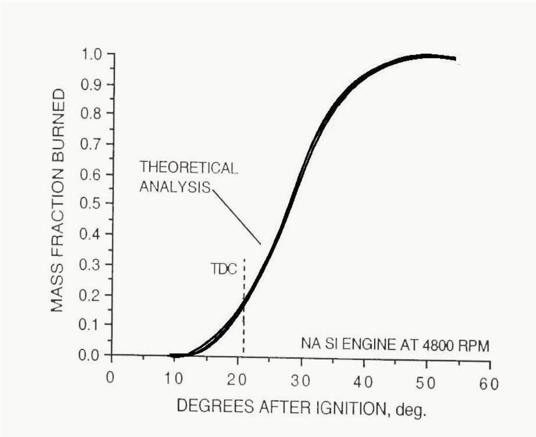
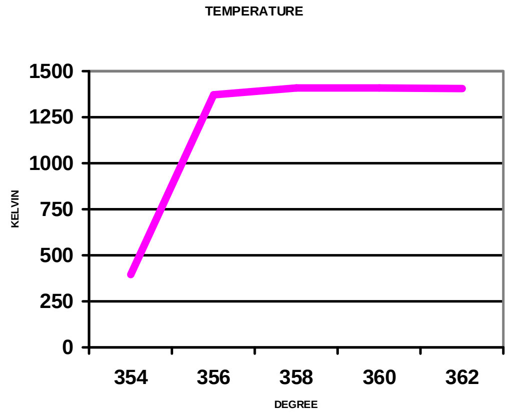
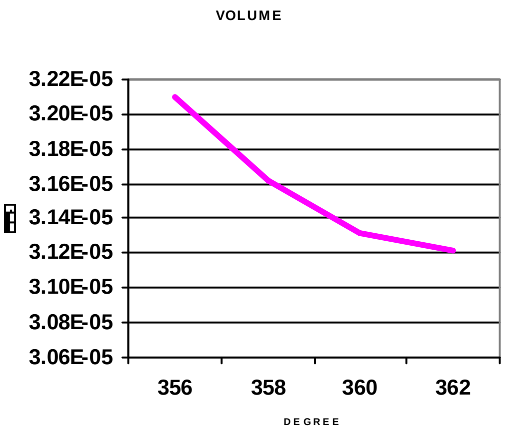
**RESULTS & DISCUSSION OF THE MODEL**






The p-θ curve shows that there is rapid rise in pressure. The pressure reaches to its peak value of 47.50 bar at 14 °atdc. This is because, at the conclusion of compression stroke combustion takes place. It is observed from the mass fraction burned curve that nearly 75% charge gets burned at 14 °atdc. After that the pressure begins to fall due to increase in cylinder volume.

The nature of T- θ curve is quite interesting. The temperature increases initially with increase in pressure. It reaches to its peak value of 2704.069 K at 21 °atdc. The heat release continues as the charge keeps on burning even after 14 °atdc when the peak pressure is reached. The rate of heat addition under these circumstances is more than the heat losses. As a result the temperature continues to rise and reaches to its peak value 21 ºatdc. the mass fraction burned curve, evaluated using vibe function. Graph shows the mass fraction burned characteristic determined from the analysis of cylinder pressure diagram from a conventional automobile naturally aspirated spark ignition engine. Both graph give comparable trend and thereby validates the combustion model used in present case.

**CONCLUSION**

From the results of simulation, it concludes that the trend of pressure and temperature with increasing crank angle is quite logical to the actual S.I. engine

- During combustion process, peak pressure reaches to 47.50 bar at 14 ˚atdc. Peak temperature of 2704.069 k is reached at 21 ˚atdc. For the naturally aspirated spark ignition engine, these results are quite relevant to the real engine. This validates the combustion model adopted in the present analysis.

- Mass fraction burned is calculated using Vibe function. The trend of curve is "s" shaped. The mass fraction burned characteristic obtained from known cylinder pressure diagram has the same "s" trend. This shows that there is a very good correspondence between the experimental data derived from the cylinder pressure diagram and the fit to that data by Vibe's analytic technique.

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