

5-27-2021

Combustion Temperature, Pressure and Products at Chemical Equilibrium of H₂-Air, NH₃-Air and C₃H₈-Air Fuel Mixtures.

Abdel-Raof Desoky

Mechanical Power Engineering Department, Faculty of Engineering, Mansoura University, Mansoura, Egypt.

Azmi Khalaf

Mechanical Power Engineering Department, Faculty of Engineering, Mansoura University, Mansoura, Egypt.

Follow this and additional works at: <https://mej.researchcommons.org/home>

Recommended Citation

Desoky, Abdel-Raof and Khalaf, Azmi (2021) "Combustion Temperature, Pressure and Products at Chemical Equilibrium of H₂-Air, NH₃-Air and C₃H₈-Air Fuel Mixtures.," *Mansoura Engineering Journal*: Vol. 13 : Iss. 1 , Article 11.

Available at: <https://doi.org/10.21608/bfemu.2021.172753>

This Original Study is brought to you for free and open access by Mansoura Engineering Journal. It has been accepted for inclusion in Mansoura Engineering Journal by an authorized editor of Mansoura Engineering Journal. For more information, please contact mej@mans.edu.eg.

COMBUSTION TEMPERATURE, PRESSURE AND PRODUCTS AT CHEMICAL EQUILIBRIUM OF H_2 -AIR, NH_3 -AIR AND C_3H_8 -AIR FUEL MIXTURES

درجات حرارة وضغوط ونواتج الاحتراق عند الاتزان الكيماوي لمخاليط الهيدروجين - الهواء -

الأمونيا - الهواء - البروبان - الهيدروجين - من الوقود

BY

A.A.DESOKY and A.S.KHALAF

Mech.Eng.Dept., EL-Mansoura University, EL-Mansoura, Egypt

الخلاصة - لدراسة التحليل الرياضي للدورات الحرارية لمحركات الاحتراق الداخلي التي تعمل بدائل الوقود من الهيدروجين - الأمونيا - البروبان - والهيدروجين فان ذلك يحتاج الى معرفة خواص غازات الاحتراق في حالة الاتزان الكيماوي . هذه الخواص اما أن تكون في صورة جداول - معادلات رياضية أو خرائط . الفرض من هذا البحث هو عمل نموذج مبدئي رياضية ثرموديناميكية لخواص الغازات الناتجة من عملية الاحتراق في حالة الاتزان الكيماوي بالإضافة الى دراسة معدلات تكوين ملوثات الهواء الجوي الناتجة من عملية الاحتراق من أول أكسيد الكربون وأكسيد النيتروجين . يستخدم هذا النموذج لمعادلة معدل تركيز نواتج الاحتراق وملوثات الهواء الجوي من أول أكسيد الكربون وأكسيد النيتروجين عند احتراق مخاليط مختلفة من بدائل الوقود والهواء عند ضغوط ودرجات حرارة مختلفة . نتائج هذا البحث أعدت في صورة خرائط وجداول عند ضغوط ودرجات حرارة ونسب خلط مختلفة . ولعمل هذه الدراسة استخدم 6 معادلات تفاعل كيماوي في حالة الاتزان بالإضافة الى معادلات التفاعل الخاصة بدراسة معادلات تكوين ملوثات الهواء الجوي مع فرضيات العناصر في حالة اتزان كيماوي .

- وسم الحصول على نتائج في الحالات المختلفة الآتية :
- ١ - مخاليط ووقود غازي من الهيدروجين - الأمونيا - البروبان على الهواء .
 - ٢ - مدى ضغوط من ١ الى ١٠٠ جو .
 - ٣ - مدى درجات الحرارة من ٢٠٠٠ الى ٥٠٠٠ ك .
 - ٤ - مدى من نسب خلط من الوقود والهواء الحقيقي الى النظري من ٠.٦ الى ٢ .

Abstract

For a thermodynamic analysis of engines and gas turbines cycles working with hydrogen, ammonia and propane as fuels, the thermodynamic properties of the combustion gases must be available in the form of equations or charts. This paper deals with the development of a thermodynamic model for the equilibrium products composition with superimposed kinetic NO and CO rates of formation. This model has been used to compare the predicted species concentration, dissociation and NO and CO rates of formation from different fuel-air mixtures combustion in engines and gas turbines.

The results of computations of the combustion products and kinetic NO and CO rates of formation at specified equilibrium temperatures, pressures, and equivalence ratios are plotted in graphs and given in tables. For calculations of the combustion products at chemical equilibrium a set of 6 equilibrium equations enlarged by the energy and mass balance equations is applied. Kinetic mechanisms for NO and CO rate of formation assuming other species at equilibrium and steady state for N atoms are also included. The results are obtained for the following conditions:-

- (1) H_2 -Air, NH_3 -Air and C_3H_8 -Air gases fuel mixtures.
 - (2) Range of pressures, $p=1-100$ ata.
 - (3) Range of temperatures, $T=2000-5000$ K.
 - (4) Range of equivalence ratios $\phi=0.6-2.0$
- Results of few selected conditions are plotted.

1-INTRODUCTION:

The subject of this research is the computation of chemical equilibrium mixture composition for systems containing C,H,O and N atoms. Mixtures of this type are encountered in the working fluid of rocket engines [1], jet engines [2] and reciprocating engines [3]. The methods and procedures of computation of combustion products and of their corresponding thermodynamic state differ according to the computation techniques employed and basic assumptions made. Our discussions will be restricted to mixtures of 10 species with P,T and ϕ known.

There are two reasons for making equilibrium mixture calculations; first, the pressure and temperature that follow combustion in internal combustion engines depend on the character of the mixture of product gases. The temperature reached in the combustion chamber of a rocket depends on the composition of the products of combustion.

On the other hand, the work produced by the working fluid in an engine and the thrust developed in a rocket depend on pressures and temperatures. The other reason for making such calculations, is for the purpose of examining the chemical nature of the product mixture. The character of exhaust emissions from combustion systems has attracted considerable attention in recent years owing to undesirable properties of carbon monoxide CO and nitric oxide NO.

Owing to the extensive production of transportation in recent years, the consumption of petroleum fuel exceeded all of the pre-estimations. Our petroleum supply cannot cope with all the growing demand for a long time. The problem taking place now in researches is the continuous reduction of the petroleum reserves of the world. Nowadays many research centers of the petroleum companies deal with the development and production of substitutes for the natural petroleum fuels. Synthetic fuels resulting from coal gasification and other processes are typical examples for these substitutes [4].

In due course the extensive research initiated by the major fuel and engine companies yielded increasing knowledge of fuel properties and the manner in which they affect engine performance, safety and reliability. This understanding helped to eliminate problems, but from time to time various new problems emerged, as in the late 1960s the growth of public concern over air pollution caused by combustion processes. The chemical equilibrium study of the combustion process with the superimposed kinetic NO and CO rates of formation presented in this paper is stimulated by the need to understand the phenomenon of combustion and emission levels from combustion systems when using alternative gases fuels.

Hydrogen appears to be an ideal fuel for 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]. The main characteristics of hydrogen [6] are listed in Table 1, along with data of other fuels of interest for combustion engines applications, namely propane and ammonia. The properties of kerosene are also listed, as a basis for comparison. From combustion viewpoint, hydrogen is characterized by high flame speeds, wide burning limits, easy ignition, and freedom from soot formation. The exhaust of the hydrogen engine has no carbon compounds. The presence of hydrogen in the mixture increases combustion speed and reduces misfiring. As a result, the lowest specific fuel consumption point is displaced towards lean mixtures. The main drawbacks of hydrogen lie in its very low density and low boiling point, which necessitate the use of large, heavy insulated storage tanks in the engine. It is also quite costly to produce.

potential as a heat sink. Because of its low heat release it is unlikely to be used in aircraft as a main fuel. However it could find application as a secondary fuel in situations where its high cooling capacity could be exploited to advantage. Unlike hydrogen, ammonia is a liquid at relatively reasonable storage pressure (7.5ata at 296K). Moreover, ammonia has been demonstrated as a practical fuel for engine application [6].

Finally, propane fuel is used as a base hydrocarbon gas fuel for comparisons. From inspection of Table 1, it is clear that the characteristics of propane are similar to those of kerosene. Compared with kerosene, it has a lower specific energy, and a lower cooling capacity. Propane has been a motor fuel, as the principal component of L.P.G., for about 50 years [7]. Emission levels with L.P.G. are reported to be less than with hydrocarbon fuels. Like ammonia, it may be stored as a liquid at ambient temperatures by modest pressurization of the fuel tank. Its higher boiling point implies easier handling. Its availability over the long term could however, be limited in some area.

2-ANALYSIS:

The equilibrium composition of the products resulting from a chemical reaction, such as the combustion process can be computed. These computation can be made according to the conditions defining mathematically the laws that govern the reaction process. In a case of chemical reaction in which the equilibrium temperature and pressure are specified constant, these laws are:-

- 1-Equilibrium equation, that is the law of chemical equilibrium.
- 2-Atomic ratio, that is the ratio of elements involved in the chemical reaction.
- 3-Concentration condition as defined by Avogadro's law, Dalton's law and state equation of a gas.

The system equation is then; equilibrium equation, this law is expressed as:

$$K_p = \frac{(n_Y)^Y * (n_Z)^Z}{(n_A)^a * (n_B)^b} * \left(\frac{P}{NT}\right)^{(Y+Z-a-b)} \quad (1)$$

Atomic ratio:--

AC=C/H no. of carbon atoms to no. of hydrogen atoms.

AD=O/H no. of oxygen atoms to no. of hydrogen atoms

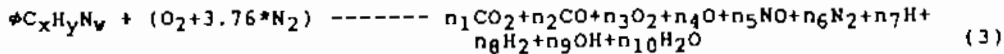
AN=N/H no. of nitrogen atoms to no. of hydrogen atoms.

The concentration condition defines the relation of number of moles n_i , to the state properties P, T of the gaseous mixture. It is derived from Avogadro's law and is expressed in general form by:--

$$n_i = \frac{P_i * V}{R * T} \quad \text{or} \quad n_i = \frac{P_i * V}{R * T} \quad (2)$$

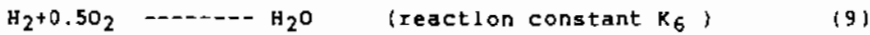
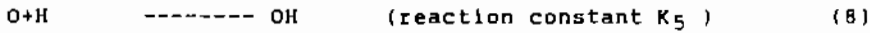
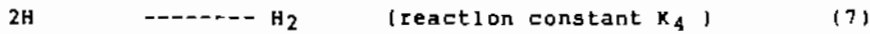
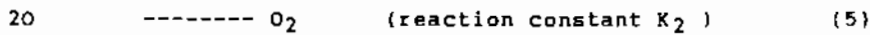
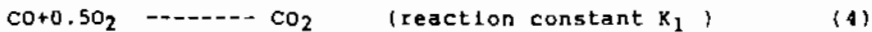
By introducing $PV=RT$, $En_i=p$ and by substituting with Dalton's law $E_{p_i}=P$, $P_i=n_i$ Consequently, in this case, all equations may be expressed either in terms of number of moles n_i or in terms of partial pressure P_i .

In this study, the fuel is represented as $C_xH_yN_w$, where x is the number of carbon atoms in the fuel, y is the number of hydrogen atoms and w is the number of nitrogen atoms. Hence, for a mixture of equivalence ratio ϕ , if one assumes the products of combustion to include only CO_2 , CO , O_2 , O , NO , N_2 , H , H_2 , OH and H_2O , the general combustion equation will be:-



where: $\phi = x + (y/4)$ is the stoichiometric AFR and $n_1, n_2, n_3, \dots, n_{10}$ represented the number of moles of CO_2, CO, O_2, \dots and H_2O respectively per ϕ moles of fuel.

To determine the number of moles $n_1, n_2, n_3, \dots, n_{10}$, the dissociation reactions are considered. In the present case there are six such independent reactions, those used being;



The equilibrium constant (K_i) for the six reactions considered (eqs. 4 to 9) by the equilibrium composition program for a given temperature and pressure are evaluated using a data in the form of fourth order polynomials for possible temperature ranges [8]. These data are shown in Table 2, and the equilibrium constant data is expressed in the form:-

$$\ln(K) = \frac{a}{T} + (b + \frac{c}{T}) * \ln(T) + d \quad (10)$$

Given the reactant mole fractions, and atomic ratios C/H, O/H and N/H, the equilibrium products mole fractions of $CO_2, CO, O_2, O, NO, N_2, H, H_2, OH$ and H_2O at the specified temperature and pressure are calculated. The equations that form the solution enter into the half interval search routine. The general notation is to the next, accumulating values for the 10 mole numbers, which are then checked in a remaining unused equation to see if it is satisfied. The search is continued until the last equation is satisfied. The iterations are started with $n_{10} = (AH/4)$, in the middle of the allowable range. The iterations continue until the change in mole fraction values between successive iterations becomes as small as we like. When the mole fraction change for any species is outside the allowable error, n_{10} is changed:

$$n_{10} = n_{10} + \frac{AH}{2(J+1)} \quad (11)$$

Figs. 1 through 7 are some illustrations of the sort of results obtained from chemical equilibrium calculations. Fig. 1 reveals the profound influence of temperature and equivalence ratio at P=6 atm for H₂-Air mixtures. From this figure it can be seen that, for temperature lower than 2000K, the dissociation has no significant effect on the composition of the combustion gases. This can be seen from figs. (1-a to 1-f), which show the composition of the combustion gases calculated under chemical equilibrium conditions for stoichiometric, weak and rich fuel-air mixtures. Although the combustion gas is assumed to consist of ten components, below 2000^oK only O₂, H₂, H₂O and N₂ exist in appreciable concentrations, so that only these components may be considered.

Writing down the combustion equation of H₂ with air for temperatures below 2000K and neglecting the components which exist in negligible small concentrations:

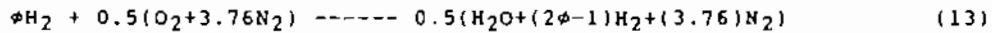
a) for $\phi \leq 1$



Thus the mole fractions of the different components are:-

$$\begin{aligned} n_{10} &= 2\phi / (\phi + 4.76) \\ n_3 &= (1-\phi) / (\phi + 4.76) \\ \text{and } n_6 &= 3.76 / (\phi + 4.76) \end{aligned}$$

b) for $\phi \geq 1$



So that the mole fractions of different components are:-

$$\begin{aligned} n_{10} &= 1 / (2\phi + 3.76) \\ n_8 &= (2\phi - 1) / (2\phi + 3.76) \\ \text{and } n_6 &= 3.76 / (2\phi + 3.76) \end{aligned}$$

Equations 12 and 13 show the influence of ϕ on the mole fraction of H₂, O₂, N₂ and H₂O. The validity of these equations can be checked by calculating the mole fractions of H₂, O, N₂ and H₂O and comparing them with their corresponding values resulting from chemical equilibrium calculations shown in Table 3. This comparison at temperature of 2000K, from this comparison it is clear that these equations can be applied with enough accuracy to calculate the mole fractions of the different components with respect to ϕ .

The results shown in fig.1 also indicated that at higher temperature the mixture will have dissociated products of H, O, NO and OH. Note that the mole fraction for H₂O, the large molecules decrease steadily with increasing temperature, while the mole fraction for the atoms O and H behave oppositely. The diatomic molecules O₂, H₂ and OH all reach maximum at some temperature. So it is not generally known whether they will increase or decrease with a temperature change of small dimension, note how rapidly the composition is changing in the region of 3500K.

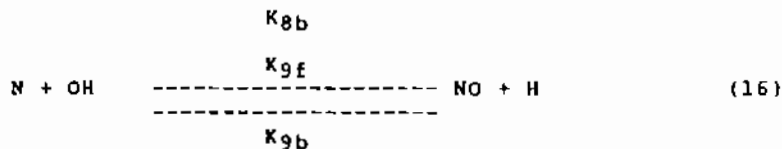
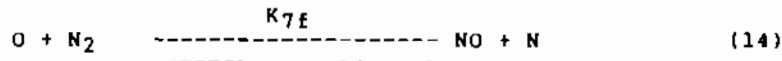
Similar shapes of the mole fraction are obtained for the combustion of NH₃-air fuel mixtures as shown in figs.(3 and 4). Note the similarity with figs.(1 and 2). At low temperatures (less than 2000K)

only the triatomic molecules H_2O , O_2 and N_2 are present, while at high temperatures H , O and OH are present. At 3500K where the composition is changing rapidly, atoms diatomic and triatomic molecules are present in more nearly equal amounts.

Figs. (5 and 6) are an illustrations of the sort of result, obtained from chemical equilibrium composition calculations. They reveal the profound influences of temperature and pressure for a reactant mixture of hydrocarbon (C_3H_8) with air. It can be seen from these figures that below 2000K the mixture consists of CO_2 , H_2O , O_2 and N_2 , but when heated to 5000K at constant pressure the mixture will have changed to comprise CO , H , OH and O . Note that the mole fraction for H_2O and CO_2 , the large molecules, decrease steadily with increasing temperature, while the mole fraction for the atoms O and H behave oppositely. The four diatomic molecules O_2 , H_2 , CO and OH all reach maximum at some temperature, so it is not generally known whether they will increase or decrease with a temperature change of small dimension. Note how rapidly the composition is changing in the region of 3500K. The results shown in fig. 7 are a comparison for the results of calculations obtained for the H_2 -Air, NH_3 -Air and C_3H_8 -Air fuel mixtures. The results reveal the influences of equivalence ratio, pressure and fuel type on chemical equilibrium composition at 3500K. More results are shown in Table 3.

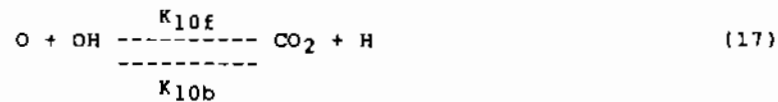
4-KINETIC NO AND CO CALCULATIONS:

The condition favourable to NO formation are those of high temperature, long residence time, high pressure and high oxygen availability. The temperature effect is predominant. Under normal condition, it is generally accepted that NO forms via the extended Zeldovich mechanism:-



The NO formation rates shown in figs. (8 and 9) and Table 3, were computed for such a mechanism, on the assumption of equilibrium concentration of $[O]$, $[O_2]$, $[OH]$, $[H]$ and $[N_2]$ and making the steady state approximation of $[N]$. These results show that for a given temperature, NO production is greatest for stoichiometric and slightly lean mixtures, while it becomes lower for rich mixture. This can be seen for all temperature and fuel type considered. It is clear from these results that nitric oxide formation rates and equilibrium concentrations depend, strongly, upon temperature and equivalence ratio. They decrease substantially as temperature is decreased or as fuel-air ratio becomes extremely fuel-rich or fuel-lean. The effect of fuel type on Nitric Oxide rates of formation is seen to be less profound.

Carbon monoxide is an inevitable intermediate in hydrocarbon combustion. Emission levels of CO can therefore only be minimized by completing as far as equilibrium allows, its oxidation to carbon dioxide. Conditions favourable to its oxidation are high temperature, oxygen availability, high pressure and long residence time. The predominant mechanism for CO oxidation is:-



Assuming this reaction and equilibrium levels of [OH] and [H] it is possible to derive the results presented in fig.9 and Table3, describing the CO production levels in terms of temperature, pressure and equivalence ratio. These results show that for temperature in excess of 2000K, equilibrium carbon monoxide concentrations should be approached rapidly. It is clear that at these temperatures equilibrium carbon monoxide levels are acceptable for equivalence ratios less than unity. As indicated, combustion temperature, pressure and equivalence ratio are major factors in determining CO rates of formation.

S- NOMENCLATURE

K	Equilibrium Constant	
K _{fi}	Forward rate constant for reaction(i)	(Cm ³ /moles)
K _{bi}	Backward rate constant for reaction(i)	(Cm ³ /moles)
n _i	number of moles of species i	
P	Pressure atm	
R	Gas constant	
ppm	Part per million	
T	Temperature °K	
V	Volume	
w	Number of nitrogen atoms in fuel molecule.	
x	Number of carbon atoms in fuel molecule.	
y	Number of hydrogen atoms in fuel molecule.	
φ	Fuel-air equivalence ratio.	
	Stoichiometric fuel-air ratio.	

REFERENCES

1. A.M. Ibrahim and M.M. El-Fawal, Thermodynamic Properties of the Combustion Gases of Hydrogen, S.A.E Paper 841401, Fuels and Lubrication Meeting, Baltimore, Oct. 1984.
2. P. Sampath and F. Shum, Combustion Performance of Hydrogen Gas in a Small Gas Turbine Combustor, 5th World Hydrogen Energy Conference, Toronto, Canada, July 1984.
3. A. Chigier, Energy and Combustion Science, Pergamon Press, 1979
4. A.A. Desoky, A Logical Basis for Advances in Combustion Technology of Spark Ignition Engines, 6th World Hydrogen Energy Conference, Vienna, Austria, July 1986
5. W. Strobl and W. Peschko, Liquid Hydrogen As a Fuel of The Future for Individual Transport, 6th World Hydrogen Energy Conference, Vienna, Austria, July 1986
6. A.H. Lefebvre, Gas Turbine Combustion, McGraw-Hill Book Company, 1976
7. E.S. Starkman, et al, Alternative Fuels for Control of Engine Emission, Journal of Air Pollution Control Association, Vol. 20, No. 2, 1970
- B.A. Campbell, Thermodynamics Analysis of Combustion Engines, John Wiley and Sons, 1979

TABLE I. PROPERTIES OF SOME ALTERNATIVE FUELS

Property	Kerosine	L.H ₂	L.C ₃ H ₈	L.NH ₃
Lower Specific Energy MJ/Kg	42.8	116	46	17.2
Cooling Capacity MJ/Kg	.38-.85	20.2	1.20	3.39
Relative Density(289K)	.80	.071	.585	.682
Specific Heat, KJ/Kg.K	1.97	7.32		
Boiling Point, K	423-573	21	231	240
Freezing Point, K	223	13	91	195
Flame Speed m/sec	.39	2.67	.43	.30

TABLE II COEFFICIENTS FOR CALCULATION REACTION CONSTANTS k_p

Reaction	a	b	c	d
$\text{CO} + .5\text{O}_2 \rightleftharpoons \text{CO}_2$	33805	.7422	165.9	-16.5739
$2\text{O} \rightleftharpoons \text{O}_2$	57126	-.0100	599.0	-16.3201
$\text{O}_2 + \text{N}_2 \rightleftharpoons 2\text{NO}$	-14096	-.6093	-1375.3	9.668
$2\text{H} \rightleftharpoons \text{H}_2$	33587	.5604	3327.	-20.8683
$\text{O} + \text{H} \rightleftharpoons \text{OH}$	44216	-.1319	1298.	-13.1303
$\text{H}_2 + .5\text{O}_2 \rightleftharpoons \text{H}_2\text{O}$	42450	-1.0740	-2147.0	3.2515

TABLE III RESULTS OF CALCULATIONS
 C₃H₈ - AIR FUEL MIXTURE EQUIVALENCE RATIO = 6
 H₂ - AIR FUEL MIXTURES

P T, K	CO ₂	CO	O ₂	Mole Fraction ¹								Mole Fraction ²								Mole Fraction ³								
				H ₂	H ₂	H ₂	H ₂	H ₂	OH	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂	H ₂
18	2000	7.0	22.7	7.42	0.002	1.38	74.4	0.001	0.05	0.57	9.5	20.7	0.05	6.80	0.00	0.004	0.09	72.0	0.43	22.3	0.006	7.39	0.00	0.003	0.08	70.0	0.45	
		3000	5.3	1.62	7.45	0.005	2.53	73.0	0.011	0.26	1.6	9.1	20.6	0.07	5.98	0.01	0.05	0.51	71.3	1.21	22.1	0.07	6.43	0.01	0.06	0.53	69.4	1.24
	4000	3.0	4.0	7.95	0.018	4.81	70.7	0.06	1.31	3.8	7.81	20.0	1.07	4.18	0.34	0.58	2.22	69.4	2.07	21.5	1.09	4.62	0.39	0.61	2.36	67.4	2.14	
	5000	0.95	5.39	4.4	7.67	4.98	63.7	4.77	1.63	4.1	2.4	17.1	4.21	3.66	2.85	2.34	5.12	61.5	3.05	18.3	4.36	3.91	2.90	2.41	5.39	59.5	3.10	
	6000	0.3	5.62	2.43	13.42	4.81	59.5	9.1	1.26	3.01	3.8	12.1	10.6	2.64	12.2	5.94	8.07	45.1	3.24	12.8	10.9	2.79	12.4	6.11	8.42	43.3	3.27	
	7000	0.1	5.56	1.1	17.83	4.0	57.1	12.0	0.64	1.58	0.1	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	8000	0.13	5.58	1.3	15.9	4.37	57.5	11.5	0.77	1.9	0.15	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	24	2000	7.1	0.9	7.25	0.001	1.28	74.5	0.001	0.04	0.05	9.5	20.7	0.05	6.80	0.00	0.004	0.09	72.0	0.43	22.3	0.004	7.39	0.00	0.004	0.08	70.0	0.45
3000			5.7	1.45	7.37	0.005	2.81	73.1	0.01	0.32	1.5	9.1	20.1	0.93	4.19	0.31	0.50	2.07	69.7	2.07	21.6	0.35	4.64	0.31	0.53	2.20	67.7	2.15
4000		3.2	3.78	7.8	0.012	4.77	70.9	0.038	1.17	3.4	8.0	17.5	3.70	3.73	2.31	2.04	4.84	62.6	3.10	18.7	3.83	4.00	2.35	2.11	5.09	60.6	3.15	
5000		1.1	5.21	4.61	6.8	5.12	64.4	4.1	1.61	4.16	2.8	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
6000		0.37	5.63	2.72	12.28	5.11	60.0	8.29	1.39	3.35	0.78	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
7000		0.13	5.58	1.3	15.9	4.37	57.5	11.5	0.77	1.9	0.15	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
8000		0.13	5.58	1.3	15.9	4.37	57.5	11.5	0.77	1.9	0.15	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
30		2000	7.2	0.08	7.32	0.001	1.37	74.5	0.001	0.039	0.05	9.53	20.7	0.04	6.80	0.00	0.003	0.08	72.0	0.43	22.3	0.004	7.39	0.00	0.004	0.08	70.0	0.45
	3000		5.5	1.33	7.3	0.004	2.8	73.2	0.006	0.28	1.4	9.16	20.6	0.09	6.00	0.01	0.07	0.58	71.3	1.21	22.1	0.10	6.42	0.01	0.07	0.61	69.3	1.24
	4000	3.4	3.61	7.65	0.012	4.74	71.0	0.04	1.1	3.2	8.12	17.8	3.34	3.77	1.97	1.84	4.63	63.4	3.14	19.0	3.46	4.04	2.00	1.90	4.87	61.3	3.19	
	5000	1.2	5.23	4.75	6.18	5.22	64.9	3.64	1.58	4.38	3.12	12.4	8.64	2.93	8.52	4.85	7.69	50.2	3.61	14.3	8.97	3.11	8.68	5.00	8.04	48.3	3.65	
	6000	0.43	5.63	2.93	11.41	5.33	60.6	7.65	1.48	3.59	0.97	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	7000	0.15	5.6	1.5	16.1	4.67	57.8	11.0	0.89	2.16	0.20	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	8000	0.15	5.6	1.5	16.1	4.67	57.8	11.0	0.89	2.16	0.20	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	40	2000	7.2	0.015	7.32	0.002	1.37	74.5	0.001	0.034	0.049	9.54	20.7	0.04	6.80	0.00	0.003	0.08	72.0	0.43	22.3	0.004	7.39	0.00	0.003	0.08	70.0	0.45
3000			6.0	1.19	7.23	0.004	2.75	73.2	0.006	0.25	1.3	9.21	20.5	0.71	4.35	0.21	0.40	1.85	70.2	2.12	22.1	0.08	5.42	0.01	0.06	0.57	69.3	1.24
4000		3.7	3.38	7.56	0.012	4.7	71.1	0.035	0.95	0.3	8.27	18.1	2.93	3.82	1.59	1.60	4.35	64.2	3.18	19.4	3.03	4.09	1.62	1.66	4.59	62.2	3.24	
5000		1.4	5.11	4.91	5.44	5.33	65.5	3.1	1.52	4.18	3.54	14.1	7.69	3.07	6.96	4.20	7.42	52.6	3.78	15.0	7.94	3.26	7.08	4.43	7.77	50.6	3.81	
6000		0.52	5.61	3.2	10.32	5.6	61.2	6.84	1.58	3.9	1.24	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
7000		0.19	5.63	1.72	15.0	5.1	58.2	10.3	1.04	2.52	0.300	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
8000		0.19	5.63	1.72	15.0	5.1	58.2	10.3	1.04	2.52	0.300	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
50		2000	7.2	0.015	7.32	0.002	1.37	74.5	0.001	0.03	0.05	9.54	20.7	0.04	6.80	0.00	0.003	0.08	72.0	0.43	22.3	0.004	7.39	0.00	0.003	0.08	70.0	0.45
	3000		6.1	1.1	7.18	0.003	2.78	73.3	0.006	0.22	1.2	9.24	20.6	0.07	5.98	0.01	0.05	0.51	71.4	1.22	22.1	0.07	6.43	0.01	0.06	0.53	69.4	1.24
	4000	3.9	3.2	7.46	0.012	4.67	71.3	0.03	0.90	0.28	8.24	18.4	2.64	3.86	1.35	1.44	4.16	64.8	3.21	19.7	2.74	4.13	1.38	1.49	4.38	62.8	3.27	
	5000	1.6	5.0	5.01	4.97	5.41	65.9	2.22	1.47	4.15	3.85	14.6	7.02	3.16	6.00	3.90	7.20	54.2	3.89	15.6	7.25	3.36	6.05	4.03	7.54	52.2	3.94	
	6000	0.59	5.6	3.39	9.51	5.78	61.8	6.22	1.63	4.05	1.48	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	7000	0.22	5.65	1.91	14.15	5.35	58.6	9.74	1.16	2.81	0.39	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	
	8000	0.22	5.65	1.91	14.15	5.35	58.6	9.74	1.16	2.81	0.39	12.9	9.45	2.81	10.0	5.31	7.87	48.2	3.46	13.6	9.73	2.98	10.1	5.47	8.23	46.2	3.49	

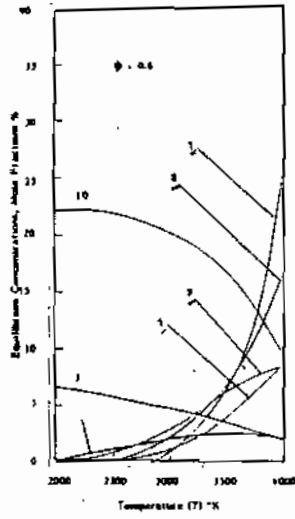


Fig. 11-a)

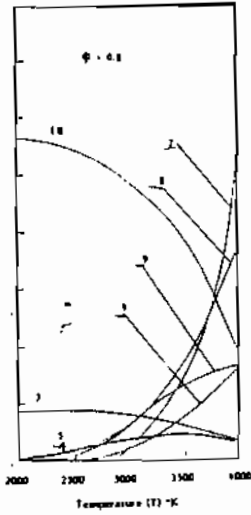


Fig. 11-b)

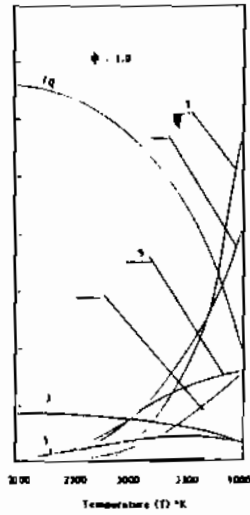


Fig. 11-c)

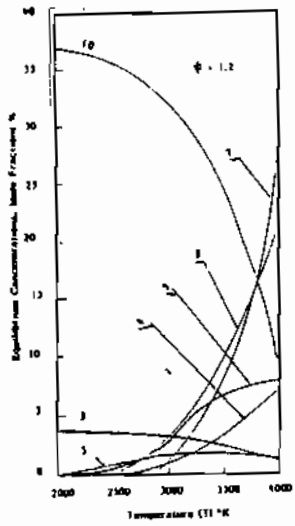


Fig. 11-d)

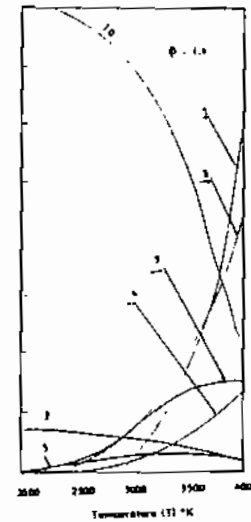


Fig. 11-e)

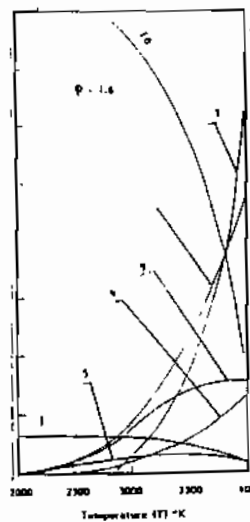


Fig. 11-f)

Figure 11) Equilibrium Composition showing the influence of Temperature and Equivalence ratio for H_2 - Air Mixtures at $p = 1$ atm.

KEY TO FIGURES

FOR C_3H_8 - AIR FUEL MIXTURES

1= nCO_2 , 2= nCO , 3= nO_2 , 4= nO , 5= nNO , 6= nN_2 , 7= nH , 8= nH_2 , 9= nOH , 10= nH_2O

FOR N_2 - AIR AND NH_3 - AIR FUEL MIXTURES,

1= nH_2O , 2= nH_2 , 3= nO_2 , 4= nN , 5= nO , 6= nOH , 7= nN_2 , 8= nNO

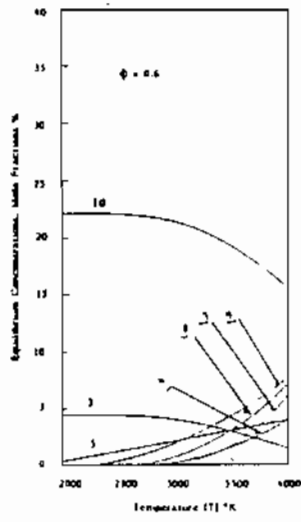


Fig. (2-a)

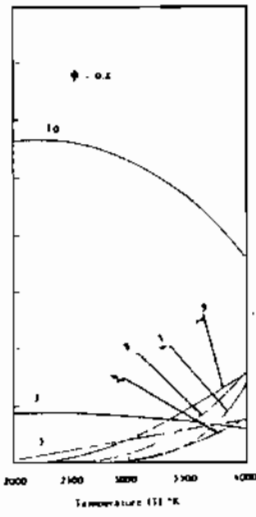


Fig. (2-b)

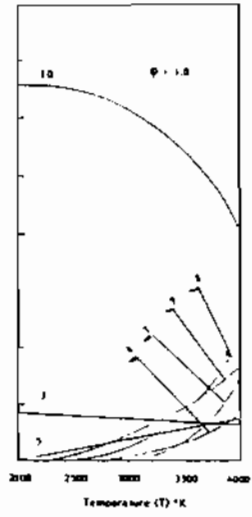


Fig. (2-c)

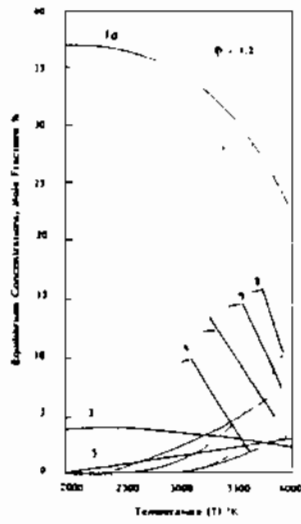


Fig. (2-d)

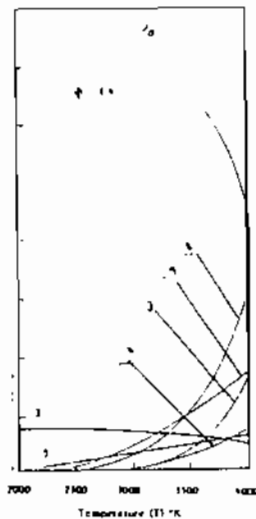


Fig. (2-e)

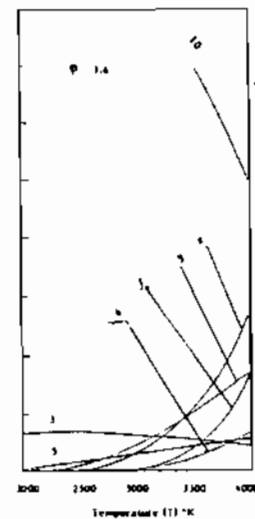


Fig. (2-f)

Figure (2) Equilibrium composition showing the influence of Temperature and Equivalence ratio for H_2 - Ar mixture at $p = 10$ atm.

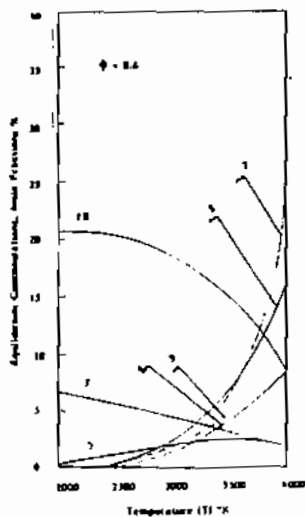


Fig. (12-a)

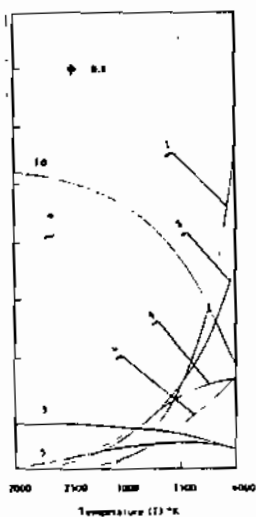


Fig. (12-b)

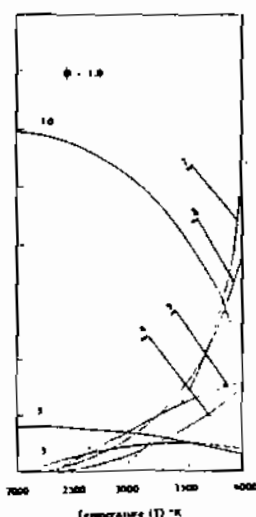


Fig. (12-c)

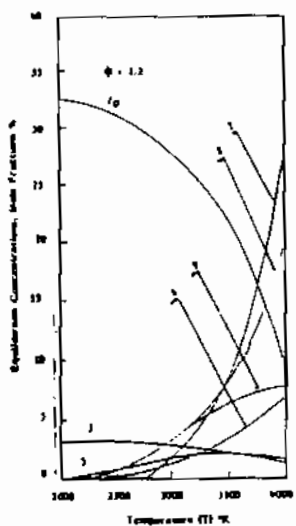


Fig. (13-a)

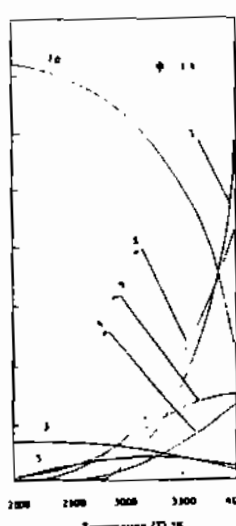


Fig. (13-b)

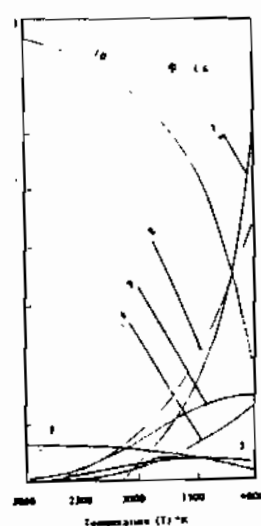


Fig. (13-c)

Figure (13) Equilibrium composition showing the influence of Temperature and Equivalence ratio for PH_2 -Air Mixture at $p=1$ atm.

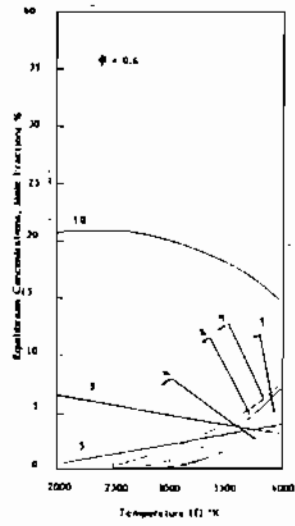


Fig. (4-a)

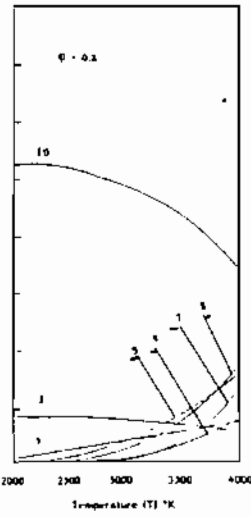


Fig. (4-b)

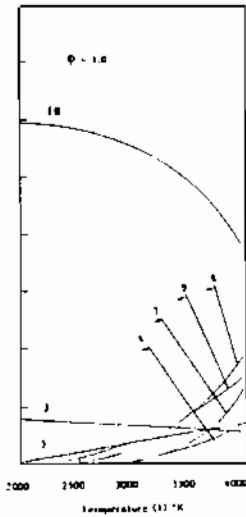


Fig. (4-c)

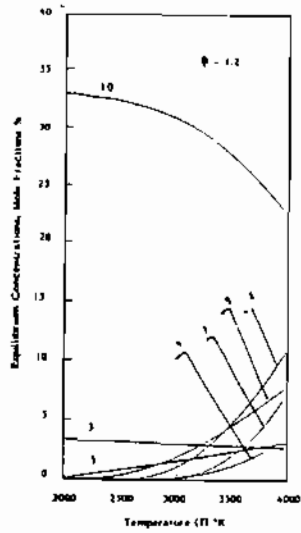


Fig. (4-d)

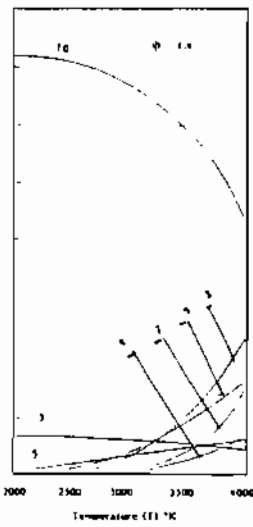


Fig. (4-e)

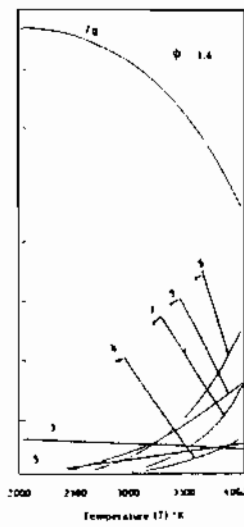


Fig. (4-f)

Figure (4) Equilibrium composition showing the influence of temperature and Equivalence ratio for $NH_3-Al_2O_3$ Mixture at $p=50$ atm.

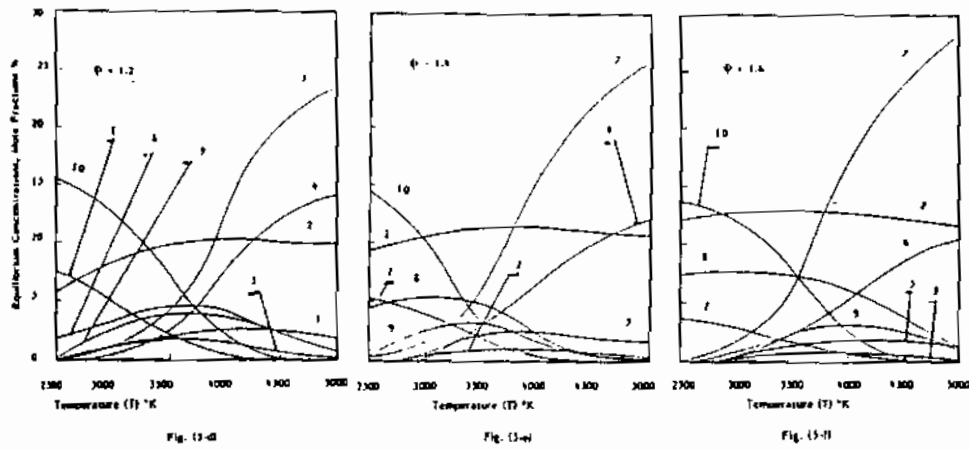
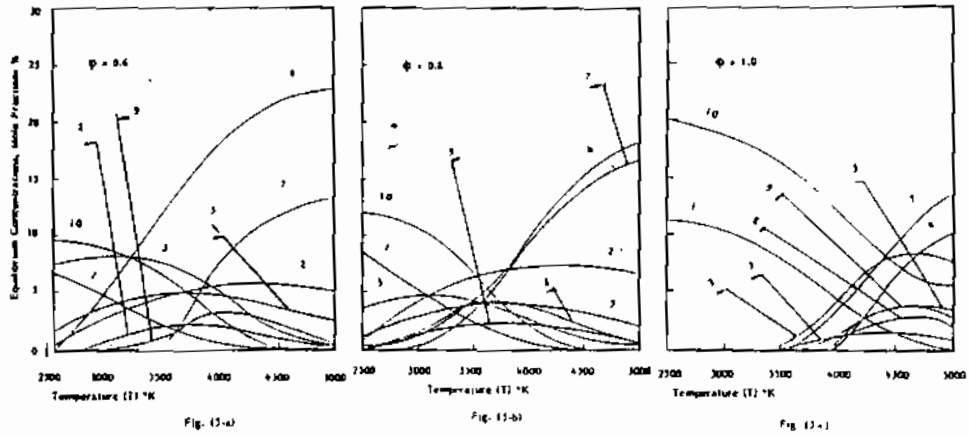


Figure 13: Equilibrium composition showing the influence of Temperature and Equivalence ratio for C₃H₈ Air Mixture at p=6 atm

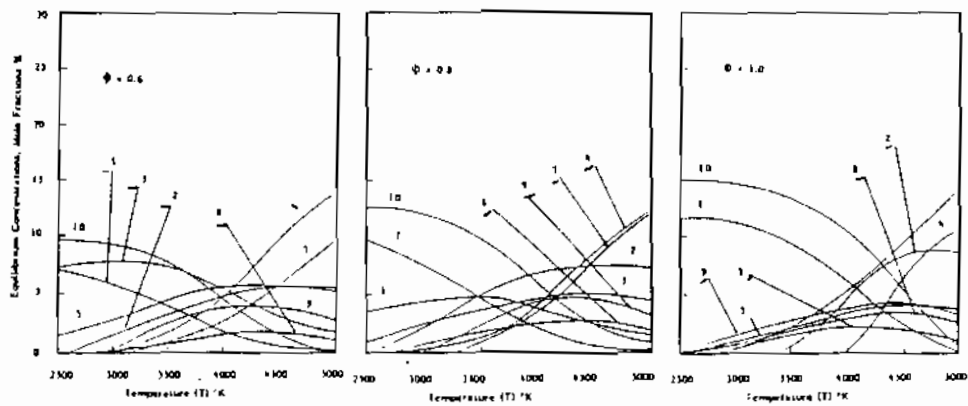


Fig. 16 (a)

Fig. 16 (b)

Fig. 16 (c)

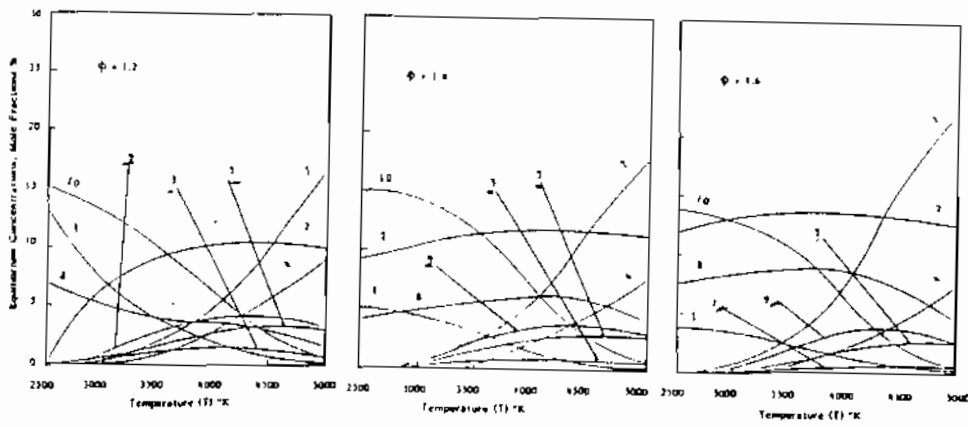


Fig. 16 (d)

Fig. 16 (e)

Fig. 16 (f)

Figure 16) Equilibrium composition showing the influence of Temperature and Equivalence ratio for C_5H_8 -Ar Mixture at p=10 atm

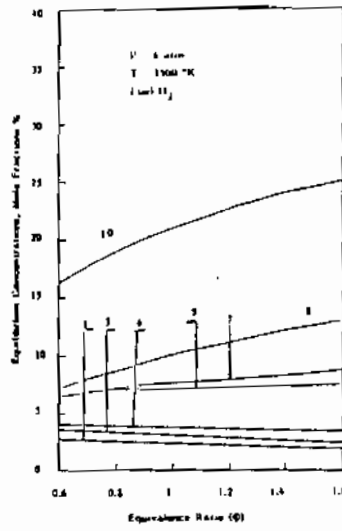


Fig. 17-a)

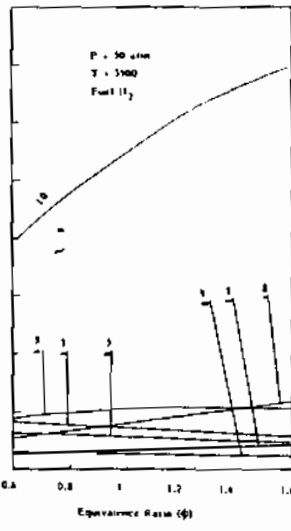


Fig. 17-b)

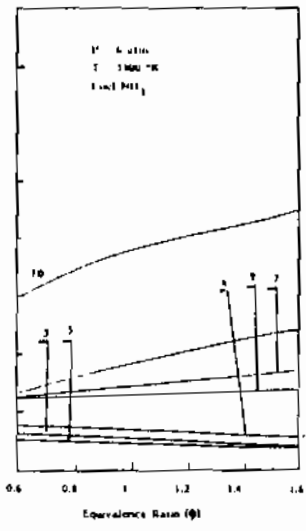


Fig. 17-c)

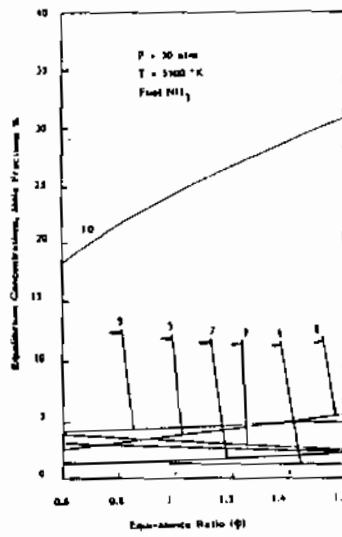


Fig. 17-d)

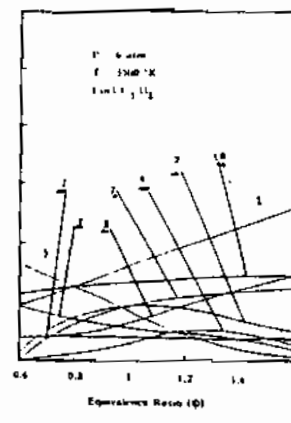


Fig. 17-e)

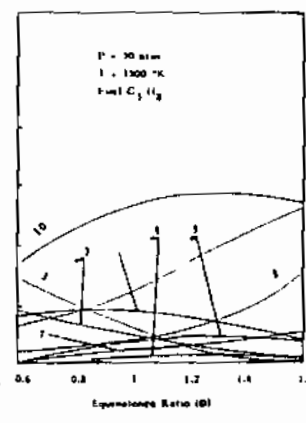


Fig. 17-f)

Figure (7) Equilibrium composition showing the influence of Fuel Type, Equivalence ratio and pressure at T=3000 °K.

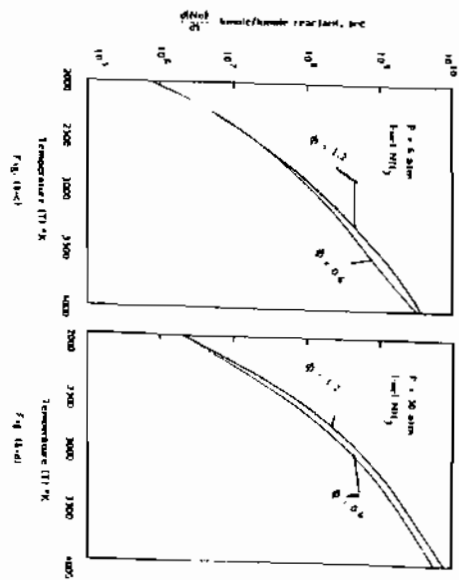
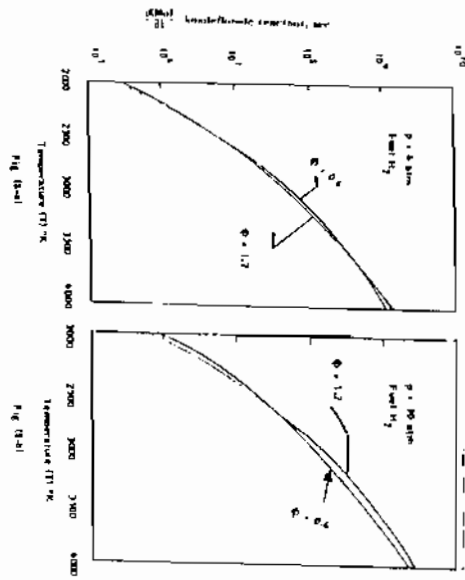


Figure 12) Variation of the rate of formation of benzene and toluene with temperature.

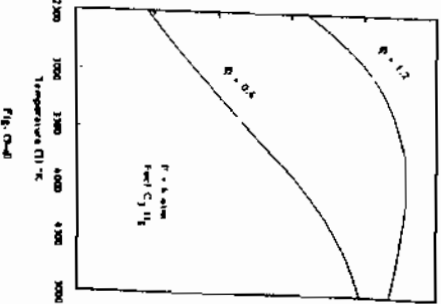
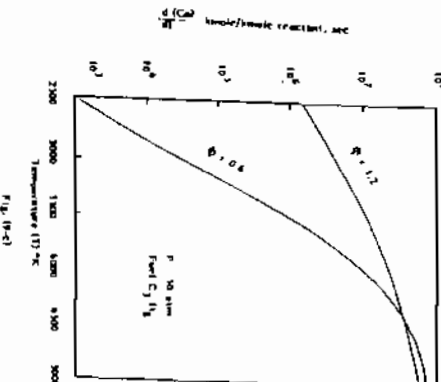
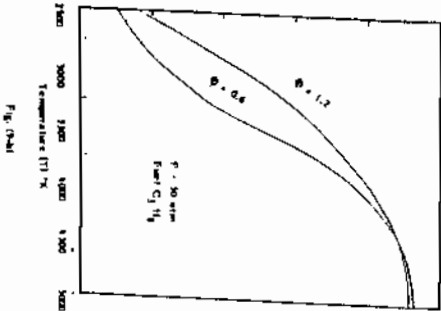
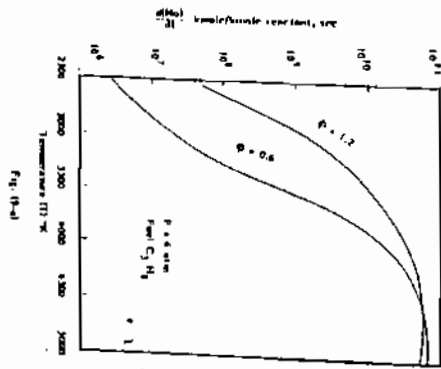


Figure (1) Rate of the CO formation as a function of Temperature and equivalence ratio for C_2H_4 -Air fuel mixture.