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# THERMODYNAMIC ANALYSIS OF A SIMPLE GAS TURBINE CYCLE WHEN DSING H2, NH3 AND C3H8 FUELS

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التحليل الشرمودت:اصيكي لدورة التوريين الخارئ النصبة عمد استعدام أيا من المهدرومين ، السروان ، الأموسا كوفسيسود

# ABSTRACT

A simple equilibrium combustion model with superimposed kinetic NO and CO rates of formation has been developed. This has been used to compute the estimated performance and emission data for a simple gas turbine cycle. The model has also been used to compare performance and emission levels of gas turbine when operating with hydrogen, ammonia and propane fuels. The analysis is mainly concerned to study the effects of equivalence ratio, pressure ratio and fuel type on the predicted performance and NO and CO emission levels. Comparison has also been made between predicted maximum cycle temperatures, NO and CO emissions with that the corresponding measured values. This comparisons indicated that the predicted trends are agree with that of the experimental trends. From the theoretical and experimental results it is found that the use of hydrogen fuel improves the performance of the gas turbine and gives higher product temperature than that of other fuels examined. The NO emission is increased as the result of increasing the product temperature. The most important engine operating variables in determining the performance and emission levels are the equivalence ratio and pressure ratio. The analysis confirms the well documented benefits of lean mixtures and low pressure ratio for lover engine emissions.

# 1-INTRUDUCTION

The gas turbine can truly be described as the primemover of the twentieth century. Its potential as a practical source was recognized in the early 1900s. The rapid development was maintained in the postware years, due to the tremendous advantages offered by the aircraft gas turbine in terms of range of, speed, fuel economy and passenger comfort. However if the gas turbine is to maintain its pre-eminence lt.

will be necessary to improve its performance in the areas of fuel economy, emissions and sensitivity to fuel type.

In recent years it has been noticed that the reserves of highly refined petroleum fuels are becoming limited. In order to conserve these stocks of fuel and to minimize power costs as the price of petroleum resources escalates, it is obviously desirable to improve the performance of gas turbines. It will also become necessary for such device to operate on a less narrow cut of the crude oil. So that a greater proportion of each barrel can be used. There are similarity obvious benefits to be obtained from making gas turbine run effliciently on alternative fuels such as, natural gas, hydrogen and ammonia fuels[1]. Thus, the need to consider the use of fuels other than highly refined petroleum products, coupled with concern for the growing level of atmospheric pollution, have tended to draw attention to our lack of understanding of the combustion process and to highlight on the object of gas turbine combustion.

Theoretical studies of combustion products at chemical equilibrium and predicting performance of combustion system are becoming important for research work in the field of rocket engines(2), jet engines[31 and reciprocating engines[4]. The method and procedures of computation of combustion products and of their corresponding thermodynamic state differ according to the Computation technique employed and basic assumptions made. Hydrogen appears to be an ideal fuel for combustion in engines. It is the cleanest possible fuel in use and it is the easiest fuel material to produce from water by using nuclear or solar energy(5). As a fuel for combustion in engines, hydrogen has a wider range of flammability than other petrolcum fuels. It can be ignited at extra lean mixtures, thus raising the combustion efficiency. The exhaust gases emitted from the hydrogen combustion device has no carbon compounds. Ammonia was selected for considerations due to 185 exhaust freedom from unburned hydrocarbon and carbon monoxide. Unlike hydrogen, with similar carbon free composition, anmonia is a liquid at relatively reasonable storage pressure and temperature (7.5 ata. and 23 oc). Finally propane fuel is considered as a base hydrocarbon gas fuel for comparisons. Propage has been used as a fuel in combustion systems as the principal component of LPG for about 50 years[6]. Emission levels with LPG are reported to be less than with hydrocarbon fuels.

Combustion characteristics of gaseous hydrogen in a "can" type gas turbine combustor is studied by Sampath, et. al.(3). Their results on combustion performance of hydrogen were compared with that of other liquid fuels using the same combustion hardware. They found that hydrogen combustion is characterized by high combustion efficiency, ease of ignition and good flame stability. However it can also result in relatively high metal temperature which can impact on liner durability and high Nox emissions. Analysis of an intercooled gas turbine cycle with hydrogen turbine and regenerative heater was made [7]. Their results indicated that the thermal efficiency and the specific output of the cycle were improved compared to the conventional cycle.

A simple model of CO exidation supported with experimental data with particular references to gas turbine combustor was developed [8]. The results concluded that the criteria for low CO emission from burners would appear that the flow of combustion gases should reside for a sufficient time in a zone where the temperature in the range of 1600

to 1800 ok.

The objective of the present investigation is to produce a mathematical model for a simple gas turbine cycle with superimposed kinetic NO and CO rates of formation. This has been used to compare the predicted performance and NO and CO emission levels of gas turbine cycle when using hydrogen, propane and ammonia fuels. Comparisons with some available experimental data are also included.

# 2-GAS TURBINE CYCLE MODEL.

The mathematical model described in this paper considers the gas turbine cycle in a manner similar to the Baryton fuel-air standard cycle. The compression and expansion processes are assumed adiabatic and the combustion process is considered steady flow constant pressure process. The combustion products is assumed to be a mixture of gases in chemical equilibrium at the appropriate temperature and pressure through out the cycle. Procedures for incorporating kinetic mechanisms for NO formation and CO exidation are also built into the model. The assumed thermodynamic cycle is shown schematically in Fig.(1). The cycle and the governing equations are outlined briefly as follows;

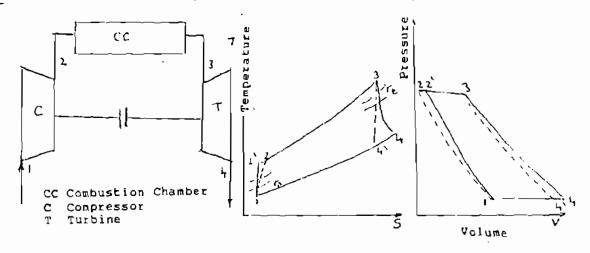


Fig.(1) Simple Gas Turbine Cycle

# 2.1-The Compression Process

This corresponds to the process 1-2 on P-V and T-S diagrams, Fig.(1). During this process an adiabatic change of state due to compression is assumed. A constant composition of oxygen and nitrogen (air) is assumed up to point 2 where the combustion begins. The process is treated in an incremental manner in pressure ratio, a 2.5 pressure ratio increment being adopted. The working fluid prior to compression is assumed to be at atmospheric pressure and a temperature of 298.15 oK. The temperature at the end of each pressure ratio increment is evaluated using the following relation;

$$Ra/^{2}c^{*}Cpam$$
T2 = T1(rp) (1)

Where, rp is the pressure ratio increment and Cpam is the mean value of molar specific heat at constant pressure. It is assumed to be constant during each pressure ratio increment and is updated at the end of each increment to allow for the change in gas temperature. Knowing the composition, pressure and temperature at any point, the thermodynamic properties (per mole of the gas mixture) are evaluated using the following relations;

$$h = \Sigma \{MFI(hT)i\}$$
 (2)

$$Cp = \Sigma \{MFi(CpT)i\}$$
 (3)

where (hT)1 and (CpT)i are the specific molar enthalpy and constant pressure molar specific heat of species i respectively. The numerical values of those thermodynamic properties are given by the following equations;

$$(hT)i = Ai, 1 + Ai, 2*T + Ai, 3*T + Ai, 4*T + Ai, 5*T$$
 (4)

Where Ai,1, Ai,2, .....,Ai,5 and Bi,1, Bi,2 .....,Bi,5 are polynomial coefficients for each species and for fuels. Those previously generated by the author(9) are used. The computations are repeated for all increments in pressure ratio until the end of compression process at point 2.

#### 2.2-The Combustion Process

Referring to Fig.(1), the mixture of fuel and air at temperature T2 and pressure P2 is assumed to burn at constant pressure. The process is considered adiabatic, and final chemical equilibrium with product species of C0, C02, O2, H2, H2O, OH, H, O, NO and N2 at point 3 is assumed. The chemical equilibrium species concentration at any temperature and pressure is calculated using the adiabatic tlame temperature program developed before[10].

The technique adopted for calculating the adiabatic flame temperature is to determine the enthalpy of the product gases at an estimated flame temperature and at equal increments in temperature above and below the estimated value. The program fits a quadratic equation in temperature to those three enthalpies, which is then solved for the temperature at which the product enthalpy is equal to the reactant enthalpy. The procedure is continued for the new estimate of temperature with half temperature increments, until the reactant and product enthalpies agree to within a set accuracy. Once TJ and the equilibrium composition have been determined by successive approximation, then all the other thermodynamic properties at point 3 are calculated using equations (2) through (5).

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# 2.3-The Expansion Process

The expansion of the products of combustion, from point 3 to point 4 in Fig.(1), is treated in an incremental manner in pressure ratio. A single expansion increment comprises two steps, these are; i) An adiabatic change of state due to decrease in pressure during the expansion increment. The temperature at the end of each expansion ratio increment (rt) is evaluated using the following relation;

$$-7t*kg/cpgm$$

$$T4 = T3*(rt)$$
 (6)

where, the value of Cpgm is assumed constant during each expansion increment and is updated at the end of each increment to allow for the change in gas temperature and composition.

i)Calculation of the revised equilibrium composition at the new pres-

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

The computation is repeated for successive increments in expansion until the end of the expansion process, i.e P= 1 ata. at point 4.

# 3-GAS TURBINE CYCLE STUDY

Computation have been performed for three fuels (H2, NH3 and C3H8), for pressure ratios (Rp) in the range of 2.5 to 40 and for equivalence ratios of .6 to 1.6. The predicted performance of these conditions has been compared on the basis of a number of parameters, including peak cycle temperature, net specific work done, thermal efficiency and the specific energy consumption. Applying the first law of thermodynamic, for a steady flow open system processes, since the compression and expansion processes are adiabatic (dq=0). Refereeing to Fig.(1) the net cycle work done may be determined as follows;

The indicated thermal efficiency is the ratio of the net work done to the energy content of the fuel supplied, i.e.

where; LHV is the lower heating value of the fuel(1). For hydrogen =116 Mj/kg, for ammonia =17.2 Mj/kg and for propane=46 Mj/kg. The indicated specific fuel consumption, ISFC is determined using the following relation:

ISFC=(MF)
$$E*ME*3600/Wnet$$
 Kgf/KWH (9)

The specific energy consumption, ISEC is calculated as follows;

# 4-KINETIC NO CALCULATION

Nitric oxide, NO can be formed in one of the following three ways i)at high temperature in flames N2 reacts with oxygen to form thermal NO II)when the fuel has nitrogen-containing compounds the nitrogen is released at comparatively low temperature to form fuel NO III)lastly NO formed in flame fronts other than that from atmospheric N2 and O2 is referred to as prompt NO. In most combustion devices, thermal NO is the dominant source of nitric oxide. Prompt NO is formed in turbulent diffusion flame when maximum temperature levels as low as 1300 oc. The principal reaction governing the formation of thermal NO during the combustion of lean, stoichiometric and rich mixtures are given by the extended Zeldovish equations[9];

$$N2 + 0 = = N0 + N$$
 (11)

$$Kf2$$
 $O2 + N ==== NO + O$ 
 $Kb2$ 
(12)

where; Kf, Kb are the forward and backward rate constant for each reaction considered. The values of Kf and Kb required for computation were taken from reference(9).

The general rate equation for NO production by these three reactions is; dNO

$$\frac{dN}{dt} = Kf1(0)(N2) - Kb1(N0)(N) + Kf2(02)(N) - Kb2(N0)(0)$$

$$\frac{dt}{dt} + Kf3(N)(OH) - Kb3(NO)(H)$$
(14)

The steady state approximation for N atoms is used;

where; () denotes mole concentration. In a high temperature combustion process, it appears to be a good assumption that the C-H-O system reaches equilibrium while NO is still negligible, so from Eq.14;

Using the temperature, pressure and the equilibrium values of O,

N2, O2, OH and B at the end of each increment in the expansion process (from the thermodynamic simulation), kinetic nitric oxide concentration is computed by integration of Eq.16 using the Euler method. It is accognized that comparison with other data should be on the basis of mass emission rates for a given power output (gm NO per sec./Kj) or per unit mass of fuel consumed (gm NO per sec./Kgf). Accordingly the data have been reset in the form of specific mass emission rates using the following expressions;

NO gm/Kj = 
$$d(NO)*$$
 MNO \* Np/Nair /Whet gm NOpersec/Kj (17)

### 5-KINETIC CO CALCULATION

Carbon monoxide, CO, is always present in the exhaust gases due to the dissociation process. With rich mixtures the carbon monoxide is further increased by incomplete combustion. It is formed as an intermediate species in the oxidation of carbon containing fuels. It is assumed that at the beginning of the expansion process 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(9);

$$KE1$$
 $CO + OH ====== CO2 + H$ 
 $Kb4$ 
(13)

Thus the rate equation for CO is simply;

$$d(CO)/dt = -Kf4(CO)(CH) + Kb4(H)(CO2)$$
 (20)

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

$$(CO) + (CO2) = (CO)e + (CO2)e$$
 (21)

The CO level through the expansion process is computed by integration of Eq.20. The specific rates of mass emission of CO gm per sec/Kj and gm per sec/Kgf are calculated using the expressions below;

CO 
$$gm/Kgf = CO gm/IKWH / ISFC Kgf/IKWH gm per sec/Kgf (23)$$

# 6-RESULTS AND DISCUSSIONS

Shown in Figs.(2)through(10), are some of the more important results of the performance and emissions calculations over a range of equivalence ratio and pressure ratio for the simple gas turbine cycle with hydrogen, propane and ammonia fuels. Some of experimental results obtained in Referencelll1 are represented for comparison. The measured and predicted results are presented now and discussed in a family of

curves as following;

Shown In Fig.(2) are the calculated peak cycle temperatures and the measured data as a function of equivalence ratio. The temperatures are vary with equivalence ratio. If dissociation were not present, the maximum peak cycle temperature would occur at the stoichiometric mixture equivalence ratio. However, due to dissociation and the influence of the different specific heats of the products of combustion, the maximum peak temperature occur with slightly rich mixtures. The diagrams also show that the fuel type can influence the calculated peak temperature. Hydrogen, for example, gives 10 to 18 percent higher peak temperature than propane, but 18 to 22 percent higher than ammonia. This can be explained due to that the less dissociation and higher heating value of hydrogen fuel than that for propane and ammonia fuels. The results shown in this figure indicate also that a higher pressure ratio increases the peak temperature. The measured combustion temperature for the three fuels examined at different equivalence ratio and at atmospheric pressure are also presented in the figure. The same observations are noted from the experimental

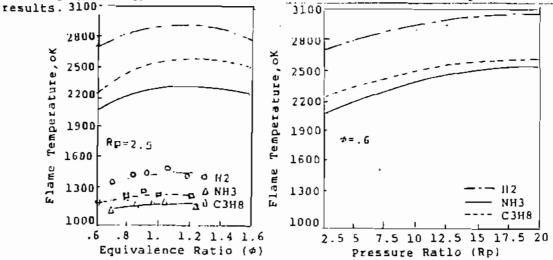


Fig.(2)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on Calculated and Measured Flame Temperature.

The net specific work done (Wnet), the indicated thermal efficiency (7th), the indicated specific fuel consumption (ISFC) and the indicated specific energy consumption (ISEC) are computed and presented in Figs.(3)through(6). These diagrams indicate that the equivalence ratio and the pressure ratio has an appreciable effect on the ideal performance. The addition of air decreases the temperature rise during the combustion process, however the temperature rise per unit of energy supplied are increased. This is because the specific heats are lower for lower temperatures, which results in higher thermal efficiency. The addition of fuel to a correct fuel-air mixture results in unliberated energy which is charged against the process in the energy supplied. This excess fuel does not increase the work in proportion to the increase in fuel, Fig.(3), and the ideal thermal ef-

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ficiency, Fig.(4), decreases while the Indicated specific energy consumption, Fig.(5), increases as the mixture is made richer.

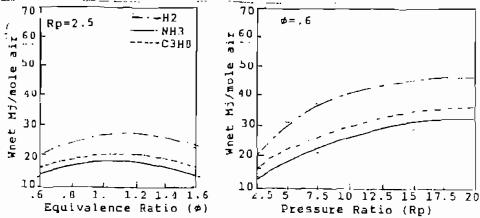


Fig.(3)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on W

The net work done, Fig.(3) is at a maximum at the same equivalence ratio as the maximum peak temperature. As noted previously the temperatures obtained for hydrogen are higher than those with propane and ammonia. This results in a higher net work done for hydrogen fuel. Also, as less dissociation occurs with hydrogen and the larger ratio of moles product - moles reactant (Np/Nair) there is a higher net work done and higher thermal efficiency for hydrogen than propane and ammonia fuels, as can be seen from Figs.(3)and(4).

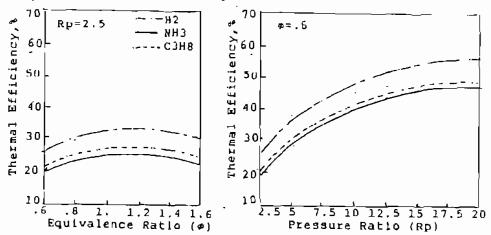


Fig.(4)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on t

Fuel consumption and specific energy consumption characteristics for the three fuels are illustrated in Figs.(5)and(6). The diagrams shows the indicated specific fuel consumption (Kgf/IKWH) and the indicated specific energy consumption (Kj/IKWH) as a function of equivalence ratio and pressure ratio. The figures highlights an ISFC for hydrogen roughly one fifth for propage and one tenth for ammonia at a comparable equivalence ratio. This is in agreement with the higher heating value for hydrogen fuel. Also, the ISEC for hydrogen is lover than those for propage and ammonia. Shown in Figs.(3)through(6) also

are the effects of pressure ratio (Rp) on colculated performance. The diagrams shown in these figures indicate that, a higher pressure ratio improves net work done, indicated thermal efficiency, indicated specific fuel consumption and indicated specific energy consumption.

The effect of equivalence ratio and pressure ratio on NO and CO pollutant emissions is shown in Figs. (7)through(8). The kinetic No rate of mass emission (gm NO per sec/Kj) and the rate of mass emission per unit mass of fuel (gm NO per sec./Kgf) as a function of equivalence ratio and pressure ratio are plotted in Fig. (7). The diagrams show that the peak nitric oxide levels occur just to the lean side of stoichiometric fuel-air mixture, because of the greater oxygen concentration and the associated relatively high temperature. For a lean mixture the rate of nitric oxide formation falls due to the attendant drop in the flame temperature. For a rich mixture the rate decreases due to oxygen deficiency and falling flame temperature. One other observation is that, hydrogen produces higher nitric oxide than that for propane and ammonia fuels with both lean and rich mixtures. This is because of the higher flame temperature for hydrogen - this higher flame temperature influences the dissociation of oxygen so that a higher atomic oxygen is formed. The results also indicate that the NO rate of mass emission is increases as the pressure ratio increased. The same observations are noted for the experimental results obtained at different equivalence ratio and at atmospheric pressure, Fig. (7).

The computed rates of mass emission of CO as a function of equivalence ratio and pressure ratio are shown in Fig.(8). The results are presented for propane fuel. The measured volumetric concentration as a function of equivalence ratio at atmospheric pressure is presented. The diagrams demonstrate that the CO rate of mass emission and the measured volumetric concentration increases steadily with increasing the equivalence ratio, as the amount of fuel in the mixture is increases. The increases of CO levels in lean mixture is a consequence of low temperatures which freezing the oxidation. It can be seen also that the CO emission level is increases as the pressure ratio is increases.

# CONCLUSIONS

On the basis of the theoretical results the following conclusions can be drawn;

- 1-It is possible to carry out gas turbine engine modeling using a simple equilibrium Brayton fuel-air cycle analysis for comparing the ideal performance and pollutant emission levels.
- 2-Hydrogen seems to be a viable alternative fuel with respect to economic, operational and emission considerations.
- 3-Hydrogen provides improved specific power output, specific fuel consumption, specific energy consumption and thermal efficiency relative to propane and ammonia fuels.
- 4-Higher NO emission is produced with the use of hydrogen
- 5-The most important engine operation variables in determining performance and emissions are the equivalence ratio and pressure ratio. The simple analysis undertaken confirms the well documented benefits of lean mixtures and lower pressure ratio for lower emission levels.
- 6-The presented experimental results are in agreement in trends with the results obtained from the thermodynamic analysis.

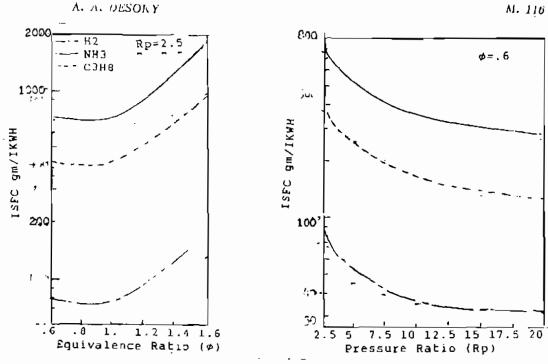


Fig.(5)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on Calculated ISFC.

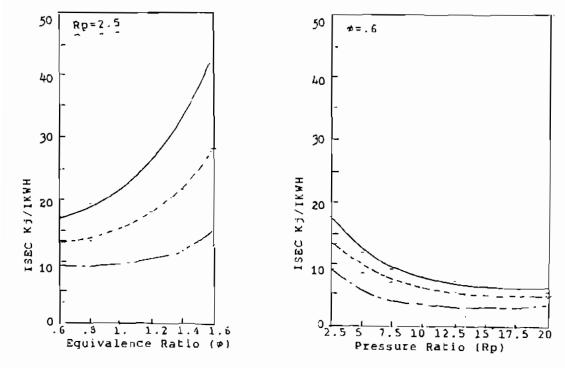


Fig.(6)Effects of Equivalence Ratic, Pressure Ratio and Fuel Type on Calculated ISEC.

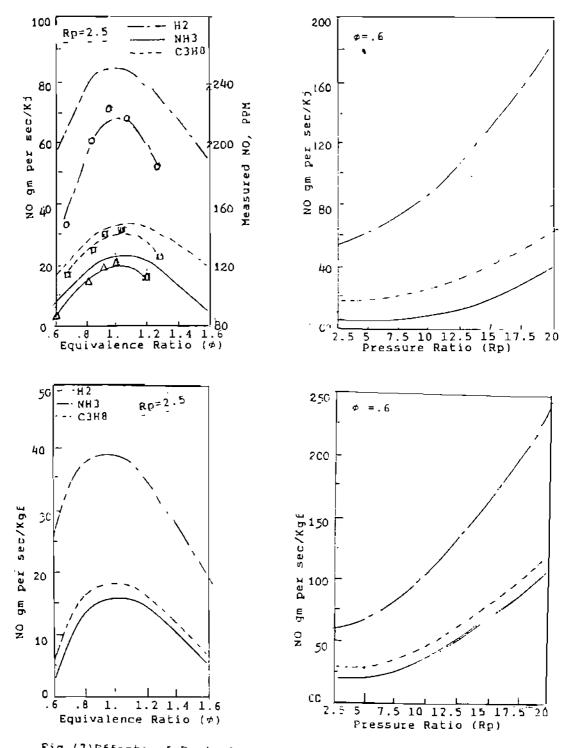


Fig.(7)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on NO Emission.

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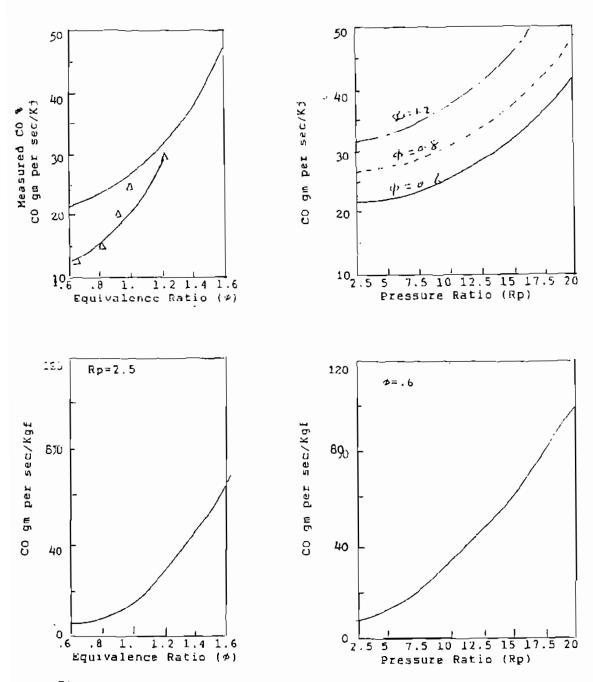


Fig.(8)Effects of Equivalence Ratio, Pressure Ratio and Fuel Type on CO Emission, Fue C3H8

#### NOMENCLATURE

Ср	Constant pressure molar specific heat	Kj/Kmol oK
-	Mean Special Meac 201 att	Kj/Kg oK
Cbdw	Mean specific heat for product gases	κj∕kg oK
hi	Molar specific outholpy for species i	Kj/Kmol
K£i	Forward rate constant for reaction i	Cm**3/mols
Kbi	Backward rate constant for reaction i	Cm**3/mols
MFi	Male fruction of species i	
MNO	Molecular weight of NO	gm/mole
HCO	Molecular weight of CO	gm/mole
ME	Fuel molecular weight	gm/mole
Nair	Number of mole of air	
Np	Number of male of products	
P	Pressure	ata.
R	Gas constant	Kj/mole oK
rt	Expansion ratio	
rр	Pressure ratio	
т	Temperature	oΚ
Wnet	Net work done	Kj/mol air
ф	Equivalence ratio	
7 th	Thermal efficiency	•
$\tau_{ m c}$	Polytropic compressor officiency (assumed 85%)	
7 t	Polytropic turbine efficiency (assumed 05%)	

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