THE CALCULATION OF ENTHALPY-ENTROPY DIAGRAMS

FOR ROCKET PROPELLANT SYSTEMS

Thesis by

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ABSTRACT

It is the purpose of this thesis to calculate the data required to construct enthalpy-entropy diagrams for propellant systems and to investigate their usefulness when applied to the determination of rocket motor performance parameters.

Diagrams which cover a range of mixture ratios bracketing the stoichiometric value are included for the following systems:

(1) Liquid Ammonia and RFNA

(2) Liquid Ammonia and Liquid Ozone

(3) Liquid Hydrogen and Liquid Ozone

Graphical performance parameter values obtained for the stoichiometric mixture of liquid ammonia and RFNA differed less than two tenths of one percent from the analytical values calculated by the Jet Propulsion Laboratory.

Performance values are determined for chamber pressures of 600 PSIA and 300 PSIA and for exhaust pressures of 14.7 PSIA, 7.35 PSIA, and .147 PSIA.

Because of the extensive calculations required to construct an h-s diagram, the graphical method of analysis is not economical unless a comprehensive study of a propellant is desired. However, if performance values are required over a wide range of boundary conditions, the h-s diagram permits the presentation of a large amount of data in a concise and readily useable form.

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INTRODUCTION

One of the chief disadvantages of determining rocket motor performance parameters by the analytical methods based on the use of isentropic flow equations is that one set of calculations yields results which are applicable for only a very limited range of physical boundary conditions. For example, values calculated for the expansion to an ambient exhaust pressure of one atmosphere cannot be applied to the evaluation of a motor which is to propel the last stage of a multiple-step rocket. Also, two sets of calculations are required to obtain the performance for both equilibrium and constant composition flow.

One solution to these problems might be the graphical presentation of the fundamental data required to calculate the theoretical performance parameters for rocket motors in such a way as to be useful over a wide range of operating conditions. This technique of using plotted data has been widely used in other fields when analytical methods have proven to be cumbersome. A notable example is the graphical analysis of high speed airplane performance.

It is the purpose of this report to provide enthalpy-entropy diagrams for the products of combustion of several propellent systems, and to investigate their usefulness when applied to the determination of the theoretical performance of rocket motors.

The basic information required for the construction of the h-s diagrams is the chemical composition of the reaction products at appropriate temperatures and pressures. The number of

these component calculations which must be made to construct a given diagram is greater than the number required for the analytical calculation of the performance parameters for one set of boundary conditions, but the diagram permits a much more comprehensive study of the specified propellent system. Also, once the basic diagram is completed, the effort required to plot a new pressure line, and thus permit the evaluation of the system for an entirely different exhaust condition, is not great.

Enthalpy-entropy diagrams for a range of mixture ratios which brackets the stoichiometric value are constructed for the NH_3-RFNA, NH_3-O_3, and H_2-O_3 propellent systems. The NH_3-RFNA system was selected in order that parameter values obtained graphically could be compared with the analytical values being calculated for this system by the Jet Propulsion Laboratory. The NH_3-O_3 and H_2-O_3 systems were chosen for two reasons: first, because of the current interest in liquid ozone as an oxidant; and second, because these systems represent, respectively, an intermediate and a very hot system, while the NH_3-RFNA system is a relatively cool one. As a result, the complete set of diagrams covers a temperature range up to $4000^{\circ}K$. The reason for the interest in liquid ozone is the large negative value of its heat of formation.

The remaining portion of the text of this report is divided into the following parts:

(1) Discussion of Assumptions and Introduction of Parameters.

(2)   Sample Calculation.

(3)   Discussion of Results.

(4)   Conclusions and Recommendations.

In part (1) the assumptions made in calculating the thermo-dynamic data used in the construction of the h-s diagrams are emphasized, and an attempt is made to clearly define the reference levels for all values used. The assumptions which must be considered when the diagrams are used to calculate performance are also included in order that the limitations of the graphical method be understood.

The sample calculation in part (2) is carried out in sufficient detail that the reader should be able to readily check any desired value by following the exact procedure used in the original computation. Because of the wide range of temperatures and pressures for which minor component calculations were made, certain trends in the computed values were noticed which probably would not show up in a single analytical calculation. Methods for utilizing these trends when making an extensive set of computations are explained.

It should be noted in connection with parts (3) and (4) that the discussion of results and the conclusions drawn from this analysis are based upon the study of theoretical maximum values of the performance parameters, and that no experimental data was available for comparison. For this reason, the construction of the diagrams themselves is emphasized rather than the particular values derived from them.

LIST OF SYMBOLS

a   Number of moles of H_2 in the reaction products

b   Number of moles of H_2O in the reaction products

c   Number of moles of CO in the reaction products

d   Number of moles of CO_2 in the reaction products

e   Number of moles of O_2 in the reaction products

f   Number of moles of N_2 in the reaction products

g   Number of moles of NO in the reaction products

h   Number of moles of OH in the reaction products

i   Number of moles of H in the reaction products

j   Number of moles of O in the reaction products

C   Number of gram atoms of carbon in the reactants

H   Number of gram atoms of hydrogen in the reactants

N   Number of gram atoms of nitrogen in the reactants

O   Number of gram atoms of oxygen in the reactants

K_p Equilibrium constant based on the ratios of partial pressures

K_n Equilibrium constant based on the ratios of mole fractions

K_1, K_2 etc.   Particular equilibrium constants based on the ratios of mole fractions of the component gases in given reactions

$n^{T^{O}K}$ Total number of moles of the reaction products at $T^{O}K$

$n_i^{T^{O}K}$ Number of moles of the i_{th} component of the reaction products at $T^{O}K$

T_c Temperature of reaction products in the rocket motor chamber before expansion through the nozzle

T_e Temperature of reaction products after expansion through the nozzle

p_c Chamber pressure in pounds per square inch absolute

p_e Exhaust pressure in pounds per square inch absolute

$\Delta H_i{}^{T^{O}K}_{300^{O}K}$ Sensible heat of the i_{th} component of the reaction products at $T^{O}K$ as referred to the defined reference state

$\Delta H^{T^{O}K}_{300^{O}K}$ Total enthalpy of the reaction products at $T^{O}K$ whose reference state is the equilibrium composition at $300^{O}K$

$Q^{T^{O}K}_{av}$ Heat released in kcals by a combustion reaction at $T^{O}K$

Q_{f_i} Heat of formation of the i_{th} component of the reaction products at $300^{O}K$

m Number of grams of propellent mixture

$\Delta h^{T^{O}K}_{300^{O}K}$ Total enthalpy per gram of the reaction products at $T^{O}K$ whose reference state is the equilibrium composition at $300^{O}K$

$S^{O}_{T^{O}K}$ Total absolute entropy of the reaction products at $T^{O}K$ and a pressure of p atmospheres

$S^{O}_{iT^{O}K}$ Absolute entropy of the i_{th} component of the reaction products at $T^{O}K$ and a pressure of one atmosphere

$s^{O}_{T^{O}K}$ Absolute entropy per gram of the reaction products at $T^{O}K$ and a pressure of p atmospheres

R_u Universal gas constant, equal to 1.986 calories per
gram mole per degree Kelvin

c   Effective exhaust velocity in feet per second

J   Mechanical equivalent of heat, equal to 4.186×10^{10}
ergs per kcal

I_{sp} Specific impulse in pounds of thrust per pound of
propellent burned per second

g   Acceleration of gravity (arbitrarily fixed at 32.16
feet per second in this report)

r   Mixture ratio. The ratio of the weight of oxidant
to the weight of fuel in a propellent system

RFNA   Red fuming nitric acid (nitric acid with 6.8% of NO_2)

PART I: DISCUSSION OF ASSUMPTIONS AND INTRODUCTION OF PARAMETERS

The assumptions upon which this analysis is based must include both those which are involved in the construction of the diagrams themselves, and any additional ones that are required when the diagrams are used in the calculation of rocket motor performance parameters. The first group includes the following:

(1) The equation of state is $pv = nRT$.

Note: The source of the enthalpy and entropy tables used is the report on "Thermochemistry and the Equation of State of the Propellent Gases" by Hirshfelder, McClure, and Curtiss, reference (2). The basic equation of state used in this report is a van der Waals equation for which corrections have been made for the overlapping of hard spheres. However, this corrected equation was not used in the calculation of enthalpy and entropy values, and the perfect gas law must be assumed.

(2) There is no Joule-Thompson effect. That is, for a constant temperature, enthalpy does not vary as the pressure changes.

(3) There is no enthalpy change on mixing.

(4) The reference state for all enthalpy values plotted

is the equilibrium composition at $300^{\circ}K$ and a pressure of one atmosphere of the gas mixture containing the reaction products, at which thermodynamic state the enthalpy of the mixture is considered to be zero. It should be noted that for all practical purposes this is equivalent to saying that at the reference state minor components have disappeared.

This qualification upon the reference state that there be no minor components present is not readily apparent because the tabulated values of enthalpy are all zero at $300^{\circ}K$. However, if we consider the equilibrium expansion through a nozzle of a specified propellent mixture to a temperature at which no significant amounts of the minor components remain, it is obvious that the heat which has appeared due to the recombination of these minor components represents an increase in energy which is available to produce an increase in the velocity of the propellent mixture. Thus, the enthalpy value of a point on the h-s diagram must represent not only the sensible heat above $300^{\circ}K$ contained in the gas mixture at the temperature corresponding to the point, but also the heat which is required to shift the equilibrium from that at the reference state to that at the thermodynamic state represented by the point. This latter increment of heat is exactly that which in an equilibrium expansion is made available for increased performance.

In a constant composition expansion the entire enthalpy drop is due to the change in the sensible heat, and in probably no actual expansion is equilibrium ever completely

maintained. In general, the enthalpy change for an expansion will be somewhat greater than the change in sensible heat due to the temperature drop but less than the sum of the sensible heat change and the heat which would be rejected from the gas mixture if equilibrium were maintained.

It is necessary to define some reference level for enthalpy values because there is no thermodynamic state at which we can say that the enthalpy of all substances is zero. For this reason, it is not possible to determine absolute enthalpy values, and any value used must be referred to some reference state.

(5) The tabulated entropy values used are absolute values of entropy of the gas components calculated at a temperature of $T^{\circ}K$ and a pressure of one atmosphere and considering the components to be pure perfect gases.

Because of the Third Law of Thermodynamics, which states that the entropy of most crystals at the absolute zero may be taken as zero, it is possible to define and to determine absolute entropies. Therefore, it is not necessary to define a reference state for entropy values in the same sense that one was defined for enthalpy values.

(6) All minor components are considered except atomic nitrogen (N). None of the adiabatic flame temperatures for the NH_3-RFNA and NH_3-O_3 systems greatly exceeds $3000^{\circ}K$, and for

this temperature range previous calculations have shown this assumption to be justified.

(7) Over a temperature range of $100^{\circ}K$ the variation of temperature dependent quantities such as gas mixture composition with temperature is assumed to be linear.

(8) The equipartition of energy among the electronic, vibrational, and rotational energy levels is assumed to be instantaneous during the combustion and expansion processes for both equilibrium and constant composition flow.

(9) The pressure lines on the h-s diagrams which represent equilibrium flow are calculated assuming that the composition of the products of the combustion reaction changes continuously to maintain the equilibrium composition corresponding to the prevailing thermodynamic state, and that the energy released by this equilibrium shift is completely available for conversion into energy of motion.

(10) The pressure lines on the h-s diagrams which represent constant composition flow are calculated assuming that the composition of the products of the combustion reaction remains constant and equal to the equilibrium composition at the adiabatic flame temperature T_c.

In using the h-s diagrams to calculate rocket motor performance parameters it is necessary to make the following additional assumptions:

(11)   The reaction of the propellent mixture proceeds to completion in the rocket motor chamber, and sufficient time is available for the equilibrium concentration of all components to be established at the adiabatic flame temperature determined by the mass and heat balance.

(12)   Viscous effects are neglected. That is, all flow is considered to be isentropic.

(13)   The gas flow through the nozzle is steady.

(14)   The gas flow leaving the nozzle is axial.

(15)   The velocity of the gas mixture in the combustion chamber is assumed to be negligible in comparison with the effective exhaust velocity.

(16)   Gravity effects are neglected.

(17)   The nozzle is always correctly expanded for the ambient exhaust pressure. If this pressure varies, the assumption of a "rubber nozzle" must be made.

The performance parameters which are considered in this report are:

(1) The effective exhaust velocity c . Unless otherwise indicated all values of the effective exhaust velocity referred to in this analysis are those defined by the equation

$$c = \text{constant } \sqrt{\Delta h}$$

where Δh is the enthalpy change for an isentropic expansion. Because of the assumptions made these are theoretical maximum values. In practical design work, an experimental value of c is obtained by dividing the measured value of thrust by the mass flow rate. This experimental value includes pressure, friction, and divergence effects, and is somewhat less than the value defined above.

(2) The specific impulse I_{sp}. The specific impulse of a propellent may be defined as the thrust per unit weight-rate of flow or the pounds of thrust per pound of propellent burned per second. It is obtained from the equation

$$I_{sp} = c/g$$

where g is the acceleration of gravity.

PART II: SAMPLE CALCULATION FOR AN OVER-OXIDIZED MIXTURE

OF LIQUID AMMONIA AND LIQUID OZONE

The objective of this section is to present in a logical
sequence the calculation of the data required to construct an
enthalpy-entropy diagram and the calculations involved in
applying the diagrams to the determination of rocket motor per-
formance parameters.

The products of reaction resulting from the combustion of
100 grams of liquid ozone and 50.0945 grams of liquid ammonia
are considered. This is an over-oxidized system (mixture ratio
1.996), and it is chosen because the minor component values for
this case are more sensitive to changes in the estimated quan-
tities than for stoichiometric and under-oxidized systems. This
sensitivity, and methods for solving the resulting complicat-
ions, are discussed.

Data for the point on the h-s diagram corresponding to a
temperature of $3200^\circ K$ and a pressure of 300 PSIA (20.408
atmospheres) is obtained. In compiling the thermodynamic data
from which to construct the charts, minor component calculations
had already been made for this pressure at $2500^\circ K$, $3000^\circ K$, and
$3500^\circ K$, and from a plot of the sensible heat of the products of
reaction and the heat available from the reaction versus temper-
ature the adiabatic flame temperature T_c had been estimated to
lie between $3200^\circ K$ and $3300^\circ K$.

STEP A: MINOR COMPONENT CALCULATIONS.

The object of this step is to obtain the equilibrium composition of the products of reaction at $3200°K$ and 300 PSIA with the value of each component correct to the nearest thousanth of a mole. The equations used are those developed by Dr. David Altman and Dr. Sidney Weinbaum of the Jet Propulsion Laboratory. This development is presented in Appendix I.

The equation for this reaction at elevated temperatures is

$$2.9412 \ NH_3 + 2.0833 \ O_3 = aH_2 + bH_2O + eO_2 + fN_2 + gNO + hOH$$
$$+ iH + jO$$
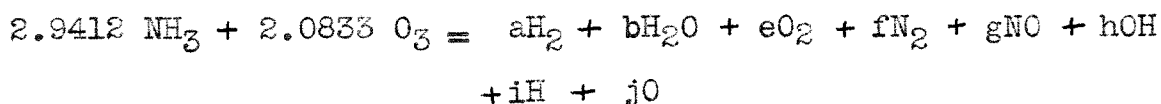
where the reactants are in the liquid state.

From Appendix I the equations to be solved are:

(I) $\quad b = \dfrac{H - 2a - K_9 a^{\frac{1}{2}}}{2 + \dfrac{K_{10}}{a^{\frac{1}{2}}}}$

(II) $\quad g = O - b \left[1 + \dfrac{K_{10}}{a^{\frac{1}{2}}} + \dfrac{K_7}{a} + \dfrac{2K_6 b}{a^2} \right]$

(III) $\quad \dfrac{2g^2 a^2}{K_3^2 \ b^2} + g - N = F(III) = 0$

$e = \dfrac{b^2}{a^2} K_6 \qquad f = \tfrac{1}{2}(N - g) \qquad h = \dfrac{b}{a^{\frac{1}{2}}} K_{10}$

$i = a^{\frac{1}{2}} K_9 \qquad j = \dfrac{b}{a} K_7$

All equilibrium constants in the above equations are those based on the ratios of mole fractions of the components in the reaction products.

From the reaction equation, the reactants represent a combined weight of 150.094 grams, and the values for the number of gram atoms of hydrogen, oxygen, and nitrogen are:

$$H = 8.8236$$
$$O = 6.2500$$
$$N = 2.9412$$

Annother equation which is used as a check for "g" is

$$\frac{g\ a}{f^{\frac{1}{2}}\ b} = K_3$$

Steps in the calculation are as follows:

(1) A value of "n", the total number of moles of the reaction products at $3200^{\circ}K$ and 300 PSIA, is assumed. Unless some data or previous results are available on which to base an estimate, this value of "n" must be a guess. However, the calculations are not too sensitive to errors in "n", and the second or third estimate based on the value obtained in previous trials should be close enough. The calculations are repeated until the derived value agrees with the estimated value to the desired degree of accuracy. In this case, component calculations for $2500^{\circ}K$, $3000^{\circ}K$, and $3500^{\circ}K$ had already been made. A plot of "n" versus temperature was prepared, and from this plot the value of "n"

at 3200°K was estimated to be 7.15. Using this value of "n",
the values of the necessary equilibrium constants based on the
ratios of mole fractions are determined from the tabulated
values of the corresponding constants based on the ratios of
partial pressures.

The resulting values are:

$$K_3 = .007659$$
$$K_6 = .002472$$
$$K_7 = .006672$$
$$K_9 = .1665$$
$$K_{10} = .06434$$

All numerical values in this calculation are carried to at
least four significant figures unless it is obvious that the de-
sired accuracy will not be sacrificed by carrying less.

(2) A value of "a", the number of moles of H_2 in the reaction
products at 3200°K is assumed. This value must also be a guess
unless previous results are available on which to base an esti-
mate. Here a plot of "a" versus temperature similar to that for
"n" was prepared, and the value at 3200°K was estimated to be
.215.

(3) Using the above estimated values of "n" and "a", equations
I, II, and III are solved with the result that F(III) is equal
to - 2.1234. This negative value of F(III) indicates that .215
is too small a value of "a". From the variation of F(III) with
"a" for previous calculations, it is estimated that "a" must be

increased by about four thousanths.

(4) The solution of equations I, II, and III is repeated for
"a" equal to .219 and for "a" equal to .220. The corresponding
values of F(III) obtained are - .2507 and   .3866. Solving for
all minor component values for these two values of "a", the
results are:

a	.219	.220
b	3.8866	3.8862
e	.7786	.7713
f	1.3940	1.3856
g	.1531	.1700
h	.5343	.5331
i	.0779	.0781
j	.1184	.1179

It is obvious from the above results that "g" and "e" are
extremely sensitive to changes in "a", while the other compon-
ents are relatively insensitive. This extreme sensitivity is not
typical of stoichiometric and under-oxidized systems, and when
"a" has been determined for these systems to the nearest thous-
anth of a mole, other component values will also be correct to
the same degree of accuracy or so nearly so that necessary cor-
rections can be made by means of an atom balance check. For this
case, however, it is necessary to estimate a new value of "a" to
four decimal places. This is done by plotting F(III) versus "a"
and linearly interpolating for F(III) equal to zero. A value of

"a" equal to .2194 is thus obtained.

(5) Solving equations I, II, and III with "a" equal to .2194, F(III) is equal to .0397, and other values are as follows:

$$
\begin{array}{ll}
a & .2194 \\
b & 3.8865 \\
e & .7756 \\
f & 1.3900 \\
g & .1611 \\
h & .5339 \\
i & .0780 \\
j & .1182 \\
n & 7.1627
\end{array}
$$

The derived value of "n" is now compared with the estimated value. The difference is .0127. Since this is larger than the arbitrarily chosen maximum allowable error of .01, a new value of "n" equal to 7.163 is assumed, and the entire process is repeated.

(6) Using the value 7.163 for "n", the equilibrium constants are:

$$
\begin{array}{ll}
K_3 = & .007667 \\
K_6 = & .002476 \\
K_7 = & .006683 \\
K_9 = & .16667 \\
K_{10} = & .06440
\end{array}
$$

(7) Since the error in the value of "n" derived above was only slightly larger than that allowable, the component values will change very little, and it is still reasonably certain that the value of "a" will lie between .219 and .220. In order to definitely determine which of these is the closer value, the calculations are now repeated with "a" equal to .2195.

(8) Using the value .2195 for "a", the value of F(III) is - .0290. The value of "a" correct to the nearest thousanth of a mole is then .220. Using the check equation for "g", the correct value is found to be .160. Final results rounded to three decimal places are:

a	.220
b	3.886
e	.776
f	1.391
g	.160
h	.534
i	.078
j	.118
n	7.163

Making an atom balance check:

$$H = 8.824$$
$$O = 6.250$$
$$N = 2.942$$

None of these values differs more than .001 from the value
as determined from the reactants. Also, "n" checks exactly with
the assumed value, and all component values can now be considered
accurate to the desired degree.

STEP B: CALCULATION OF THE ADIABATIC FLAME TEMPERATURE T_c.

When the procedure as outlined in step A is carried out
for 3300°K, the following results are obtained:

	3200°K	3300°K
a	.220	.286
b	3.886	3.751
e	.776	.767
f	1.391	1.385
g	.160	.172
h	.534	.634
i	.078	.116
j	.118	.159
n	7.163	7.270

The adiabatic flame temperature T_c is defined as that tem-
perature at which the sensible heat of the combustion reaction
products is equal to the heat released by the reaction at 300°K.

The sensible heat is defined by:

$$\text{Sensible Heat} = \sum n_i^{T°K} \; \Delta H_i {}^{T°K}_{300°K}$$

where "n_i" is the number of moles of the i_{th} component of the

combustion reaction products at the temperature indicated by the superscript ("n_i" = "a", "b", "e" etc.), and "ΔH_i" is the sensible heat of the i_{th} component of the reaction products at the temperature indicated by the superscript and as referred to the defined reference state. The values of "ΔH_i" as defined here are the enthalpy values tabulated in Table II.

The heat released by the combustion reaction is defined by:

$$Q_{av}^{T^\circ K} = \sum n_i^{T^\circ K} Q_{f_i} - Q_f \text{ (Reactants)}$$

where "Q_{f_i}" is the heat of formation of the i_{th} component of the reaction products.

In this case:

$$\sum n_i^{3200^\circ K} \Delta H_{i\,300^\circ K}^{3200^\circ K} = .220 \times 22.927 + 3.886 \times 33.006$$
$$+ .776 \times 25.344 + 1.391 \times 23.947$$
$$+ .160 \times 24.519 + .534 \times 23.227$$
$$+ .078 \times 14.405 + .118 \times 14.405$$

$$= 205.432 \text{ kcals per } 7.163 \text{ moles}$$
$$\text{or per } 150.094 \text{ grams.}$$

$$\sum n_i^{3300^\circ K} \Delta H_{i\,300^\circ K}^{3300^\circ K} = .286 \times 23.818 + 3.751 \times 34.362$$
$$+ .767 \times 26.308 + 1.385 \times 24.837$$
$$+ .172 \times 25.421 + .634 \times 24.121$$
$$+ .116 \times 14.901 + .159 \times 14.901$$

$$= 214.044 \text{ kcals per } 7.270 \text{ moles}$$
$$\text{or per } 150.094 \text{ grams.}$$

$$Q_{av}^{3200°K} = 3.886 \times 57.798 + .160 \times (-21.6) + .534 \times (-10.06)$$
$$+ .078 \times (-52.089) + .118 \times (-59.159)$$
$$- 2.9412 \times 16.07 - 2.0833 \times (-31.6)$$

$$= 223.090 \text{ kcals per } 7.163 \text{ moles}$$
$$\text{or per } 150.094 \text{ grams.}$$

$$Q_{av}^{3300°K} = 3.751 \times 57.798 + .172 \times (-21.6) + .634 \times (-10.06)$$
$$+ .116 \times (-52.089) + .159 \times (-59.159)$$
$$- 2.9412 \times 16.07 - 2.0833 \times (-31.6)$$

$$= 209.617 \text{ kcals per } 7.270 \text{ moles}$$
$$\text{or per } 150.094 \text{ grams.}$$

Using a linear interpolation to find at what temperature the heat released is equal to the sensible heat of the reaction products, the result is

$$T_c = 3280°K.$$

STEP C: CALCULATION OF ENTHALPY VALUES.

The enthalpy of a gas mixture at a temperature of $T^O K$ whose reference state is the equilibrium composition at $300^O K$ is given by:

$$\Delta H_{300^O K}^{T^O K} = \sum n_i^{T^O K} \Delta H_{i 300^O K}^{T^O K} + \sum \left(n_i^{300^O K} - n_i^{T^O K} \right) Q_{f_i}$$

where all symbols are the same as previously defined.

$$\Delta H_{300^O K}^{3200^O K} = 205.432 + (4.412 - 3.886) \times 57.798$$
$$- .160 \times (-21.6) - .534 \times (-10.06)$$
$$- .078 \times (-52.089) - .118 \times (-59.159)$$

$$= 255.705 \quad \text{kcals per 7.163 moles}$$
$$\text{or per 150.094 grams.}$$

The enthalpy value plotted is defined by:

$$\Delta h_{300^O K}^{T^O K} = \Delta H_{300^O K}^{T^O K} \Big/ m$$

where "m" is the number of grams of propellent mixture, in this case 150.094 grams.

$$\Delta h_{300^O K}^{T^O K} = \Delta h_{300^O K}^{3200^O K} = \frac{255.705}{150.094}$$

$$= 1.704 \quad \text{kcals per gram.}$$

Pressure lines on the h-s diagram whose enthalpy values are calculated using $\Delta H_{300^{\circ}K}^{T^{\circ}K}$ as defined above correspond to equilibrium flow because the value $n_i^{T^{\circ}K}$ continuously changes as the equilibrium shifts. If pressure lines corresponding to constant composition flow are desired, it is necessary only to replace $n_i^{T^{\circ}K}$ by $n_i^{T}c$ in the equation for $\Delta H_{300^{\circ}K}^{T^{\circ}K}$. The second summation term becomes a constant value which is always greater than the value when $n_i^{T^{\circ}K}$ is used. The enthalpy value for a temperature of $T^{\circ}K$ and corresponding to constant composition flow is therefore larger than the value at $T^{\circ}K$ corresponding to equilibrium flow. Because the heats of formation of the minor components are negative, the fact that the minor components do not disappear in a constant composition flow means that less of the total heat present in the gas mixture during such a flow is sensible, and as a result T_e and the exhaust velocity are both less than the values for equilibrium flow.

It should also be noted that when equilibrium flow is being considered and enthalpy values are being calculated for temperatures less than $2000^{\circ}K$, the second summation term in the equation for $\Delta H_{300^{\circ}K}^{T^{\circ}K}$ is zero because for these temperatures the composition of the gas mixture is assumed to be the same as the equilibrium composition at $300^{\circ}K$.

STEP D: CALCULATION OF ENTROPY VALUES.

The total absolute entropy of a gas mixture at $T^{\circ}K$ and an absolute pressure of "p" atmospheres is given by:

$$S^{\circ}_{T^{\circ}K} = \sum n_i^{T^{\circ}K} S^{\circ}_{i_{T^{\circ}K}} - n^{T^{\circ}K} R_u \ln p$$

$$- \sum n_i^{T^{\circ}K} R_u \ln \left(n_i/n \right)^{T^{\circ}K}$$

where $S^{\circ}_{i_{T^{\circ}K}}$ is the absolute entropy of the i_{th} component of the reaction products, and R_u is the universal gas constant.

Values of the absolute entropy for the gas components are tabulated in Table III. For this report, the values of n_i/n were carried to four decimal places, and the natural logs of these fractions were taken from Volume III of the tables compiled by the Works Progress Administration, which lists the entering argument from .0001 to 5.0000 in steps of .0001.

For $3200^{\circ}K$ and 20.408 atmospheres pressure:

$$\begin{aligned}
S^{\circ}_{3200^{\circ}K} = \quad & .220 \times 49.04 + 3.886 \times 69.01 + .776 \times 68.57 \\
& + 1.391 \times 64.31 + .160 \times 69.47 + .534 \times 61.97 \\
& + .078 \times 39.13 + .118 \times 49.79 \\
& - 7.163 \times 1.986 \times \ln 20.408 - 1.986 \Big[.220 \ln .220/7.163 \\
& + 3.886 \ln 3.886/7.163 + .776 \ln .776/7.163 \\
& + 1.391 \ln 1.391/7.163 + .160 \ln .160/7.163 \\
& + .534 \ln .534/7.163 + .078 \ln .078/7.163 \\
& + .118 \ln .118/7.163 \Big]
\end{aligned}$$

$$S^O_{3200^O K} = 474.762 - 42.898 \quad 19.820$$

$$= 451.684 \quad \text{cals per degree Kelvin per } 7.163$$

moles or per 150.094 grams.

The entropy value plotted is given by:

$$s^O_{T^O K} = S^O_{T^O K} \Big/ m$$

For $3200^O K$ and 300 PSIA:

$$s^O_{3200^O K} = \frac{451.684}{150.094}$$

$$= 3.009 \quad \text{cals per gram per degree Kelvin.}$$

To calculate entropy values for pressure lines correspon- ding to constant composition flow it is necessary only to re- place $n_i^{T^O K}$ by $n_i^{T_c}$ in the equation for $S^O_{T^O K}$.

STEP E: CALCULATION OF EFFECTIVE EXHAUST VELOCITY AND
SPECIFIC IMPULSE.

The effective exhaust velocity is given by:

$$c = \sqrt{\frac{2 \Delta H^{T_c}_{T_e} \times J}{m}} \quad \text{cm per second}$$

where "J" is the mechanical equivalent of heat equal to 4.186×10^{10} ergs per kcal.

Since the plotted enthalpy value is $\Delta H/m$ the equation
for "c" can be written as follows:

$$c = \sqrt{2 \, \Delta h_{T_e}^{T_c} \times 4.186 \times 10^{10}} \qquad \text{cm per second}$$

The numerical factor .03281 converts cm per second to
feet per second. The equation for "c" then becomes:

$$c = .03281 \times 2.89345 \times 10^5 \sqrt{\Delta h_{T_e}^{T_c}} \qquad \text{feet per second}$$

Finally:

$$c = 9493.41 \sqrt{\Delta h_{T_e}^{T_c}} \qquad \text{feet per second}$$

The value of $\Delta h_{T_e}^{T_c}$ is very simply determined from the
h-s diagram. A vertical line is dropped from T_c on the pressure
line corresponding to the chamber pressure to the pressure line
corresponding to the ambient exhaust pressure. The value of en-
thalpy for this latter intercept is $\Delta h_{300^\circ K}^{T_e}$. The enthalpy
drop is then given by:

$$\Delta h_{T_e}^{T_c} = \Delta h_{300^\circ K}^{T_c} - \Delta h_{300^\circ K}^{T_e}$$

For the sample calculation the isentropic expansion from
300 PSIA to 14.7 PSIA is considered. For this case:

$$\Delta h_{T_e}^{T_c} = 1.821 - 1.022 = .799 \text{ kcals per gram}$$

from Figure 22.

$$c = 9493.41 \sqrt{.799} \quad \text{feet per second}$$

$$c = 8486 \quad \text{feet per second}$$

I_{sp} is determined by dividing the value of the effective exhaust velocity by the value of the acceleration of gravity. For this calculation:

$$I_{sp} = \frac{8486}{32.16} = 264 \text{ seconds}$$

STEP F: DETERMINATION OF THE EXHAUST TEMPERATURE T_e .

The value of the exhaust temperature T_e can be determined roughly from the h-s diagram. It is the temperature value at the intercept of the isentropic expansion line and the pressure line representing the ambient exhaust pressure. A more accurate value is obtained from a plot of entropy versus temperature, and all values reported in this analysis are determined in this manner. On the T-s diagram a vertical line is dropped from T_c on the pressure line representing the chamber pressure to the pressure line corresponding to the ambient exhaust pressure. The temperature value of this intercept is T_e .

PART III: DISCUSSION OF RESULTS.

There is no basis for an extended discussion of the per-
formance values reported in this analysis. No experimental
data for the propellent systems considered here was available,
and the only analytically determined values available for com-
parison were those for the stoichiometric mixture of liquid
ammonia and RFNA calculated by the Jet Propulsion Laboratory.
The results obtained by both methods are as follows:

A. Equilibrium Flow:

Parameter	JPL Value	Graphical Value
T_c	$2600^{\circ}K$	$2599^{\circ}K$
T_e	$1631^{\circ}K$	$1630^{\circ}K$
c	7315 ft/sec	7323 ft/sec
I_{sp}	227.2 sec	227.7 sec

B. Constant Composition Flow:

Parameter	JPL Value	Graphical Value
T_c	$2600^{\circ}K$	$2599^{\circ}K$
T_e	$1505^{\circ}K$	$1505^{\circ}K$
c	7217 ft/sec	7199 ft/sec
I_{sp}	224.1 sec	223.8 sec

It should be noted that T_c is determined in the same way for both analytical and graphical solutions. For the graphical solution, however, T_e is read directly from the appropriate T-s diagram, and the values of "c" and I_{sp} depend only on the value of the enthalpy change for the expansion considered. The value of this enthalpy change is taken directly from the h-s diagram. The fact that the above values agree to within two tenths of one percent is considered a positive check on the accuracy of the graphical method.

Pressure lines on the h-s and T-s diagrams corresponding to constant composition flow are constructed only for the expansion from a chamber pressure of 300 PSIA to an ambient exhaust pressure of one atmosphere. These pressure lines are indicated on the diagrams by dashed lines, and should be used only for the above specified expansion. The error, however, will not be great if they are used to approximate the constant composition flow parameter values for a chamber pressure of 600 PSIA. The fact that exhaust pressure lines for constant composition flow are included for only this one condition is not intended to convey the impression that the actual expansions of these propellent systems conform to the assumptions for equilibrium flow. It was originally intended to calculate complete constant composition flow data, but time limitations prevented this. In the absence of more complete data, no definite conclusions can be drawn as to which type of flow would result from the combustion of the propellent systems considered.

For very hot systems, such as H_2-O_3 , the position of the exhaust pressure lines representing constant composition flow on the h-s and T-s diagrams is quite different from that of the corresponding pressure lines for equilibrium flow. This displacement on a percentage basis is greatest on the T-s diagram, and as a result T_e is the performance parameter whose equilibrium flow value differs most from its constant composition flow value. For the H_2-O_3 system the T_e value for constant composition flow is several hundred degrees lower than the equilibrium flow value.

The plots of specific impulse versus mixture ratio show one significant tendency. The mixture ratio for which the maximum value of the specific impulse is obtained apparently shifts towards the over-oxidized side as the exhaust pressure approaches absolute zero. If this effect is general, it will be an important factor in the design of the latter stages of multiple-step rockets.

PART IV: CONCLUSIONS AND RECOMMENDATIONS.

Because of the extensive calculations which are required
to construct even a skeleton enthalpy-entropy diagram for a
propellent system, this graphical method is not recommended
unless a comprehensive study of the system is to be made. It
does, however, have several definite advantages over analyti-
cal methods. The h-s diagram makes possible the presentation
of a large amount of data in a concise and readily useable
form. If the diagram is a fairly complete one, an almost infi-
nite variation of the physical boundary conditions defining
the expansion process is possible, whereas one set of analyti-
cal calculations is limited to one combustion condition and
one exhaust condition.

The graphical method does not require that attention be
focused on either the assumptions of equilibrium flow or of
constant composition flow to the exclusion of the other since
exhaust pressure lines for both conditions can be plotted on
the same diagram. Neither is it necessary to assume isentropic
flow if some criteria for estimating a "condition curve" are
available.

In order to better evaluate the usefulness of the h-s
and T-s diagrams in calculating performance parameters, this
graphical method should be applied to a propellent system for
which complete experimental data is available. If a complete
set of pressure and temperature lines are constructed, not

only for the thermodynamic conditions in the rocket motor
chamber and at the nozzle exhaust, but also for conditions
near the throat, the h-s diagram could be applied to the cal-
culation of the characteristic velocity and the nozzle thrust
coefficient as well as the parameters determined in this
analysis. It is believed that a thorough investigation of one
propellent system in this manner would be of great value.

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Table XXL. __Equilibrium constants.__*

Temp-(°K)	K₁	K₂	K₃	K₄	K₅	K₆	K₇	K₈	K₉	K₁₀
298.1	1.007×10^{-5}	7.82×10^{24}	5.736×10^{-8}	7.260×10^{2}	1.56×10^{24}	8.13×10^{-8}	2.08×10^{-7}	8.650×10^{-7}	1.629×10^{-3}	1.644×10^{-4}
700	0.1110	3.637×10^{3}		9.150×10^{-3}	9.68×10^{13}					8.698×10^{-4}
800	.2478	31.25		2.909×10^{-3}	9.84×10^{11}					6.072×10^{-4}
900	.4546	0.7513		1.177×10^{-3}	1.46×10^{11}					1.567×10^{-3}
1000	.7266	.03720		5.638×10^{-4}	3.29×10^{10}					2.951×10^{-3}
1100	1.058	3.147×10^{-3}	1.495×10^{-5}	3.070×10^{-4}	9.55×10^{9}	3.45×10^{-7}	8.65×10^{-7}	2.460×10^{-6}	3.119×10^{-3}	5.230×10^{-3}
1200	1.435	3.994×10^{-4}	3.69×10^{-5}	1.847×10^{-4}	3.39×10^{9}	1.308×10^{-6}	3.34×10^{-6}	6.846×10^{-6}	5.610×10^{-3}	
1300	1.844	6.975×10^{-5}	6.89×10^{-5}	1.196×10^{-4}	1.40×10^{9}	4.19×10^{-6}	1.066×10^{-6}	1.560×10^{-5}	9.663×10^{-3}	
1400	2.270	1.553×10^{-5}	1.685×10^{-4}	8.239×10^{-5}	6.56×10^{8}	1.260×10^{-5}	3.305×10^{-5}	3.475×10^{-5}	1.592×10^{-2}	
1500	2.704	4.218×10^{-6}	3.512×10^{-4}	5.948×10^{-5}	3.38×10^{8}	3.452×10^{-5}	8.121×10^{-5}	7.231×10^{-5}	2.514×10^{-2}	
1600	3.135	1.348×10^{-6}	6.74×10^{-4}	4.469×10^{-5}	1.89×10^{8}	8.85×10^{-5}	2.34×10^{-4}	1.426×10^{-4}	3.897×10^{-2}	6.995×10^{-3}
1700	3.555	4.925×10^{-7}	1.188×10^{-3}	3.479×10^{-5}	1.13×10^{8}	2.08×10^{-4}	5.85×10^{-4}	2.673×10^{-4}	5.675×10^{-2}	1.442×10^{-2}
1800	3.975	2.029×10^{-7}	2.05×10^{-3}	2.783×10^{-5}	7.08×10^{7}	4.64×10^{-4}	1.243×10^{-3}	4.797×10^{-4}	1.185×10^{-1}	2.312×10^{-2}
1900	4.393	9.211×10^{-8}	3.42×10^{-3}	2.293×10^{-5}	4.66×10^{7}	8.90×10^{-4}	2.65×10^{-3}	8.280×10^{-4}	1.148×10^{-1}	3.586×10^{-2}
2000	4.782	4.545×10^{-8}	5.479×10^{-3}	1.923×10^{-5}	3.19×10^{7}	1.983×10^{-3}	5.336×10^{-3}	1.373×10^{-3}	0.1579	5.290×10^{-2}
2100	5.149	2.393×10^{-8}	8.525×10^{-3}	1.641×10^{-5}	2.26×10^{7}	3.808×10^{-3}	1.027×10^{-2}	2.210×10^{-3}	.2125	7.677×10^{-2}
2200	5.420	1.320×10^{-8}	1.294×10^{-2}	1.421×10^{-5}	1.65×10^{7}	7.055×10^{-3}	1.904×10^{-2}	3.482×10^{-3}	.2813	1.087×10^{-1}
2300	5.853	7.902×10^{-9}	1.859×10^{-2}	1.247×10^{-5}	1.24×10^{7}	1.248×10^{-2}	3.389×10^{-2}	5.253×10^{-3}	.3654	1.513×10^{-1}
2400	6.140	4.873×10^{-9}	2.758×10^{-2}	1.107×10^{-6}	9.48×10^{6}	2.157×10^{-2}	5.657×10^{-2}	7.798×10^{-3}	.4662	2.060×10^{-1}
2500	6.440	3.138×10^{-9}	3.894×10^{-2}	9.95×10^{-6}	7.40×10^{6}	3.363×10^{-2}	9.778×10^{-2}	1.182×10^{-2}	.5910	2.763×10^{-1}
2600	6.668	2.089×10^{-9}	5.404×10^{-2}	8.00×10^{-6}	5.88×10^{6}	8.85×10^{-3}	2.34×10^{-1}	1.611×10^{-2}	.7367	8.014×10^{-1}
2700	6.954	1.435×10^{-9}	7.355×10^{-2}	8.21×10^{-6}	4.74×10^{6}	2.08×10^{-3}	5.85×10^{-1}	2.248×10^{-2}	.9084	4.691×10^{-1}
2800	7.185	1.018×10^{-9}	9.821×10^{-2}	7.56×10^{-6}	3.87×10^{6}	4.64×10^{-3}	1.243×10^{-1}	3.066×10^{-2}	1.107	5.984×10^{-1}
2900	7.376	7.360×10^{-10}	1.300×10^{-1}	6.96×10^{-6}	3.21×10^{6}	8.90×10^{-3}	2.65×10^{-1}	4.166×10^{-2}	1.336	7.569×10^{-1}
3000	7.582	5.458×10^{-10}	1.683×10^{-1}	6.49×10^{-6}	2.69×10^{6}	3.157×10^{-2}	5.336×10^{-1}	5.544×10^{-2}	1.597	9.495×10^{-1}
3100	7.748		2.162×10^{-1}		2.27×10^{6}	4.526×10^{-1}	1.258	7.258×10^{-2}	1.893	1.164
3200	7.929		2.760×10^{-1}		1.94×10^{6}	6.519×10^{-1}	1.806	9.423×10^{-2}	2.226	1.426
3300	8.078		3.483×10^{-1}		1.66×10^{6}	9.139×10^{-1}	2.537	1.206×10^{-1}	2.598	1.730
3400	8.192	1.621×10^{-10}	4.302×10^{-1}	4.86×10^{-6}	1.44×10^{6}	1.263	3.508	1.588×10^{-1}	3.012	2.089
3500	8.304		5.291×10^{-1}		1.26×10^{6}	1.718	4.778	1.916×10^{-1}	3.470	2.478
3600	8.440		5.404		1.10×10^{5}	5.821×10^{-1}	1.591	7.258×10^{-2}	.7367	
3700	8.535		7.355		9.68×10^{5}	8.896×10^{-1}	2.516	9.423×10^{-2}	.9084	
3800	8.664		9.821		8.59×10^{5}	1.412	3.876	1.206×10^{-1}	1.107	
3900	8.712		1.300		7.64×10^{5}	2.134	5.878	1.588×10^{-1}	1.336	
4000	8.732	6.88×10^{-11}	1.683	3.94×10^{-6}	6.83×10^{5}	3.157	8.711	5.544×10^{-2}	1.597	
4100	8.819		2.162×10^{-1}		6.12×10^{5}	4.526×10^{-1}	1.258	7.258×10^{-2}	1.893	1.164
4200	8.884		2.760×10^{-1}		5.52×10^{5}	6.519×10^{-1}	1.806	9.423×10^{-2}	2.226	1.426
4300	8.898		3.483×10^{-1}		5.01×10^{5}	9.139×10^{-1}	2.537	1.206×10^{-1}	2.598	1.730
4400	8.929		4.302×10^{-1}		4.51×10^{5}	1.263	3.508	1.588×10^{-1}	3.012	2.089
4500	8.952	3.36×10^{-11}	5.291×10^{-1}	3.38×10^{-6}	4.10×10^{5}	1.718	4.778	1.916×10^{-1}	3.470	2.478
4600	8.974		6.451×10^{-1}		3.74×10^{5}	2.307	6.431	2.379×10^{-1}	3.969	2.923
4700	8.984		7.799×10^{-1}		3.41×10^{5}	3.068	8.545	2.927×10^{-1}	4.520	3.432
4800	8.994		9.344×10^{-1}		3.12×10^{5}	3.915	11.21	3.570×10^{-1}	5.118	3.992
4900	9.003		1.119		2.86×10^{5}	5.228	14.59	4.321×10^{-1}	5.764	4.637
5000	9.012	2.02×10^{-11}	1.317	3.00×10^{-6}	2.63×10^{5}	6.693	18.77	5.193×10^{-1}	6.461	5.317

* See next page for definitions of K_1, K_2 ....

Table XXX. [Concluded.]

Temp. (°K)	K_{11}	K_{12}	K_{13}	K_{14}	K_{15}	K_{16}	K_{17}
298.1							
400							3.976×10^{-5}
500							1.822×10^{-5}
600							1.026×10^{-5}
700							6.660×10^{-6}
800							4.724×10^{-6}
900							3.603×10^{-6}
1000	2.11×10^{-10}					2.226×10^{-15}	2.888×10^{-6}
1100							2.416×10^{-6}
1200							2.081×10^{-6}
1300	2.98×10^{-11}						1.835×10^{-6}
1400	1.13×10^{-11}						1.653×10^{-6}
1500	6.62×10^{-12}				2.77×10^{-6}	9.078×10^{-16}	1.510×10^{-6}
2000					2.37×10^{-6}	7.290×10^{-16}	1.136×10^{-6}
2500					2.23×10^{-6}	7.446×10^{-16}	9.87×10^{-7}
3000		8.27×10^{-8}	3.55×10^{-7}	1.90×10^{-4}	2.16×10^{-6}		9.93×10^{-7}
3500		3.80×10^{-7}	8.45×10^{-7}	7.61×10^{-4}	2.16×10^{-6}		9.89×10^{-7}
4000		1.20×10^{-6}	1.65×10^{-6}	2.15×10^{-3}	2.17×10^{-6}		9.88×10^{-7}
4500		2.92×10^{-6}	2.62×10^{-6}	4.80×10^{-3}	2.22×10^{-6}		9.87×10^{-7}
5000		5.96×10^{-6}	4.41×10^{-6}	9.09×10^{-3}	2.28×10^{-6}		9.88×10^{-7}

$K_1 = P_{CO} P_{H_2O} / P_{CO_2} P_{H_2}$; $K_2 = P_{CH_4} P_{H_2O} / P^3_{H_2} P_{CO}$; $K_3 = P_{NO} P_{H_2} / P^{1/2}_{N_2} P_{H_2O}$;

$K_4 = P_{NH_3} / P^{1/2}_{N_2} P^{3/2}_{H_2}$; $K_5 = P_{CO} / P^{1/2}_{O_2}$; $K_6 = P_{O_2} P^2_{H_2} / P^2_{H_2O}$;

$K_7 = P_O P_{H_2} / P_{H_2O}$; $K_8 = P_N / P^{1/2}_{N_2}$; $K_9 = P_H / P^{1/2}_{H_2}$; $K_{10} = P_{OH} P^{1/2}_{H_2} / P_{H_2O}$.

$K_{11} = P_{C_2H_2} P^2_{H_2O} / P^2_{CO} P^3_{H_2}$; $K_{12} = P_{CH} P_{H_2O} / P_{CO} P^{1/2}_{H_2}$;

$K_{13} = P_{CN} P_{CO_2} / P^2_{CO} P^{1/2}_{N_2}$; $K_{14} = P_{NH} / P^{1/2}_{N_2} P^{1/2}_{H_2}$; $K_{16} = P_{C_2N_2} P^2_{CO_2} / P^4_{CO} P_{N_2}$;

$K_{15} = P_{HCN} P_{H_2O} / P_{CO} P^{3/2}_{H_2} P^{1/2}_{N_2}$; $K_{17} = P_{H_2CO} / P_{H_2} P_{CO}$.

TABLE II   ENTHALPY TABLE
$\Delta H^{T°K}_{300°K}$ kcals/gram mole

T°K	H_2	H_2O	CO	CO_2	O_2	N_2	OH	NO	H,N,O	RΔT
300	0.0	0.0	0.0	0.0	0.0	0.0			0.0	0.0
400	0.695	0.811	0.699	0.942	0.721	0.697			0.497	0.199
500	1.393	1.641	1.404	1.970	1.447	1.399			0.993	0.397
600	2.093	2.496	2.125	3.072	2.203	2.112			1.490	0.596
700	2.796	3.380	2.862	4.232	2.981	2.840			1.987	0.795
800	3.502	4.292	3.615	5.441	3.778	3.582			2.484	0.993
900	4.212	5.234	4.386	6.692	4.594	4.343			2.981	1.192
1000	4.931	6.208	5.171	7.976	5.421	5.118	4.985	5.308	3.477	1.390
1100	5.657	7.211	5.973	9.291	6.278	5.907	5.725	6.133	3.974	1.589
1200	6.393	8.247	6.785	10.629	7.135	6.709	6.465	6.958	4.471	1.788
1300	7.138	9.312	7.606	11.989	7.990	7.520	7.233	7.800	4.967	1.986
1400	7.895	10.399	8.437	13.367	8.847	8.342	8.002	8.643	5.464	2.185
1500	8.664	11.519	9.275	14.760	9.704	9.173	8.783	9.499	5.961	2.384
1600	9.439	12.660	10.120	16.168	10.592	10.009	9.584	10.355	6.457	2.582
1700	10.226	13.821	10.972	17.587	11.481	10.854	10.390	11.221	6.954	2.781
1800	11.023	15.006	11.829	19.017	12.369	11.703	11.197	12.088	7.451	2.980
1900	11.828	16.206	12.689	20.455	13.257	12.558	12.015	12.957	7.947	3.178
2000	12.644	17.424	13.554	21.902	14.146	13.417	12.834	13.827	8.444	3.377
2100	13.466	18.659	14.423	23.358	15.061	14.279	13.643	14.700	8.941	3.576
2200	14.295	19.909	15.294	24.820	15.974	15.143	14.506	15.598	9.438	3.774
2300	15.132	21.171	16.169	26.290	16.889	16.013	15.360	16.480	9.935	3.973
2400	15.975	22.446	17.045	27.760	17.802	16.883	16.213	17.364	10.430	4.171
2500	16.827	23.733	17.923	29.242	18.717	17.758	17.080	18.249	10.928	4.370
2600	17.683	25.031	18.807	30.729	19.659	18.636	17.936	19.143	11.425	4.569
2700	18.542	26.338	19.691	32.218	20.601	19.516	18.807	20.036	11.921	4.767
2800	19.410	27.656	20.576	33.712	21.543	20.399	19.678	20.929	12.418	4.966
2900	20.282	28.980	21.464	35.211	22.486	21.284	20.563	21.823	12.915	5.165
3000	21.160	30.315	22.353	36.712	23.427	22.170	21.447	22.716	13.411	5.363
3100	22.041	31.658	23.242	38.222	24.384	23.058	22.335	23.617	13.908	5.562
3200	22.927	33.006	24.136	39.734	25.344	23.947	23.227	24.519	14.405	5.761
3300	23.818	34.362	25.028	41.244	26.308	24.837	24.121	25.421	14.901	5.959
3400	24.712	35.723	25.923	42.764	27.276	25.729	25.021	26.325	15.398	6.158
3500	25.611	37.092	26.818	44.281	28.247	26.622	25.920	27.229	15.894	6.356
3600	26.512	38.466	27.715	45.808	29.219	27.516	26.822	28.135	16.392	6.555
3700	27.416	39.845	28.613	47.332	30.198	28.412	27.730	29.041	16.889	6.754
3800	28.326	41.231	29.512	48.862	31.178	29.307	28.640	29.948	17.385	6.952
3900	29.236	42.619	30.412	50.394	32.164	30.205	29.552	30.856	17.882	7.151
4000	30.153	44.010	31.313	51.930	33.153	31.104	30.467	31.761	18.379	7.350
4100	31.069	45.413	32.215	53.471	34.139	32.006	31.390	32.682	18.875	7.548

SOURCE OF DATA:

"THERMODYNAMIC PROPERTIES OF PROPELLANT GASES", HIRSCHFELDER, CURTIS, MCCLURE, AND OSBORNE, O. S. R. D. REPORT # 547.

NOTE: FOR USE OF THIS TABLE IN CALCULATING THEORETICAL PROPELLANT PERFORMANCE.
cf: PROGRESS REPORT 1-25

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TABLE III   ENTROPY TABLE ($S^o_{T^oK}$)

(cal/degree/mole)

T°K	H$_2$O	CO	CO$_2$	O$_2$	N$_2$	NO	OH	H	N	O	H$_2$
300	44.80	47.30	50.20	49.00	45.80	50.40		27.40	36.62	38.06	31.27
400	47.12	49.31	52.89	51.06	47.79	52.45		28.82	38.04	39.48	33.27
500	48.96	50.38	55.17	52.67	49.35	54.06		29.92	39.14	40.58	34.83
600	50.52	52.19	57.17	54.05	50.65	55.40		30.82	40.04	41.48	36.10
700	51.88	53.32	58.96	55.25	51.77	56.57		31.59	40.81	42.25	37.18
800	53.10	54.32	60.57	56.31	52.76	57.60		32.25	41.47	42.91	38.12
900	54.21	55.23	62.04	57.27	53.66	58.53		32.84	42.06	43.50	38.96
1000	55.24	56.06	63.39	58.14	54.48	59.38	52.51	33.36	42.58	44.02	39.72
1100	56.20	56.82	64.64	58.96	55.23	60.17	53.21	33.83	43.05	44.49	40.41
1200	57.10	57.53	65.80	59.71	55.93	60.89	53.86	34.26	43.48	44.92	41.05
1300	57.95	58.19	66.89	60.39	56.58	61.56	54.47	34.66	43.88	45.32	41.65
1400	58.76	58.81	67.91	61.03	57.19	62.18	55.04	35.03	44.25	45.69	42.21
1500	59.53	59.39	68.87	61.62	57.76	62.77	55.58	35.37	44.59	46.03	42.74
1600	60.27	59.94	69.78	62.19	58.30	63.32	56.10	35.69	44.91	46.35	43.24
1700	60.97	60.46	70.64	62.73	58.81	63.85	56.58	35.99	45.21	46.65	43.72
1800	61.65	60.95	71.46	63.24	59.30	64.35	57.05	36.27	45.49	46.93	44.17
1900	62.30	61.42	72.24	63.72	59.76	64.82	57.49	36.54	45.76	47.20	44.61
2000	62.93	61.86	72.98	64.18	60.20	65.27	57.91	36.80	46.02	47.46	45.03
2100	63.53	62.28	73.69	64.63	60.62	65.70	58.30	37.04	46.26	47.70	45.43
2200	64.11	62.69	74.37	65.06	61.02	66.12	58.70	37.27	46.49	47.93	45.81
2300	64.67	63.08	75.02	65.47	61.41	66.51	59.08	37.49	46.71	48.15	46.19
2400	65.21	63.45	75.65	65.86	61.78	66.89	59.45	37.70	46.92	48.36	46.54
2500	65.74	63.81	76.26	66.23	62.14	67.25	59.80	37.90	47.12	48.56	46.89
2600	66.25	64.16	76.84	66.60	62.48	67.60	60.14	38.10	47.32	48.76	47.23
2700	66.74	64.49	77.40	66.96	62.81	67.94	60.47	38.29	47.51	48.95	47.55
2800	67.22	64.81	77.94	67.30	63.13	68.27	60.78	38.47	47.69	49.13	47.87
2900	67.69	65.12	78.47	67.63	63.44	68.58	61.09	38.64	47.86	49.30	48.17
3000	68.14	65.42	78.98	67.95	63.74	68.88	61.39	38.81	48.03	49.47	48.47
3100	68.58	65.71	79.48	68.26	64.03	69.18	61.68	38.97	48.19	49.63	48.76
3200	69.01	65.99	79.96	68.57	64.31	69.47	61.97	39.13	48.35	49.79	49.04
3300	69.43	66.26	80.43	68.87	64.58	69.75	62.24	39.28	48.50	49.94	49.32
3400	69.84	66.53	80.88	69.16	64.85	70.02	62.51	39.43	48.65	50.09	49.57
3500	70.24	66.79	81.32	69.44	65.11	70.28	62.77	39.57	48.79	50.23	49.84
3600	70.63	67.04	81.75	69.71	65.36	70.54	63.03	39.71	48.93	50.37	50.01
3700	71.01	67.29	82.17	69.98	65.61	70.79	63.28	39.85	49.07	50.51	50.34
3800	71.38	67.53	82.58	70.24	65.85	71.03	63.52	39.98	49.20	50.64	50.59
3900	71.74	67.76	82.98	70.50	66.08	71.27	63.76	40.11	49.33	50.77	50.82
4000	72.09	67.99	83.37	70.75	66.31	71.50	63.99	40.24	49.46	50.90	51.05
4100	72.44	68.21	83.75	70.99	66.53	71.73	64.22	40.36	49.58	51.02	51.28

TABLE IV

HEATS OF FORMATION AT CONSTANT PRESSURE- USED IN THIS ANALYSIS

Constituent	Heat of Formation in Kilocalories per Mole
H_2O	+57.798
NO	-21.600
OH	-10.060
H	-52.089
O	-59.159
$NH_3(1)$	+16.070
NO_2	- 6.100
HNO_3	+41.660
$O_3(1)$	-31.500
$H_2(1)$	+ 1.848

TABLE V

ATOMIC WEIGHTS USED

Element	Atomic Weight
N	14.008
H	1.008
O	16.000
H_2	2.016
H_2O	34.016
NH_3	17.032
HN_3	63.016
NO_2	46.008
O_3	48.000

TABLE VI
SAMPLE CALCULATION SHEET (A)

H-8.8236
O-6.2500
N-2.9412

$NH_3 - O_3$
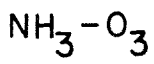
P=300 PSIA
T=3200°K

OVER—OXIDIZED (r=1.996)

h	7.150				7.163		
Kn 3	.007659				.007667		
6	.002472				.002476		
2K6	.004944				.004952		
7	.006672				.006683		
9	.16650				.16667	ATOM BALANCE	
10	.06434				.06440		
a	.215	.219	.220	.2194	.2195	H	8.824
2a	.430	.438	.440	.4388	.4390	O	6.250
a½	.4626	.4680	.4690	.4684	.4685	N	2.942
a²	.0462	.04796	.0484	.04814	.04818		
X K10/a½	.1391	.1375	.1372	.13736	.13746		
2+K10/a½	2.1391	2.1375	2.1372	2.13736	2.13746		
K9a½	.0770	.0779	.0781	.0780	.0781		
H-2a-K9a½	8.3166	8.3077	8.3055	8.3068	8.3065		
b	3.8879	3.8866	3.8862	3.88648	3.8861		
b²	15.1158	15.1057	15.1026	15.1047	15.1018		
y 2K6b/a²	.41583	.4007	.3970	.3991	.3994		
z K7/a	.03103	.0305	.0303	.0304	.0304		
A 1+X+y+z	1.58596	1.5687	1.5645	1.5667	1.5670		
bA	6.1661	6.0969	6.0800	6.0889	6.0907		
g	.0839	.1531	.1700	.1611	.1593		
g²	.007039	.02344	.0289	.02595	.02536		
K3²	.00005866				.00005878		
2g²a²/K3²b²	.73393	2.5374	3.1578	2.8198	2.7529		
F(II)	-2.1234	-.2507	+.3866	+.0397	-.0290		
a		.219	.220	.2194	.2195		.220
b		3.8866	3.8862	3.8865	3.8861		3.886
e		.7786	.7713	.7756	.7761		.776
f		1.3940	1.3856	1.3900	1.3909		1.391
g		.1531	.1700	.1611	.1593		.160
h		.5343	.5331	.5339	.5342		.534
i		.0779	.0781	.0780	.0781		.078
j		.1184	.1179	.1182	.1183		.118
n				7.1627	7.1625		7.163

TABLE VII
SAMPLE CALCULATION SHEET (B)

NH_3-O_3 (m = 150.094 GRAMS)   P = 300 PSIA

OVER-OXIDIZED (r = 1.996) Q_F (REACTANTS) = –18.3589 KCALS

T° K		2500	3000	3200	T_c 3280	3300	3500	
a H_2		.016	.120	.220	.273	.286	.453	
b H_2O		4.343	4.093	3.886	3.778	3.751	3.411	
e O_2		.865	.799	.776	.769	.767	.752	
f N_2		1.438	1.406	1.391	1.386	1.385	1.366	
g NO		.065	.130	.160	.170	.172	.209	
h OH		.104	.366	.534	.614	.634	.853	
i H		.002	.032	.078	.108	.116	.242	
j O		.008	.063	.118	.151	.159	.273	
n		6.841	7.009	7.163	7.249	7.270	7.559	
$\Sigma n_i \Delta H_i$		148.140	188.584	205.432		214.044	231.716	
Q_{av}				223.090		209.617		
ΔH		155.156	218.905	255.705		277.790	331.423	
Δh		1.034	1.458	1.704	1.821	1.851	2.208	
$\Sigma n_i S_i^o$		443.960	464.406	474.762		480.758	494.845	
$nR_L N P$		40.970	41.976	42.898		43.539	45.270	
$\Sigma n_i R_{LN} \frac{n_i}{n}$		13.725	17.381	19.820	20.974	21.262	24.648	
S^o		416.715	439.811	451.684		458.481	474.223	
s^o		2.776	2.930	3.009	3.046	3.055	3.160	
			ATOM	BALANCE	CHECK			
H		8.824	8.824	8.824		8.824	8.823	
O		6.250	6.250	6.250		6.250	6.250	
N		2.941	2.942	2.942		2.942	2.941	

TABLE VIII

ENTHALPY - ENTROPY SUMMARY

P = pressure in psia
h = kcal per gram
s = cal per gram per $^\circ K$

RFNA - NH_3 OVER-OXIDIZED (r = 3.00)

Temp$^\circ K$		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3000	Δh	1.381	1.422			
	s	2.811	2.886			
2500	Δh	1.004	1.012			
	s	2.674	2.739			
2400	Δh	0.943	0.948			
	s	2.649	2.713			
2300	Δh	0.885	0.888			
	s	2.624	2.688			
2000	Δh	0.723	0.724	0.730		
	s	2.549	2.611	2.884		
1500	Δh			0.479	0.479	0.479
	s			2.740	2.802	3.152
1300	Δh			0.390	0.390	
	s			2.677	2.739	
1000	Δh			0.261	0.261	0.261
	s			2.564	2.626	2.976
500	Δh				0.070	0.070
	s				2.362	2.712
400	Δh					0.035
	s					2.634
300	Δh				0.0	0.0
	s				2.185	2.535

RFNA – NH_3 STOICHIOMETRIC ($r = 2.21$)

Temp°K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3000	Δh	1.517	1.57			
	s	2.946	3.033			
2700	Δh	1.233				
	s	2.846				
2600	Δh	1.154	1.171			
	s	2.817	2.889			
2500	Δh	1.080	1.092			
	s	2.788	2.858			
2000	Δh	0.770	0.772	0.783		
	s	2.650	2.716	3.005		
1200	Δh			0.610		
	s			2.911		
1500	Δh			0.510	0.510	0.510
	s			2.849	2.914	3.282
1400	Δh			0.462		
	s			2.815		
1300	Δh				0.414	
	s				2.845	
1000	Δh			0.278	0.278	0.277
	s			2.661	2.726	3.094
500	Δh					0.074
	s					2.813
300	Δh					0.0
	s					2.626

RFNA - NH$_3$ UNDER-OXIDIZED (r = 1.50)

Temp°K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3000	Δh	1.548	1.583			
	s	3.272	3.362			
2500	Δh	1.169	1.172			
	s	3.134	3.213			
2100	Δh	0.920	0.921			
	s	3.026	3.103			
2000	Δh	0.861	0.861	0.864		
	s	2.997	3.074	3.413		
1500	Δh			0.577	0.577	0.577
	s			3.248	3.326	3.764
1400	Δh			0.418		
	s			3.130		
1000	Δh			0.317	0.317	0.317
	s			3.038	3.116	3.553
900	Δh			0.268	0.268	
	s			2.987	3.064	
800	Δh				0.221	
	s				3.008	
500	Δh				0.086	0.086
	s				2.797	3.234
400	Δh					0.042
	s					3.138
300	Δh					0.0
	s					3.017

$NH_3 - O_3$ OVER-OXIDIZED (r = 2.00)

Temp°K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3500	Δh	2.041	2.208			
	s	3.044	3.160			
3400	Δh	1.888				
	s	2.999				
3300	Δh	1.749	1.850			
	s	2.958	3.055			
3200	Δh		1.704			
	s		3.009			
3000	Δh	1.415	1.458	1.940		
	s	2.852	2.930	3.379		
2500	Δh		1.034	1.107		
	s		2.776	3.080		
2000	Δh			0.747	0.747	
	s			2.920	2.984	
1500	Δh			0.488	0.488	0.488
	s			2.773	2.835	3.187
1000	Δh					0.266
	s					3.008
500	Δh					0.071
	s					2.739

NH_3 - O_3 STOICHIOMETRIC (r = 1.41)

Temp°K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3500	Δh	2.351	2.554			
	s	3.278	3.412			
3400	Δh	2.167				
	s	3.225				
3300	Δh	2.001	2.132			
	s	3.175	3.288			
3200	Δh		1.956			
	s		3.233			
3000	Δh	1.597	1.658	2.267		
	s	3.046	3.137	3.657		
2500	Δh		1.146	1.260	1.311	
	s		2.951	3.294	3.383	
2000	Δh			0.819	0.824	
	s			3.099	3.169	
1800	Δh			0.691	0.691	
	s			3.031	3.098	
1500	Δh			0.533	0.533	0.533
	s			2.934	3.001	3.380
1000	Δh					0.289
	s					3.183

$NH_3 - O_3$ UNDER-OXIDIZED (r = 1.10)

Temp$^{\circ}$K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3500	Δ h	2.275	2.469			
	s	3.508	3.647			
3200	Δ h	1.810	1.892			
	s	3.369	3.474			
3100	Δ h	1.692	1.750			
	s	3.332	3.429			
3000	Δ h	1.588	1.628	2.164		
	s	3.297	3.389	3.919		
2500	Δ h		1.195	1.249		
	s		3.232	3.590		
2000	Δ h			0.878	0.879	
	s			3.426	3.504	
1700	Δ h			0.699	0.699	
	s			3.329	3.406	
1500	Δ h			0.585	0.585	0.585
	s			3.258	3.335	3.770
1000	Δ h					0.320
	s					3.556
500	Δ h					0.086
	s					3.233

NH$_3$ – O$_3$ UNDER-OXIDIZED (r = 0.80)

Temp^{o}K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
3500	Δh		2.563			
	s		3.994			
3000	Δh	1.754	1.771			
	s	3.660	3.752			
2600	Δh	1.391	1.398			
	s	3.526	3.619			
2500	Δh	1.317	1.321	1.377		
	s	3.497	3.589	4.004		
2000	Δh			0.975		
	s			3.826		
1500	Δh			0.653	0.653	0.653
	s			3.641	3.731	4.238
1400	Δh			0.592		
	s			3.599		
1300	Δh			0.532	0.533	
	s			3.555	3.648	
1200	Δh			0.474	0.474	
	s			3.508	3.599	
1100	Δh				0.417	
	s				3.548	
1000	Δh			0.360	0.360	0.360
	s			3.404	3.494	4.002
500	Δh					0.098
	s					3.640

$H_2 - O_3$ OVER-OXIDIZED (r = 9.92)

Temp$^\circ$K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
4000	Δh	3.935	4.555			
	s	3.839	4.087			
3800	Δh	3.274				
	s	3.670				
3700	Δh	2.993	3.350			
	s	3.595	3.774			
3600	Δh		3.028			
	s		3.686			
3500	Δh	2.516	2.746	5.345		
	s	3.462	3.607	4.745		
3000	Δh	1.706	1.765	2.431	2.777	
	s	3.213	3.306	3.858	4.055	
2500	Δh			1.334	1.383	2.367
	s			3.464	3.555	4.380
2000	Δh			0.885	0.889	0.943
	s			3.266	3.338	3.764

H$_2$ - O$_3$ STOICHIOMETRIC (r = 7.94)

Temp°K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
4000	Δh	4.580	5.293			
	s	4.217	4.499			
3800	Δh	3.819				
	s	4.023				
3700	Δh	3.495	3.912			
	s	3.936	4.141			
3600	Δh		3.542			
	s		4.037			
3500	Δh	2.936	3.213	6.204		
	s	3.780	3.947	5.246		
3000	Δh	1.965	2.046	2.869	3.278	
	s	3.481	3.588	4.229	4.457	
2500	Δh		1.397	1.549	1.617	2.825
	s		3.352	3.752	3.859	4.821
2000	Δh			0.992	0.999	1.092
	s			3.507	3.587	4.069
1800	Δh					0.833
	s					3.930

$H_2 - O_3$ UNDER-OXIDIZED (r = 6.61)

Temp $^\circ$K		P = 600	P = 300	P = 14.7	P = 7.35	P = .147
4000	Δh	4.680	5.454			
	s	4.600	4.910			
3800	Δh	3.861				
	s	4.391				
3700	Δh	3.516	3.957			
	s	4.298	4.522			
3600	Δh		3.561			
	s		4.411			
3500	Δh	2.933	3.213	6.460		
	s	4.136	4.314	5.738		
3000	Δh	2.000	2.058	2.836	3.267	
	s	3.850	3.960	4.632	4.880	
2500	Δh		1.490	1.565	1.611	2.778
	s		3.754	4.177	4.286	5.294
2000	Δh			1.086	1.090	1.124
	s			3.966	4.057	4.582
1500	Δh					0.719
	s					4.350
1000	Δh					0.391
	s					4.084

$H_2 - O_3$ UNDER-OXIDIZED (r = 4.96)

Temp°K		P=600	P = 300	P = 14.7	P = 7.35	P = .147
4000	Δh	5.108	5.949			
	s	5.367	5.717			
3600	Δh	3.569				
	s	4.960				
3500	Δh	3.299	3.560	7.072		
	s	4.886	5.083	6.690		
3400	Δh		3.256			
	s		4.994			
3000	Δh	2.359	2.411	3.125	3.556	
	s	4.598	4.732	5.490	5.760	
2500	Δh		1.781	1.863	1.908	3.023
	s		4.503	5.037	5.171	6.297
2000	Δh			1.307	1.308	1.357
	s			4.791	4.907	5.579
1500	Δh					0.870
	s					5.301
1000	Δh					0.477
	s					4.983
800	Δh					0.332
	s					4.822

TABLE IX

PERFORMANCE SUMMARY

RFNA – NH$_3$(l)

r		Pc	Pe	C	Isp	Tc $^\circ$K	Te $^\circ$K
3.00		300	14.7	6645	207	2325	1360
2.21	(stoic.)	300	14.7	7323	228	2599	1630
1.50		300	14.7	6898	214	2062	1110
3.00		600	14.7	7161	223	2331	1170
2.21	(stoic.)	600	14.7	7942	247	2621	1425
1.50		600	14.7	7384	230	2063	955
3.00		300	7.35	7167	223	2325	1190
2.21	(stoic.)	300	7.35	7914	246	2599	1425
1.50		300	7.35	7384	230	2062	955
3.00		600	7.35	7576	236	2331	1010
2.21	(stoic.)	600	7.35	8437	262	2621	1240
1.50		600	7.35	7782	242	2063	810
3.00		300	.147	8721	271	2325	480
2.21	(stoic.)	300	.147	9751	303	2599	615
1.50		300	.147	8869	276	2062	350
3.00		600	.147	8854	275	2331	400
2.21	(stoic.)	600	.147	9920	308	2621	515
1.50		600	.147	8996	280	2063	300

TABLE IX

PERFORMANCE SUMMARY

$NH_3(1) - O_3(1)$
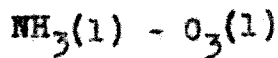
r		P_c	P_e	C	I_{sp}	T_c K	T_e K
2.00		300	14.7	8486	264	3280	2400
1.41	(stoic.)	300	14.7	8930	278	3285	2460
1.10		300	14.7	8901	277	3124	2050
0.80		300	14.7	8292	258	2564	1423
2.00		600	14.7	9233	287	3352	2200
1.41	(stoic)	600	14.7	9749	303	3362	2290
1.10		600	14.7	9649	300	3179	1802
0.80		600	14.7	8910	277	2573	1220
2.00		300	7.35	9199	286	3280	2200
1.41	(stoic.)	300	7.35	9692	301	3285	2280
1.10		300	7.35	9621	299	2124	1805
0.80		300	7.35	8921	277	2564	1230
2.00		600	7.35	9873	307	3352	2185
1.41	(stoic.)	600	7.35	10414	324	3362	2100
1.10		600	7.35	10233	318	3179	1580
0.80		600	7.35	9412	293	2573	1050
2.00		300	.147	11684	363	3280	1100
1.41	(stoic.)	300	.147	12409	386	3285	1220
1.10		300	.147	11872	369	3124	796
0.80		300	.147	10786	335	2564	465
2.00		600	.147	11936	371	3352	1140
1.41	(stoic.)	600	.147	12721	396	3362	1060
1.10		600	.147	12132	377	3179	665
0.80		600	.147	10972	341	2573	380

TABLE IX

PERFORMANCE SUMMARY

$$H_2(1) - O_3(1)$$

r		P_c	P_e	c	I_{sp}	$T_c \, ^oK$	$T_e \, ^oK$
9.92		300	14.7	10129	315	3634	2870
7.94	(stoic.)	300	14.7	10613	330	3640	2900
6.61		300	14.7	11107	345	3607	2820
4.96		300	14.7	11762	366	3447	2500
9.92		600	14.7	11059	344	3752	2770
7.94	(stoic.)	600	14.7	11665	363	3760	2815
6.61		600	14.7	12227	380	3721	2710
4.96		600	14.7	12816	398	3537	2280
9.92		300	7.35	11021	343	3634	2735
7.94	(stoic.)	300	7.35	11629	362	3640	2765
6.61		300	7.35	12113	377	3607	2670
4.96		300	7.35	12768	397	3447	2275
9.92		600	7.35	11856	368	3752	2625
7.94	(stoic.)	600	7.34	12521	389	3760	2675
6.61		600	7.35	13081	407	3721	2550
4.96		600	7.35	13651	424	3537	2010
9.92		300	.147	14391	447	3634	1920
7.94	(stoic.)	300	.147	15217	473	3640	2015
6.61		300	.147	15768	490	3607	1650
4.96		300	.147	16081	500	3447	1080
9.92		600	.147	14819	461	3752	1710
7.94	(stoic)	600	.147	15739	489	3760	1910
6.61		600	.147	16214	504	3721	1430
4.96		600	.147	16442	511	3537	910

TABLE X

FROZEN PERFORMANCE SUMMARY

RFNA - NH_3

r		P_c	P_e	c	I_{sp}	$T_c \, ^oK$	$T_e \, ^oK$
3.00		300	14.7	6563	204	2325	1315
2.21	(stoic.)	300	14.7	7199	224	2599	1505
1.50		300	14.7	6898	214	2062	1110

NH_3 - O_3

2.00		300	14.7	8155	254	3200	1882
1.41	(stoic.)	300	14.7	8544	266	3285	1900
1.10		300	14.7	8643	269	3124	1780
0.80		300	14.7	8232	256	2564	1395

H_2 - O_3

9.92		300	14.7	9578	298	3634	2095
7.94	(stoic.)	300	14.7	10091	314	3640	2100
6.61		300	14.7	10566	329	3721	2060 -
4.96		300	14.7	11306	352	3447	1960

- F1 -

SOLID LINES: EQUILIBRIUM FLOW
DASHED LINE: CONSTANT COMPOSITION FLOW

SPECIFIC IMPULSE – I_{SP} – SECONDS

320

300

280

260

240

220

200

180

$Pe = .147$ PSIA

$Pe = 7.35$ PSIA

$Pe = 14.7$ PSIA

STOIC. MIXTURE RATIO
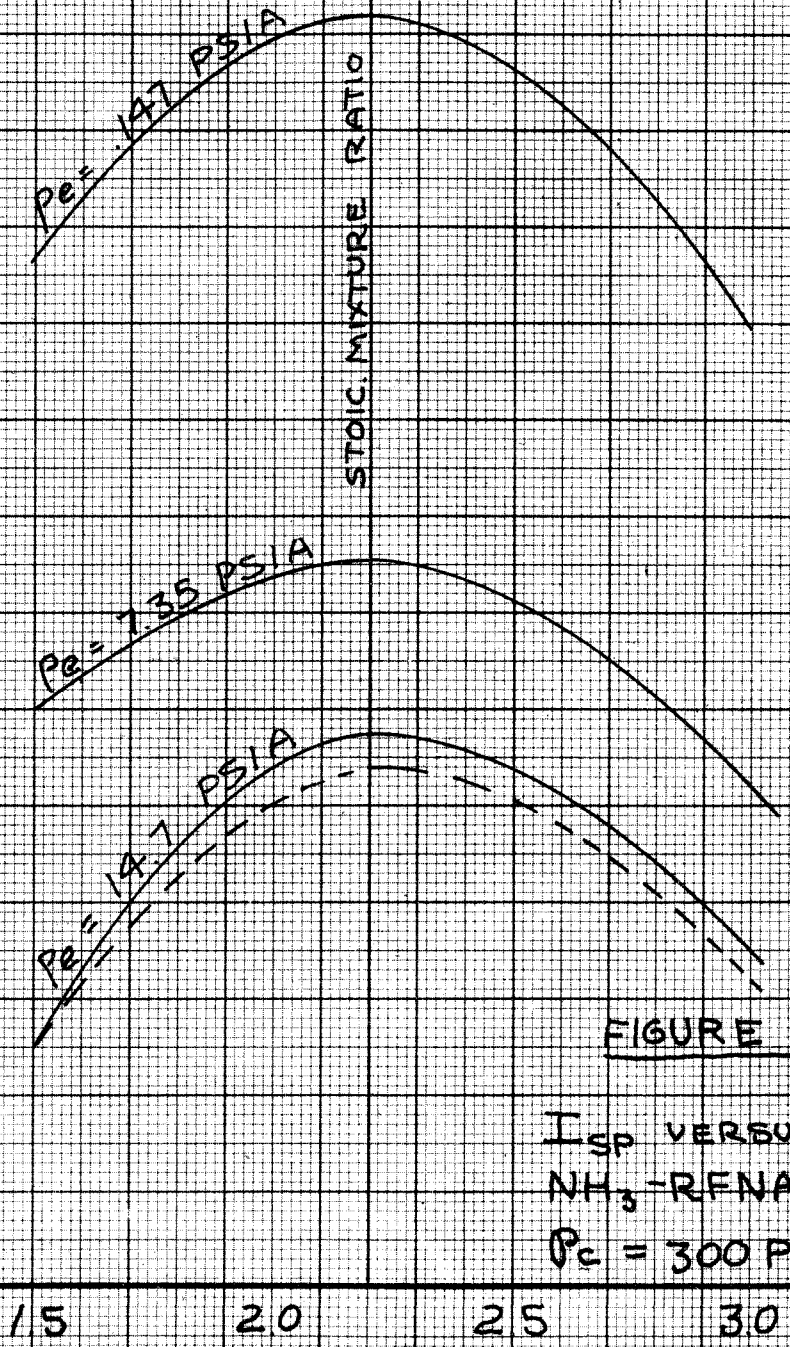
FIGURE 1

I_{SP} VERSUS r
NH_3-RFNA SYSTEM
$P_c = 300$ PSIA

MIXTURE RATIO r

15   20   25   30

FIGURE 2

I_{SP} VERSUS r

NH_3-RFNA SYSTEM

P_C = 600 PSIA
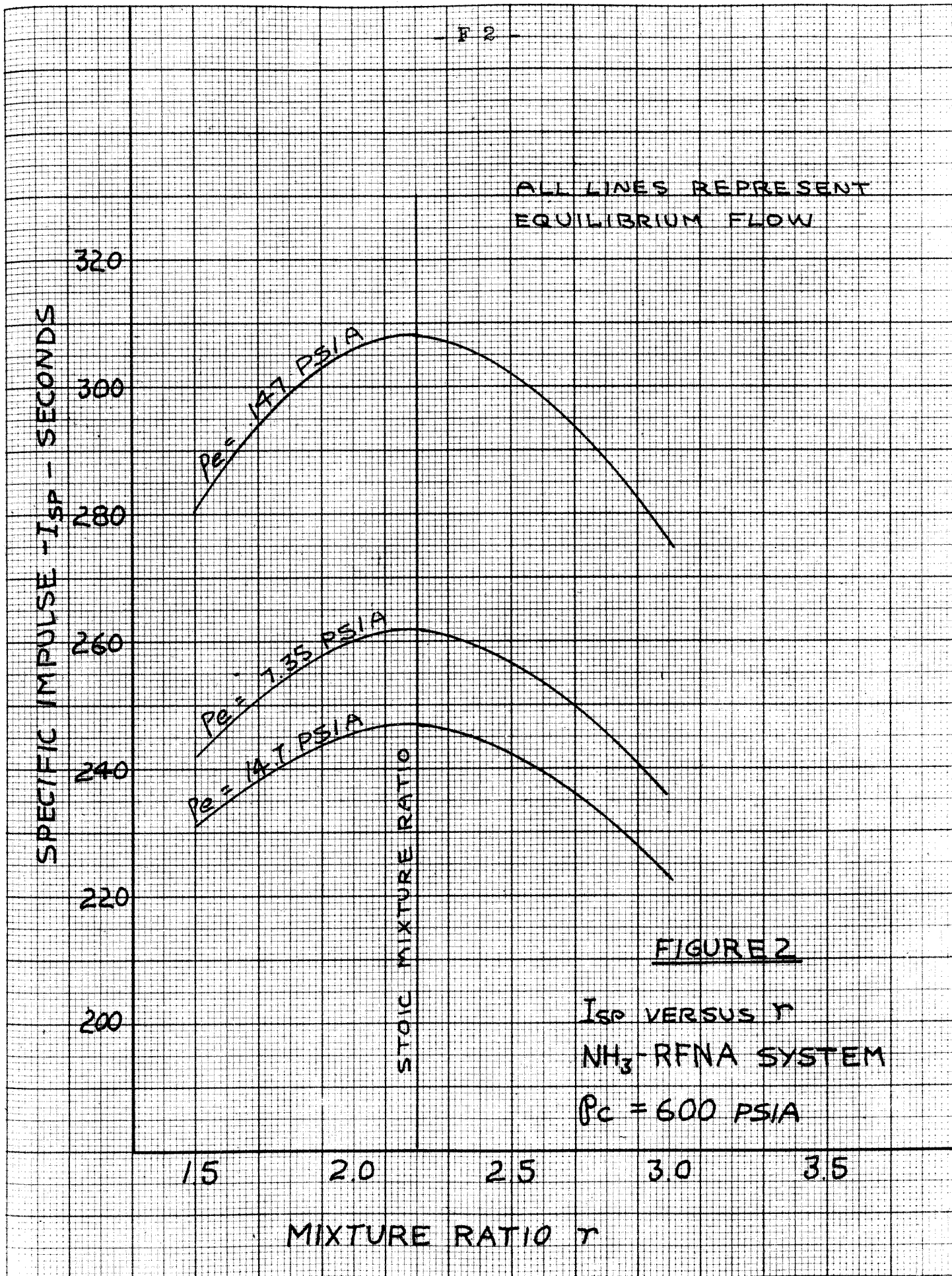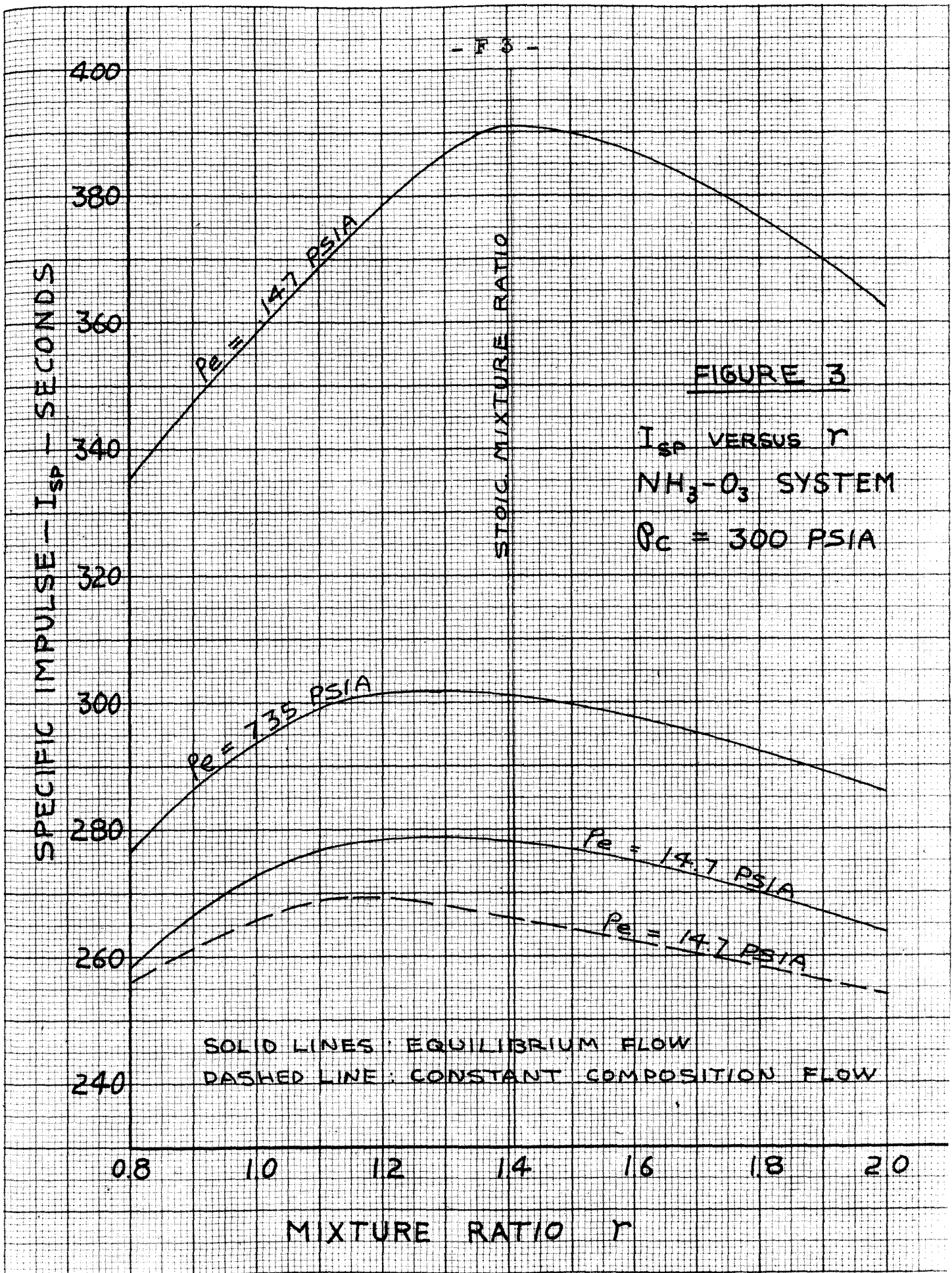
FIGURE 3

I_{sp} VERSUS r

NH_3-O_3 SYSTEM

P_c = 300 PSIA

SOLID LINES : EQUILIBRIUM FLOW

DASHED LINE : CONSTANT COMPOSITION FLOW

FIGURE 4

I_{SP} VERSUS r

NH_3-O_3 SYSTEM

$P_C = 600$ PSIA

FIGURE 5

I_{SP} VERSUS r

H_2-O_3 SYSTEM

$P_C = 300$ PSIA

FIGURE 6

I_{SP} VERSUS r

H_2-O_3 SYSTEM

P_c = 600 PSIA

ALL LINES REPRESENT EQUILIBRIUM FLOW
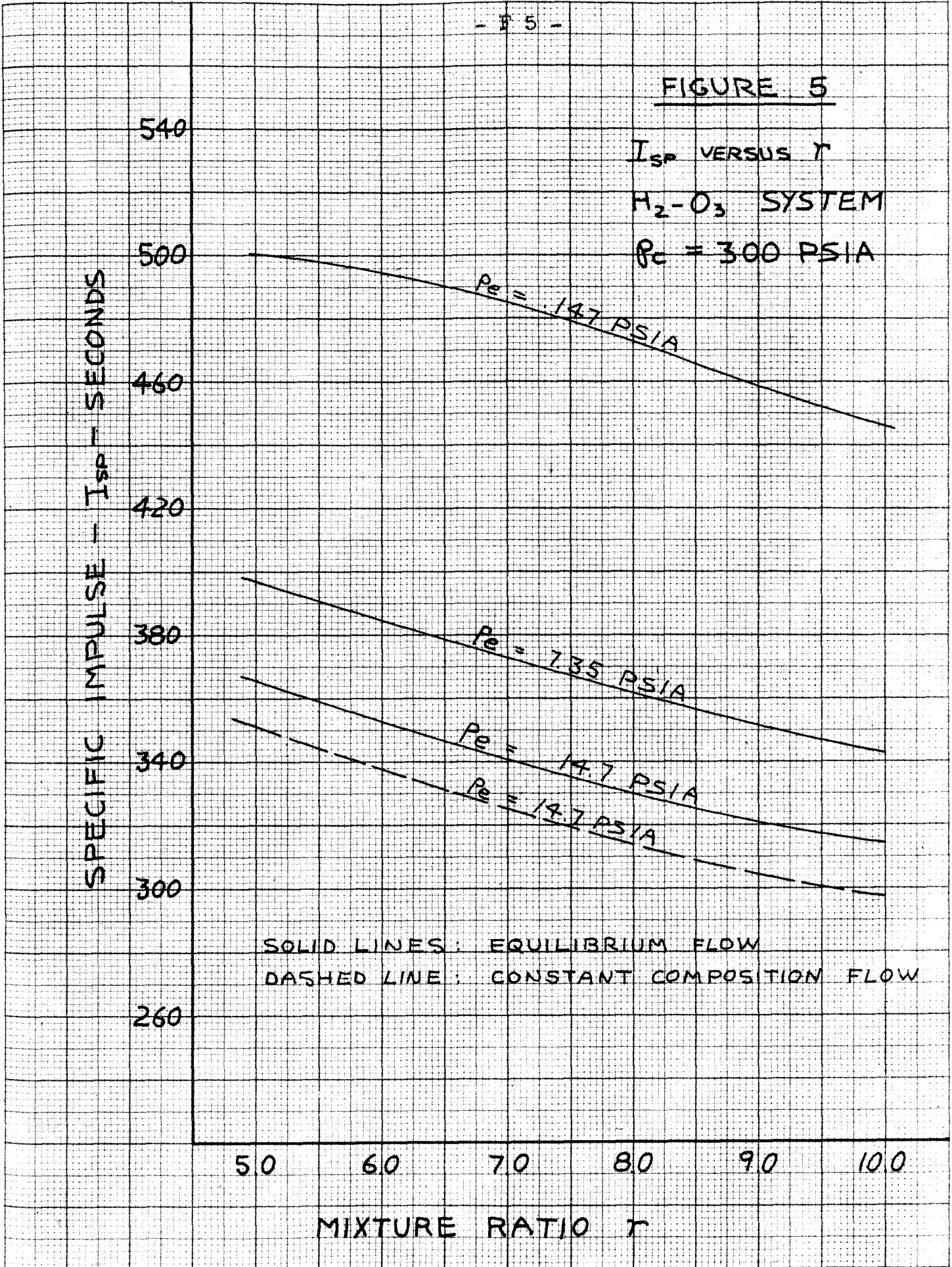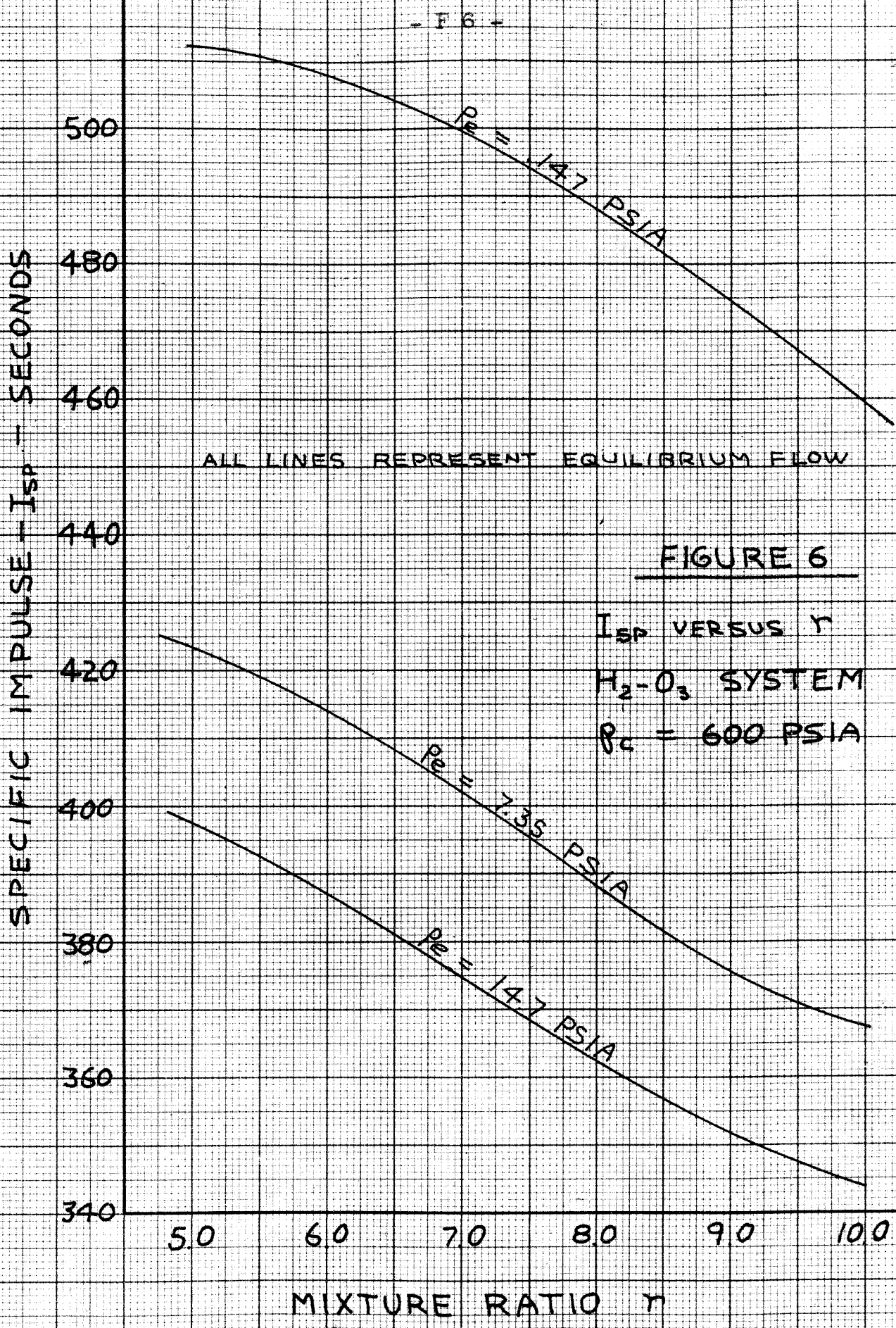
- F 7 -
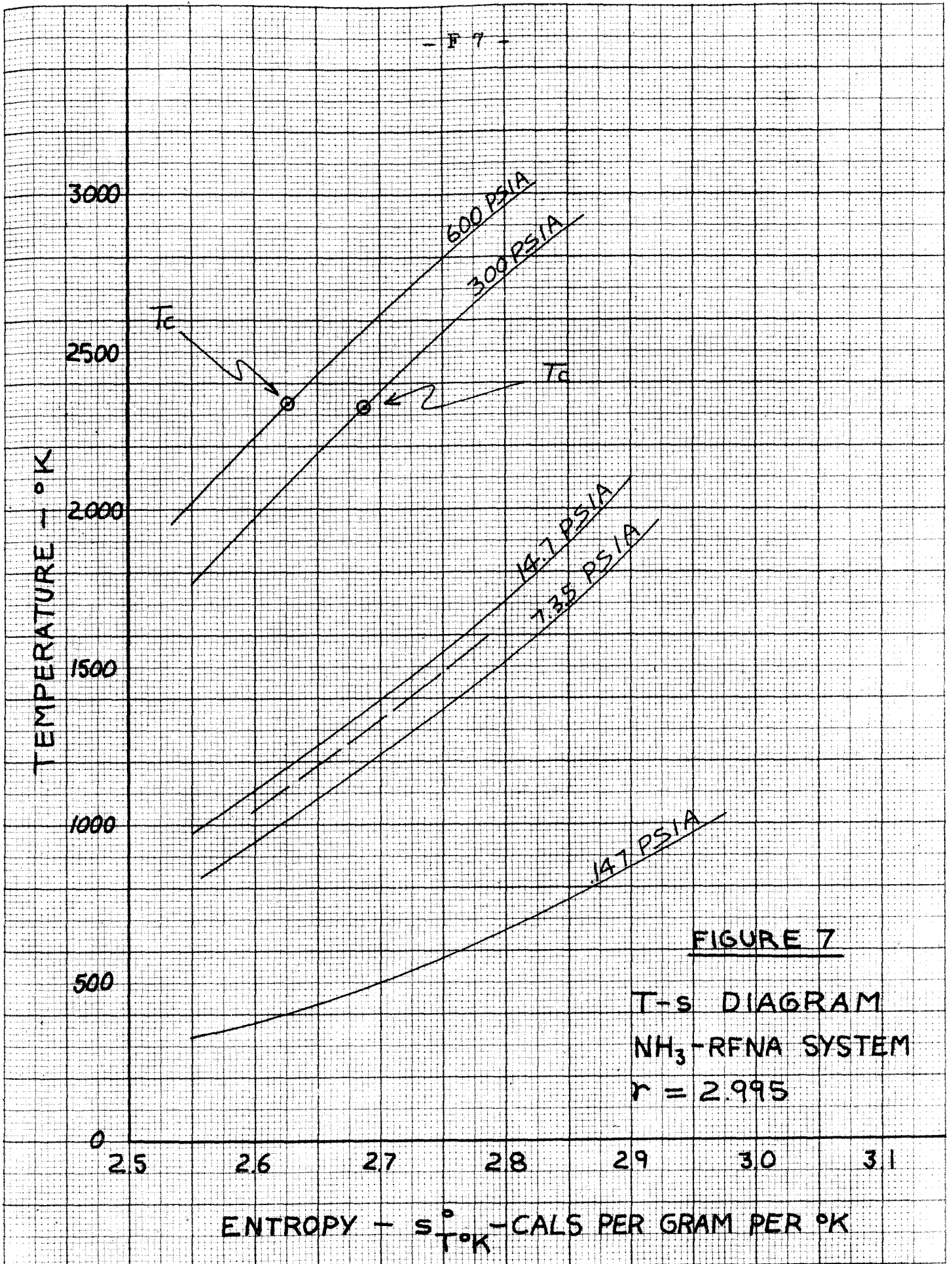
FIGURE 7

T-s DIAGRAM

NH₃-RFNA SYSTEM

$r = 2.995$

- F 8 -

FIGURE 8

T-S DIAGRAM

NH₃-RFNA SYSTEM

STOIG. r = 2.206

FIGURE 8. T-s DIAGRAM, NH₃-RFNA SYSTEM, STOIG. r = 2.206

Axis labels: TEMPERATURE - °K (vertical), ENTROPY - S°/T°K - CALS PER GRAM PER °K (horizontal)

Curves labeled: 600 PSIA, 300 PSIA, 14.7 PSIA, 7.35 PSIA, 14.7 PSIA, with points marked Tc.

FIGURE 9

T-s DIAGRAM

NH$_3$-RFNA SYSTEM

$r = 1.498$

- F 10 -
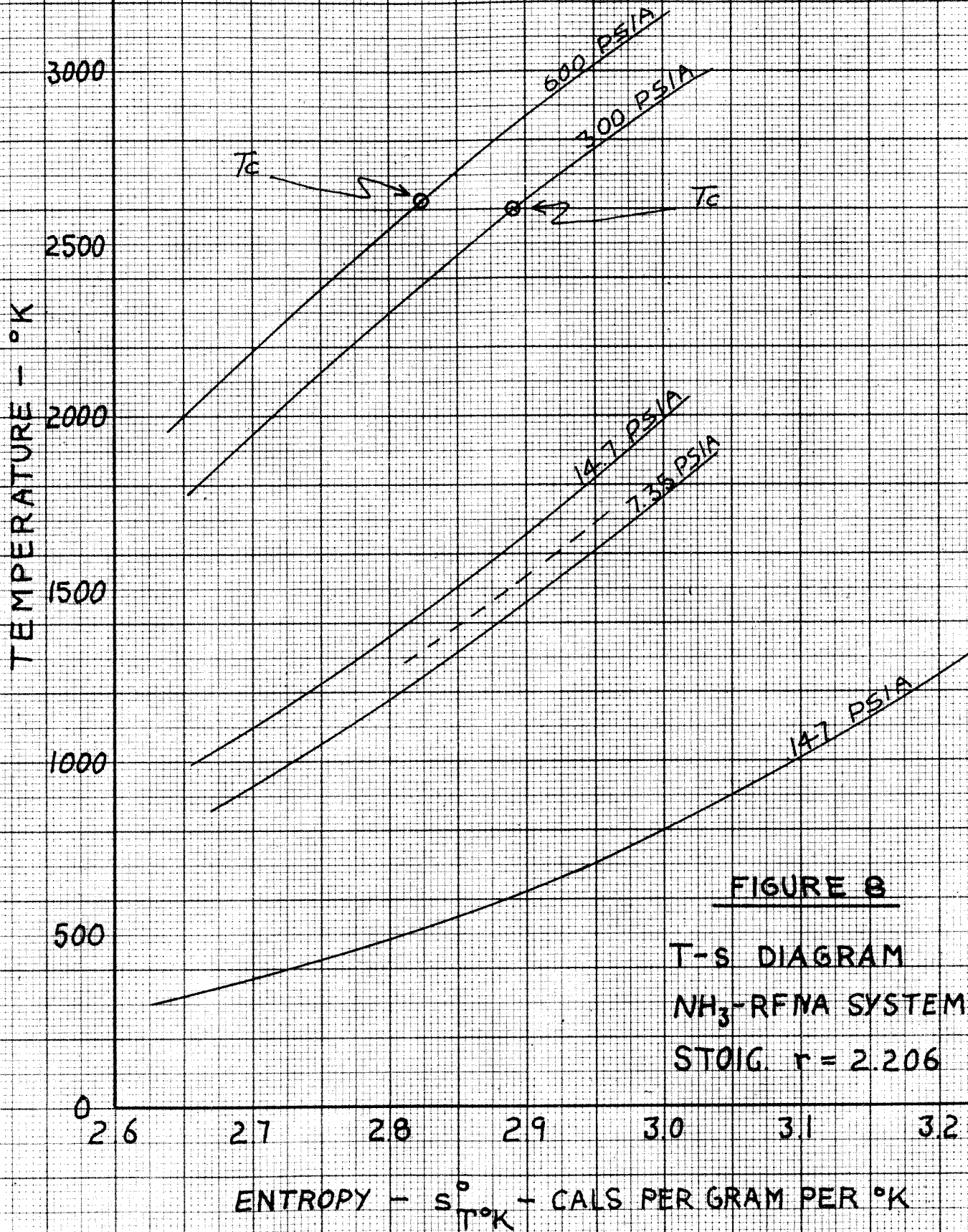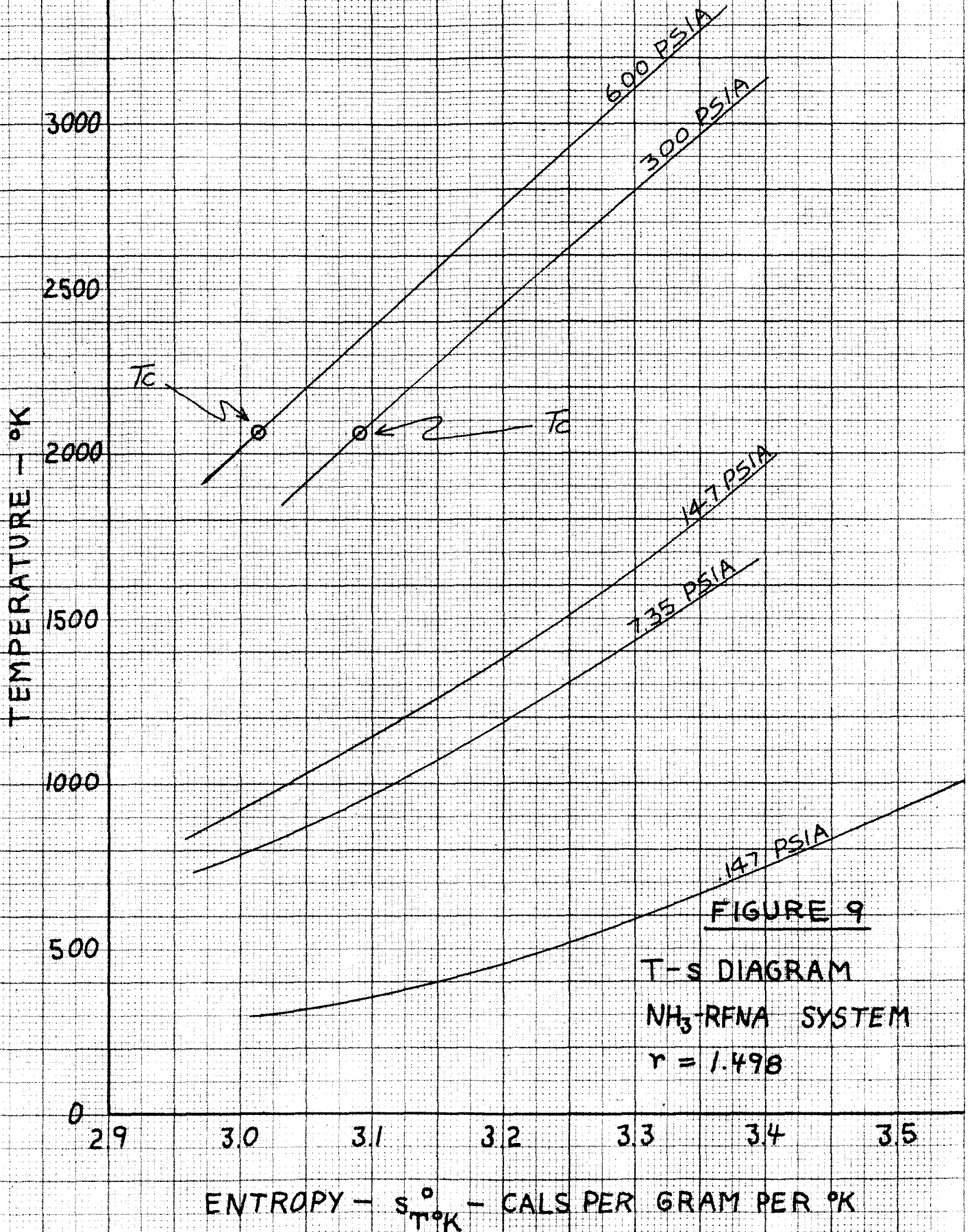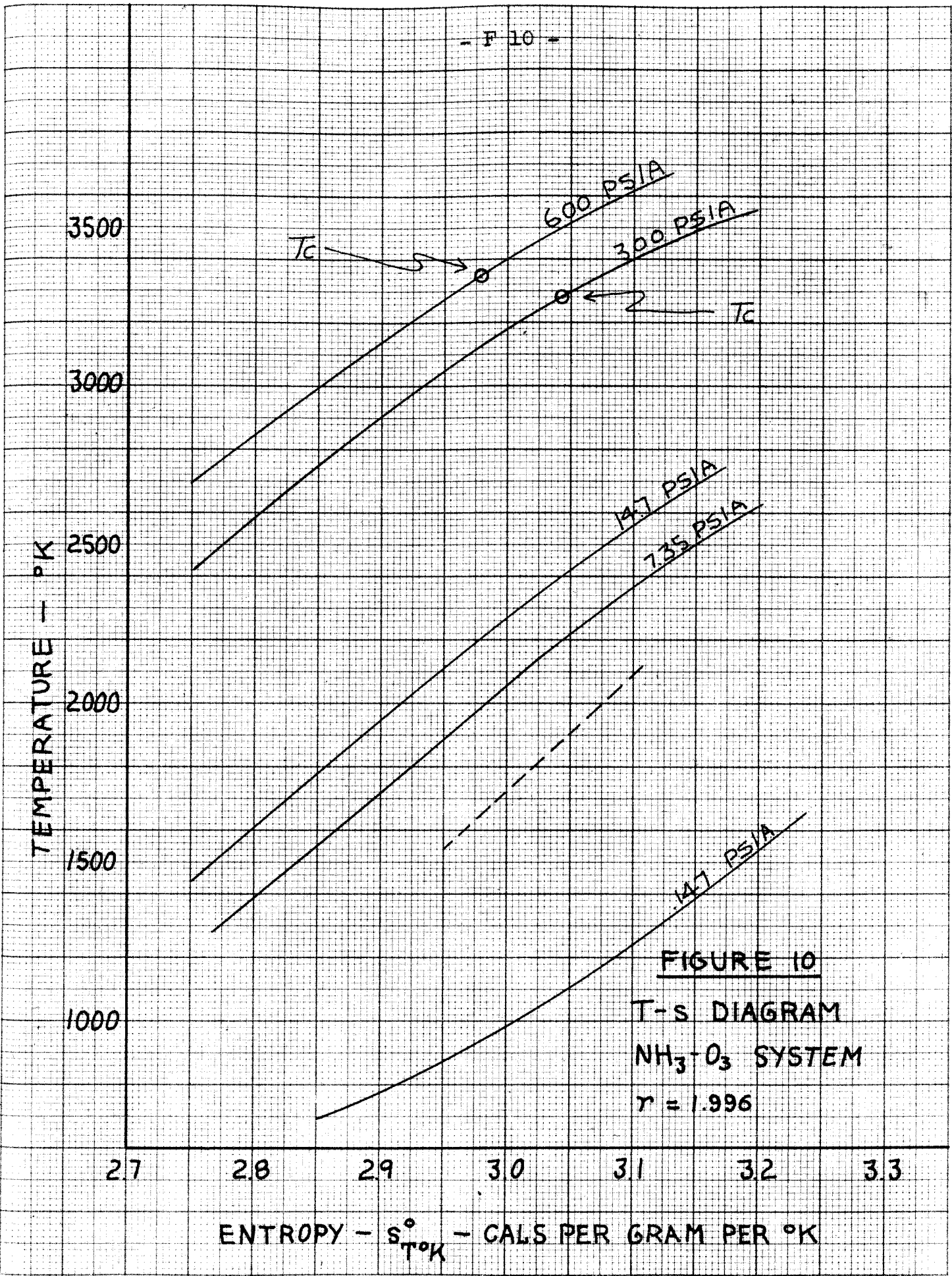
FIGURE 10

T-s DIAGRAM

NH₃-O₃ SYSTEM

r = 1.996

FIGURE 11

T-S DIAGRAM

$NH_3 - O_3$ SYSTEM

STOIC. $r = 1.409$

- F 12 -

FIGURE 12

T-s DIAGRAM

NH_3-O_3 SYSTEM

$r = 1.098$

FIGURE 13

T-s DIAGRAM

NH$_3$-O$_3$ SYSTEM

r = 0.798
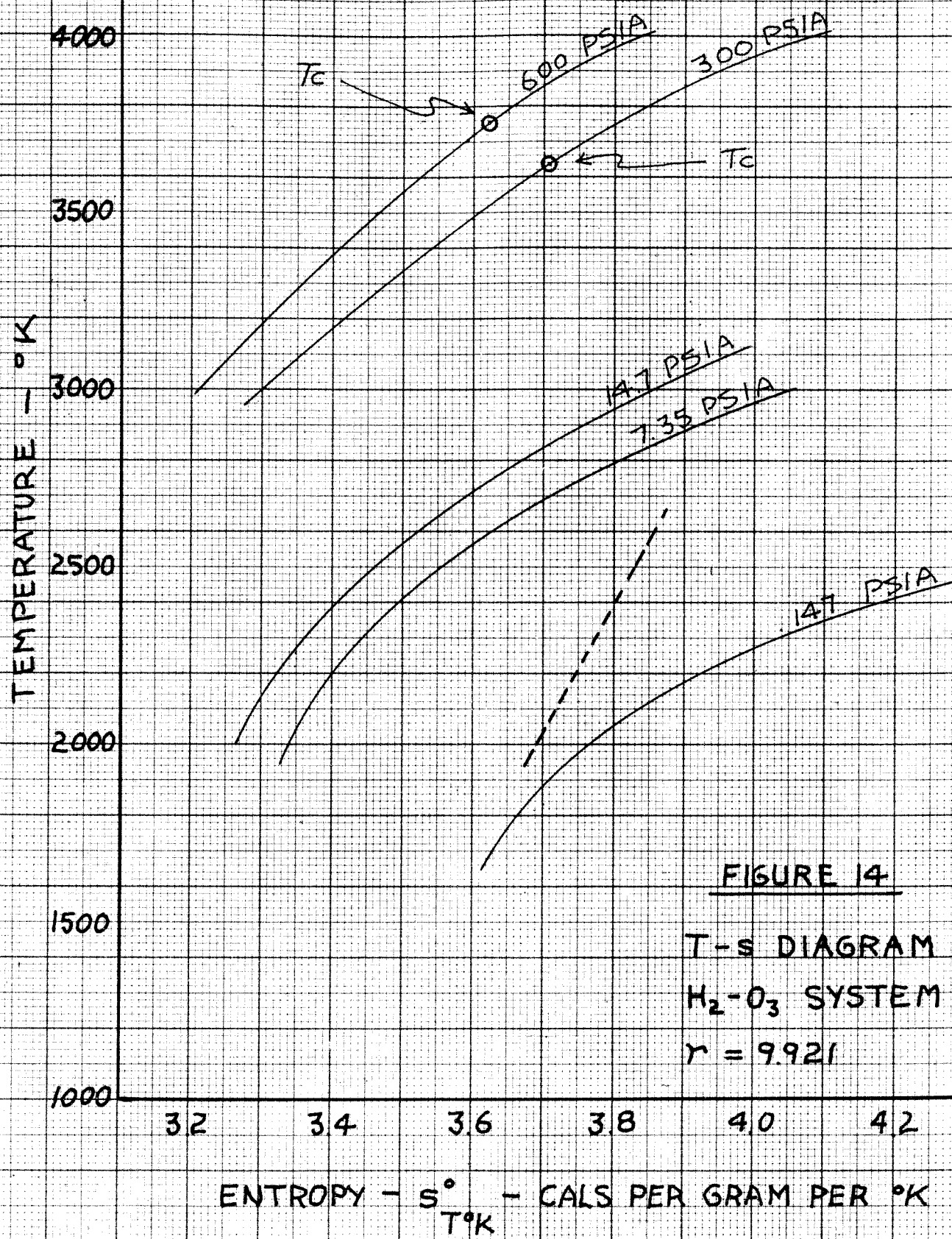
FIGURE 14

T-s DIAGRAM

$H_2 - O_3$ SYSTEM

$r = 9.921$

- F 15 -
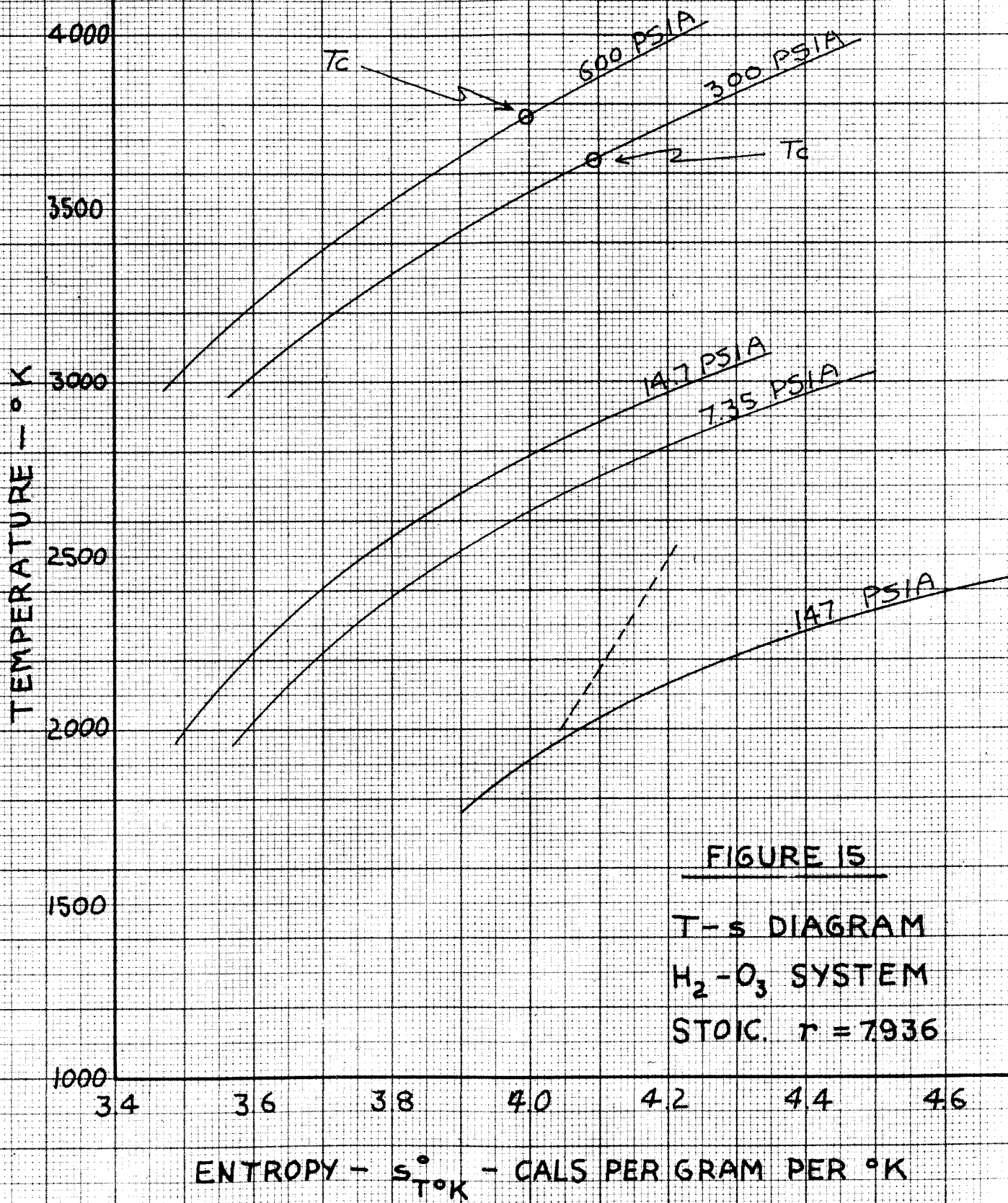
FIGURE 15

T-s DIAGRAM

$H_2 - O_3$ SYSTEM

STOIC. $r = 7.936$

TEMPERATURE - °K

600 PSIA

300 PSIA

Tc

Tc

14.7 PSIA

7.35 PSIA

.147 PSIA

4000

3500

3000

2500

2000

1500

1000

3.4   3.6   3.8   4.0   4.2   4.4   4.6

ENTROPY - $s^o_{T°K}$ - CALS PER GRAM PER °K

- F 16 -

FIGURE 16

T-s DIAGRAM

H_2-O_3 SYSTEM

$r = 6.614$

FIGURE 17

T-s DIAGRAM

H₂-O₃ SYSTEM

$r = 4.960$
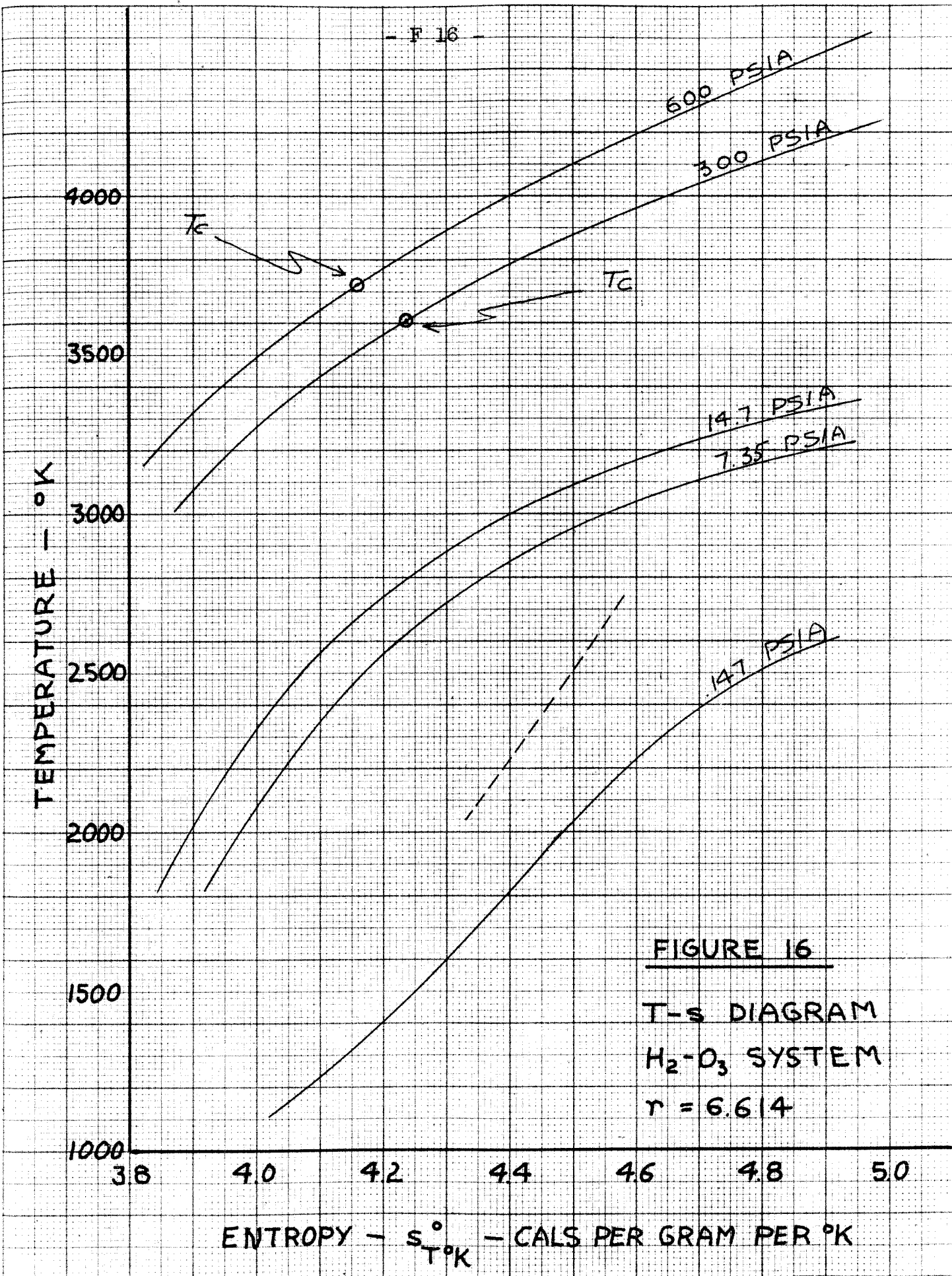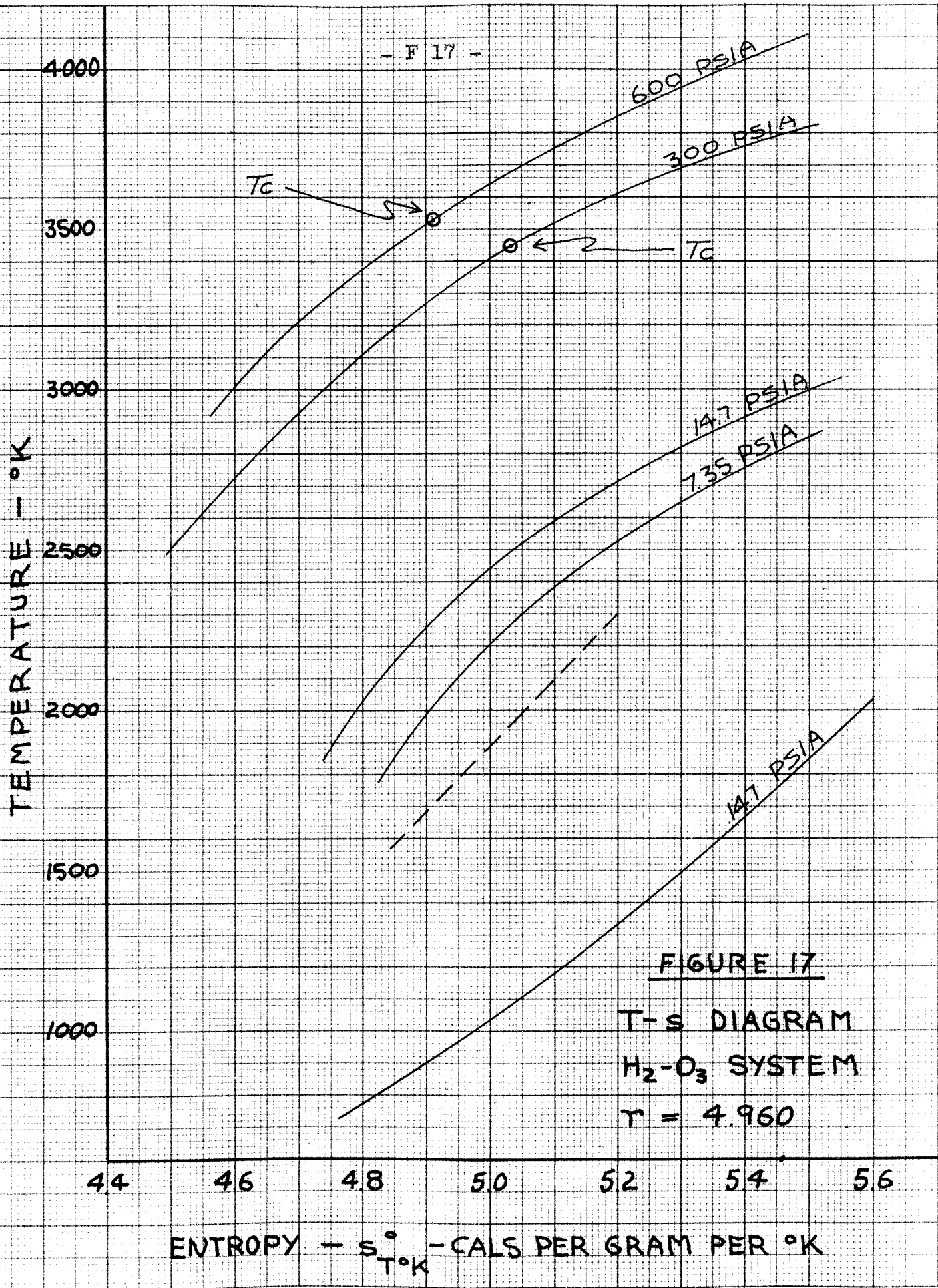
FIGURE 18

THEORETICAL SPECIFIC IMPULSE FROM h-s DIAGRAM

$$c = 9493 \sqrt{\Delta h} \; \text{ft/sec}$$

$$I_{sp} = c/g \quad \text{seconds}$$

h-s DIAGRAM

NH₃ - RFNA SYSTEM

r = 2.995

ENTHALPY - Δh T_{0K}^{3000K} - KCALS PER GRAM

ENTROPY - $s_{T_{0K}}^{0}$ - CALS PER GRAM PER ^{0}K
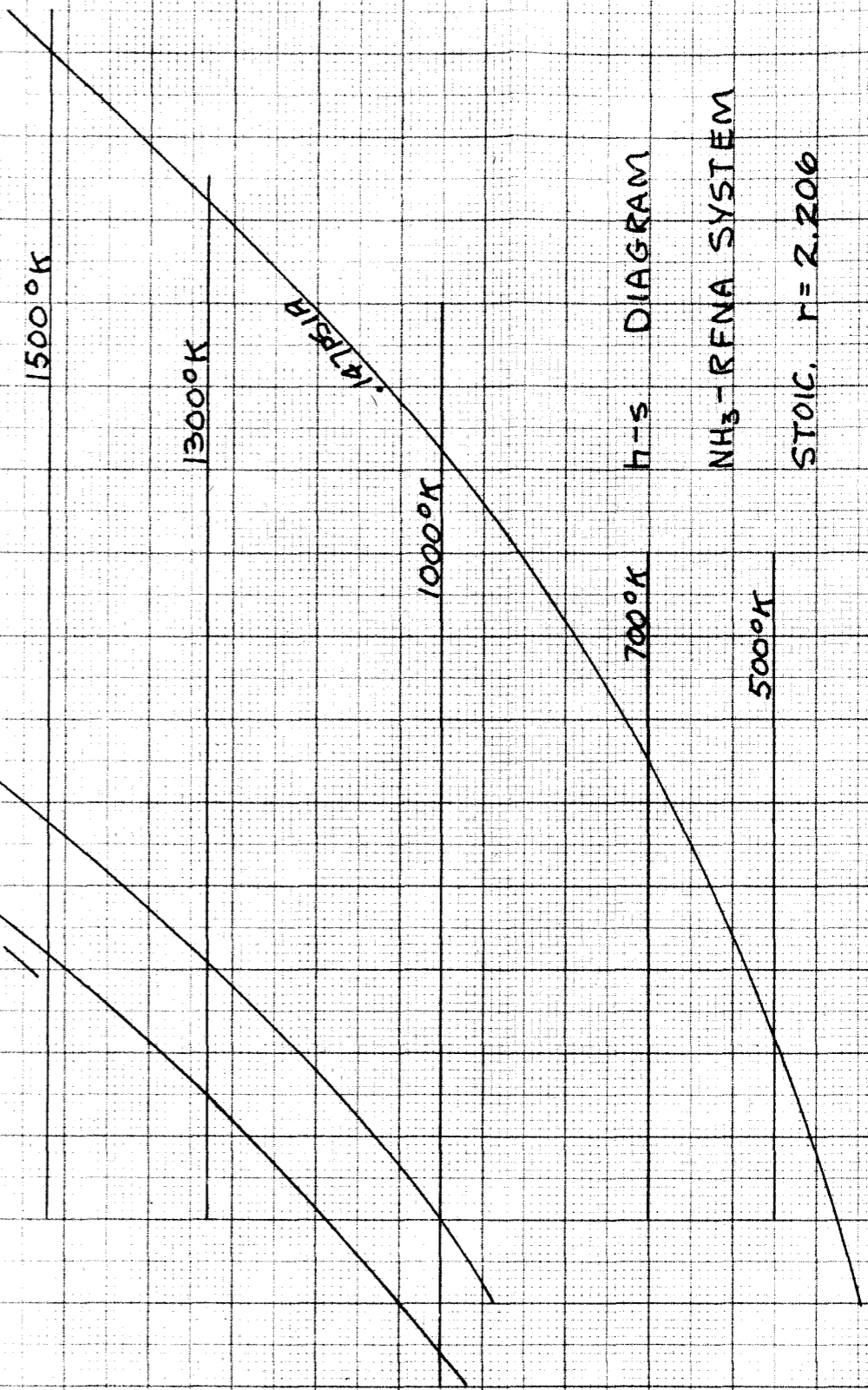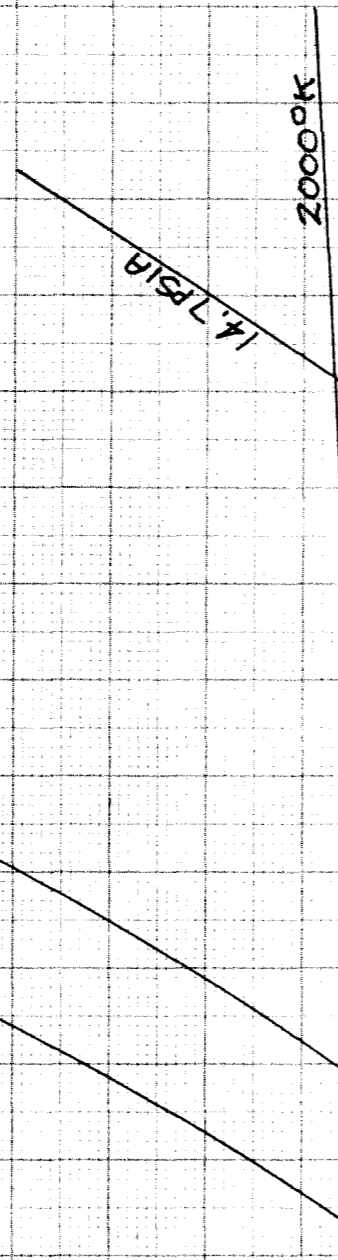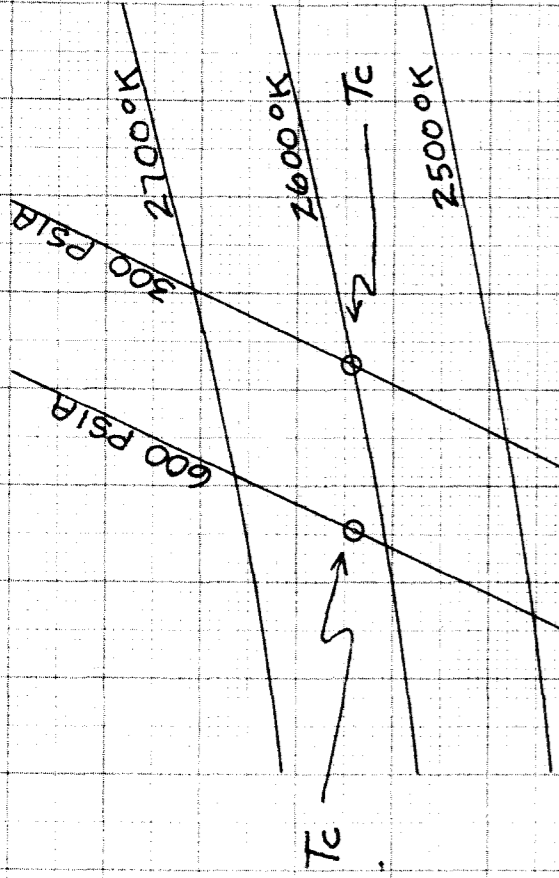
h - s   DIAGRAM

NH_3 - RFNA SYSTEM

STOIC. r = 2.206
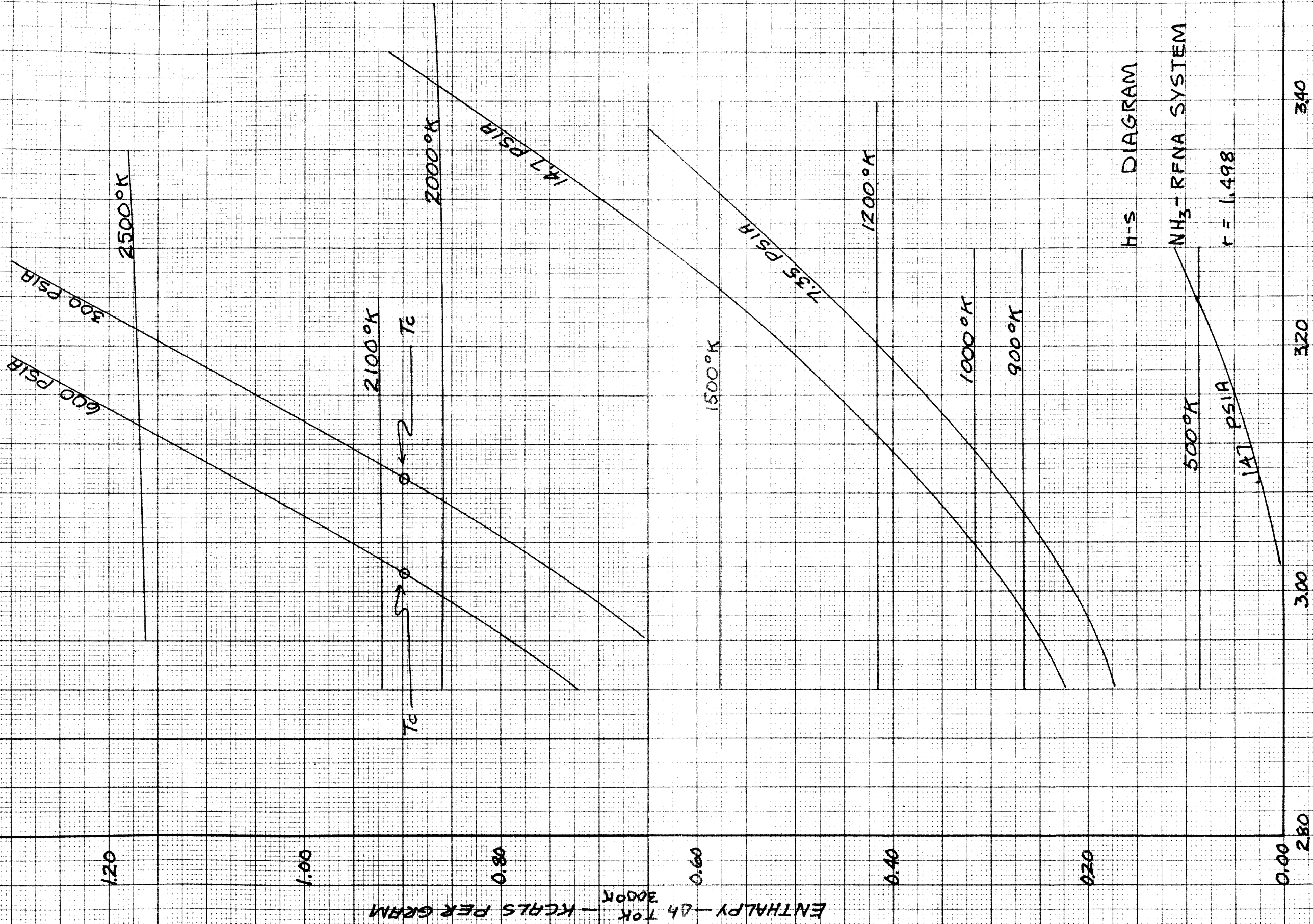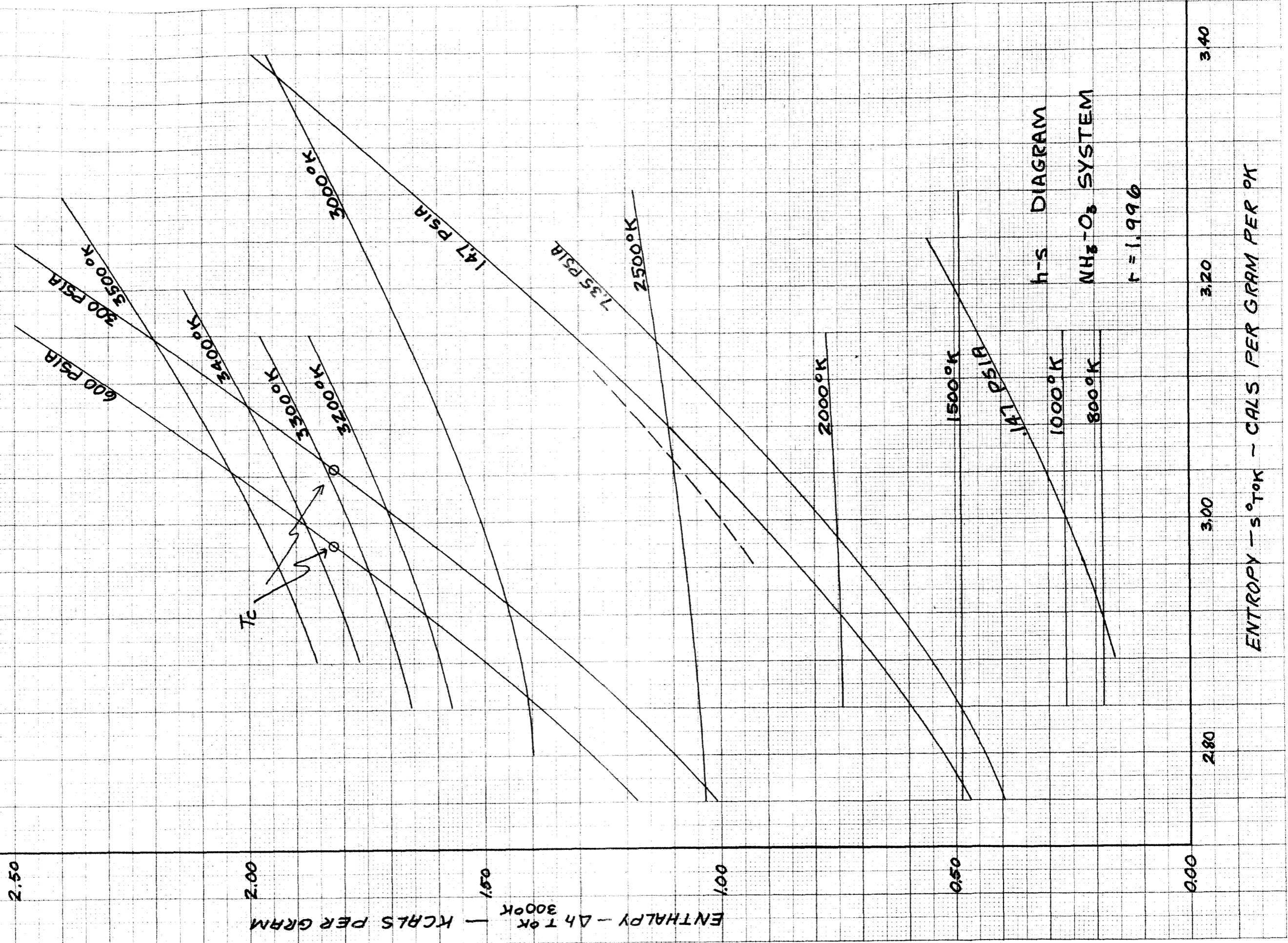
h-s DIAGRAM

NH₃ - RFNA SYSTEM

r = 1.498
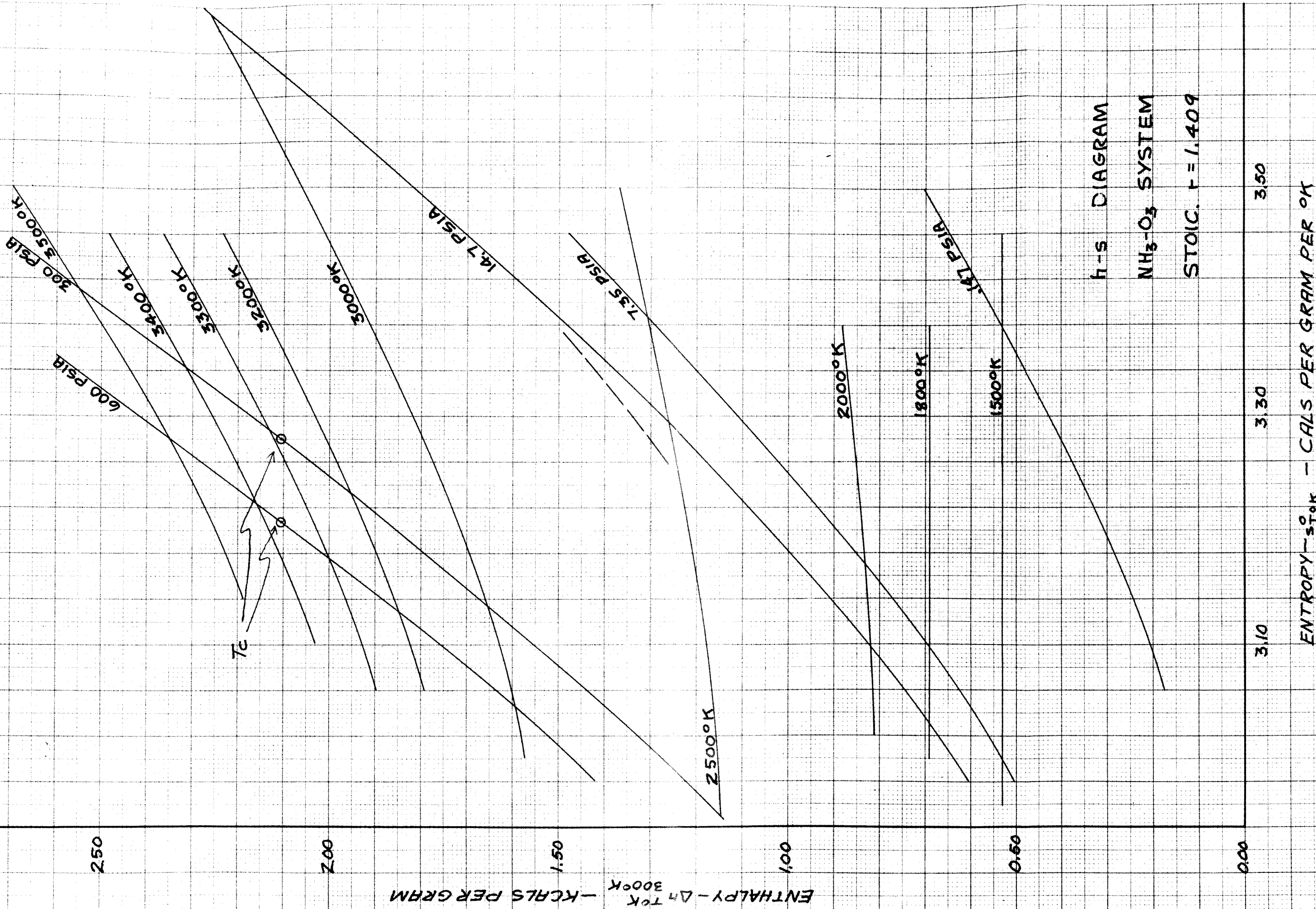
ENTROPY — s°K — CALS PER GRAM PER °K

ENTHALPY — Δh T°K — KCALS PER GRAM
         300°K

h-s DIAGRAM

NH₃-O₃ SYSTEM

r = 1.996

ENTHALPY — Δh T°K — KCALS PER GRAM
                    3000°K

ENTROPY — s°T°K — CALS PER GRAM PER °K

h-s DIAGRAM

NH₃-O₃ SYSTEM

STOIC. r = 1.409

ENTROPY—s°₀ₖ — CALS PER GRAM PER °K

ENTHALPY—Δh T°K / 3000°K — KCALS PER GRAM

600 PSIA

200 PSIA

4000°K

3400°K

3300°K

3200°K

3000°K

14.7 PSIA

7.35 PSIA

14.7 PSIA

2500°K

2000°K

1800°K

1500°K

Tc

2.50

2.00

1.50

1.00

0.50

0.00

3.10

3.30

3.50

ENTROPY — $s°_{T°K}$ — CALS PER GRAM PER °K

ENTHALPY — $\Delta h°_{T°K}_{300°K}$ — KCALS PER GRAM

h-s DIAGRAM
NH_3-O_3 SYSTEM
r = 1.098
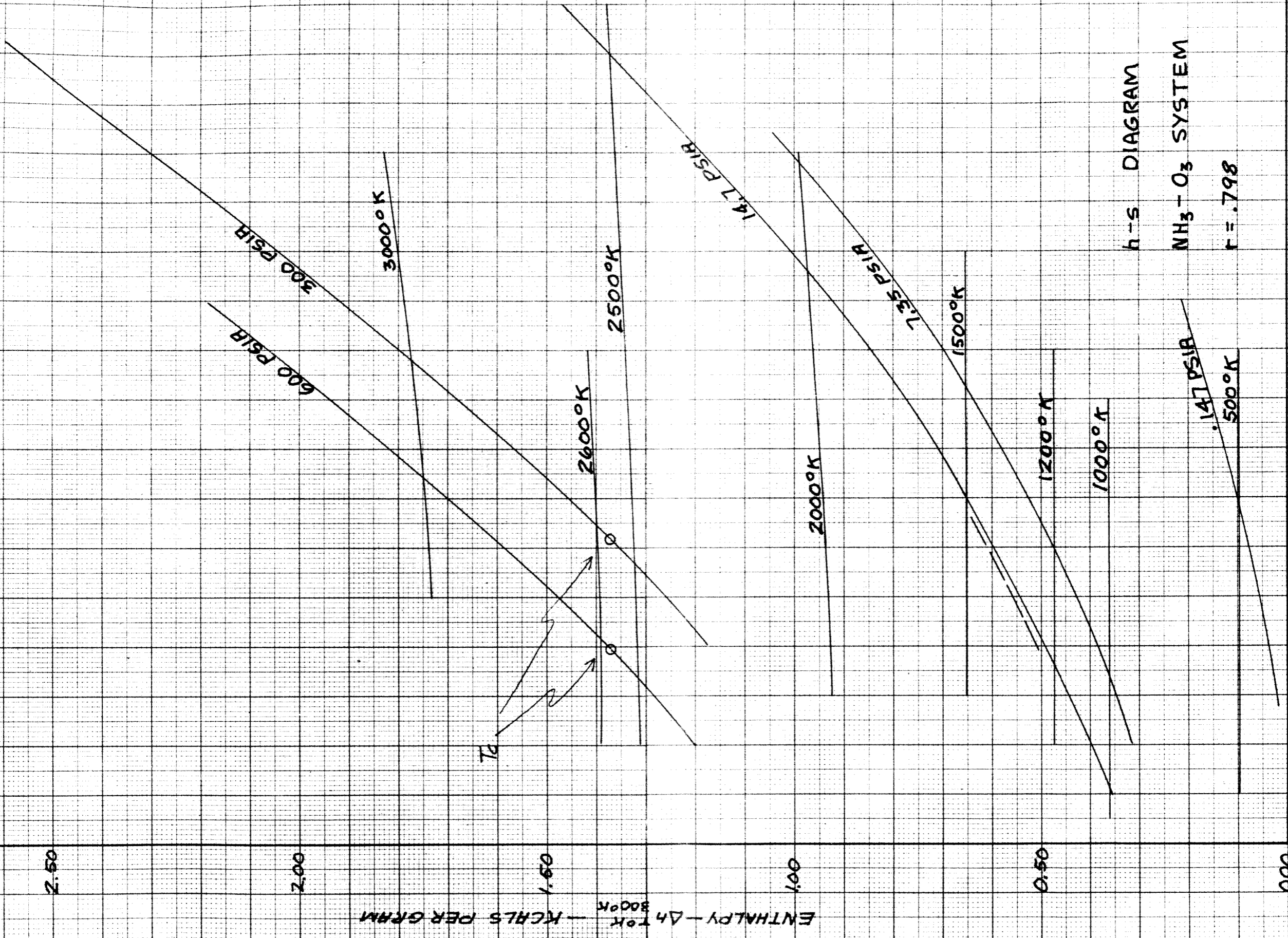
h-s DIAGRAM

$NH_3 - O_3$ SYSTEM

r = .798

ENTROPY - $S^0_{T^oK}$ - CALS PER GRAM PER ^oK

ENTROPY — $s^o_{T^oK}$ — CALS PER GRAM PER °K

ENTHALPY — $\Delta h_{T^oK}^{3000^oK}$ — KCALS PER GRAM

h-s. DIAGRAM

$H_2 - O_3$ SYSTEM

$r = 9.921$

h-s DIAGRAM

$H_2 - O_3$ SYSTEM

STOIC. r = 7.936

ENTROPY — $s^o_{T^oK}$ — CALS PER GRAM PER ^oK

ENTHALPY — $\Delta H \frac{T^oK}{3000^oK}$ — KCALS PER GRAM

ENTROPY — $s^o_{T^oK}$ — CALS PER GRAM PER ^oK

h-s DIAGRAM

H_2-O_2 SYSTEM

r = 6.614
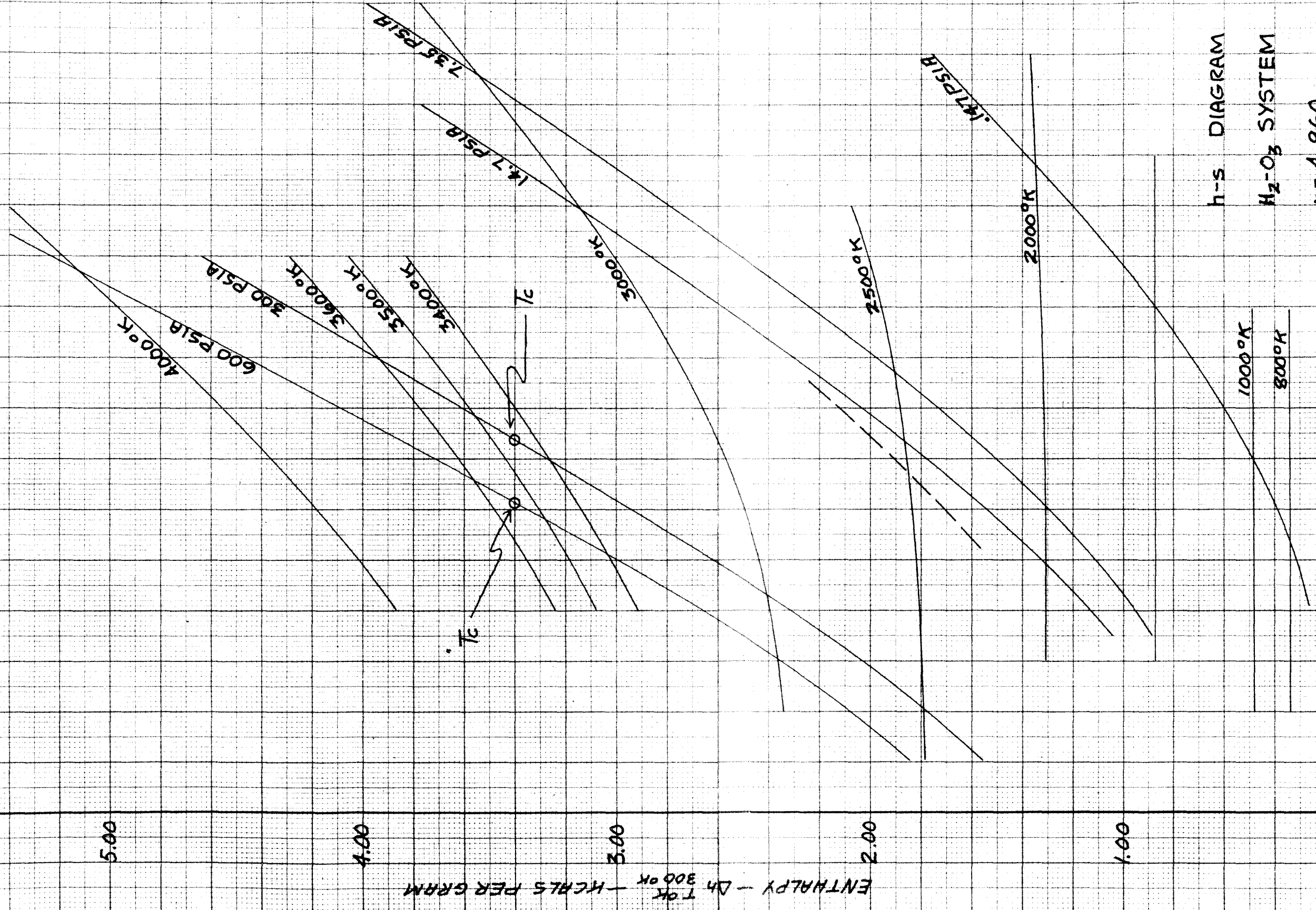
ENTHALPY — $\Delta h_{T^oK}^{3000^oK}$ — KCALS PER GRAM

ENTROPY — $s°_{T°K}$ — CALS PER GRAM PER °K

h-s DIAGRAM

H_2-O_3 SYSTEM

r = 4.960

ENTHALPY — $\Delta h_{300°K}^{T°K}$ — KCALS PER GRAM

APPENDIX I

MINOR COMPONENT CALCULATIONS OF
C, H, O, N SYSTEMS

The most tedious part of a performance calculation for high temperature systems is the solution for the gas composition at chamber and exit conditions. For systems containing carbon, hydrogen, oxygen, and nitrogen, there are ten components to solve for if the chamber temperature exceeds about $2500^\circ K$ and an eleventh (atomic nitrogen) if the temperature exceeds about $3000^\circ K$. Trial and error solutions require many cycles of operations and so are fairly long. It is possible, however, to set up ten equations involving the ten unknown components in terms of the equilibrium constants and the mass balance equations. These equations can then be reduced in number by eliminating unknowns and the resulting equations can be solved directly for the components. One such scheme is the following:

Let the number of moles of the components be represented by the following symbols:

$$a = n_{H_2} \qquad f = n_{N_2}$$
$$b = n_{H_2O} \qquad g = n_{NO}$$
$$c = n_{CO} \qquad h = n_{OH}$$
$$d = n_{CO_2} \qquad i = n_{H}$$
$$e = n_{O_2} \qquad j = n_{O}$$

These ten unknowns are related by the following equations:

(1) $\dfrac{bc}{ad} = K_1$　　　　　(6) $\dfrac{ha^{\frac{1}{2}}}{b} = K_{10}$

(2) $\dfrac{ga}{f^{\frac{1}{2}}b} = K_3$　　　　(7) $c + d = C$

(3) $\dfrac{a^2e}{b^2} = K_6$　　　(8) $b + c + 2d + 2e + g + h + j = 0$

(4) $\dfrac{aj}{b} = K_7$　　　(9) $2a + 2b + h + i = H$

(5) $\dfrac{i}{a^{\frac{1}{2}}} = K_9$　　　　(10) $2f + g = N$

where C, O, H, and N represent the total number of gram atoms of the element in the sample chosen for the calculation. The K's are given in terms of the number of moles of the constituents and are related to the K_p's (in terms of pressures) by the relation:

$$K = K_p(n/P)^{n_p - n_R}$$

where n is the total number of moles, P, the total pressure, and $n_p - n_R$ represents the difference in the number of moles between the products and reactants for the particular reaction under consideration.

The elimination of the unknowns may now be accomplished as follows. Solve Eqn. for c:

$$c = C - d$$

Substitute into Eqn. (1) to yield

$$bC - bd - K_1 ad = 0$$

This gives for $\underline{d}$:

$$d = \frac{bC}{b + K_1 a}$$

Substitute back into Eqn. (7) and obtain for $\underline{c}$:

$$c = C - \frac{bC}{b + K_1 a} = \frac{C}{1 + \frac{b}{K_1 a}}$$

The remaining unknowns are now readily solved for in terms of $\underline{a}$ and $\underline{b}$ to yield:

$$d = \frac{bC}{b + K_1 a} \qquad\qquad h = \frac{b}{a^{\frac{1}{2}}} K_{10}$$

$$e = \frac{b^2}{a^2} K_6 \qquad\qquad i = a^{\frac{1}{2}} K_9$$

$$f = \tfrac{1}{2}(N-g) \qquad\qquad j = \frac{b}{a} K_7$$

Substitute for $\underline{h}$ and $\underline{i}$ into Eqn. (9) and obtain for $\underline{b}$:

$$(\text{I}) \qquad b = \frac{H - 2a - K_9 a^{\frac{1}{2}}}{2 + \frac{K_{10}}{a^{\frac{1}{2}}}}$$

Solve for $\underline{g}$ from Eqn. (8) to yield:

$$(II) \quad g = 0 - C \left[\frac{K_1 a + 2b}{K_1 a + b} \right] - b \left[1 + \frac{K_{10}}{a^{\frac{1}{2}}} + \frac{K_7}{a} \right]$$

$$- 2K_6 \frac{b^2}{a^2}$$

Another equation for g is obtained by eliminating f from Eqn's. (2) and (10) to give:

$$(III) \quad \frac{2g^2 a^2}{K_3^2 b^2} + g - N = 0 = F(III)$$

The equations I, II, and III form the basis for the solution of the unknowns. This is accomplished as follows:

PROCEDURE

(1) Choose a likely value of a.

(2) Calculate the corresponding value of b from (I).

(3) Calculate the corresponding value of g from (II).

(4) Substitute the values of a, b, and g into Eqn. (III) to obtain F(III).

(5) Repeat calculations and interpolate to those values which make F(III) equal to zero.

In general, it will be found that if F(III) is greater than zero, a should be decreased, and vice versa.

The following are special cases:

A. Case where there is no C in the system $\left[N, H, O \right]$:

Eqn's. (I) and (III) are the same but (II) becomes:

(II) $g = 0 - b \left[1 + \dfrac{K_{10}}{a^{\frac{1}{2}}} + \dfrac{2K_6 b}{a^2} + \dfrac{K_7}{a} \right]$

The procedure is the same.

B. Case where there is no N in the system $\left[C, H, O \right]$:

Eqn. (I) is the same, (III) is eliminated, and (II) becomes:

(II) $b \left[1 + \dfrac{K_{10}}{a^{\frac{1}{2}}} + \dfrac{K_7}{a} + \dfrac{2K_6 b}{a^2} \right] + C \left[\dfrac{K_1 a + 2b}{K_1 a + b} \right]$

$$- 0 = F(II) = o$$

The proper $\underline{a}$ will make $F(II)$ equal to zero.

C. Case where both C and N are absent $\left[H, O \right]$:

Eqn. (I) is the same, (III) is eliminated, and (II) becomes:

$$(II) \qquad b \left[1 + \frac{K_{10}}{a^{\frac{1}{2}}} + \frac{K_7}{a} + \frac{2K_6 b}{a^2} \right] - 0 = F(II) = o$$

The proper $\underline{a}$ makes F(II) equal to zero.