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Theoretical and Experimental Studies on the Combustion of Synthetic Fuels in Spark Ignition Engines.

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THEORETICAL AND EXPERIMENTAL STUDIES ON THE COMBUSTION OF SYNTHETIC
FUELS IN SPARK IGNITION ENGINES.

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ABSTRACT

A theoretical and experimental investigation on the performance
and emission of spark ignition engine have been made using gasoline,
alcohol and gasoline-alcohol mixture as fuels. A thermodynamic model
has been developed with superimposed pseudo-kinetic NO and CO forma-
tion. This has been used to compute estimated performance and emis-
sion data for a spark ignition engine. The model has also been used
to compare the prediction performance and emission data when operat-
ing the engine with methanol, ethanol and gasoline fuels.

A series of an experimental tests were carried out on a single
cylinder spark ignition engine to confirm the theoretical results of
the mathematical model. Comparison of results indicates that alcohol
seems to be a viable alternative fuel to gasoline with respect to
efficient, operational and emission considerations.

INTRODUCTION

The incentives for studying the combustion of alternative fuels
in engines are, some fuel or fuel additive may solve the problem of
emissions, knock, derivability and efficiency. Also an alternative
fuel may help conserve the world's petroleum supplies as well as be-
ing available when those supplies are exhausted. Transportations is
unique among the energy consuming sectors of the economy of industr-
ialized nations, because it is totally dependent on one source of
fuel crude oil. It has therefore imparative to investigate the cons-
equences of using non-petroleum fuels for transportation application.

Alcohol has been proposed as a clean-burning synthetic fuel,
that could have many applications, and its advantages have been wid-
ely acclaimed [1,2]. It can be obtained either from the distillation
of wood products or, more efficiently, by combining hydrogen and
carbon monoxide which are available from coal gasification processes.
Alcohol has a research octane number of 106 [3] compared to 90:100
normal gasoline, and a blending octane value of 130. Thus a 20% mix-
ture of methanol with 90 octane gasoline gives a blend fuel with an
octane number of 98. It could therfore be used as an effective sub-
stitute for tetraethyl lead as an anti-knock agent.

Information in the lirerature is plentiful for automotive use
of methanol: however, few systematic studies exist on combusrion and
emission properties of an engine fueled with the highe alcohols and
alcohols-gasoline blends [4,5]. The objective of this study is to
obtain more quantitatlve information on the combustion and emission

properties of sprak ignition engines using gasoline, methanol, etha-
nol, methanol-gasoline blends and ethanol-gasoline blends fuels.

THEORETICAL ANALYSIS

The availability of a mathematical model would obviously be most
helpful in the further development of the spark ignition engine. A
simple equilibrium cycle model with superimposed "Pseudo Kinetic" NO
and CO formation has been developed. This model is used to compare
likely engine performance with gasoline, metanol and ethanol fuell-
ing. The cycle synthesis is concerned with the progressive step by
step calculations of the physical and thermodynamic states of the
charge in the combustion chamber at succeeding points around the re-
levant parts of the engine cycle.

The compression and expansion processes are considered isentro-
pic , and the combustion process is assumed to occur instantaneou-
sly at constant vulum at TDC. The working fluid is assumed to be a
homogeneous fuel-air mixture in chemical equilibrium at the appropria-
te temperature and pressure at each point in the cycle. An elementa-
ry treatment of the exhaust and induction processes is included and
provision for a degree of exhaust gas residual is incorporated. The
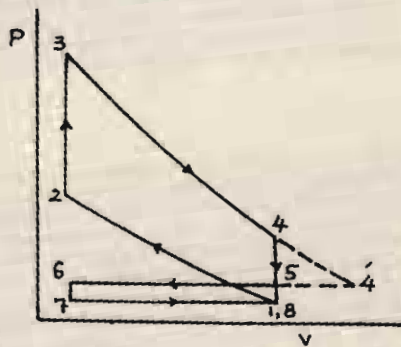assumed thermodynamic cycle is illustrated in Fig. 1.
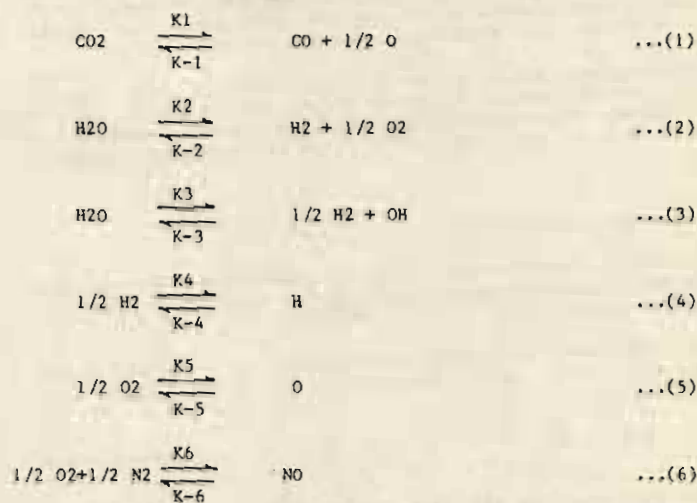

Fig.1 The assumed thermodynamic cycle.

1. Thermodynamic Cycle Analysis

During the compression process,the fuel-air mixture is compres-
sed adiabatically from "1" to "2". Initially the working fluid prior
to compression is assumed to consist only of fuel vapour + air at at-
mospheric pressure and a temperature of 298 K. At the end of one co-
mplete cycle, recycled residual gas is included and the cycle compu-
tation is repeated. The cycle is completed at point "1" which is cor-
responding to point "8". The process is considered in an incremental
manner, a 10 degree crankangle increment being adopted. The working
fluid composition is considered to be constant during the compress-
ion process . The thermodynamic properties (enthalpy, entropy ,
and constant pressure specific heat) were evaluated from sixth
order polynomial equations [5] . The value of specific heat
ratio is assumed constant during each crank angle incremerr and is

updated at the end of each increment to allow for the change in mixture pressure and temperature. During each increment in compression, an isentropic change of state due to piston motion is assumed. At this stage in the development of the model the working fluid during the compression process is assumed to be completely vaporized . This assumption can be improved later by assuming some of the fuel to be in the liquid state.

The compressed mixture at temperature T2 and pressure P2 is assumed to burn adiabatically at constant volume. In this analysis, the products of combustion are assumed in chemical equilibrium and comprises , CO, CO2, O2, H2, H2O, OH, H, O, NO and N2.

To determine the number of moles of products of combustion , dissociation reactions are considered.   In the present study there are six such independent reactions, those used are:

$$CO_2 \xrightleftharpoons[K-1]{K1} CO + 1/2\ O \qquad\qquad ...(1)$$

$$H_2O \xrightleftharpoons[K-2]{K2} H_2 + 1/2\ O_2 \qquad\qquad ...(2)$$

$$H_2O \xrightleftharpoons[K-3]{K3} 1/2\ H_2 + OH \qquad\qquad ...(3)$$

$$1/2\ H_2 \xrightleftharpoons[K-4]{K4} H \qquad\qquad ...(4)$$

$$1/2\ O_2 \xrightleftharpoons[K-5]{K5} O \qquad\qquad ...(5)$$

$$1/2\ O_2 + 1/2\ N_2 \xrightleftharpoons[K-6]{K6} NO \qquad\qquad ...(6)$$

The expansion of the products of combustion from point "3" to point "4" (Fig.1), is again treated in an incremental manner. A single expansion increment comprises two steps, these are :

i)   An isentropic change of state due to piston motion during the increment .

ii)   Calculation of the revised equilibrium composition at the new pressure and temperature at the end of the increment.

The exhaust process is represented from "4" to "6" in Fig. 1. The process is treated in two stages. The first stage corresponds to the period from "4" to "5", which represents the event where the exhaust value opens and the products of combustion expelled into the atmosphere. The process is irreversible and is accompanied by an increase

in entropy. However, the condition at point "5" can be found by all-
owing the burned gas remaining in the cylinder to expand isentropi-
cally, and do work in pushing out the expelled portion. The tempera-
ture, pressure and entropy at point "5"then correspond to the condi-
tion at point "4'". The process $4 \rightarrow 5$ is computationally treated in
two steps. In the first of these steps, the gases remaining in the
cylinder at the end of expansion are allowed to expand isentropic-
ally tn an intermediate pressure P_x, where $P_x = \sqrt{P4}$. Then in the
second step the gases expand from P_x down to the exhaust pressure,
P5 = 1 atm. The second stage of the exhaust process corresponds to
step $5 \rightarrow 6$ in Fig.1. During this period, it is assumed that the pis-
ton is returned to TDC, with expulsion of most of the residual gas
remaining in the cylinder at BDC.

The induction process corresponds to the period $7 \rightarrow 8$ in Fig.1.At
the current stage in the model's development equal exhaust and indu-
ction pressure have been assumed. At point"7"the intake valve opens
and fresh completely vaporized charge is inducted and mixed with the
residual gases remaining in the cylinder from the previous cycle.The
pressure is considered to remain constant throughout this process
and it is assumed that no chemical reaction occurs.

The complete camputation cycle outlined above is then repeated
using the values obtained for point "8" as the new initial point in
the cycle. The whole procedure is repeated until correspondence bet-
ween conditions at point "1" and point "8" is obtaied in successive
cycles.

2. Performance Calculations

Computation have been performed for three fuels (C8H18 , CH3OH
and C2H5OH), for a compression ratios in the range 6 to 16 and for
equivalence ratios in the range 0.6 to 1.6.

Applying the first low of thermodynamic, for a closed system,
the net work done of the cycle is obtained by the following relation
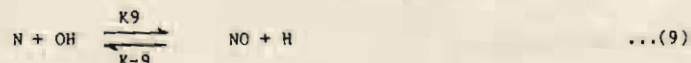
$$W_{net} = \frac{RO}{PO} (\overline{U}_3 - \overline{U}_4) - (U_2 - U_1) \qquad \text{J/mole. charge}$$

The indicated mean effective pressure is determined by dividing
the net work done by the displacement volume . The indicated ther-
mal efficiency is the ratio of the net work done to the energy cont-
ent of the fuel supplied.

3. Emission Calculation

The kinetic mechanism proposed for NO calculation is the extended
Zeldovish mechanism, which is comprised of the following reactions :

$$N2 + O \underset{K-7}{\overset{K7}{\rightleftharpoons}} NO + N \qquad \qquad ...(7)$$

$$O2 + N \underset{K-8}{\overset{K8}{\rightleftharpoons}} NO + O \qquad\qquad\qquad ...(8)$$

$$N + OH \underset{K-9}{\overset{K9}{\rightleftharpoons}} NO + H \qquad\qquad\qquad ...(9)$$

The differential equation governing the formation of NO is;

$$\frac{d(NO)}{dt} = K7(O)(N2) - K-7(NO)(N) + K8(O2)(N) - K-8(NO)(O)$$
$$+ K9(N)(OH) - K-9(NO)(H). \qquad\qquad ...(10)$$

Taking the temperature, pressure and equllibrium values of O, N2,O2, OH and H at the end of each crankangle increment during the expansion process, kinetic NO formation is computed using Euler integration method for eq. (10). The initisl value for NO concentration at TDC is assumed to be zero. In the present study, it is assumed that at TDC all carbon content of the fuel is instantaneously converted to CO which is subsequently oxidized to CO2 during the expansion process via the following reaction:

$$CO + OH \underset{K-10}{\overset{K10}{\rightleftharpoons}} CO2 + H \qquad\qquad\qquad ...(11)$$

Thus the rate equation for CO is simply aa follows:

$$\frac{d(CO)}{dt} = - K10(CO)(OH) + K-10(H)(CO2) \qquad\qquad ...(12)$$

The CO level through the expansion stroke is computed from eq. (12) and by involving the carbon conservation equation:

$$(CO) + (CO2) = (CO2) + (CO) \qquad\qquad\qquad ...(13)$$

EXPERIMENTAL STUDY

The engine utilized in this work was a single cylinder air cooled standard spark igntion engine. It was equipped with standard throttled carburetor and thermocouple to monitor the exhaust temperature. A needle valve was used to precisely control the fuel rate. Since the engine was operated at wide open throttle and differenr throttle positions in these tests, adjustment of this valve wss the means for obtaining different air fuel ratins. Spark adavance was adjusted in all tests for maximum power, while compression ratio was kept constant at 6.5:1.

Air flow rate to the engine was determined with the aid of an air box , calibrated orifice and manomter. The power ourput of the engine was absorbed by a dc dynamometer unit coupled directly to the engine shaft. This dynamometer is also used in motoring tests to determine the friction horsepower. Measurements of the engine speed was performed with a speed indicator.

The fuels used in experiments were gasoline, methanol, ethanol, a 10 % methanol-90 % gosoline and a 10 % ethanol-90 % gasoline. To avoid problems of cold starting with alcohol fuels , a dual fuel system is used. The engine was started on gasoline and then switched over to the alcohol fuels when warmed up.

RESULTS AND DISCUSSIONS

Computation have been performed for three fuels (C8H18, C2H5OH and CH3OH) for different compression ratios and different equivalence ratios. Shown in Figs.2 through 7 some of the more important computed results of the performance and emission levels.

Figure 2 shows the effects of fuel type and equivalence ratio on theoretical peak cycle temperature and pressure. The cycle peak pressures and temperatures vary with equivalence ratio. Because of the dissociation and the influence of different specific heats of CO and CO2, the maximum peak pressure and temperature occurs with rich
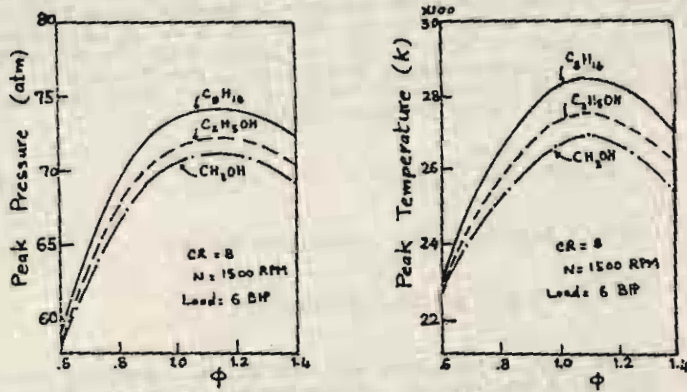

Fig.2 Effect of fuel type and equivalence ratio on calculated peak pressure and peak temperature.
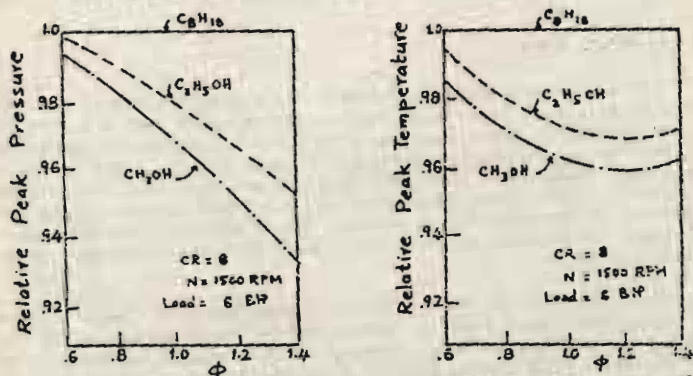

Fig.3 Effect of fuel type and equivalence ratio on calculated relative peak pressure and peak temperature.
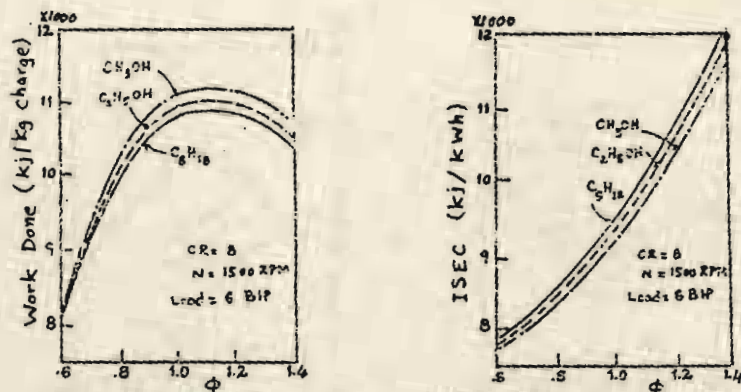
Fig.4   Effect of fuel type and equivalence ratio on calculated work
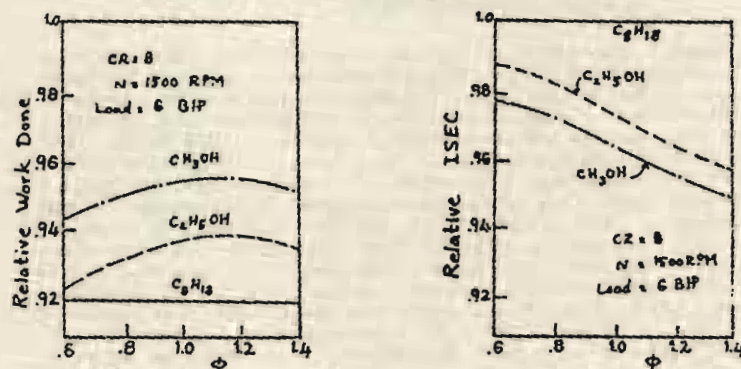   done and specific energy consumption.

Fig.5   Effect of fuel type and equivalence ratio on calculated rela-
        tive work done and specific energy consumption.

mixtures. The diagram also show that the fuel composition can influ-
ence the calculated peak pressure and peak temperature   Alcohols has
a lower proportion of carbon in the fuel molecule than isooctane.
This leads to a lower peak pressure and peak temperature for alcoho-
ls fuel than isooctane.   More ready comparison of the results shown
in Fig.3 can be made if normlized with isooctane as the datum.

    Shown in Fig.4 are the effects of fuel type and equivalence ratio
on calculated net output per unit mass of chage and indicated speci-
fic energy consumption such a quantity is importance when comparing,
since the cost of producing fuel is generally reported as cost per
energy unit. For these reasons we define the indicated specific ene-
rgy consumption as the rate of energy consumed divided by the indi-
cated power. As a less dissociation occurs with alcohol, resulting
in a lower ratio of moles product-moles reactant,there is a slightly
higher net output per unit mass of charge and alightly lower idica-
ted specific energy consumption for alcohol fuels than isooctane.
This results can be easly ahown in Fig.5, when the results are norm-
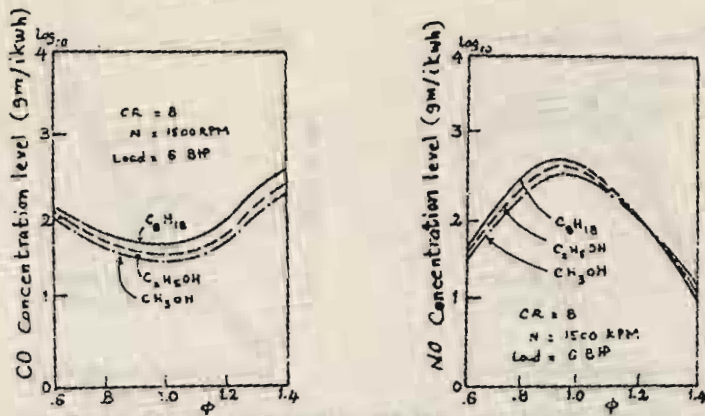alized with the results obtained for isooctane as a datum.

Fig.6 Calculated CO and NO emission levels for gasoline, methanol and ethanol fuels.

Figure 6 illustrates the influences of fuel type and equivalence ratio on calculated kinetic NO and CO mass emission levels (gm/ikwh) In order to include the range of equivalence ratios to be considered the NO and CO mass emission levels have been plotted on a log scale. These diagrams show that the peak NO levels occur just to the lean side of stoichiometric because of the greater oxygen concentration and the associated high temperature. For lean mixture, the rate of NO formation falls due to the attendant drop in the adiabatic flame temperature. For a rich mixture, the rate decreases due to oxygen defficiency and falling adiabatic flame temperature. One other observation is that the nitric oxide concentration is mainly dependent on the equivalence ratio(ϕ). The effect of fuel type is less important. However, alcohols produces slightly less nitric oxide than isooctane with both lean and slightly above stoichiometric. This is because of the lower adiabatic flame temperature for alcohols as shown in Fig. 2.
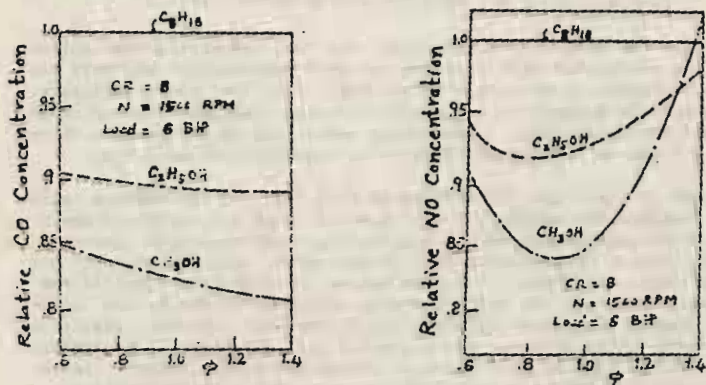

Fig.7 Relative calculated CO and NO emission levels for gasoline, methanol and ethanol fuels.

Also shown in Fig.6 the computed CO levels from the kinetic me-
chanism as a function of equivalence ratio.   The diagram demonest-
rates that, for fuel rich mixture , the CO concentration increases
steadily with increasing   as the amount of excess fuel incresses.
With fuel lean mixture (0.7< ϕ < 1.0),CO concentration varies little
with ϕ . Also, it can be seen that the effects of fuel type on CO
concentration is less important. However, alcohol fuels produces a
slightly lower CO level as a result of a lower ratio of. carbon in
the fuel molecules, and its more favorable diasociation properties.
This can be shown in Fig. 7, where the results were normalized to
isooctane results as a datum.
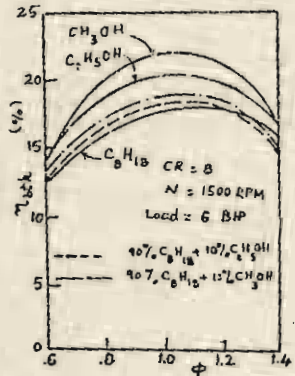
Fig.8 Measured brake thermal
       efficieney for used fuels,
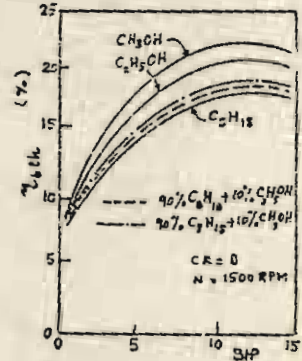   at different equivalence
       ratios.

Fig.9 Measured brake thermal
       efficiency for used fuels,
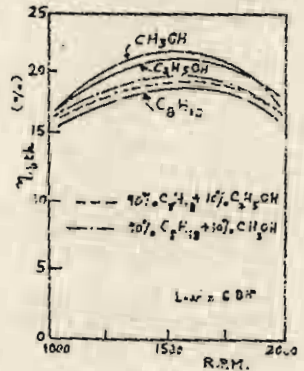   at differerent BHP .

Fig.10 Measured brake thermal efficienvy
       for used fuels, at different speeds.

Figures 8-12 show the experimental results using gasoline, methanol, ethanol, gasoline-methanol and gasoline-ethanol mixtures as a running fuels. Fig. 8 shows the relation between the engine brake thermal efficiency and fuel air equivalence ratio at constant speed of 1500 RPM. It can be noted that the efficiency is higher for alcohol fuels rather than gasoline and gasoline-alcohol blends. Fig. 9 and Fig.10 also represents the engine brake thermal efficiency versus engine brake hotsepower and engine speed respectively. The brake thermal efficiency for ethanol and methanol is higher than for gasoline. This is attributed to the lower heating value of those fuels than gasoline.

Measured levels of CO and NO in the engine exhaust gases when using gasoline, methanol, ethanol, gasoline-methanol and gasoline-ethanol blend fuels are shown in Fig. 11 and Fig. 12 respectively. From Fig. 11 it can be noted that CO concentration levels are higher than that for alcohol fuels. also Fig. 12 shows that for lean mixture (equivalence ratio $\phi < 1$), NO concentration levels are higher for gasoline than that for alcohol and gasoline-alcohol blends fuels.
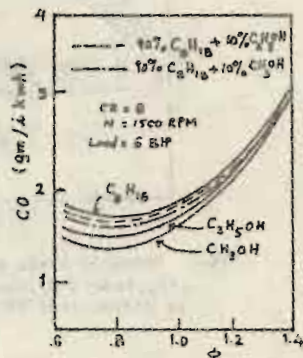
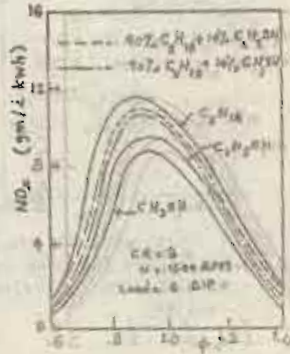Fig.11 Measured CO concentration levels for different fuels.

Fig.12 Measured NO concentration levels for different fuels.

CONCLUSION

On the basis of the theoretical and experimental results, the following conclusions can be offered:

1- The fuels which are still regarded today as unconventional will become increasingly important in the future, such fuels which relatively well suited to rhe autembile sentor, are alcohol and gasoline-alcohol blends.

2- Alcohol as a motor fuel provides improved power output, specific energy consumption and highly thermal efficiency relative to gasoline.

3- The concentration levels of CO and NO emissions in the exhaust gas are reduced with alcohol and gasoline-alcohol blends as fuels.

NOMENCLATURE

CR	Compression ratio
F/A	Fuel to air mass ratio
Pm	Maximum pressure in atm.
SEC	Specific energy consumption (kj/kwh)
TDC	Top dead center
Tm	Maximum temperature
V	Volume
Ki	Forward rate constant for reaction i (cm^3 / mole. S).
K-i	Backward rate constant for reaction i(cm^3 / mole. S).
RO	No of moles of O_2 in reactants.
PO	No of moles of O_2 in products.
u	Internal energy in j/mole.
W	Net work done per cycle.
η_{bth}	Brake thermal efficiency
ϕ	Equivalence ratio, (actual F/A ratio to stoichiometric F/A ratio).

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