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THE EFFECT OF COMBUSTION DURATION ON THE PERFORMANCE AND EMISSION CHARACTERISTICS OF PROPANE-FUELED 4-Stroke S. I. ENGINES

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ان ازدياد القلق من النضوب السريع لمصادر الطاقة و بخاصة الأحفورية منها ولتأثيرها السيئ على البيئة و خاصة عند احتراقها كان لهما الأثر الكبير في تحفيز الباحثين للبحث عن مصادر بديلة للطاقة تكون أكثر ملائمة للبيئة وذات مصادر متجددة. قبل البدء في تصنيع أي محرك يعمل إلى الوقود البديل يجب ان يتم اختيار العوامل التصميمية المثلى والمناسبة له بناء على خصائص هذا الوقود البديل اولا. هنا يعتبر علم التمثيل التشبيهي باستخدام المعادلات الرياضية المناسبة والتي تستطيع محاكاة النظام المراد دراسته، تعتبر أهم أداة تساعد المصممين والباحثين على تصميم و تحسين عمل المحرك الجديد. في ظل هذه المعطيات تم عمل برنامج لتمثيل العمليات التي تحدث داخل المحرك الذي يدار بطاقة الغاز (غاز البروبان المسال) وتم التأكد من نجاح البرنامج في محاكاة العمليات التي تحدث داخل المحرك بنسبة خطأ مقبولة. ثم تم عمل دراسة لتأثير فترة الاحتراق علي أداء و نسبة الملوثات في العادم لهذا المحرك. لقد وجد بأن هناك قيمة مثلى لهذه الفترة والتي تعطي أفضل أداء للمحرك.

The growing concern about the fast depletion of petroleum-based fuels and the environmental pollution caused by their combustion has been a compelling incentive to all researchers to find ways to use environmentally friendly and renewable sources of energy. Before bringing an engine to the production line, it is expected that the engine using alternative fuels must be properly designed and optimized for this alternative fuel. Mathematical modeling is such an effective tool available to the designer which not only helps in designing new engines but also allows optimization of the performance of old engines. Keeping this in mind, a computer model of a 4-stroke spark ignition engine was developed using LPG as a fuel. This paper is an attempt to predict the mutual effect of combustion duration and engine performance on each other using propane as a fuel. It showed that there exists certain duration for the combustion that has to be maintained in order that the desired output may be achieved.

1. INTRODUCTION

Oil reserve all over the world is depleting at an alarming rate. In addition to this, the deteriorating quality of air we breathe is becoming another great public concern. Emissions of sulfur dioxide, hydrocarbons, carbon monoxide, nitrogen oxides, lead ...etc. have compelled scientists to find ways to reduce these emissions because of their impact on human health and ecological imbalance. These factors along with the oil crisis in the 1970s have led scientists and researchers to search for clean and environmentally friendly alternatives to the conventional fuels used to power I. C. Engines. Among the alternatives found to be superior to the present Gasoline are: Natural gas (Methane CH_4), Hydrogen (H_2), LPG. (i.e. Liquefied Petroleum Gas in the form of either Propane C_3H_8 , Butane C_4H_{10} or a mixture of both).

In the present paper Propane as a fuel has been considered. The advantages of propane over gasoline are many and are well known and documented in the literature [1, 2, 3], hence no need to mention them here.

However, the introduction of electronic injectors and availability of lead-free gasoline have eroded these advantages in efficiency and emissions previously enjoyed by propane fueled engines. Thus, future use of propane in the automobile field depends upon further improvements in utilization of propane in I. C. Engines.

This paper is an attempt to shed some light on the effect of combustion duration (which was varied by varying the equivalence ratio) on engine performance using analytical model. The analytical model developed was tested and verified against experimental data of several engines. It was used to study the effect of various operating parameters on the combustion duration as well as the effect of combustion duration on the engine performance and emission characteristics to try to get a better understanding of the interaction between these parameters.

2. BRIEF DESCRIPTION OF SIMULATION MODEL

The main program consists of two main stages: (1) The pipe calculations and (2) the cylinder calculations. The cylinder calculations are subdivided into two main stages: (1) power cycle and, (2) gas exchange process. The power cycle is further subdivided into three main stages: (1) compression, (2) ignition or combustion and (3) expansion or power stroke. Finally, the expansion stroke is subdivided into (1) expansion with two zones (burned and unburned) and (2) expansion of full products.

The power stroke simulation model is based on the model developed by Gupta *et.al*. [4], Raine *et.al*. [5] and Yamin *et.al.* [6] for a disk-type piston-cylinder design. The verification of this model has been done by simulating a Vaxhaul engine [see Appendix (B) for technical data]. The calculated and experimental results are shown in references [4 & 6].The model was modified with the inclusion of the gas exchange model which is described in details in [7] & [8], the turbulent combustion model described in [9,10] and the inclusion of the calculation of the friction parameters of various parts of the engine as given in [11]. Since describing the complete model would make this paper extremely lengthy and would bring it out of scope of the main topic, a brief description of the model is presented in appendix (A).

3. MODEL VERIFICATION

Though this model was verified for gasoline-fueled engines [8], there was however a need to verify it for the case of propane-fueled engines. This was the first part of this study. For this part certain thermodynamic properties and coefficients of internal energies of the reaction for propane fuel were introduced. In the second part, the experimental data of the performance of certain engines like Vaxhaul, and two different models of Ricardo Variable Compression Ratio engines (as available in the user manual) were compared with the calculated data. The results presented in Figures (1-a & 1-b) are for the Vaxhaul engine. These figures that the model can predict the performance of the engine by showing similar trends within certain acceptable accuracy.

4. RESULTS AND DISCUSSION

To start with, the fuel properties for propane are shown in Appendix (B). Before proceeding further with the results, let us have an idea about the methodology followed in this study. The study was carried out by first finding the Maximum Brake Torque (here and after referred to as MBT) angle for each engine speed and at WOT. This is done to eliminate the effect of ignition angle. Furthermore, since most of the cars today run with compression ratio (here and after referred to as CR) near CR=9, hence the compression ratio was chosen to be equal to 9. The combustion duration was then varied by varying the equivalence ratio of the mixture. This was chosen by the authors as it is known that the equivalence ratio has an influence on the duration covered by the combustion process.

Fist, the effect of some engine design parameters on combustion duration (in milliseconds) is studied. Second the effect of varying the combustion duration on engine performance and emission characteristics is studied. Discussion of the results is presented in three parts:

I Effect of operating conditions on the combustion duration.
II Effect of combustion duration on performance parameters.
III Effect of combustion duration on emission characteristics.

I. Effect of operating conditions on the combustion duration.

I.1 Effect Of Engine Speed on Combustion Duration.

Figure (2) shows that the combustion duration (in milliseconds) decreases as the engine speed (in rpm) increases. This is a clear effect of turbulence. As the engine speed increases, the turbulence inside the cylinder increases, leading to a better heat transfer between the burned and unburned zones.

I.2. Effect of Equivalence Ratio on the Combustion Duration.

Referring to Figure (2) it can be observed that operating at lean or rich mixtures the combustion duration tends to increase. This effect is more predominant at lower speeds. This is because of the less thermal energy liberated from the leaner mixture which increases the ignition delay and slows the flame propagation. The flame temperature is low at lean and rich mixtures. Further, the incomplete combustion due to oxygen deficiency at rich mixtures also has an adverse effect over the flame speed. From this figure it can also be seen that the combustion duration is minimum at equivalence ratios (here and after denoted by "Φ" and in the graphs referred to as "EQVR") close to 1.1 i.e. 10% rich for all engine speeds.

I.3 Effect of Compression Ratio on Combustion Duration.

Figure (3) shows that the combustion duration decreases as the compression ratio increases. This is because of the increase in the end-of-compression temperature and pressure and decrease in the fraction

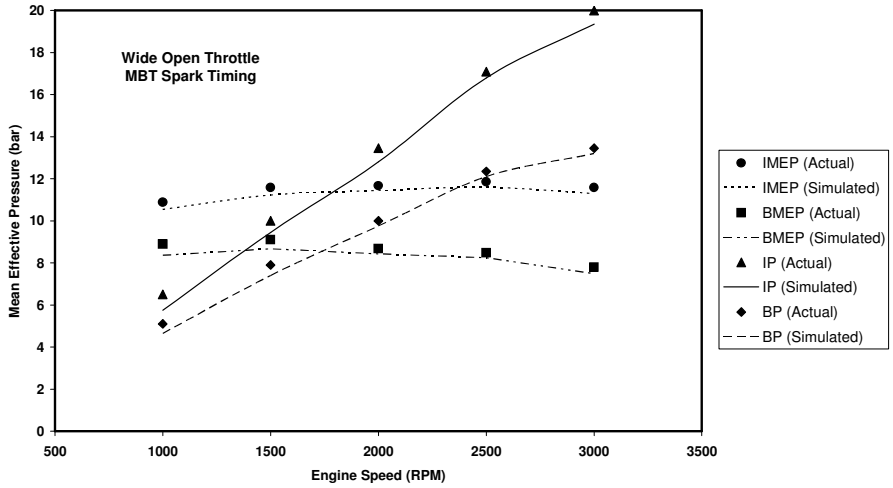

Figure 1-A. Performance Comparison between the experimental & theoretical results.

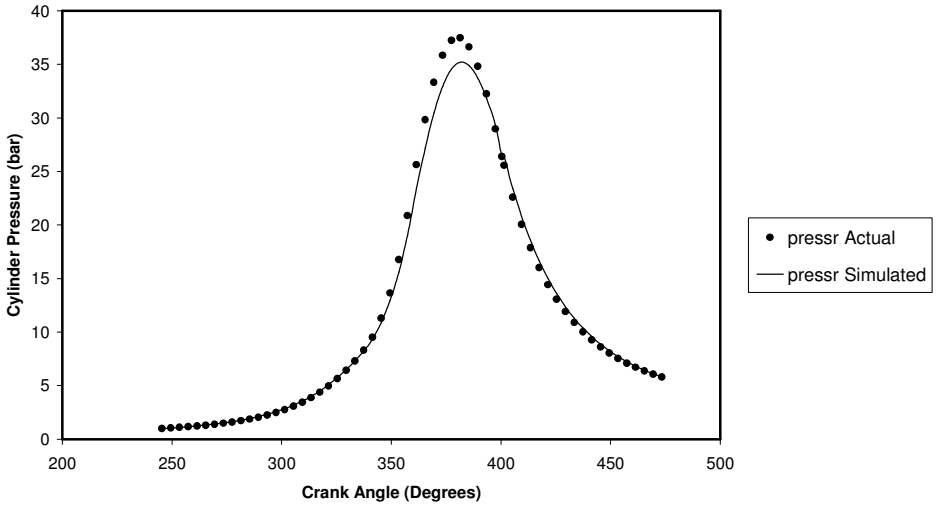

Figure 1-B. Pressure-Crank Angle comparison the experimental & theoretical results

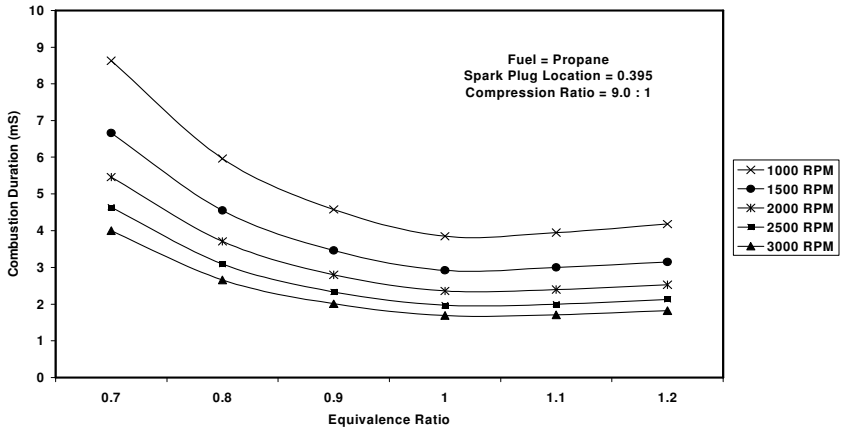

Figure 2. Variation of Combustion Duration with Equivalence Ratio at different engine speeds.

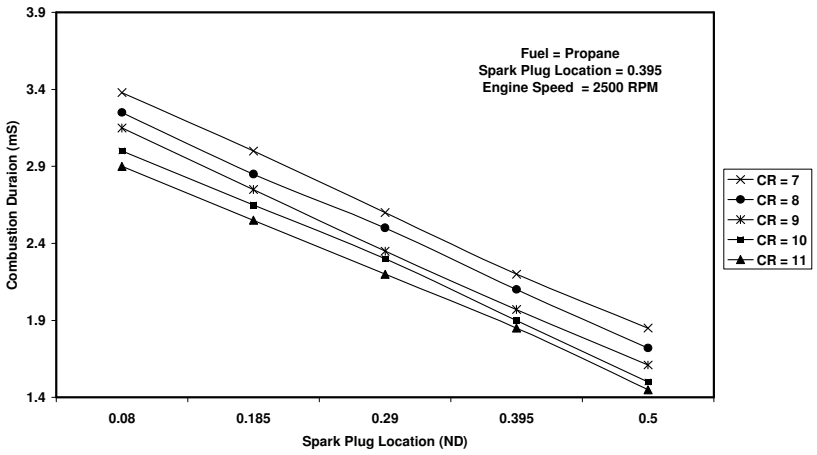

Figure 3. Variation of Combustion Duration with Spark Plug Location at different compression ratios

residual gases. This creates a favorable condition for the reduction of ignition lag and increase in the flame speed. In the present analysis compression ratio equal to 9.0 has been chosen for further analysis because most of the present day automobiles (S. I. Engines) have compression ratio near this range.

I.4. Effect of Spark Plug Location on Combustion Duration.

Before proceeding with the discussion it would be appropriate to define the term XSP used in the program. XSP is a non-dimensional parameter referring to the ratio of the distance between the spark plug location from the nearest wall to the cylinder diameter. Figure (3) shows the effect of compression ratio and spark plug location on the combustion duration. The graph has been plotted for $\Phi = 1.0$ and engine speed = 2500 rpm.

Referring to Figure (3) it can be seen that as the spark is shifted from the peripheral position (i.e. XSP = 0.08) to the center (i.e. XSP = 0.5), the combustion duration decreases. This is because of the decrease in the distance traveled by the flame. The spark location has greater effect on suppressing detonation. For selecting the best location for the present study an analysis on the effect of XSP on some engine performance and emission parameters was made.

Referring to Figures (4 a, b, c & d) it can be observed that there is no significant change in the power and economy parameters between XSP=0.395 and XSP=0.5. However, from the emissions point of view, location XSP = 0.29 is most favorable. Taking the possibility of detonation into account, location XSP = 0.395 has been selected for further analysis.

I.5. Effect of Spark Advance on Combustion Duration.

Figure (5) shows the effect of spark advance angle on combustion duration. It is observed that shortest combustion duration is obtained at maximum brake torque angle (here and after referred to as MBT). This spark timing is selected for further studies.

II. Effect of Combustion Duration on Engine's Performance Parameters.

After studying the effect of operating parameters on the combustion duration, the effect of combustion duration on engine performance has been examined. Before proceeding further, let us discuss some aspects of the combustion process.

Theoretically, the rate of combustion should be such that the combustion duration is minimum with high rate of pressure rise. Pressure should be maximum at TDC to produce greater force acting through a large period of the power stroke. This, however, means that the products will have enough time to lose some of its heat to the coolant resulting in poor performance in addition to the rough engine operation. Therefore, in practice, engines are so designed that only 50 % of the pressure rise is completed by the TDC resulting in peak pressure and temperature occurring at 10^o - 15^o after TDC which reduces the heat loss and makes the engine operation smooth. Therefore, for best results, the combustion has to be completed within 15^o after TDC.

Figures (6,7 & 8) show that an increase in the combustion duration causes the peak temperature (both burned and unburned) as well as the brake mean effective pressure to decrease. This is because

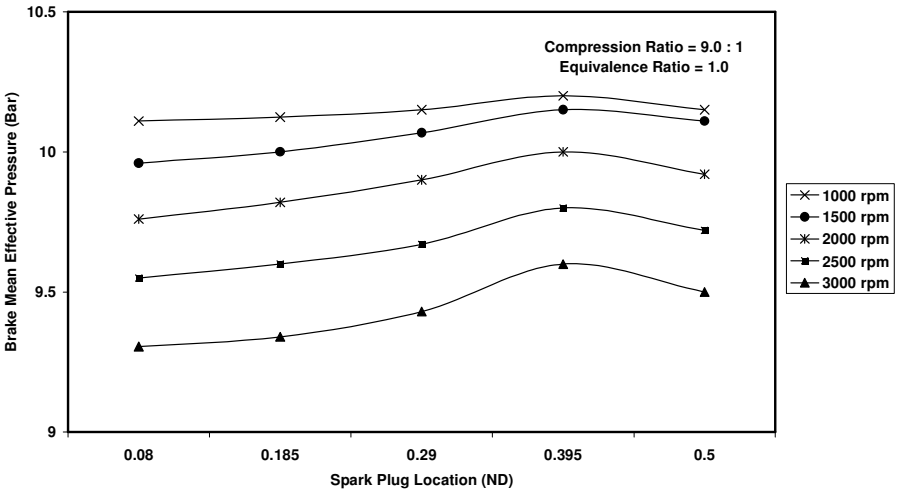

Figure 4-A. Variation of Brake Mean Effective Pressure with Spark Plug Location at different engine speeds.

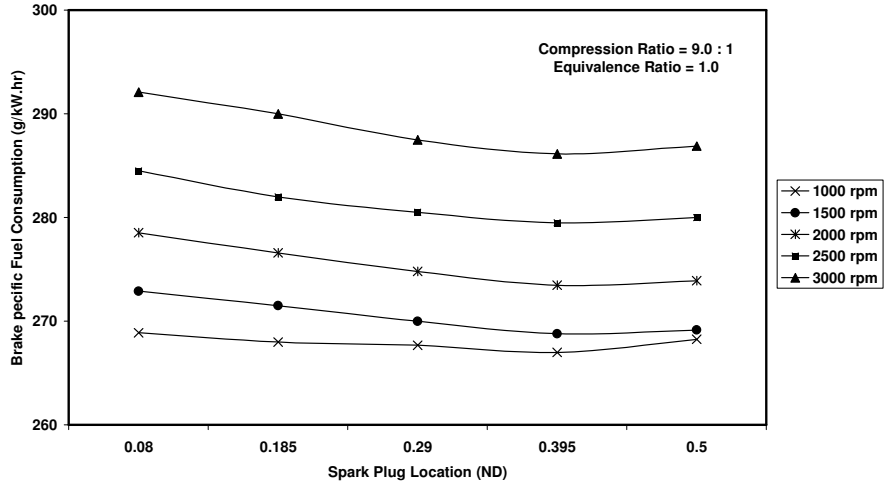

Figure 4-B. Variation of Brake Specific Fuel Consumption with Spark Plug Location at different engine speeds.

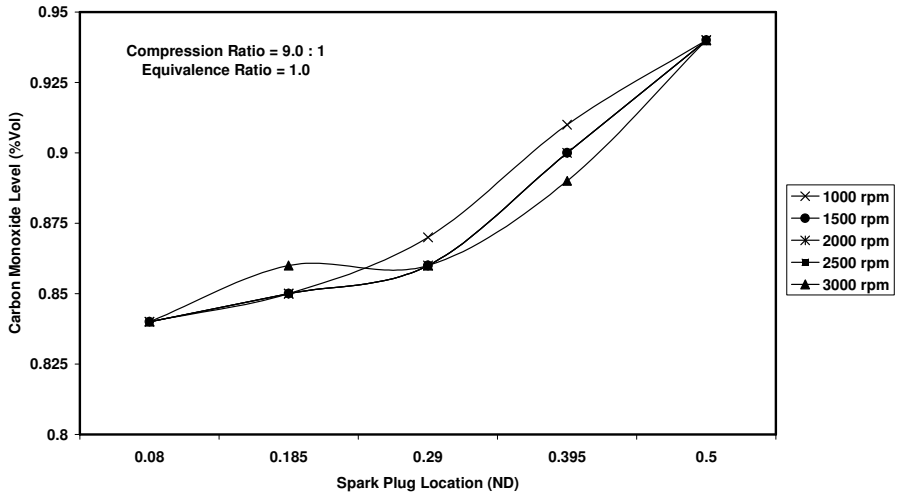

Figure 4-C. Variation of Carbon Monoxide Level with Spark Plug Location at different engine speeds.

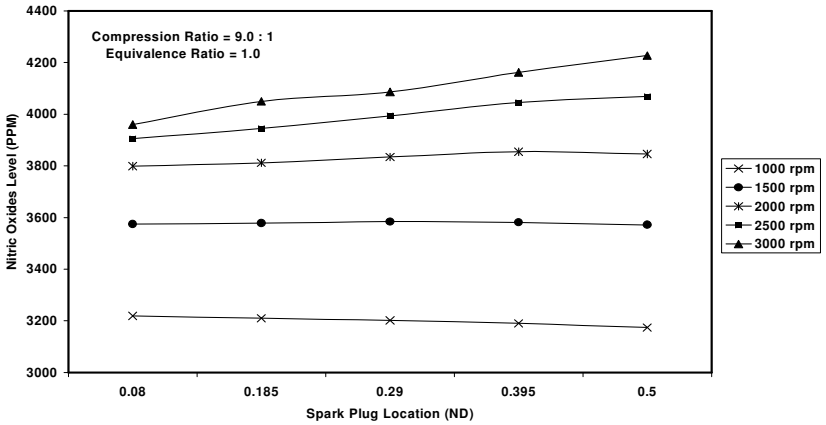

Figure 4-D. Variation of Nitric Oxide Level with Spark Plug Location at different engine speeds.

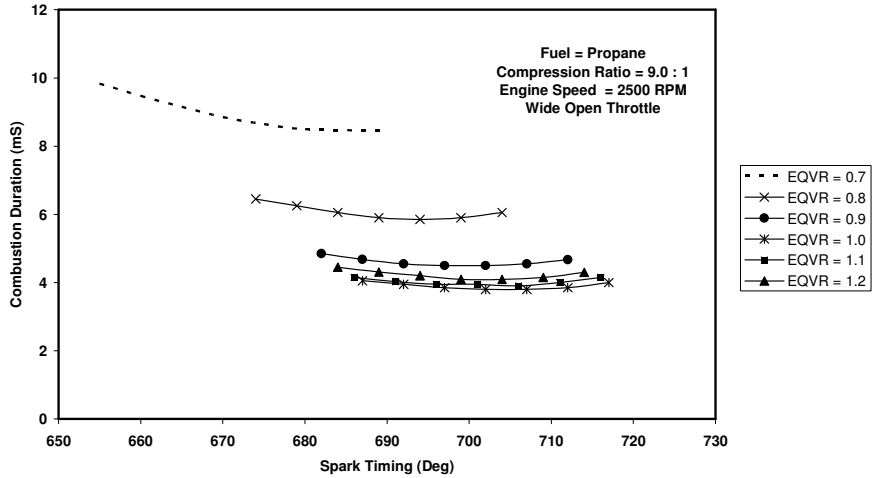

Figure 5. Variation of Combustion Duration with Spark Timing at different equivalence ratios.

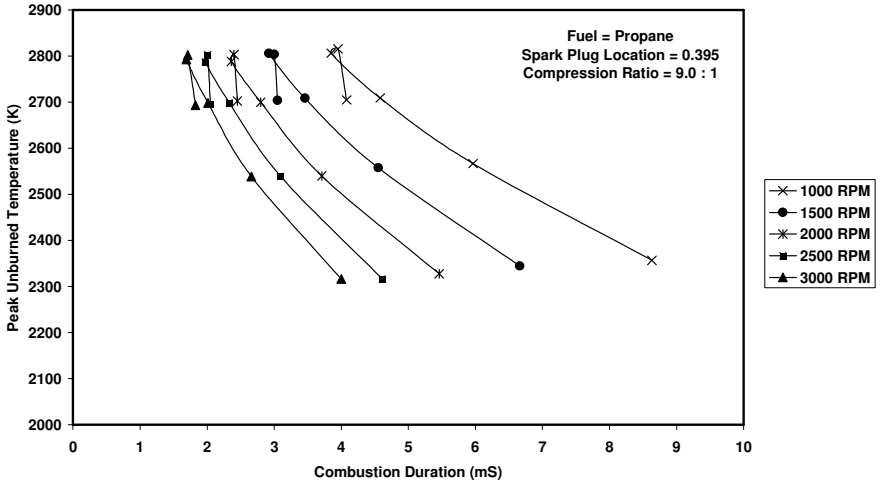

Figure 6. Variation of Peak Unburned Temperature with combustion duration at different engine speeds.

of the increased percentage heat loss, which is shown in Figure (9). On the other hand, because increasing the combustion duration increases the lean misfire limit, there is a decrease in the BSFC to certain limit as shown in Figure (10) and improvement of the thermal efficiency as shown in Figure (11). Therefore, it becomes clear that any attempt to increase the combustion duration either by reducing the compression ratio, locating the spark near the periphery or operate at leaner mixtures, though is going to improve the engine economy, but, is going to reduce the power output.

Further examination of the figures lead to a conclusion that for better performance in terms of power and economy, the combustion duration has to be between 4-6 milliseconds which mean that the engine should run on mixtures within stoichiometric.

III. Effect of Combustion Duration on Emission Characteristics.

From the emission point of view, it may be seen from Figures (12 & 13) that both CO and NO_X emissions are lower when the combustion duration is higher than that for best performance. This imlies that the conditions for minimum emissions are not the same as those for best performance. Further, though thye range of 4-6 milliseconds looks favorable for all engine speeds regarding CO it is not the case at lower speeds for NO emissions. Also noticed that CO & NO emissions are lower when the combustion duration is high, this is because it allows more time for the combustion to complete, hence the concentration of CO is reduced. Further, at higher combustion duration (Figures 6 & 7), the peak burned and unburned temperature is low and therefore the formation of NO is reduced. On the other hand, decreasing the combustion duration beyond certain limit, reduces the concentration of NO because of the less time of exposure of products of combustion to cylinder's peak temperature. If the mixture is made progressively rich, the combustion duration decreases. Due to rich mixture, formation of CO increases.

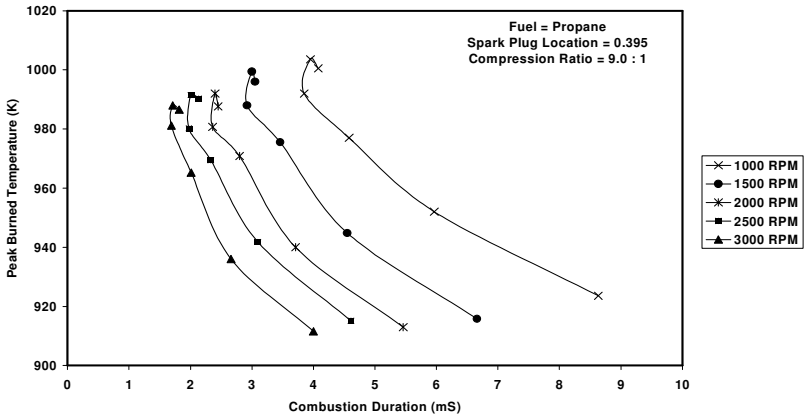

Figure 7. Variation of Peak Burned Temperature with combustion duration at different engine speeds.

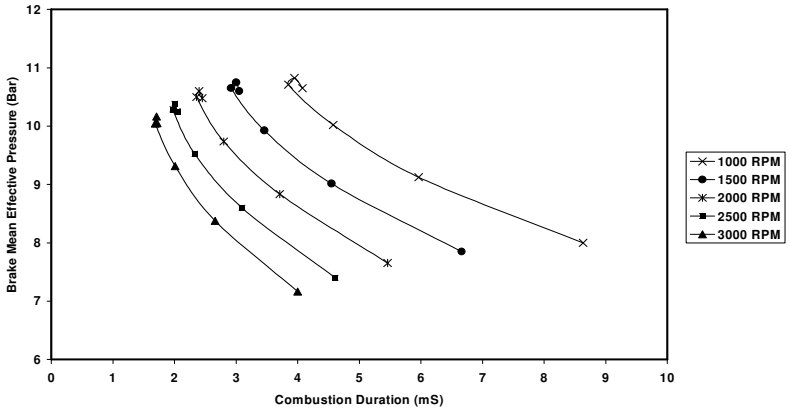

Figure 8. Variation of Brake Mean Effective Pressure with combustion duration at different engine speeds.

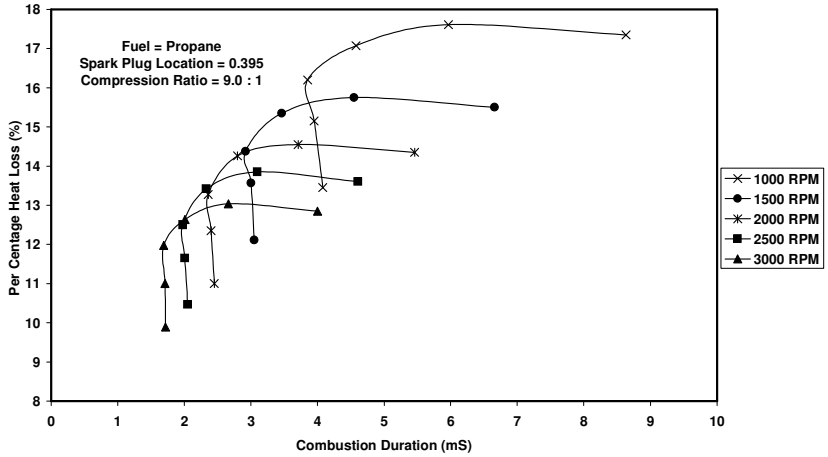

Figure 9. Variation of Per Cent Heat Loss with combustion duration at different engine speeds.

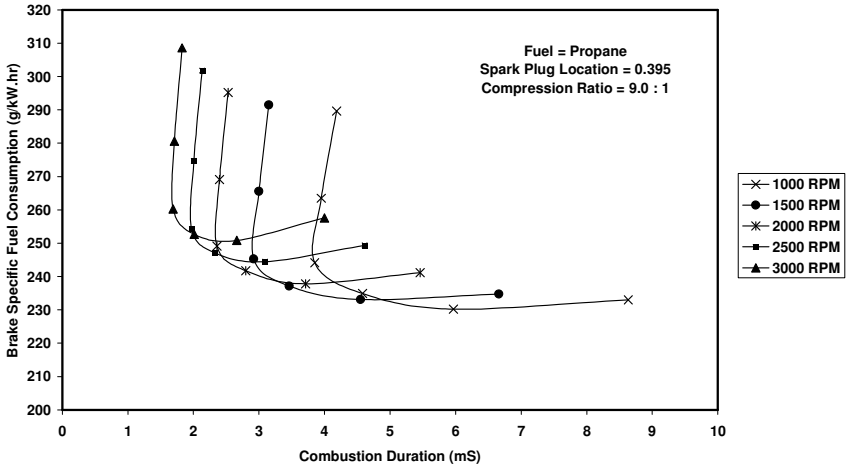

Figure 10. Variation of Brake Specific Fuel Consumption with combustion duration at different engine speeds.

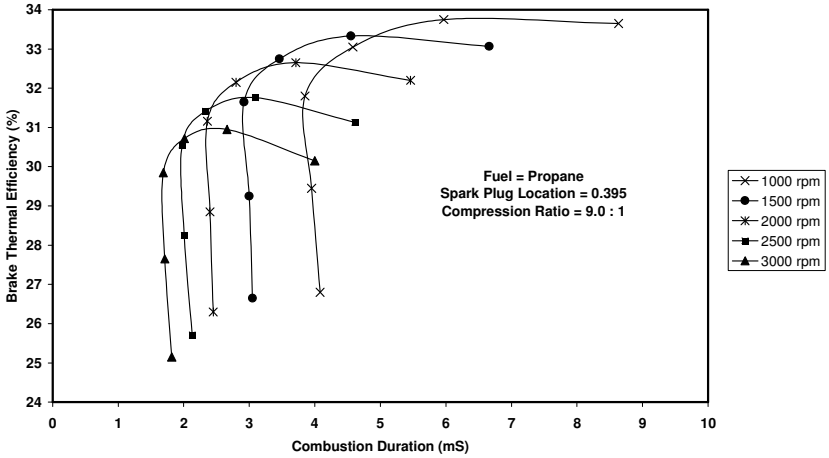

Figure 11. Variation of Brake Thermal Efficiency with combustion duration at different engine speeds.

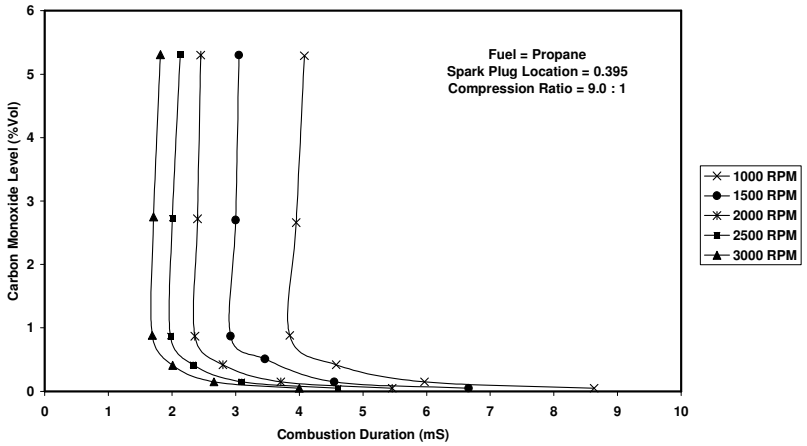

Figure 12. Variation of Carbon Monoxide Level with combustion duration at different engine speeds.

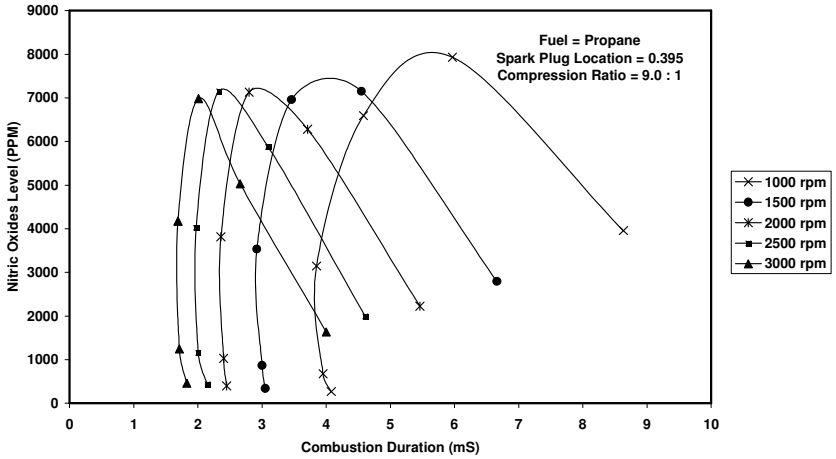

Figure 13. Variation of Nitric Oxide Level with combustion duration at different engine speeds.

5. CONCLUSION

1. Engines operating parameters have to be carefully chosen by the designer taking into account their effect on the combustion duration.
2. Any attempt to control the emissions by operating the engine at leaner mixtures have to take into account their effect on other variables like B.M.E.P. and B.S.F.C.
3. Combustion duration has a significant effect on both performance and emission characteristics of the engine and has to be carefully designed for to achieve the best engine performance characteristics.

6. NOMINATORS

a,b	: Annand's constants
A	: piston cross-sectional area
C_v	: specific heat at constant volume
D	: diameter (bore)
fi	: fraction of fresh mixture
m	: mass
p	: pressure
Q	: total heat flux
r	: compression ratio
r_f	: flame radius
R	: gas constant
R_e	: Reynolds number

T : gas temperature
u : specific internal energy
U_t : turbulent flame speed
U_{in} : mean inlet gas velocity
U_p : mean piston speed
V : volume
V_f : Volume occupied by flame front
W : work
WOT : wide open throttle
Φ : equivalence ratio
θ : crank angle
μ : dynamic viscosity
ρ : gas density
γ : specific heat ratio
η_{vol} : volumetric efficiency

Suffixes

1 : mixture at inlet conditions
2 : mixture after compression
b : burnt product
f : final
p : product
u : unburned
i : inlet
w : cylinder wall

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APPENDIX (A)

BRIEF DESCRIPTION OF THE MODEL.

Compression

The following assumptions have been made during the calculations of compression stroke: (1) The mixing between fresh charge and residual gases is perfect, (2) No chemical reaction occurs during

compression. The calculation procedure starts with the trapped mass of fuel, air and residuals. The pressures and temperatures in this stroke are then calculated using the first law of thermodynamics equations and the equation of state :

$$\frac{dp}{d\theta} = \left\{ \frac{R}{C_v}\left(\frac{dQ}{d\theta}\right) - p\frac{dV}{d\theta}\left(\frac{R}{C_v}+1\right)\right\}/V \qquad (1)$$

$$\frac{dT_u}{d\theta} = T_u\left(\frac{1}{V}.\frac{dV}{d\theta} + \frac{1}{p}.\frac{dp}{d\theta}\right) \qquad (2)$$

$$\frac{dW}{d\theta} = p\frac{dV}{d\theta} \qquad (3)$$

This continues till the nominal spark time, when combustion period is said to commence. The heat transfer rate from the gas to wall is calculated using Annand's [12] equation for convective heat transfer:

$$\frac{Q}{A} = \frac{a\,k_q}{D}(R_e)^b(T_u - T_w) \qquad (4)$$

where $$K_q = \frac{C_p\mu}{0.7}$$

"A" is the piston's cross-sectional area,

"K_q " is the thermal conductivity, and,

"C_p" is the specific heat at constant pressure.

The variables are continuously updated during calculation using the general formula:

$$x_{n+1} = x_n + \frac{dx}{d\theta}\Delta\theta \qquad (5)$$

where "x" is the variable. The numerical procedure used for this purpose is the Runge-Kutta Method.

Ignition

The calculations then proceed in three phases. Firstly, the initiation of the combustion, then the subdivision of the combustion chamber into two zones separated by spherical flame front and, finally a single zone encompassing the whole of the combustion chamber.

To initiate combustion a unit mass of the cylinder content is considered to burn at constant volume. The internal energy of the initial reactants are set equal to the internal energy of the products. The first guessed value is calculated using the Annand's equation [4] as below:

$$T_b = T_m + 2500^* \Phi * f_i \quad \text{for } \Phi \le 1.0 \qquad (6)$$

$$T_b = T_m + 2500^* \Phi * f_i - 700 * (\Phi - 1.0)^* f_i \quad \text{for } \Phi > 1.0 \qquad (7)$$

$$T_b = T_b - \delta T_b \qquad (8)$$

where, $\delta T_b = (e_p - e_m) / C_{vb}$, "e_b" and "e_m" are specific internal energies for the burnt and unburnt mixture respectively.

Now, balancing the internal energies for burned products at the guessed temperature with that of the unburned mixture at current unburned temperature using iterative techniques until $\delta T_p < 5\ ^oK$.

Initiation of Two-Zone Calculation

The calculation and geometrical representation of the enflamed volume is given in details by Baruah [13]. From the burnt and unburnt mixture properties the turbulent flame speed is then calculated using Keck's equation [9] :

$$U_t = BU_{in}\left(\frac{\rho_u}{\rho_b}\right)^C \qquad (9)$$

where "B" and "C" are constants depending on engine design conditions, " U_{in}" is the inlet gas speed and is given by :

$$U_{in} = \eta_{vol}\, U_P\left(\frac{A_P}{A_{IV}}\right) \qquad (10)$$

where "A_{IV}" is the maximum opening area of the inlet vale, "A_P" is the piston's cross-sectional area, and "U_P" is the mean piston speed.

The radius of the burnt zone "R_b" centered on the spark point is given by:

$$R_b = \left(\frac{U_t\,\Delta\theta}{360\,N}\right) \qquad (11)$$

where; "N" is the engine speed in RPS, "$\Delta\theta$'' is the cank angle step in degrees.

The corresponding volume of the burnt mixture "V_b" is given by:

$$V_b = \frac{2}{3}\pi R_b^3 \qquad (12)$$

In order to initiate the two zones, a finite product volume $V_b = (10^{-3}$ cylinder volume) is assumed. If "V_b" is less than this value, combustion is said not to have been initiated. Hence the delay period is given by:

$$(\Delta\theta)_{Delay} = \left(\frac{360N}{U_t}\right)\left(\frac{0.0015V_C}{\pi}\right)^{\frac{1}{3}} \qquad (13)$$

where "V_C" is the cylinder volume.

If the total time step Δ from the nominal ignition of the spark is less than the delay period $(\Delta\theta)_{Delay}$ the compression stroke is continued. Once Δθ is measured from the nominal spark time is greater than $(\Delta\theta)_{Delay}$ we enter the second phase when the cylinder is divided into two zones separated by a spherical flame front centered on the spark plug.

Now, to initiate the two-zone calculations, the temperature in the burnt and unburnt zones must be adjusted to ensure uniform pressure distribution in the cylinder. The subscripts "u" and "b" represent the initial values and subscripts "uf" and "bf" represent the final values for the unburnt and burnt zone pressures and temperatures respectively. The procedure followed is as follows : a unit mass of the cylinder content is considered. The temperature "T_b" is calculated from the first law, allowing for heat losses and dissociation from the initial pressure and temperature of the unburnt mixture "P_u & T_u". This will give a second pressure "P_b" for the burnt gases from the expression :

$$P_b = \left(\frac{M_b}{M_u}\right)\left(\frac{T_b}{T_u}\right)P_u \qquad (14)$$

Where "M_b" and "M_u" are the number of moles per unit mass for the products and initial reactants, respectively. From the volume of the initial nucleus of the burnt zone "V_b" the burnt mass "m_b" can be calculated from "P_b & T_b". From the total mass in the cylinder "m_c" the unburnt mass "m_u" can be calculated by subtracting the burnt mass from the total cylinder mass ($m_u = m_c - m_b$), and hence the internal energies of the cylinder contents obtained, thus,

$$E = m_b e_b + m_u e_u \qquad (15)$$

The complete procedure and analysis is given in reference [14].

Expansion

The expansion process has also been considered in sets of two domains:

(1) Two Zone, and (2) Full product.

Two zones expansion :

The major assumptions for this model are :

(I) The original charge is homogeneous.

(II) At any time, the pressure is uniform throughout the cylinder.

(III) Volume occupied by non-equilibrium chemical reaction zone is negligibly small.

(IV) Burned gas is at full thermodynamic equilibrium.

(V) Burned gas is frozen at its original composition, and,

(VI) There is no heat transfer between burned and unburned zones.

Full product :

Once the combustion process is completed, the variables are organized to calculate for single zone only. The Runge-Kutta method is used, while the heat transfer coefficient is calculated using Annand's equation [12].

Species Formation

It is assumed that only 12 species are present in the combustion products both inside the cylinder as well as the exhaust. These are: H_2O, H_2, OH, H, N_2, NO, CO_2, CO, O_2, O and A. The governing equations for the mechanism of NO formation are (based on Lavoie et.al. [15]):

(1) $N + NO \Leftrightarrow N_2 + O$ $K_{f1} = 3.1*10^{10} * E^{(-160/T)}$ m^3/kmols

(2) $N + O_2 \Leftrightarrow NO + O$ $K_{f2} = 6.4*10^6 * T * E^{(-3125/T)}$ m^3/kmols

(3) $N + OH \Leftrightarrow NO + H$ $K_{f3} = 4.2*10^{10}$ m^3/kmols

(4) $H + N_2O \Leftrightarrow N_2 + OH$ $K_{f4} = 3.0*10^{10} * E^{(-350/T)}$ m^3/kmols (17)

(5) $O + N_2O \Leftrightarrow N_2 + O_2$ $K_{f5} = 3.2*10^{12} * E^{(-18900/T)}$ m^3/kmols

(6) $O + N_2O \Leftrightarrow NO + NO$ $K_{f6} = K_{f5}$

(7) $N_2O + M \Leftrightarrow N_2 + O + M$ $K_{f7} = 10^{12} * E^{(-30500/T)}$ m^3/kmols

In these equations the rate constants (K_{fi}) are all in m^3/kmols. M is a third body which may be involved in the reactions, but is assumed to be unchanged by the reactions. M can be assumed to be N_2. These equations can be applied to the zone containing "burned" products, which exists after the passage of the flame through the unburned mixture. It will be assumed that H and OH, and O and O_2 are in equilibrium with each other; these values can be calculated by the methods described in [15].

The rate of formation of the NO can be derived in the following manner. Consider reaction "j"; let K_{fj} be the forward reaction rate, K_{bj} be the backward rate, and R_j the 'one way' equilibrium rate. Also let

$$\frac{[NO]}{[NO]_e} = \alpha \qquad \frac{[N]}{[N]_e} = \beta \qquad \frac{[N_2O]}{[N_2O]_e} = \gamma$$

where suffix 'e' denotes equilibrium values. Then the following expressions are obtained for the burned gas, or product, volume.

Referring to equations (17) the net rate for NO can be derived as follows:

K_{f1} [N] [NO] + K_{b1} [N_2] [O] = - α β K_{f1} [N]$_e$ [NO]$_e$ + K_{b1} [N_2]$_e$ [O]$_e$ (18)

But,

K_{f1} [N]$_e$ [NO]$_e$ = K_{b1} [N_2]$_e$ [O]$_e$ = R_1

So the net rate from the first equation of the set equations (17) becomes - α β R_1 + R_1.

Using similar procedure for the rest of equations of (17) involving NO gives the following expression, which also allows for the change in volume over the time step 't' :

$$\frac{1}{V}\frac{d}{dt}([NO]V) = -\alpha(\beta R_1 + R_2 + R_3 + 2\alpha R_6) + R_1 + \beta(R_2 + R_3) + 2\gamma R_6 \quad (19)$$

where 'V' is the volume of the products zone.

Repeating the same procedure as above to find the net rate for 'N' from all equations of (17) involving N we get the following expression, which also allows for the change in volume over the time step 't':

$$\left.\begin{aligned}\frac{1}{V}\frac{d}{dt}([N]V) &= -\beta(\varepsilon R_1 + R_2 + R_3) \\ &\quad + R_1 + \alpha(R_2 + R_3)\end{aligned}\right\} \quad (20)$$

And similarly for N_2O :

$$\left.\begin{aligned}\frac{1}{V}\frac{d}{dt}([N_2O]V) &= -\gamma(R_4 + R_5 + R_6 + R_7) \\ &\quad + R_4 + R_5 + \alpha^2 R_6 + R_7\end{aligned}\right\} \quad (21)$$

A finite time is required for the reactions to reach their equilibrium values; this is called the Relaxation Time. Lavoie [15] found that the relaxation times for the formation of atomic Nitrogen and Nitrous Oxide are several orders of magnitude shorter than those of NO, and hence it can be assumed that the [N] and [N_2O] values are at steady state, which means that the right-hand sides of the equations (20) and (21) are zero. Then from equations (20) and (21):

$$\beta = \frac{R_1 + \alpha(R_2 + R_3)}{(\alpha R_1 + R_2 + R_3)}$$

$$\gamma = \frac{R_4 + R_5 + \alpha^2 R_6 + R_7}{(R_4 + R_5 + R_6 + R_7)}$$

These values can be substituted into equation (19) to give the rate of formation of (NO) as:

$$\frac{1}{V}.\frac{d}{dt}[[NO].V] = 2.(1-\alpha^2)\left[\frac{R_1}{1+\alpha\frac{R_1}{R_2+R_3}} + \frac{R_6}{1+\frac{R_6}{R_4+R_5+R_7}}\right] \quad (22)$$

The detailed method is given in reference [16].

CO Formation:

The formation of CO inside the cylinder is assumed to be at equilibrium condition up to the peak value. After that, the concentration of CO is assumed to lie between the peak equilibrium and the current equilibrium. This is because, at lower temperature during the expansion process, the actual chemical reaction rates for the formation of CO lag behind the equilibrium value leading to a higher value than obtained at equilibrium.

Since the actual value of CO lies between the peak and exhaust equilibrium values, a multiplication factor called "COFAC" is introduced to obtain a more realistic value at exhaust. The following relation is used to calculate the concentration of CO:

$$X_{co} = X_{co_{eq}} + COFAC.(X_{co_{max}} - X_{co_{eq}}) \quad (23)$$

where,

X_{co} = Corrected concentration of CO

$X_{co_{eq}}$ = Concentration of CO at equilibrium

$X_{co_{max}}$ = Maximum value of CO concentration at equilibrium condition

COFAC = Scale factor for CO formation.

The value of COFAC is adjusted with experimental results. This simplified model for calculating the CO concentration is used to obtain a reasonably correct value for CO because the other models developed by Annand [16] and Daneshyar et al. [17] not only deviate considerably with experimental results, but also consumes considerable amount of time for computation. Therefore, these are not used in the present work.

APPENDIX (B)

DATA USED FOR COMPUTATION

(A) ENGINE DATA FOR VAXHAUL 4-CYLINDER ENGINE:

Cycle	: 4-Stroke
Cylinder Bore	: 95.25 mm
Stroke Length	: 69.24 mm
Connecting Rod Length	: 136.50 mm
Cylinder Volume	: 1975 cc
Compression Ratio	: 8.5:1
Angle of Ignition	: 9^o BTDC at Idling
Spark Plug Location cylinder edge	: 33.5 mm from the nearest
Mean Inlet Valve Diameter	: 42.0 mm
Mean Exit Valve Diameter	: 38.0 mm
Valve Timing	:
EVO	: 114.57^o ATDC
EVC	: 393.43^o ATDC
IVO	: 326.57^o ATDC
IVC	: 605.43^o ATDC

(B) FUEL DATA:

	PETROL	PROPANE
Fuel Specification:	C_7H_{13}	C_3H_8
Internal Energy Coefficients for Polynomial Expression as in [4]:		
U_2	-1.0715E04	5.70E02
U_3	2.8955E02	4.03E01
U_4	-0.80E-01	-0.006E01
U_5	1.665E-05	0.00E00
Viscosity Coefficient (Kg/m.s):	2.0E-07	0.2E-06
Calorific Value (kJ/Kg):	42000	46300
Annand's Constants:		
a	0.40	
b	0.70	
c	0.4284E-011	(kW/m^2K^4)