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THEORETICAL STUDIES ON THE COMBUSTION OF HYDROGEN, ALCOHOL AND ISOOCTANE FUELS IN DIVIDED CHAMBER SPARK IGNITION ENGINE

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ABSTRACT

A mathematical model of the compression, combustion, and expansion phases of the divided chamber sprak ignition engine is reported here. This model has been developed in an attempt to combine as many as possible the basic characteristics of the divided chamber sprak ignition engine combustion. It is used to compare the predicting performance and emission levels when operating the engine with hydrogen, alcohol and isooctane fuels. A procedure for incorporating simple kinetic mechanisms for NO formation and CO oxidation is built into the model.

The divided chamber engine is treated as a pair of two thermodynamic sub-systems (prechamber and mainchamber systems) coupled by mutual mass flow. The results obtained are related to such important practical questions, as the effect of prechamber volume ratio, connecting orifice size, fuel type and degree of charge stratification, on prediciting performance and emission levels. This study shows that the divided chamber engine performance and emission levels are strongly affected by these design parameters. The results also indicated that improvement in engine performance and emission levels have been fullfilled when using hydrogen and alcohol fuels than that with isooctane Moreover, two stage combustion results in a loss of power compared to conventional spark ignition engine. This might be more compensated in practice. The reasons for this power loss and possible means of compensating are discussed here,

INTRODUCTION

This work is based upon the premise that the interaction between engine design and operating variables is sufficiently complex, that a fundamental model is essential in interpreting the resulting engine performance. Dale (1982) indicated that the most desirable advances in engine technology would transfer a good deal of the functions served by controlling the chemistry and mechanics of combustion processes, taken place in the engine cylinder. Overington (1981) found that ethanol, methanol and propane are all viable fuels for higher compression ratio engines. The use of these fuels offers improved torque, thermal efficiency and lower exhaust emissions. It is considered that a thermodynamic equilibrium combustion model can be used to good advantage and quick screening various concepts prior to elaborate hardware development program.

Based on theoretical viewpoint, operation at lean fuel-air ratios should produce 1- improved engine thermal efficiency due to favorable thermodynamic properties of the charge and reduced

throttling losses, 2- Low HC and CO emissions due to excess oxygen available for oxidation and 3- Low NO emission due to reduced peak cycle temperature. This is confirmed in current practice with compression ignition engine. However, conventional spark ignition engine actually reaches the lowest specific fuel consumption at air-fuel ratios not very far from the stoichiometric when the fuel used is gasoline. This is because, with leaner mixtures combustion becomes too slow and erratic (Young, 1981). Adams (1978) and Desoky (1981) demonestrated that much accelerated burning rates can be achieved by adopting the divided chamber concept. The lean limit can also be extended by using hydrogen fuels due to its higher combustion speed, it can also reduce misfiring (Gentili, 1984). As a result, the lowest specific fuel consumption point can be displaced towards the leaner mixtures by using hydrogen fuels.

A large number of designs have been proposed to implement the charge stratification concept. Several of them have been under active development for more than 20 years. Moreover, each design includes several parameters which can be varied over broad ranges so that great freedom of selection is available. Such a selection cannot be made simply through trial and error experimental procedures. It is well known that it takes many years of research and development even to assess the actual potential of a given engine. We are attempting to use computer modelling techniques to help design a combustion process which will be optimized for low emissions and high fuel economy. The purpose of this research is to demonestrate that the indicated performance and emission levels of divided chamber engine may be predicted with a degree of accuracy if a fundamental analysis is made of the engine cycle. The analytical procedure represented here under more development ... will be modified to include additional phenomena especially in the area of combustion and fluid mechanics.

MODEL DESCRIPTION AND ASSUMPTIONS

The purpose of the current model of divided chamber combustion is to estimate, qualitatively rather than quantitatively, the relative effect of a number of design and operating parameters on the comparative cycle and emissions performance of such engines. The model is also used to compare the predicted performance and emission levels of such engines when using isooctane, alcohol and hydeogen fuels. The model is evolved from the calculation procedure for single chamber combustion as previously described (Desoky, 1984). The assumed thermodunamic model representing the divided chamber engine is shown in Fig. 1. The model consists of two thermodynamic subsystems, one of a fixed volume representing the prechamber, and the other of prescribed variable volume representing the mainchamber. The two systems communicate via an orifice of cross section area Ao. The model is similar to two one-system models each capable of handling its own reactants and products. Initially both systems are assumed to contain a homogeneous reactants. Mixing is allowed between the mass transfer through the connecting orifice during compression, combustion and expansion phasses.

The pressure in each system is assumed to be uniform with values Pp and Pm, where subscripts p and m refer to quantities in the prechamber and mainchamber respectively. During the compression process, the mixture strengh of the homogeneous charge drawn in and mixed with the residuals has to be determined for the set overall equivalence ratio and required prechamber equivalence ratio and volume ratio. Combustion event is considered to occur at top dead centre in two steps, both adiabatic instantaneous constant volume processes. Initially combustion is permitted in the prechamber, this is followed by a flow of mass into the mainchamber. Then combustion is allowed in the mainchamber, followed by an associated reverse flow into the prechamber Compression and expansion processes within the systems in response to mass flows and piston movement are assumed to be isentropic. Variation in composition between the two systems can of course occur as a result of the different reactants composition in the two systems and the generated temperature difference. A brief mathematical formulation of the model will then follow.

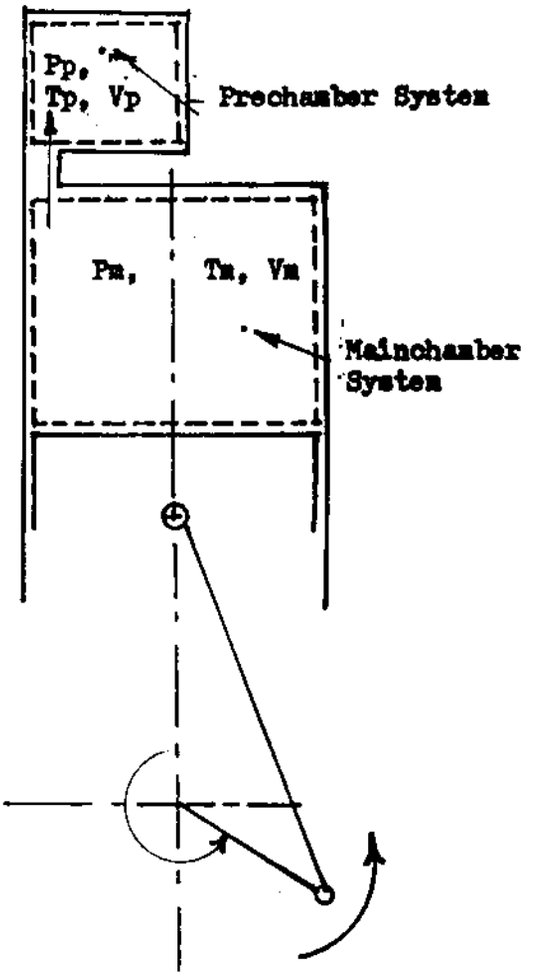

Fig. 1 Thermodynamic model of Divided Chamber Engine.

The Compression Process

During the compression process, the model is concerned with the properties of the fluid system contained in an divided chamber engine cylinder when all valves are closed. Thus the model treats a fixed mass of homogeneous mixture of fuel and air and residual gases. The pressure in each system is assumed to be uniform. The working fluid during this process is considered to be invariable composition, and thus needs to be calculated only once at the starting of the cycle. The fluid composition is computed from the known fuel composition, set of equivalence ratio, Ø and the residual mole fraction determined from the analysis of the exhaust and intake processes. The process is treated in an incremental manner, a 10 degree crankangle increment being adopted. At the beginning of compression identical subsystems pressures and temperatures are assumed. An estimate of the mainchamber pressure and temperature at the end of each crankangle increment is determined by assuming isentropic compression due to piston motion ignoring any transfer of mass into the prechamber. The values of temperature and pressure derived are then modified to allow for reultant transfer of mass through the connecting orifice into the prechamber. This transfer, is assumed to occur at the end of the crankangle increment

according to the time of 10 degree crankangle rotation and the pressure difference between the two systems. An isentropic compression and expansion of the gases within the systems in response to mass flows are assumed.

The mass flow through the connecting orifice is calculated using the isentropic quasisteady flow equation,

$$\frac{dM}{dt} = Cd.\ Pm\ .\ Ao \left\{ \frac{2Y}{Y-1} \frac{g_c}{R\ Tm} \left\{ (Pp/Pm)^{\frac{2}{Y}} - (Pp/Pm)^{\frac{Y+1}{Y}} \right\} \right\}^{\frac{1}{2}} \quad (1)$$

Where, Ao is the connecting orifice cross section area, Cd is the coefficient of discharge from the crifice, g_c is the dimensional constant, R is the mixture gas constant and Y is the mixture specific heat ratio. The time step used in the integration of mass transfer equation is taken as that equivalent to the cranangle increment (10°).

The mainchamber volume which changes as a result of piston motion is calculated at the end of each increment from the following relation,

$$Vm_j = \frac{1}{2} \left\{ 1+1/r - \cos \theta_j - \left\{ (1/r)^2 - \sin^2 \theta_j \right\}^{1/2} + \frac{2(1-VR)}{(CR-1)} \right\} \quad (2)$$

Where, Vm_j is the ratio of mainchamber volume at successive crankangle increment to the total displacement volume, CR, compression ratio, VR, prechamber volume ratio.

The Combustion Process

Following the compression process, combustion is considered to proceed in two stages at TDC (top dead cntre). Combustion is first allowed within the prechamber with an attendant flow of mass into the mainchamber. Then in the second stage, combustion is permitted in the mainchamber, with an associated reverse flow into the prechamber. Final chemical equilibrium with the product species, CO, CO_2, O_2, H_2, H_2O, OH, H, O, NO and N_2 is assumed. To determine the number of moles of the products of combustion dissociation reactions are considered. In the present study there are six such independent reactions, these used are

$$CO_2 \underset{K_{-1}}{\overset{K_1}{\rightleftharpoons}} CO + 1/2\ O_2 \quad (3)$$

$$H_2O \underset{K_{-2}}{\overset{K_2}{\rightleftharpoons}} H_2 + 1/2\ O2 \quad (4)$$

$$H_2O \underset{K_{-3}}{\overset{K_3}{\rightleftharpoons}} 1/2\ H_2 + OH \quad (5)$$

$$1/2\ H_2 \underset{K_{-4}}{\overset{K_4}{\rightleftharpoons}} H \quad (6)$$

$$1/2\ O_2 \underset{K_{-5}}{\overset{K_5}{\rightleftharpoons}} O \qquad (7)$$

$$1/2\ O_2 + 1/2\ N_2 \underset{K_{-6}}{\overset{K_6}{\rightleftharpoons}} NO \qquad (8)$$

Where, K_i is the forward rate constant for reaction i, Cm^3/mole S), $^1K_{-i}$ is the backward rate constant for reaction i.

Following combustion in the prechamber, an isentropic mass flow through the connecting orifice into the mainchamber is assumed to occur untill equality in pressure between the two sub-systems is achieved. Then, the transferred products are allowed to mix with the reactants in the mainchamber. A further instantaneous constant volume reaction is assume to result in the mainchamber. As a result the mainchamber pressure now exceeds that in the prechamber. Therefore reverse flow is allowed, with associated isentropic expansion of the mainchamber products and isentropic compression of the prechamber gases. Such a reverse flow is observed experimentally in the engine tests (Desoky, 1981).

The Expansion Process

The expansion process is treated in a fashion similar to the compression process. A 10 degree crankangle increment is again adopted. Each successive increment in crankangle comprises two steps. Those two steps comprise an isentropic expansion of the products of combustion in the mainchamber due to piston motion followed by a mass flow from the prechamber. An isentropic change of state within the two sub-systems due to mass transfer is assumed. Changes in fluid composition in both chambers (including mass transfer region) are allowed at each step in calculation. Chemical equilibrium at the relevant pressure and temperature is considered throughout the process.

In addition to calculating equilibrium CO and NO concentrations, a pessudo kinetic NO and CO during the expansion process is made. The kinetic mechanism proposed for NO calculation is the extended Zeldovish mechanism which comprised the following reactions,

$$N_2 + O \underset{K_{-7}}{\overset{K_7}{\rightleftharpoons}} NO + N \qquad (9)$$

$$O_2 + N \underset{K_{-8}}{\overset{K_8}{\rightleftharpoons}} NO + O \qquad (10)$$

$$N + OH \underset{K_{-9}}{\overset{K_9}{\rightleftharpoons}} NO + H \qquad (11)$$

The differential equation governing the formation rate of NO is;

$$\frac{d(NO)}{dt} = K_7(O)(N_2)-K_{-7}(NO)(N)+K_8(O_2)(N)-K_{-8}(NO)(O) + K_9(N)(OH)-K_{-9}(NO)(H) \qquad (12)$$

Using the temperature pressure and equilibrium values of O, N_2, O_2, OH and H at the end of each crankangle increment during the expansion process, kinetic NO formation is calculated by integration of equation (12). The steady state approximation for N atoms is used. The initial value for NO at TDC is assumed to be zero.

To calculate the kinetic CO, it is assumed that at TDC all the carbon content of the fuel is instantaneously converted to CO which is subsequently oxidized to CO_2 during the expansion process via the following reaction,

$$CO + OH \underset{K_{-10}}{\overset{K_{10}}{\rightleftharpoons}} CO_2 + H \qquad (13)$$

Thus the rate equation for CO is simply,

$$\frac{d(CO)}{dt} = - K_{10}(CO)(OH) + K_{-10}(H)(CO_2) \qquad (14)$$

The product temperature and pressure, and the concentrations of other species are assumed to remain the same as predicted from the full equilibrium model. Thus by invoking the carbon conservation equation,

$$(CO) + (CO_2) = (CO)_e + (CO)_e \qquad (15)$$

The CO levels throughout the expansion stroke is computed by integration of eqn. (14).

The rate controlled equations for calculating the kinetic NO and CO are numerically integrated throughout the expansion stroke using Eueler's method. The time step used is taken as that equivalent of 1 degree crankangle rotation. The kinetic levels for NO and CO are estimated for the two chambers separately. In addition, an average concentration, weighed for the total number of moles in each chamber is calculated. At the end of the expansion process, the two systems are assumed to combine to form one system having averaged thermodynamic properties.

Exhaust and Induction Processes

An elementary treatment of the exhaust and induction processes is included. The exhaust process is treated in two stages. The first represents the event where the exhaust valve is open and the products of combustion expelled into the atmosphers. The process is irreversible and is accompanied by an increase in entropy. In the second stage, it is assumed that the piston is returned to TDC, with expulsion of most of the residual gas remaining in the cylinder at BDC (bottom dead centre). The composition during the second stage is considered to be invariable,

and is also assumed to be adiabatic frictionless and of constant pressure. At the end of this process, the volume and the mole fraction of the residual gases at TDC is calculated.

At the current stage of the model development equals exhaust and induction pressure has been assumed. During the induction process and at TDC the intake valve is assumed to open and fresh completely vaporized charge is inducted. The fresh charge and residual gases trapped in the cylinder are assumed to be perfectly mixed. The pressure is considered constant throughout this process and it is assumed that no chemical reaction occurs. The internal energy of the mixed system is equal to the sum of the internal energies of vaporized fresh charge and residual gases. This enables the mixture temperature to be calculated by successive approximation.

The complete cycle computation outlined above is then repeated using the values obtained at BDC as the new initial point in calculation. The whole procedure is repeated untill correspondence between the assumed initial values and the calculated values at BDC is obtained at successive cycles.

RESULTS AND DISCUSSIONS

In present analysis, performance and emission levels of CO and NO are calculated for isooctane ($C_8 H_{18}$), methanol ($CH_3 OH$), ethanol ($C_2 H_5 OH$) and hydrogen (H_2) fuels. The volume ratios varying from 10% to 50% and the connecting orifice area ratios (connecting orifice cross section area/stroke volume) varying from 0.00175 to .00575. The minimum and maximum torch opening area are calculated by the techniques proposed by Adams (1978). Two series of results are obtained, in the first series the calculations are carried out with the modelling of homogeneous mixture, i.e both chambers have the same equivalence ratio. In the second series, the effect of charge stratification is examined. The overall equivalence ratios varying from .6 to 1.0 and the maximum allawable richness in the prechamber is taken to be 1.4. All the results presented here are obtained at engine compression ratio of 8 and an engine speed of 2400 rpm.

Shown in Figs.2 through 4, are the way that theoretical peak pressures and temperatures are affected by the combustion in divided chamber engine, equivalence ratio and fuel type. The data obtained from the one stage combustion model (VR=0.0) are included for comparison. For a given volume ratio, connecting orifice size and fuel type the curves are seen to follow the pattern predicted for one stage combustion. However, lower pressures and temperatures are predicted from the two stage combustion model. This is seen to be due to the effect of flow through the connecting orifice and subsequent mixing. The results also show that the theoretical peak cycle pressure and temperature are influnced by the fuel type. More ready comparison of the results shown in Fig. 4, if the results are normalized with isooctane as a datum. From this figure it can be noted that, hydrogen gives 5 to 10% higher peak temperature than isooctane, but 10 to 15% lower peak pressures. The characteristics of

methanol and ethanol are predicted to yield lower pressures and temperatures than isooctane.

Illustrated in Figs. 5 through 7, are the effects of equivalence ratio, volume ratio, connecting orifice size and fuel type on calculated indicted mean effective pressure (IMEP) and indicated thermal efficiency. The curves again follow similar trends to those obtained for single stage combustion, although lower values are predicted for the divided chamber engine. This is seen to be due to irreversibilities generated by the flow through the connecting orifice and subsequence mixing. The effect of fuel type on calculated IMEP and thermal efficiency are shown in Fig. 7. From these diagrams it can be seen that, the hydrogen fuel yield to predict higher IMEP than all other fuels, and alcohol fuels yields to predict higher thermal efficiency.

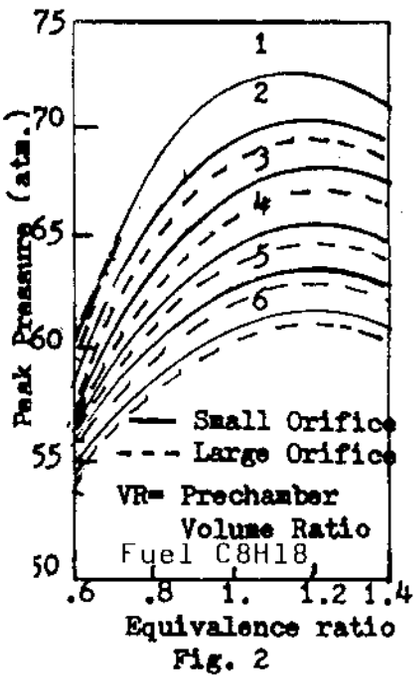

Fig. 2

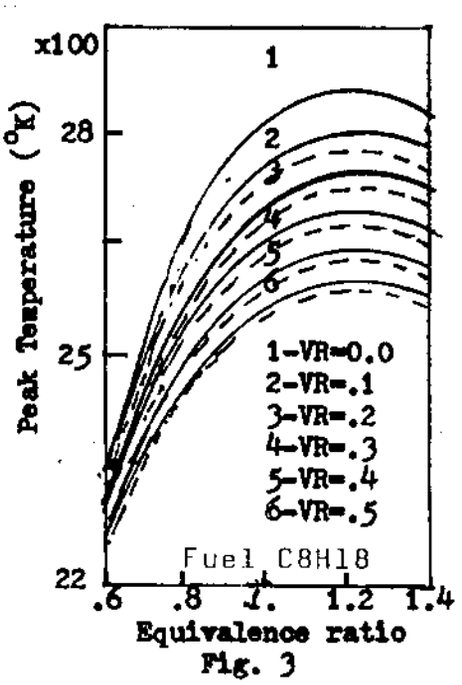

Fig. 3

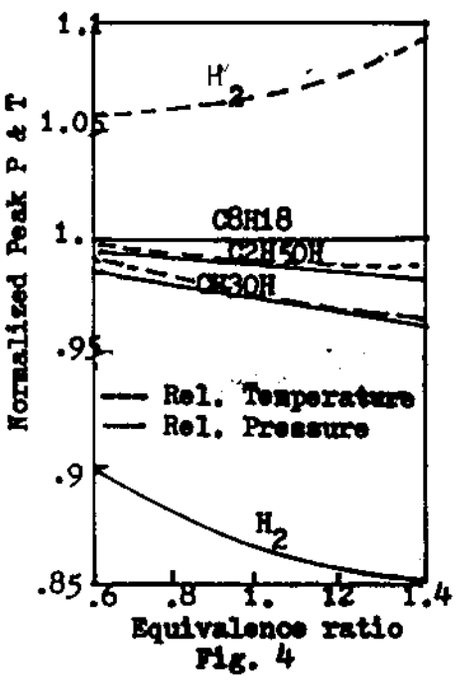

Fig. 4

Figs. 2 through 4, Effects of Volume Ratio, Connecting Orifice Size, Fuel Type and Equivalence Ratio on Peak Cycle Pressures and Temperatures.

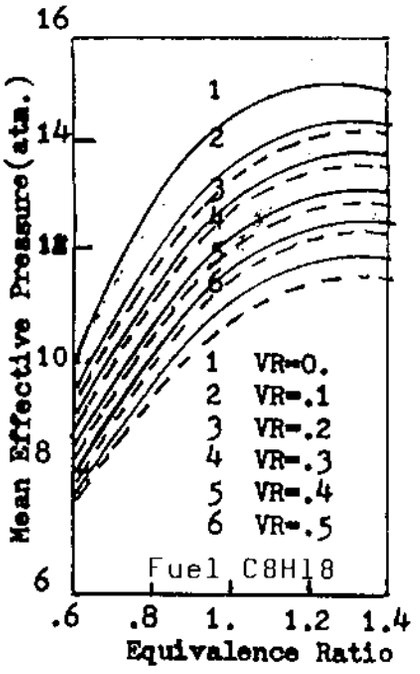

Fig. 5

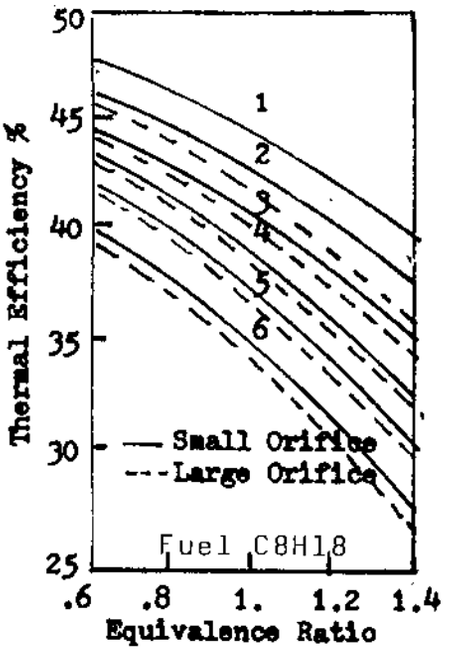

Fig. 6

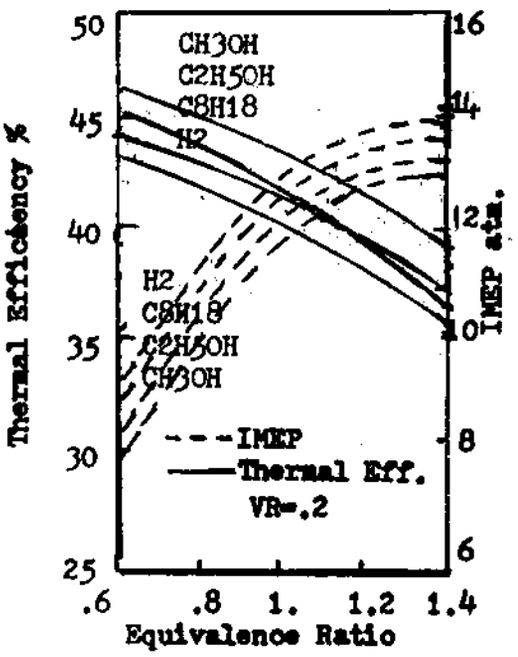

Fig. 7

Figs. 5 through 7, Effects of Volume Ratio, Connecting Orifice Size, Fuel Type and Eqyivalence Ratio on Indicated Mean Effective Pressure and Thermal Efficiency.

In Figs. 8 through 10, the average kinitically calculated NO and CO mass emission rates (gm/IKWH) are plotted versus equivalence ratio. The volume ratio is taken as a parameter. The peak NO levels becomes lower as the volume ratio increases. However, for rich mixtures a slightly increased in NO levels may be obtained with the higher volume ratio. The same figures indicated also that a slightly higher NO levels are predicted for large connecting orifice cross section area. The results presented in Fig. 10, shows that the type of fuel has a little influence on NO and CO emissions.

In the second series of results, the effectiveness of charge stratification on performance and NO & CO emission levels are studied. Presented in Figs. 11 and 12, are the effects of overall equivalence ratio, volume ratio and fuel type at prechamber equivalence ratio of 1.2, on calculated peak pressures and temperatures. The peak pressures and temperatures becomes lower as the volume ratio increases or the overall equivalence ratio decreases. The decreases in peak pressures and temperatures are significant at lower overall equivalence ratio.

As the rsulting of lower temperature in the mainchamber and the fast decay in pressure during the expansion stroke in the case of stratified charge engine, the engine cycle gives incomplete combustion, lower IMEP and poorer fuel economy. This can be seen from Figs. 13 and 14. As the volume ratio becomes higher and the overall mixture becomes leaner, a marked decrease in IMEP is observed. As the volume ratio increases than 30% the trends in the indicated thermal efficiency reverse its known pattern and the thermal efficiency becomes lower as the overall

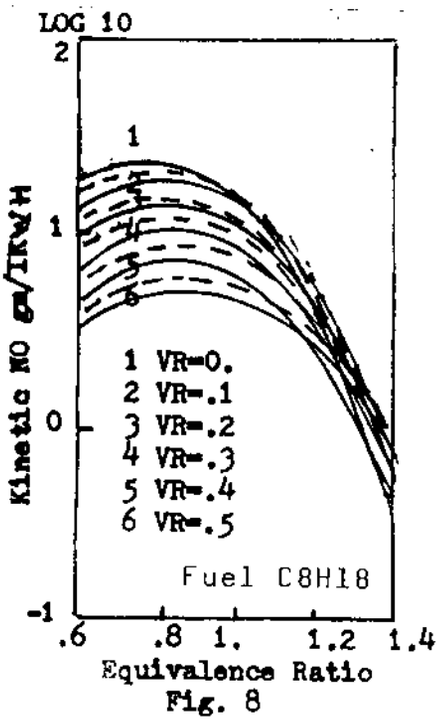

Fig. 8

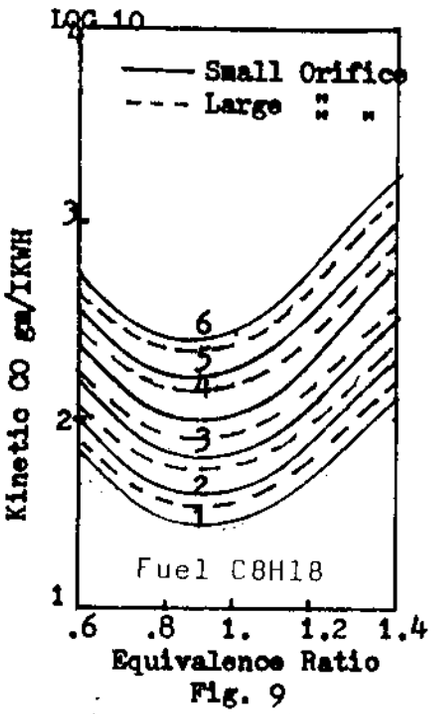

Fig. 9

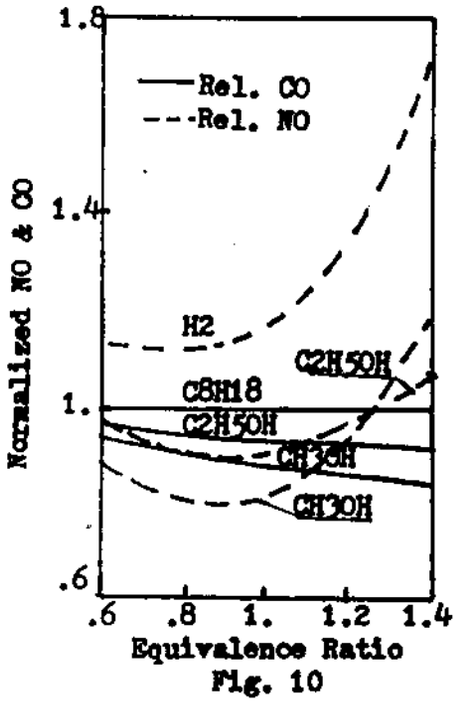

Fig. 10

Figs. 8 through 10, Effects of Volume Ratio, Connecting Orifice Size, Fuel Type and Equivalence Ratio on Kinetic NO and CO Emission (gm/IKWH).

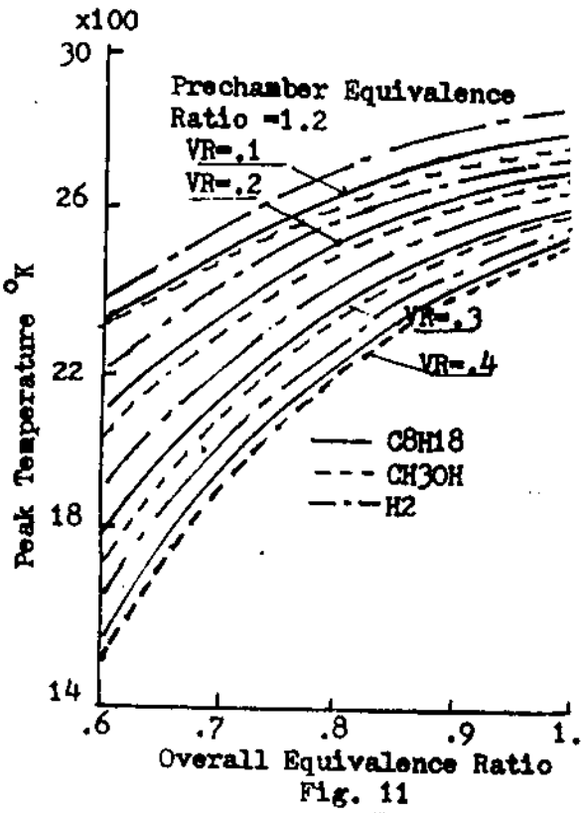

Fig. 11

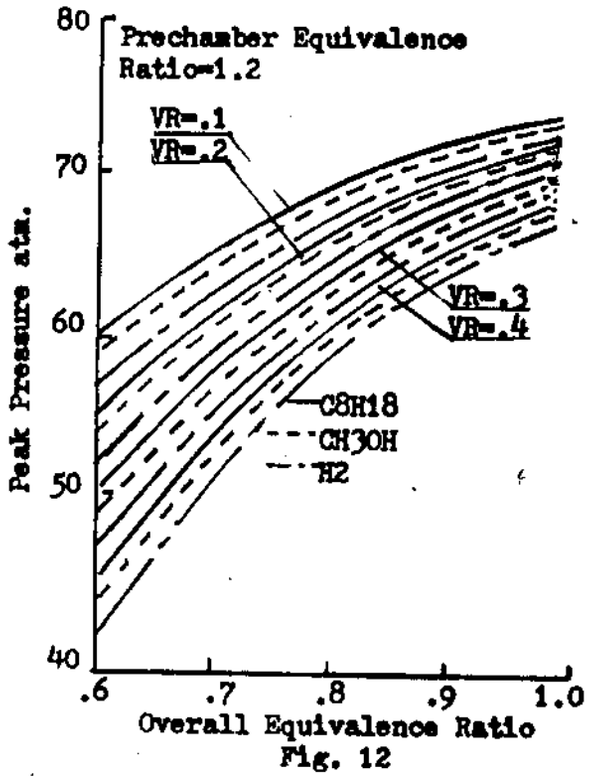

Fig. 12

Figs. 11 and 12, Effects of Volume Ratio, Overall Equivalence Ratio and Fuel Type on Calculated Peak Pressures and Temperatures.

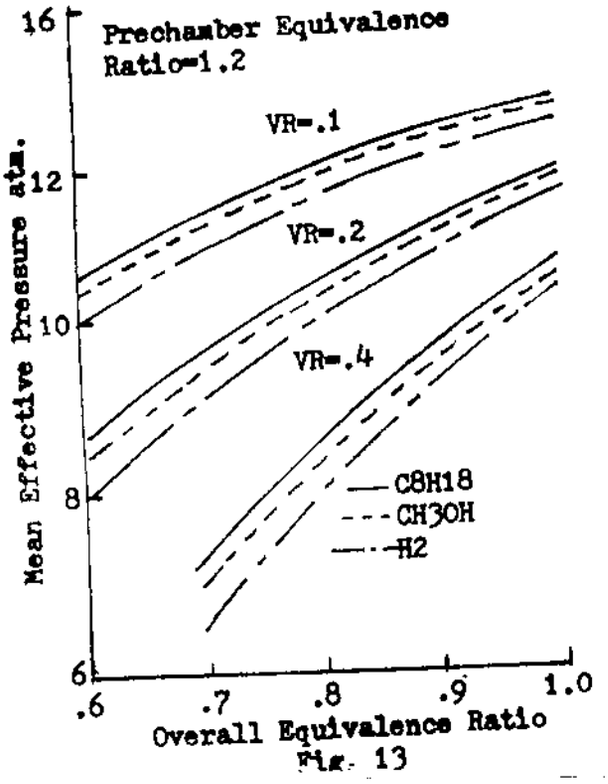

Fig. 13

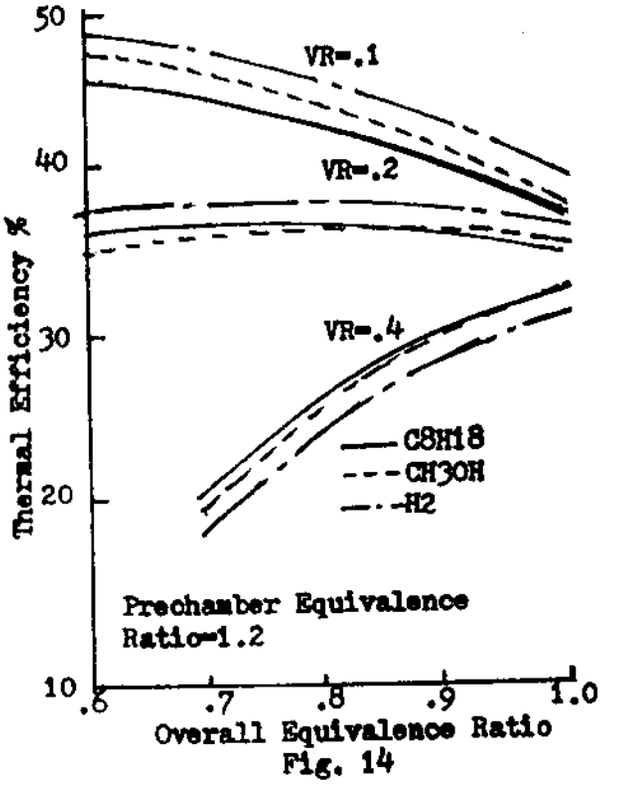

Fig. 14

Figs. 13 and 14, Effects of Volume Ratio, Overall Equivalence Ratio and Fuel Type on Calculated Mean Effective Pressure and Thermal Efficiency.

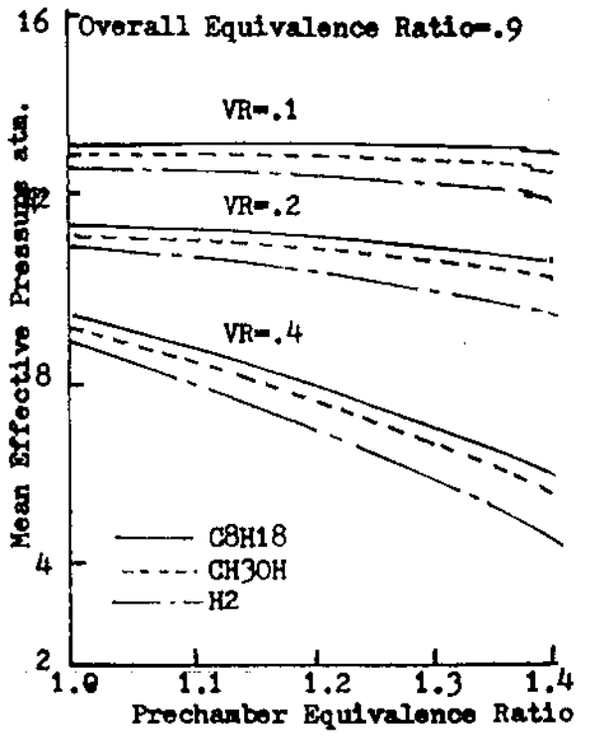

Fig. 15

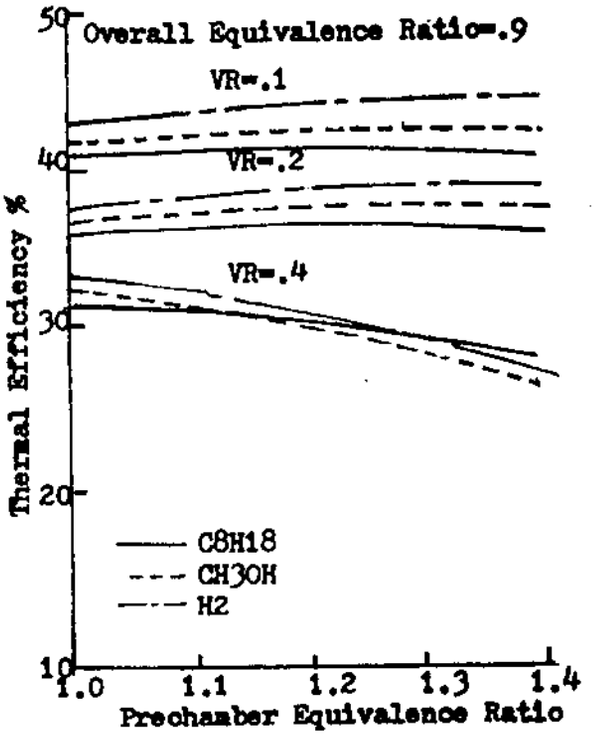

Fig. 16

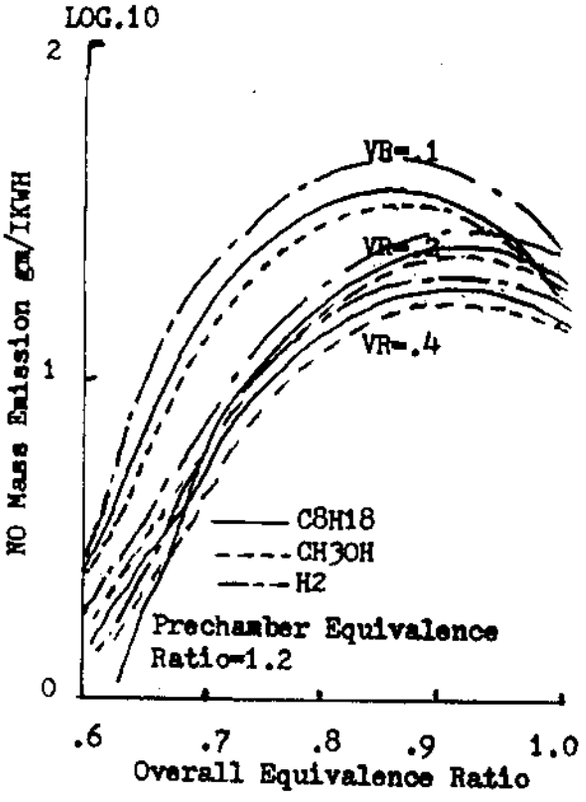

Fig. 17

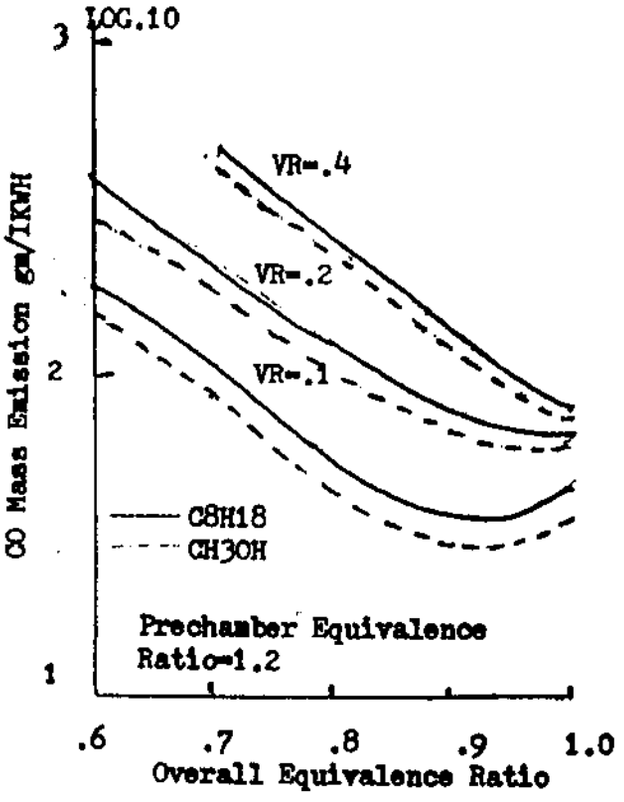

Fig. 18

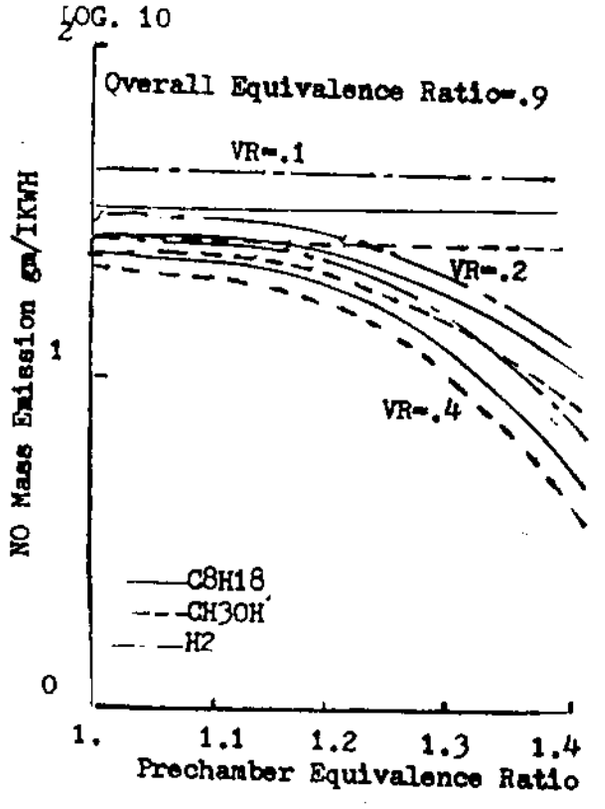

Fig. 19

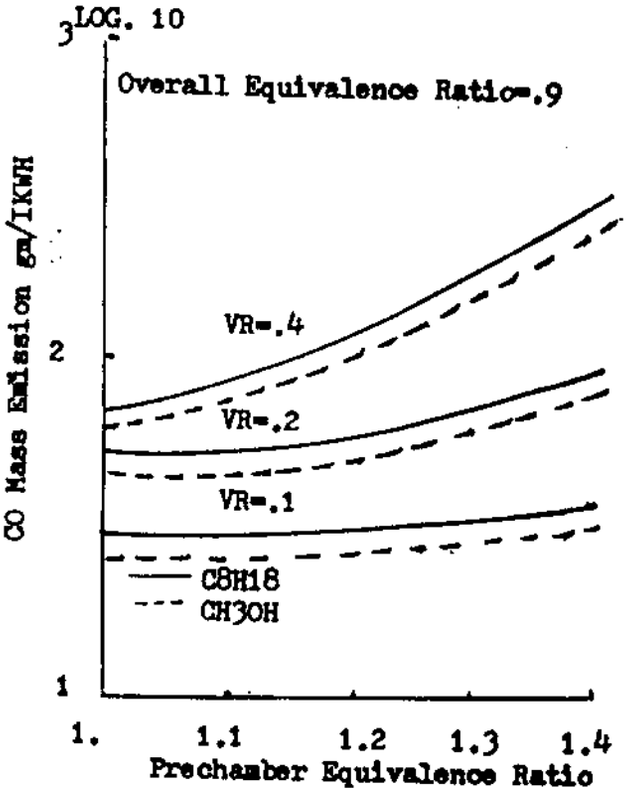

Fig. 20

mixture is made leaner. At higher volume ratio and lower overall equivalence ratio, there is a sharp decline in indicated theranal efficiency. This is the result of the incomplete oxidation of the fuel in the rich region of the charge with subsequent loss of power. However, this will be more compensated by an ability to run at leaner overall mixture strength. Equally, in practice, the faster combustion rates result with charge stratification would allow the theoretical maximum performance to be more closely approached.

Given in Figs. 15 and 16, are the calculated IMEP and thermal efficiency at an overall equivalence ratio of 0.9 as a function of prechamber equivalence ratio. The prechamber volume ratio is taken as a parameter. According to the result predicted in these figures, slight decrease in IMEP and thermal efficiency is noted for stratified charge at small volume ratios. As the volume ratio increases, or prechamber mixture becomes richer, there is a great loss in power and poor thermal efficiency is predicted.

The emission data on the basis of rates of mass emission per unit power are presented in Figs. 17 through 20. The CO emission results shows a marked increased with increasing volume ratio or prechamber degree of richer. Also these results shows that the NO mass emission rates increases as the volume ratio increase or degree of prechamber richer is increaeses.

CONCLUSIONS

The simulation of the thermodynamic cycle of a divided chamber engine has been described. Based on the results obtained, the following conclusions may be drawn;

1- The developed cycle model is adequate for analyzing the performance of divided chamber stratified charge engine.
2- Divided chamber combustion engine results in a loss of power compared to single stage combustion. This is as a result of irreversibilities associated with the flow through the connecting orifice and subsequent mixing.
3- Charge stratification leads to a further loss of power. However, this might be more compensated by the ability to run at leaner mixitures. Equally in practice, the faster combustion rates could be ashieved with charge stratification. This would allow the theoretical maximum performance to be more closely approached. In addition, lower pollutants emissions are predicted.
4- It is considered that the model reported in this work is most useful in providing an understanding of the sometimes disappointing performance of stratified charge engines reported in literature. The model gives an upper limit for the performance.
5- On the basis of the model developed, engine performance and emission levels are profoundly influenced by fuel composition, Alcohols and hydeogen fuels provide improved engine performance and emission levels relative to isooctane.

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NOMENCLATURE

CR	Compression Ratio.
TDC	Top dead centre
IMEP	Indicated mean effective pressure (ata.)
Pp	Prechamber pressoin (ata.)
Pm	Mainchamber pressure (ata.)
Tp	Prechamber Temperature (^{o}K)
Tm	Mianchamber Temperature (^{o}K)
Vp	Prechamber Volume
Vm	Mainchamber Volume
VR	Volume ratio (Prechumber volume to total clearance volume at TDC)
ϕ	Fuel-air equivalence ratio
θ	Crank position (deg.)
r	Crank radius
l	Connecting rod length