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⑥ COMPUTER CALCULATIONS OF ROCKET  
ENGINE COMBUSTION PROPERTIES,

⑩ by

Roy C. Robinette, Jr.

Captain, USAF

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G.C.



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## ACKNOWLEDGEMENT

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## NOMENCLATURE

The following symbols are employed in the derivations of this thesis.

<u>Symbol</u>	<u>Explanation</u>
$A_1$	Total number of atoms of a particular species in the reactants.
$a_1$	The number of atoms of a particular species contained in a product of combustion.
$a_j$	The stoichiometric coefficient in the equilibrium equation.
(a/G)	Mole fraction of species a.
(a/G)P	Partial pressure of species a.
C	Centigrade temperature scale.
CONV	Convergence.
Cal	Calorie.
$C_p$	The value of specific heat measured at constant pressure.
$C_v$	The value of specific heat measured at constant volume.
CH2	$C_p$ value for hydrogen at some T.
CH2A	$C_p$ value for hydrogen at $T + 100$ K.
F	Fahrenheit temperature scale.
G,g	Gibb's free energy function.
G	Total number of moles when used in the equations of combustion.
gmole	Gram mole.
H,h	Enthalpy.
Hf	Heat of formation (chemical).
Hr	Heat of reaction (chemical).
H2	Enthalpy of hydrogen at T.

## NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
H2A	Enthalpy of hydrogen at T + 100 K.
H2S	Enthalpy of hydrogen at 298.16 K.
K	Kelvin temperature scale.
Kcal	One thousand calories.
Kp	Equilibrium constant based on partial pressure.
k	Isentropic exponent (Cp/Cv).
L	Work other than expansion work.
Log	Naperian logarithm.
M	Molecular weight.
m	Mass.
N	Number of moles.
n <sub>1</sub>	The number of moles of a product of combustion.
O/F	Oxidizer/fuel molar ratio.
P, p	Pressure.
PS	Combustion pressure (atmospheres).
PK1	Logarithm value of Kp1 at some T.
PK1A	Logarithm value of Kp1 at T + 100 K.
Q	Thermodynamic heat.
Ru	Universal gas constant (1.98718 $\frac{\text{Cal}}{\text{gmole-K}}$ ).
RS	Fractional value between hundreds of degrees.
S, s	Entropy.
S	Molar ratio (oxidizer/fuel).

## NOMENCLATURE (continued)

<u>Symbol</u>	<u>Explanation</u>
T,t	Temperature degrees absolute.
Tc	Adiabatic flame temperature.
TOLER	Tolerance level for the matrix solution.
U,u	Thermodynamic enternal energy.
V,v	Volume.
X <sub>i</sub>	Error function of substance i.
(3,7)	(Row 3, Column 7) of the matrix.
(2:148)	(Reference 2: Page 148)

CHAPTER I  
INTRODUCTION

A rocket engine is a device for converting the thermochemical energy of one or more propellants into exhaust jet kinetic energy. The term propellant is applied to any material, solid or liquid, consumed in the rocket motor for producing high-pressure, high-temperature gases. It is generally assumed, and there is some evidence to support the assumption, that, under the pressure and temperature occurring in a rocket-motor combustion chamber and nozzle, the chemical reaction takes place under conditions which approach chemical equilibrium. Accordingly, in the ensuing discussions the thermodynamic properties of the gas flowing through the rocket motor are assumed to be those from thermochemical equilibrium calculations.

(1:426)\*

↘ The scope of this paper will be limited to the equilibrium calculations of combustion products and the resulting adiabatic flame temperature. The problem of attempting to determine the equilibrium constituents as the gases progress through the rocket nozzle <sup>is</sup> will not be attempted <sup>here</sup> ~~at this time although this author realizes the very pronounced problem which exists.~~ Jo p. 2

As the static temperature decreases during the systematical progression of the gases through the nozzle, the molecules of the propellant which have dissociated due to the high temperature in the combustion chamber tend to reassociate. In a basic rocketry problem frozen flow is assumed, that is, the equilibrium combustion of the

\* Numbers in parentheses refer to items in the bibliography and the related page number.

1

gases in the combustion chamber is unaltered during the expansion process in the nozzle. (1:436) In the condition of equilibrium flow the equilibrium composition corresponding to the local conditions of pressure and temperature is obtained in each section of the nozzle. The preceding statements correspond to the two extreme cases of frozen or equilibrium flow. In the case of real flow, at a temperature often exceeding 3000 K near the chamber, reactions of recombination take place. (2:179) However, the residence time in the nozzle is very small and these reactions may not have sufficient time for completion. Equilibrium flow, therefore, is not obtained and the real flow is situated at some intermediate point between the two extreme cases.

Before the age of electronic computers, the problem of calculating the combustion properties of a rocket engine was very tedious and almost impossible to solve. Since the present day engineers have access to the electronic computers, it is only fitting that a thesis be presented in a form illustrating the solution of combustion problems by use of the electronic computers.

~~The following presentation is~~ a solution of a relatively simple combustion problem consisting of only six products of combustion. <sup>is presented.</sup> By ~~simply~~ understanding and following the illustrated procedures a problem consisting of any number of products of combustion may be computed and solved to any desired degree of accuracy.

CHAPTER II  
HEAT OF REACTION ( $\Delta H_r$ )

The energy released or absorbed in a chemical reaction, under the condition that the products are returned to the initial temperature of the reactants, is defined as the Heat of Reaction. If the reaction takes place at constant pressure, the heat of reaction is equal to the change in enthalpy during the reaction, i.e.,  $(H)_{\text{products}} - (H)_{\text{reactants}}$ . Of course, these enthalpy values must include the energy associated with the chemical bonds of each substance as well as its thermal energy which is due to the random motion of the molecules. (4:1)

The heat of reaction at constant pressure is related to the heat of reaction at constant volume by the following thermodynamic relationships

$$dq = du + pdv = dh - vdp = dH_r \quad (1)$$

The internal energy ( $U$ ) for an ideal gas is a function of temperature only. From this fact it is possible to make the assumption that for an ideal gas, the finite difference of internal energy ( $\Delta U$ ) at constant pressure is equal to the same value at constant volume, which defines

$$(\Delta U)_p = (\Delta U)_v \quad (2)$$

However

$$(\Delta H_r)_v = \Delta U + P\Delta V^0 \quad (3)$$

and

$$(\Delta H_r)_p = \Delta H - V\Delta P^0 \quad (4)$$

Since by definition

$$H = U + PV \quad (5)$$

then

$$\Delta H = \Delta U + \Delta(PV) \quad (6)$$

on rearranging

$$\Delta U = \Delta H - \Delta(PV) \quad (7)$$

Then by substitution

$$(\Delta Hr)_v = (\Delta Hr)_p - \Delta(PV) = (\Delta U)_p = (\Delta U)_v \quad (8)$$

which can be written as

$$(\Delta Hr)_v = (\Delta Hr)_p - (\Delta N_{gas}) RT \quad (9)$$

Standard Heat of Formation is the heat of reaction when a compound is formed from its elements in their standard state. The standard state of an element is its stable form at a temperature of 298.16 K or 25 C and a pressure of one atmosphere. The standard state is sometimes referred to as being 0 C and one atmosphere. The standard-state temperature is really artificial, for, if the reaction were to take place isothermally, it would require a perfect heat sink which removes heat from the system as fast as it is liberated by the chemical reaction.

When a substance is combined with oxygen the heat of reaction is called the heat of combustion since the reaction is one in which the oxygen is the oxidizer. The formation of carbon dioxide from its elements in their standard state is as follows



Here the carbon must be in the graphite state since that is the stable form of carbon at 25 C, likewise the oxygen and the carbon dioxide must be in the gaseous state. Under these conditions the heat of reaction is the standard heat of formation of  $CO_2$ . In this case

the heat of reaction can also be called the heat of combustion.

The sign associated with the heat of reaction is an indication as to whether the reaction is endothermic (takes up heat) or exothermic (gives off heat). In this country normally a minus or negative sign is associated with an exothermic reaction. This convention is not true all over the world. An easy way to determine which convention is used for any particular set of tables is to check the heat of formation of water. Water will always have an exothermic heat of formation and from this, the correct sign convention can be determined for the remaining substances.

## CHAPTER III

### CHEMICAL EQUILIBRIUM AND THE EQUILIBRIUM CONSTANT

There are several different ways of defining and expressing the equilibrium constant. For example, depending upon the circumstances, the equilibrium constant can be based on concentrations, activities, fugacities, or partial pressures of the constituents present in the equilibrium mixture. In situations where the perfect gas law is closely followed by the constituents of the mixture, the equilibrium constant based on partial pressures is the most useful, i.e., the most easily applied.

An arbitrary thermodynamical system which is separated from its surroundings by a control surface which is a perfect thermal insulator, will now be considered. It is desired to determine from the thermodynamic characteristics of the system whether or not the system is in equilibrium or undergoing a spontaneous change of state. As a first step in the consideration of the aforementioned problem, it is necessary to determine what information can be derived by applying the first and second laws of thermodynamics to the system. The only information furnished by the first law is that one type of energy can be converted into another, and the ratio of the conversion is constant. The first law gives no information regarding the direction in which an energy transformation will proceed. As far as the first law is concerned, it is possible for the conversion to proceed in any direction that is permitted by the constraints imposed on the thermodynamic system. Thus the first law gives no information whatsoever regarding either the spontaneity or the

direction of a physical or chemical process. (2:529)

The second law established the principle that it is impossible to take heat from a system and convert it into work without simultaneous changes occurring in the system or in its environment. From the second law it is learned that only for a reversible adiabatic (isentropic) process is the entropy constant. From the entropy principle it is deduced that the only changes of state (processes) that are possible are those which produce an increase in the entropy of an isolated system. The second law gives no information indicating whether or not a process will take place if the constraints imposed on the system do allow the entropy of the system to increase. Thus it is seen that neither the first nor the second law provides the information for determining (1) whether a thermodynamic system is in equilibrium, and (2) if a spontaneous change of state can occur in a thermodynamic system.

The internal energy ( $U$ ) of a thermodynamic system is analogous to the potential energy of a dynamic system. A dynamical system which is at rest can be set into motion spontaneously if the constraints imposed on it permit the potential energy of the system to diminish. The potential energy of the system tends to convert itself spontaneously into kinetic energy. Studies show that, assuming conditions permit, a dynamical system will be in equilibrium when its potential energy is a minimum. It is a fundamental principle of dynamics that a dynamical system tends to attain the state where its potential energy is a minimum, subject, of course, to the geometrical constraints imposed on the system. Thus, the internal energy ( $U$ ) of a thermodynamical system, if permitted to do so, will be transformed into other forms of energy

having a nonpotential energy nature, until the equilibrium condition for the system is attained. Hence, a spontaneous change of state can take place in a thermodynamic system only if it occurs in the direction which tends to make the internal energy of the system a minimum, and the system will not be in equilibrium until the minimum value of  $U$  is attained. Hence, one fundamental principle that gives spontaneity of a process is that the process must proceed in the direction that will result in the  $U$  of the system proceeding to a condition of  $U$ -min.

From the second law the change of state for an isolated thermodynamic system must result in an increase in the entropy of the system. Since the entropy of the system must increase, the equilibrium condition will be attained only when no further increase in entropy is possible, that is, when the entropy of the system is a maximum, subject to the constraints imposed on it. Hence, a natural process can proceed only in the direction allowing  $S$  of the system to approach  $S$ -max.

From the preceding it follows that the necessary and sufficient conditions for a thermodynamical system to be in equilibrium are: (1) its internal energy must be a minimum, and (2) its entropy must be a maximum. Hence, a spontaneous process is possible only if the change of state can proceed so that the conditions of  $U \rightarrow U$ -min and  $S \rightarrow S$ -max are satisfied.

The free-energy denoted by  $G$  (Gibbs Function) is defined by

$$G = H - TS = U - TS + PV \quad (11)$$

Since  $H$ ,  $U$ ,  $T$ , and  $S$  are thermodynamic point properties, the free-energy function  $G$  is likewise a point property. Hence, a finite change, such as  $\Delta G$  depends only on the final and initial states of the system.

The exact differential  $dg$  is given by

$$dg = du - tds - sdt + pdv + vdp \quad (12)$$

Combining the first and the second laws of thermodynamics results in the following familiar equations

$$tds = dq = du + pdv = dh - vdp \quad (13)$$

One very important statement which is quite often overlooked by the student of thermodynamics is that these equations are based on a pure substance, that is, a substance which is chemically homogeneous and fixed in chemical composition. If the state of the system is such that no chemical reaction can occur without an external stimulus, then the system is in complete (mechanical, thermal, and chemical) equilibrium. When in such a state, the system is chemically homogeneous and invariant; so it is a pure substance and the preceding relationships will apply. However, when a spontaneous chemical reaction occurs it is an irreversible process of a nonpure substance and the equations become (6:482)

$$tds > du + pdv \quad (14)$$

or

$$tds > dh - vdp \quad (15)$$

In the statement of the first law for a closed system, where

$$du = dq - dw \quad (16)$$

it is considered that  $dw$  is equal to  $pdv + dL$ , and defines  $dL$  as work other than expansion work; the  $tds$  equations for a chemical reaction may then be written as

$$tds = du + pdv + dL \quad (17)$$

or

$$tds = dh - vdp + dL \quad (18)$$

The free-energy equation is then stated as

$$dg = du + pdv + vdp - tds - sdt \quad (19)$$

Then substituting for  $t ds$  from equation (17)

$$dg = du + pdv + vdp - (du + pdv + dL) - sdt \quad (20)$$

which results in

$$dg = vdp - sdt - dL \quad (21)$$

In the special case where  $dp = 0$  and  $dt = 0$ , the finite change in free-energy for such a process is denoted by

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} = -\Delta L \quad (22)$$

This equation shows that the change in the free-energy function  $(\Delta G)_{tp}$  represents the maximum (nonexpansion) useful work obtained from a constant temperature and pressure process. It also shows that, for a process conducted so that  $dp = 0$  and  $dt = 0$ , the useful work  $\Delta L$  is equal to the decrease in the value of the free-energy function.

The free-energy function finds its principal use in establishing the criteria for predicting the equilibrium of chemical and physical processes. For a system that is in equilibrium at a given temperature and pressure, the value of the free-energy function is a minimum. Moreover, for a process to take place spontaneously without change in temperature and pressure, the corresponding change in the free-energy function must be negative. Hence, for a spontaneous change (with  $dp = 0$  and  $dt = 0$ )

$$(\Delta G)_{tp} = (G_2 - G_1)_{tp} < 0 \quad (23)$$

The foregoing provides a criterion for the possible existence of equilibrium. If  $(\Delta G)_{tp} = 0$ , a spontaneous change of state is impossible. The foregoing shows that, if the free-energy function at a second state (state 2) is less than it is in the initial state (state 1), the system must eventually pass to state 2. Thus the change in the free-energy function is a measure of the tendency of a system to change its state; that tendency is called the escaping tendency.

From the discussion of the free-energy function the following conclusions may be drawn.

1. The only chemical reaction that can proceed spontaneously are those for which the free-energy function decreases.

2. If a chemical reaction gives no change in the free-energy function, then the reaction is in the equilibrium state.

3. Since the direction of a chemical reaction depends on the concentrations of the chemical species involved, the values of the free-energy function for the different species are related to their concentrations.

4. If the reactants in a chemical process cannot form the desired products by a given isothermal process, they cannot form them by any other process, because the change in the free-energy function is independent of the path since it is a property.

When  $H_2O$  and  $CO_2$  and other products of combustion are subject to temperatures of 4300 F and higher they tend to dissociate in a manner and to a degree determined solely by the temperature of the mixture. When the products of combustion dissociate, heat is absorbed, which decrease the energy available to accelerate the combustion gases

through the rocket engine. Dissociation is a reversible reaction, that is, one that will go in either direction. In any mixture of products and reactants both dissociation and combustion are constantly occurring. When the rate of dissociation equals the rate of combustion the reaction is in chemical equilibrium and an equilibrium constant exists.

In the general chemical reaction



A, B, C, D represent various substances and a, b, c, d represent the corresponding stoichiometric coefficients. (9:498)

For this example it will be assumed that all the substances involved represent ideal gases. The double arrow indicates that when equilibrium is achieved each substance will be present in a certain amount, and each substance will exist at its partial pressure. As previously stated for a system to be in equilibrium  $dL$  must equal 0, that is, no work is being done. From this, equation (21) becomes

$$dg = vdp - sdt \quad (25)$$

which for a isothermal process reduces to

$$dg = vdp = \frac{RuT}{p} dp \quad (26)$$

Then upon intergrating from  $p^0$  to  $p$  and  $g^0$  to  $g$ , equation (26) becomes

$$g - g^0 = RuT \log \frac{p}{p^0} \quad (27)$$

By letting subscript zero refer to standard conditions at one atmosphere

$$g - g^0 = RuT \log p \quad (28)$$

where  $p$  is in atmospheres.

From the mixture of gases as given in the previous general

equation (24), the following can be written

$$g_A - g_A^{\circ} = RuT \log p_A \quad (29)$$

$$g_B - g_B^{\circ} = RuT \log p_B \quad (30)$$

$$g_C - g_C^{\circ} = RuT \log p_C \quad (31)$$

$$g_D - g_D^{\circ} = RuT \log p_D \quad (32)$$

Now by writing an expression for the change in Gibb's free-energy function as the reaction goes to completion, that is, starting with reactants A and B and ending with products C and D and since

$$\Delta G = G \text{ products} - G \text{ reactants} \quad (33)$$

then

$$\Delta G = cg_C + dg_D - ag_A - bg_B \quad (34)$$

Substitution in the pressure equations (29) through (32), gives

$$\begin{aligned} \Delta G &= cg_C^{\circ} + c RuT \log p_C + dg_D^{\circ} + d RuT \log p_D \\ &\quad - ag_A^{\circ} - a RuT \log p_A - bg_B^{\circ} - b RuT \log p_B \end{aligned} \quad (35)$$

However,  $\Delta G^{\circ}$  is defined as

$$\Delta G^{\circ} = cg_C^{\circ} + dg_D^{\circ} - ag_A^{\circ} - bg_B^{\circ} \quad (36)$$

and equation (35) then reduces to

$$\Delta G = \Delta G^{\circ} + RuT \log \frac{p_C^c p_D^d}{p_A^a p_B^b} \quad (37)$$

When the reaction is in equilibrium ( $\Delta G = 0$ ), and since  $\Delta G^{\circ}$  is a constant and  $RuT$  is a constant, the quantity

$$\log \frac{P_C^c P_D^d}{P_A^a P_B^b} \quad (38)$$

must be equal to a constant which is defined as

$$\log K_p \quad (39)$$

This results in the following equality

$$K_p = e^{\frac{-\Delta G^\circ}{R_u T}} \quad (40)$$

where  $K_p$  is the equilibrium constant expressed by the partial pressures of the combustion gases.

For this paper no attempt will be made to consider the equilibrium constant which is expressed in values of concentrations, activities, or fugacities.

## CHAPTER IV

### CALCULATION OF THE ADIABATIC FLAME TEMPERATURE

All methods for determination of the adiabatic flame temperature and the composition of the combustion products are based on two principles: the First Law of Thermodynamics and the Law of Conservation of Mass. These two principles when used in conjunction with experimentally determined chemical equilibrium data, yield a system of simultaneous equations in terms of the gas composition. The various methods of determining the gas composition differ in the manner in which the simultaneous equations are set up and solved.

By applying the First Law of Thermodynamics and the Law of Conservation of Mass to a chemical reaction it is possible to define the term Adiabatic Flame Temperature. Assuming that the chemical reaction is at constant pressure and adiabatic, and that there is no shaft work performed, the First Law of Thermodynamics states that the enthalpy of the reactants at their temperature prior to the reaction ( $T_b$ ) is equal to the enthalpy of the products of the reaction at the flame temperature ( $T_c$ ). Here the enthalpy must include the chemical energy of the molecules of each specie as well as their energy due to random motion, since changes in internal energy occur as a result of the rearrangement of the molecules during reaction.

The Law of Conservation of Mass applied to a chemical reaction requires that the number of atoms of each element remain constant. For example, the number of atoms of a single element in the products after the reaction must be equal to the number of atoms of the same element

in the reactants prior to the reaction, and the same is true for all other elements. Thus in accordance with the definition of a mole, it can be said that the number of atoms of any particular species is constant.

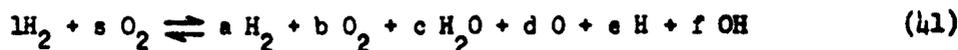
With the aforementioned laws of natural response, the necessary equations and calculations may now be presented for solving any possible system of combustion. For this combustion problem liquid hydrogen and liquid oxygen will be burned. However, by simply rearranging some of the basic steps, any oxidizer - fuel combination, may be used.

Now before the reaction equations can be written, a decision must be made as to what products of combustion are likely to be present in the combustion gas. For the adiabatic reaction, the equilibrium flame temperature will be very high and a considerable amount of dissociation can be expected.

A basic knowledge of chemistry is required to determine the possible products. By comparing the equilibrium constants of the selected products, some may be eliminated by observing that their  $K_p$  value is several orders of magnitude less than the values listed for the other reactions. The presence of other combinations may be discounted when the experimental fact is considered that a chemical system will tend to adjust itself so that the constituents are in their lowest energy state. After a decision has been reached with regard to the products of combustion, the reaction equations can then be written.

In the combustion of liquid oxygen and liquid hydrogen, a possible assumption of probable products are,  $H_2$ ,  $O_2$ ,  $H_2O$ ,  $O$ ,  $H$ ,  $OH$ ,  $O_3$ , and  $H_2O_2$ .  $O_3$  and  $H_2O_2$  can be eliminated by applying the above-mentioned rules as these are both high energy forms.

The following equation



list the six assumed products of combustion. The value of  $s/l$  will give the molar, oxidizer to fuel ratio. This can easily be converted to mass ratio, if desired, by use of the following equation

$$m = N M \quad (42)$$

However, for this problem only the molar ratio will be considered.

In the development of the system for solving for the molar values of the products of combustion it is necessary to regress a moment to discuss the selected system. "The errors are distributed among all the species" is the title of reference (2:142). This method is completely general and can be used irrespective of the number of substances present in the combustion products. The system is well suited for solution by electronic computers, which is the primary reason it was selected.

The system of equations used to determine the equilibrium composition at a given pressure and temperature is formed by linear equations representing the conservation of the species and by non-linear equations which can be written in logarithmic form and represent the various equilibria.

By referring to equation (41) and utilizing the basic equation for the balance of individual species

$$A_1 = \sum_1^i n_1 \quad (43)$$

the first three equations may be formed.

1. Equation for hydrogen balance

$$2 = 2a + 2c + e + f \quad (44)$$

2. Equation for oxygen balance

$$2s = 2b + c + d + f \quad (45)$$

3. Equation for total moles

$$G = a + b + c + d + e + f \quad (46)$$

For any combustion problem, the number of products of combustion is equal to I, and the number of different species (atoms) is equal to J. Then from the equation

$$Y = I - J \quad (47)$$

the value of Y will determine the absolute number of independent equilibrium equations.

For this problem

$$Y = 6 - 2 \quad (48)$$

or

$$Y = 4 \quad (49)$$

Therefore, the number of independent equilibrium equations is 4. The basic equation for equilibrium in logarithmic form is

$$\log z_1 = \sum_{ij} a_j \log n_i \quad (50)$$

which allows the formation of the following four additional equations.

The values of  $K_p$  listed in NACA Report 1037 and also in the Appendix are based on the constituents being formed from their atoms. Therefore, the equations become

4. H<sub>2</sub>O Equilibrium Equation, which is formed from



and results in

$$K_p(H_2O) = \frac{((c/G)P)}{((e/G)P)^2 (d/G)P} \quad (52)$$

which by rearranging becomes

$$K_p(\text{H}_2\text{O}) = \frac{c}{e^2 d} \frac{G^2}{P^2} \quad (53)$$

Then by equating

$$K_p(\text{H}_2\text{O}) = K_{p1} \quad (54)$$

In logarithmic form equation (53) may be stated as

$$2 \log P + \log K_{p1} = \log c - 2 \log e - \log d + 2 \log G \quad (55)$$

5. H<sub>2</sub> Equilibrium Equation, which is formed from



and results in

$$K_p(\text{H}_2) = \frac{(a/G)P}{((e/G)P)^2} \quad (57)$$

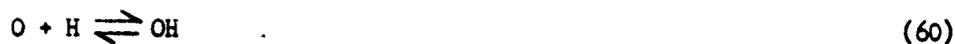
which by rearranging becomes

$$K_p(\text{H}_2) = \frac{a}{e^2} \frac{G}{P} \quad (58)$$

Then by defining  $K_p(\text{H}_2)$  as  $K_{p2}$  and writing in logarithmic form, equation (58) may be stated as

$$\log P + \log K_{p2} = \log a - 2 \log e + \log G \quad (59)$$

6. OH Equilibrium Equation, which is formed from



and results in

$$K_p(\text{OH}) = \frac{(f/G)P}{(d/G)P (e/G)P} \quad (61)$$

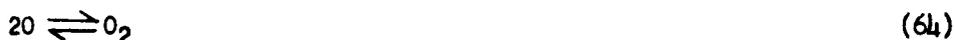
which by rearranging becomes

$$K_p(\text{OH}) = \frac{f}{de} \frac{G}{P} \quad (62)$$

Then by defining  $K_p(\text{OH})$  as  $K_{p3}$  and writing in logarithmic form, equation (61) may be stated as

$$\log P + \log K_{p3} = \log f - \log d - \log e + \log G \quad (63)$$

7.  $\text{O}_2$  Equilibrium Equation, which is formed from



and results in

$$K_p(\text{O}_2) = \frac{(b/G) p}{((d/G)P)^2} \quad (65)$$

which by rearranging becomes

$$K_p(\text{O}_2) = \frac{b}{d^2} \frac{G}{P} \quad (66)$$

Then by defining  $K_p(\text{O}_2)$  as  $K_{p4}$  and writing in logarithmic form, equation (65) may be stated as

$$\log P + \log K_{p4} = \log b - 2 \log d + \log G \quad (67)$$

This results in an array of mathematical logic consisting of seven equations and seven unknowns. Such a system can be solved by trial and error. It can be linearized by choosing arbitrary values for the number of moles ( $n_1^0$ ) and then solving for an error function ( $X_1^0$ ). The error functions are used in the following equation

$$n_1 = n_1^0 (1 + X_1^0) \quad (68)$$

If  $X_1^0$  is sufficiently small, equation (68) in logarithmic form may be written as

$$\log n_1 \approx \log n_1^0 + X_1^0 \quad (69)$$

This is true by considering the fact that the  $\log(1 + \text{small number})$  is approximately equal to the small number.

Equations (43), (44), (45), and (46) can thus be written in

the form

$$\sum_i a_i n_i^o X_i^o = A_1 - \sum_i a_i n_i^o = A_1 - A_1^o \quad (70)$$

where

$$A_1^o = \sum_i a_i n_i^o \quad (71)$$

Equations (55), (59), (63), and (67) can be written in the form

$$\sum_{ij} a_j X_i^o = \log z_1 - \sum_{ij} a_j \log n_i^o = \log \frac{z_1}{z_1^o} \quad (72)$$

where

$$\log z_1^o = - \sum_{ij} a_j \log n_i^o \quad (73)$$

The transformation of the variables is now complete. The new system is linear with respect to the error function ( $X_i$ ) and can thus be solved by any standard method of solving simultaneous linear equations. The selected method is well suited for solution by electronic computers.

A complete description for the selected method to solve simultaneous linear equations is presented in the Appendix. The program is a partial replica of a method listed in the IBM listing of selected programs for the 1620 computer. (5.0.007) The original program was based on the original FORTRAN system and had to be completely rewritten so as to be suitable for use with the present FORTRAN program.

Table I, on the following page, consists of the seven linear equations of combustion consolidated into a matrix form. A detailed example is attached to Table I. It is available for additional reference, as required, to complete the formation of a similar system of equations necessary to solve other combustion problems.

TABLE I  
COMBUSTION PROBLEM IN MATRIX FORM

	1.	2.	3.	4.	5.	6.	7.																
	$\frac{H_2}{a}$	$\frac{O_2}{b}$	$\frac{H_2O}{c}$	$\frac{O}{d}$	$\frac{H}{e}$	$\frac{OH}{f}$	$\frac{G}{g}$	$a^0 \ b^0 \ c^0 \ d^0 \ e^0 \ f^0 \ g^0$															
H																							
1. Bal.	2a	XA	0	XB	2c	XC	0	XG	=	2 - (2a	+2c	+e	+f	) = A1									
0																							
2. Bal.	0	XA	2b	XB	c	XC	d	XD	0	XE	f	XF	0	XG	=	2S - (	2b	+c	+d	+f	) = A2		
M																							
3. Total	a	XA	b	XB	c	XC	d	XD	e	XE	f	XF	-GH	XG	=	G - (	a	+b	+c	+d	+e	+f	) = A3
4.	0	XA	0	XB	1	XC	-1	XD	-2	XE	0	XF	+2	XG	=	2log p	+ Pk1	- (log c	- 2log e	- log d	+ 2log G)	=	A4
5.	1	XA	0	XB	0	XC	0	XD	-2	XE	0	XF	+1	XG	=	log p	+ Pk2	- (log a	- 2log e	+ log G)	=	A5	
6.	0	XA	0	XB	0	XC	-1	XD	-1	XE	1	XF	+1	XG	=	log p	+ Pk3	- (log f	- log e	- log d	+ log G)	=	A6
7.	0	XA	+1	XB	0	XC	-2	XD	0	XE	0	XF	+1	XG	=	log p	+ Pk4	- (log b	- 2log d	+ log G)	=	A7	

The following examples illustrate how the above matrix is set up:

$$A_1 = \sum_i a_i n_i \quad ** \quad n_i = n_i^0(1 + X_i) \quad ** \quad \sum_i a_i n_i^0 X_i^0 = A_1 - \sum_i a_i n_i^0$$

$$2 = 2a + 2c + e + f = 2a^0 + 2a^0 XA + 2c^0 + 2c^0 XC + e^0 + e^0 XE + f^0 + f^0 XF$$

$$2 = 2a^0 XF + f^0 XF - 2 - (2a^0 + 2c^0 + e^0 + f^0)$$

$$\log z_1 = \sum_{ij} a_j \log n_i \quad ** \quad \log n_i = \log n_i^0 + X_i \quad ** \quad \sum_{ij} a_j X_i = \log z_1 - \sum_{ij} a_j \log n_i^0$$

$$2 \log P + Pk1 = \log c - 2 \log e - \log d + 2 \log G$$

$$2 \log P + Pk1 = \log c^0 + XC - 2 \log e^0 - 2 XE - \log d^0 - XD + 2 \log G^0 + 2 XG$$

$$XC - 2 XE - XD + 2 XG = 2 \log P + Pk1 - (\log c^0 - 2 \log e^0 - \log d^0 - \log G^0)$$

The value of  $X_1$  obtained from the solution of the matrix provides the new value of  $n_1^1$  which is computed, for the second approximation, from the equation

$$n_1^1 = n_1^0 (1 + X_1) \quad (74)$$

A very important consideration is that the first approximation may not be very close to the correct value. It is probable that during the first few trials a value for  $X_1$  of less than -1.00 may be computed. The program will not accept a value for  $X_1$  of -1.00 or less; a value greater than -1.00 must then be used. In this problem -0.995 was utilized for such cases with complete success. After the assumed values are within the correct range a value of less than -1.00 will never be calculated and the calculated values of  $X_1$  may be used completely. At this time the computer may be set to compute continuously until the desired convergence is obtained.

When the calculated error functions have a value of equal to or less than -1.00 and are then used in equation (74), a negative or zero value is calculated for  $n_1$ . This creates errors in the calculation resulting from the computer attempting to take the log of a negative or zero number. By inserting -0.995, a very small positive value of  $n_1$  is calculated. This answer is approximately correct since it would be impossible to actually have a negative value of a constituent.

The initial selected values for the number of moles of the products of combustion are completely arbitrary; however, if any information on the approximate values is available, it should be utilized. After the problem is solved one time it is advisable to use the calculated values

as the original selected values for the number of moles in solving the problem for the new temperature selection as determined by Figure 4-1. This will allow the problem to converge quicker and save having to replace the error functions that are equal to or less than -1.00. Another suggestion is to require the sum of the first selected values not to exceed the value of the number of moles of the reactants.

The convergence of the system is given by the expression

$$\text{CONV} = /A_1 - A_1^0/ + /...../ + / \ln \frac{z_1}{z_1^0} / + /.....? \quad (75)$$

In the computer program, the value of  $A_1 - A_1^0$  is set equal to A1 and the value of the  $\log \frac{z_1}{z_1^0}$  is set equal to A4. By reference to the initial equations (44) and (55), it is quite apparent that when the correct values for the number of moles of the products have been computed A1, A2, A3, A4, A5, A6, and A7 will all be equal to zero.

When the computer does not have the ability to add absolute values, a simple method that may be used calls for adding the sum of  $\sqrt{x \cdot x}$ . The system is solved when the value of C becomes sufficiently small.

The method described above will now be applied in the solution of a problem involving the selected propellants of liquid oxygen and liquid hydrogen.

The Kp values listed in NACA 1037 are presented in logarithmic form to the base 10. The logarithmic program on the 1620 computer is based on the Napierian Logarithm Scale. To be consistent the values for Kp are multiplied by the natural logarithm of 10.

The computer program is subdivided into four parts:

1. Solution of the coefficients and the values for the solution column of the matrix.

2. Assignment of the appropriate values to columns and rows of the matrix program.
3. Solution of the matrix program.
4. Solution of the difference in enthalpies.

The value for the total number of moles has been assigned to G and GH in the computer program. The matrix coefficient (GH) in position (3, 7) of the developed matrix created some confusion, during the early stages of the problem. By experimentation it was found that by letting GH be equal to the new value for the total number of moles calculated from the value of XG and by letting the G equal the sum of the new values for the  $n_1$ 's the problem would converge. However, by reversing the value of G and GH the problem would not converge.

The computer program is designed to automatically replace any undesired error function with -0.995. This ability is dependent on the position of Sense Switch 3 which also controls the type out of solutions. When Sense Switch 3 is in the off position all values are typed out by the typewriter. During the type-out of the solution of the error functions, if one has a value of -1.00 or less, it is changed to -0.995. A message that this step has been completed is also typed out.

When the operator desires, Sense Switch 3 may be turned on to eliminate typing of all values except the value of convergence. This also eliminates the ability to change the error functions; therefore, it is important that the convergence value must be observed to be decreasing before this step is performed. If Sense Switch 3 is turned on prematurely and an undesired value of an error function is computed, an error statement will be typed out indicating that the computer has

been requested to take the logarithm of a negative number. The solution must be restarted as all values are then incorrect.

As the convergence approaches the desired limit, Sense Switch 3 may be turned off. This allows all values to be typed out which are then the correct solutions for the number of moles of each of the products of combustion.

By turning on Sense Switch 2, the computer branches to the fourth subdivision, where the difference in enthalpies is computed.

The computer also has been programed to interpolate linearly, as necessary, all values of input data. The value of RS is the fractional value between hundreds of degrees. If it is desired to compute for 3528 K, values for 3500 K and 3600 K are read into the computer. The value of RS is then 0.28.

The present computer, with 20,000 storage locations, did not have sufficient locations to compute the value of the molecular weight and the isentropic exponent. A second program was written to perform this computation. The last step of the first program is the command to punch out on data cards, the solution for the number of moles of each of the products. These solution cards are then used in the second program with the necessary additional data to compute the molecular weight and the isentropic exponent. This program also has the ability to interpolate linearly the necessary data.

For the design calculations in this problem the reactants will be assumed to be at standard conditions (298.16 K). The problem is then solved for a particular molar ratio and a selected chamber or total pressure (23 atmospheres). The necessary values are taken from

NACA 1037 by assuming a particular combustion temperature. The combustion products and the change in enthalpies ( $\Delta H$ ) are then calculated.  $\Delta H$  is defined as the enthalpy of the products taken at the combustion temperature minus the enthalpy of the reactants taken at the temperature prior to combustion. If the assumption for the combustion temperature is correct,  $\Delta H$  will be equal to zero. If  $\Delta H > 0$  the assumed temperature was too high; a lower value must be chosen, and combustion of the gas must be recalculated for the new temperature. Of course, if  $\Delta H < 0$  then a larger value for the temperature must be selected. Repetition of this procedure two or three times will usually yield the correct value of temperature, by graphical interpolation.

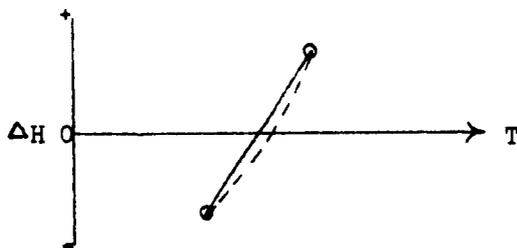


Figure 4-1. Interpolation for adiabatic flame temperature.

If the first two assumed values of temperature give values of  $\Delta H$  on each side of the zero line as shown in Figure 4-1, an approximate value of the combustion temperature may be determined by linear interpolation; however, since the curve of  $\Delta H$  vs  $T$  is usually concaved up, the value so determined will usually be less than the actual temperature.

Linear interpolation for the proper values of  $H$  and  $K_p$  is acceptable. It should be noted that linear interpolation for  $K_p$  over a wide temperature ranges is not accurate, and logarithmic interpolation is required for adequate approximations. However, the equilibrium constants in

NACA 1037 are tabulated for every one hundred degrees Kelvin and linear interpolation within this range of temperature yields sufficiently accurate results.

The following pages consisting of Table II and Table III have the complete computer program for liquid hydrogen and liquid oxygen. With the previous explanations and a basic knowledge of the IBM 1620 FORTRAN system, no problem should exist in setting up the program to compute the combustion properties for any propellant combination.

TABLE II  
FIRST COMPUTER PROGRAM

```

DIMENSION X(7,8)
81 FORMAT(//(F12.8))
32 FORMAT(//8HSOLUTION)
33 FORMAT(44HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34 FORMAT(2HIS I3)
40 FORMAT(EL1.8)
  READ40, PK1,PK2,PK3,PK4,PS,S,TOLER,RS
  READ40,PK1A,PK2A,PK3A,PK4A
  READ40,A,B,C,D,E,F
  READ 40,XA,XB,XC,XD,XE,XF,XG
  PK1=PK1 - RS*(PK1 - PK1A)
  PK2=PK2 - RS*(PK2 - PK2A)
  PK3=PK3 - RS*(PK3 - PK3A)
  PK4=PK4 - RS*(PK4 - PK4A)
27 G=A+B+C+D+E+F
  A=A*(1.+XA)
  B=B*(1.+XB)
  C=C*(1.+XC)
  D=D*(1.+XD)
  E=E*(1.+XE)
  F=F*(1.+XF)
  GH=G*(1.+XG)
  G=A+B+C+D+E+F
  H=LOG(10.)
  A1=2.-(2.*A+2.*C+E+F)
  A2=2.*S-(2.*B+C+D+F)
  A3 = G-(A+B+C+D+E+F)
  A4=2.*(LOG(PS))+H*PK1-(LOG(C)-2.*LOG(E)-LOG(D)+2.*LOG(G))
  A5=(LOG(PS))+H*PK2-(LOG(A)-2.*LOG(E)+LOG(G))
  A6=(LOG(PS))+H*PK3-(LOG(F)-LOG(E)-LOG(D)+LOG(G))
  A7=(LOG(PS))+H*PK4-(LOG(B)-2.*LOG(D)+LOG(G))
  CONV=SQRT(A1*A1)+SQRT(A2*A2)+SQRT(A3*A3)+SQRT(A4*A4)+SQRT(A5*A5)
  CONV=CONV+SQRT(A6*A6)+SQRT(A7*A7)
  IF (SENSE SWITCH 3)50,51
51 PRINT81,A1,A2,A3,A4,A5,A6,A7
  PRINT 81,A,B,C,D,E,F,G,GH
50 PRINT 81,CONV
  IF(SENSE SWITCH 2)30,31
31 X(1,1)=2.*A
  X(2,1)=0.
  X(3,1)=A
  X(4,1)=0.
  X(5,1)=1.
  X(6,1)=0.
  X(7,1)=0.
  X(1,2)=0.

```

```
X(2,2)=2.*B
X(3,2)=B
X(4,2)=0.
X(5,2)=0.
X(6,2)=0.
X(7,2)=1.
X(1,3)=2.*C
X(2,3)=C
X(3,3)=C
X(4,3)=1.
X(5,3)=0.
X(6,3)=0.
X(7,3)=0.
X(1,4)=0.
X(2,4)=D
X(3,4)=D
X(4,4)=-1.
X(5,4)=0.
X(6,4)=-1.
X(7,4)=-2.
X(1,5)=E
X(2,5)=0.
X(3,5)=E
X(4,5)=-2.
X(5,5)=-2.
X(6,5)=-1.
X(7,5)=0.
X(1,6)=F
X(2,6)=F
X(3,6)=F
X(4,6)=0.
X(5,6)=0.
X(6,6)=1.
X(7,6)=0.
X(1,7)=0.
X(2,7)=0.
X(3,7)=-GH
X(4,7)=2.
X(5,7)=1.
X(6,7)=1.
X(7,7)=1.
X(1,8)=A1
X(2,8)=A2
X(3,8)=A3
X(4,8)=A4
X(5,8)=A5
X(6,8)=A6
X(7,8)=A7
N = 7
N1 = N + 1
DO 14 I = 1, N, 1
```

```

DIAG = X(I,I)
IF (DIAG) 3, 20, 4
3 IF (DIAG + TOLER) 5, 19, 19
4 IF (DIAG - TOLER) 19, 19, 5
5 DO 6 J = I, N1
6 X(I,J) = X(I,J) / DIAG
K = 1
9 IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
DO 12 J = I, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
IF (K-N) 9, 9, 14
14 CONTINUE
IF (SENSE SWITCH 3)1,28
28 J = N1
TYPE 32
DO 18 I=1, N
TYPE 40, X(I,J)
IF (X(I,J) + 1.0) 65, 65, 18
65 X(I,J) = -.995
TYPE 66
66 FORMAT(41HTHE ABOVE VALUE HAS BEEN CHANGED TO -.995)
18 CONTINUE
GO TO 1
19 TYPE 33
TYPE 34,I
GO TO 5
20 STOP
1 XA=X(1,8)
XB=X(2,8)
XC=X(3,8)
XD=X(4,8)
XE=X(5,8)
XF=X(6,8)
XG=X(7,8)
GO TO 27
30 READ 40,H2S, O2S,H2,O2,H2O,O,H,OH
READ 40,H2A,O2A,H2OA,OA,HA,OHA
OH = OH + RS*(OHA - OH)
H = H + RS*(HA - H)
O = O + RS*(OA - O)
H2O = H2O + RS*(H2OA - H2O)
O2 = O2 + RS*(O2A - O2)
H2 = H2 + RS*(H2A - H2)
HTS=H2S+S*O2S
HTC=A*H2 + B*O2 + C*H2O + D*O + E*H + F*OH
DELH=HTC-HTS
PRINT 41,HTC,HTS,DELH
41 FORMAT (//(E14.8))
PUNCH 40,A,B,C,D,E,F
STOP
END

```

## TABLE III

## SECOND COMPUTER PROGRAM

```

67 FORMAT (//(35HTHE MOLECULAR WEIGHT OF THE MIX IS F10.5))
68 FORMAT(28HTHE CP VALUE FOR THE MIX IS F10.5)
69 FORMAT (23HTHE VALUE FOR CP/CV IS F10.5)
40 FORMAT(E11.8)
  READ 40,A,B,C,D,E,F,S,RS
  READ 40, CH2, CO2, CH2O, CO, CH, COH
  READ 40, CH2A, CO2A, CH2OA, COA, CHA, COHA
  U=A+B+C+D+E+F
  CH2 = CH2 + RS*(CH2A - CH2)
  CO2 = CO2 + RS*(CO2A - CO2)
  CH2O = CH2O + RS*(CH2OA - CH2O)
  CO = CO + RS*(COA - CO)
  CH = CH + RS*(CHA - CH)
  COH = COH + RS*(COHA - COH)
  CPM = CH2*A/G + CO2*B/G + CH2O*C/G + CO*D/G + CH*E/G + COH*F/G
  CVM = CPM - 1.98718
  CK = CPM/CVM
  CMOL = 2.*A/G + 32.*B/G + 18.*C/G + 16.*D/G + 1.*E/G + 17.*F/G
  PRINT 67,CMOL
  PRINT 68,CPM
  PRINT 69,CK
  STOP
  END

```

## CHAPTER V

### RESULTS OF CALCULATIONS

The results based on a combustion pressure of 23 atmospheres are the primary concern of this report. A graph relating the flame temperature, isentropic exponent, and molecular weight of the products, to the oxidizer-fuel ratio, is presented in Figure 5-2. In addition a very interesting theory of rocketry is proven - the temperature of the gases depends primarily on the oxidizer-fuel ratio, and to a small extent on combustion pressure. The latter depends, of course, on the rate at which the propellants are being consumed and the throat area of the exhaust nozzle. The curve of the flame temperatures based on a combustion pressure of 20 atmospheres is presented for demonstration of the effect resulting from varying the combustion pressure.

The program is set up for the IBM 1620 computer as described in Chapter IV. To facilitate the calculations of the initial constants and coefficients for the matrix program, the value of zero must be read in for the error functions XA, XB, XC, XD, XE, XF, and XG. A temperature is selected for which the equilibrium constants are taken from NACA 1037. In addition to the four Kp constants, values for the molar ratio (S), combustion pressure (PS), tolerance level (TOLER), and a value for the fractional number of degrees (RS) have to be read in to the computer. The tolerance level and its use are explained in the Appendix.

Subdivision three of the first computer program, consisting of the solution of the seven linear equations, has almost entirely been taken from the program listed in the Appendix. The input section has been

deleted, since each individual position of the matrix has been identified in subdivision two. The portion evaluating a zero diagonal has been amended because the only way to adjust the rows or columns of the matrix is to rewrite the program. Care should be taken in the original writing of the computer program to prevent a zero major diagonal. Specific instructions are given in the Appendix.

A tolerance level value of 0.00001 was read in at the beginning of the program. The section permitting changing of the tolerance level was omitted from the computer program. The tolerance level in this program is not very important since the calculated values of the error functions are only used to create new assumed selections for the products of combustion. As long as the convergence continues to decrease the program is successful.

The computer program has been written to interpolate, when necessary, the input data for a selected temperature falling between hundreds of degrees. An example may be illustrated by assuming the desired temperature is 3528 K. A value for RS of 0.28 must be entered in the computer along with the appropriate input data selected at 3600 K and 3500 K. The data consisting of the four Kp constants, and the enthalpy of the constituents are taken from the NACA 1037 tables in the Appendix.

The values listed in Table IV are computed from an oxidizer/fuel molar ratio of 0.5 and with a combustion pressure of 23 atmospheres. The computation was completed for temperatures of 3400 K, 3500 K, and 3600 K. The calculated values of the moles of the products are given in Table II along with the value of  $\Delta H$  computed for each of the three temperatures. These values of  $\Delta H$  are plotted on the graph in Figure 5-1, and then

graphically interpolated for the temperature for which  $\Delta H$  is zero. The temperature was determined to be 3528 K. The problem was then computed again for a temperature of 3528 K and the resulting  $\Delta H$  was within the required accuracy. As proof, the problem was then computed at 3525 K to get an estimate of the change of  $\Delta H$  per degree Kelvin. The  $\Delta H$  at 3528 K was +0.06076 while the  $\Delta H$  at 3525 K was -0.10568. This was sufficient proof that the temperature of 3528 K was within the experimental accuracy possible in the combustion chamber of a rocket engine.

TABLE IV  
RESULTS OF CALCULATIONS  
FOR O/F RATIO OF (0.5) AND 23 ATMOSPHERES

Temp. K	3400	3500	3525	3528	3600
H <sub>2</sub>	0.1325	0.1545	0.1602	0.1609	0.1779
O <sub>2</sub>	.0429	.0491	.0506	.0508	.0554
H <sub>2</sub> O	.8015	.7629	.7527	.7515	.7199
O	.0183	.0257	.0279	.0281	.0354
H	.0375	.0518	.0560	.0565	.0704
OH	<u>.0944</u>	<u>.1132</u>	<u>.1182</u>	<u>.1188</u>	<u>.1338</u>
G	1.1271	1.1572	1.1656	1.1666	1.1928
$\Delta H$	-6.5760	-1.4671	-0.1057	+0.0608	+4.2998

Since the second computer program was also written to compute a linear interpolation for necessary input data, it is only required to read into the computer Cp values for the six products of combustion at temperatures of 3600 K and 3500 K. In addition, as stated before, the

computed values taken from the first program for the number of moles, the value of S, and the value of RS have to be entered as input data into the computer. The particular values of molecular weight were permanently written into the program.

The value for the molecular weight of the mixture is computed from the following equation

$$M = (a/G)M_{H_2} + (b/G)M_{O_2} + (c/G)M_{H_2O} + (d/G)M_O + (e/G)M_H + (f/G)M_{OH} \quad (76)$$

This value, for an O/F ratio of 0.5 and a combustion pressure of 23 atmospheres, was computed as

$$M = 15.42976 \quad (77)$$

The value for Cp of the mixture is computed from the following equation

$$C_p \text{ mixture} = (a/G)C_p_{H_2} + (b/G)C_p_{O_2} + (c/G)C_p_{H_2O} + (d/G)C_p_O + (e/G)C_p_H + (f/G)C_p_{OH} \quad (78)$$

This value was determined to be

$$C_p \text{ mixture} = 11.44081 \frac{\text{Cal}}{\text{gmole-K}} \quad (79)$$

From the thermodynamic identity which relates the specific heat at constant volume (Cv) to that at constant pressure (Cp), Cv will now be computed from the equation

$$C_v = C_p - R_u \quad (80)$$

where

$$R_u = 1.98718 \frac{\text{Cal}}{\text{gmole-K}} \quad (81)$$

Then from equation (79) and (80)

$$C_v = 11.44081 - 1.98718 \quad (82)$$

or

$$C_v = 9.45363 \frac{\text{Cal}}{\text{gmole-K}} \quad (83)$$

The isentropic exponent ( $k$ ) is the ratio of the specific heats and is

$$k = \frac{C_p}{C_v} \quad (84)$$

or

$$k = \frac{11.44081}{9.45363} \quad (85)$$

then

$$k = 1.21020 \quad (86)$$

Table V consists of tabulated values from the calculations at different O/F ratio while holding the combustion pressure constant at 23 atmospheres. These values were computed with the same procedures as have been illustrated for an O/F ratio of 0.5

The tabulated results of the change in adiabatic flame temperature, caused by changing the combustion pressure to 20 atmospheres, is presented in Table VI. Only the variation of the flame temperature is available in Table VI as this is the only variation of importance.

TABLE V  
FINAL RESULTS OF CALCULATIONS  
COMBUSTION PRESSURE 23 ATMOSPHERES

O/F Molar Ratio	0.2	0.3	0.4	0.5	0.6	0.7	
Tc K	<u>2777</u>	<u>3300</u>	<u>3492</u>	<u>3528</u>	<u>3495</u>	<u>3440</u>	
Moles in Products	H <sub>2</sub>	0.5950	0.3942	0.2476	0.1609	0.1099	0.0788
	O <sub>2</sub>	.0000	.0013	.0139	.0508	.1106	.1865
	H <sub>2</sub> O	.3979	.5679	.6830	.7515	.7961	.8270
	O	.0001	.0023	.0131	.0281	.0395	.0460
	H	.0121	.0486	.0627	.0565	.0448	.0345
	OH	<u>.0020</u>	<u>.0272</u>	<u>.0761</u>	<u>.1188</u>	<u>.1432</u>	<u>.1541</u>
	G	1.0071	1.0415	1.0964	1.1666	1.2441	1.3269
M	8.3405	11.1377	13.4985	15.4298	17.0399	18.3909	
Cal g-mole-K	Cp	10.2839	11.0239	11.3384	11.4408	11.4600	11.4360
	Cv	8.2967	9.0367	9.3512	9.4536	9.4728	9.4488
	k	1.2395	1.2199	1.2125	1.2102	1.2098	1.2103

TABLE VI  
FINAL RESULTS OF CALCULATIONS  
COMBUSTION PRESSURE 20 ATMOSPHERES

O/F Molar Ratio	0.2	0.3	0.4	0.5	0.6	0.7
Tc K	2758	3280	3470	3505	3476	3411

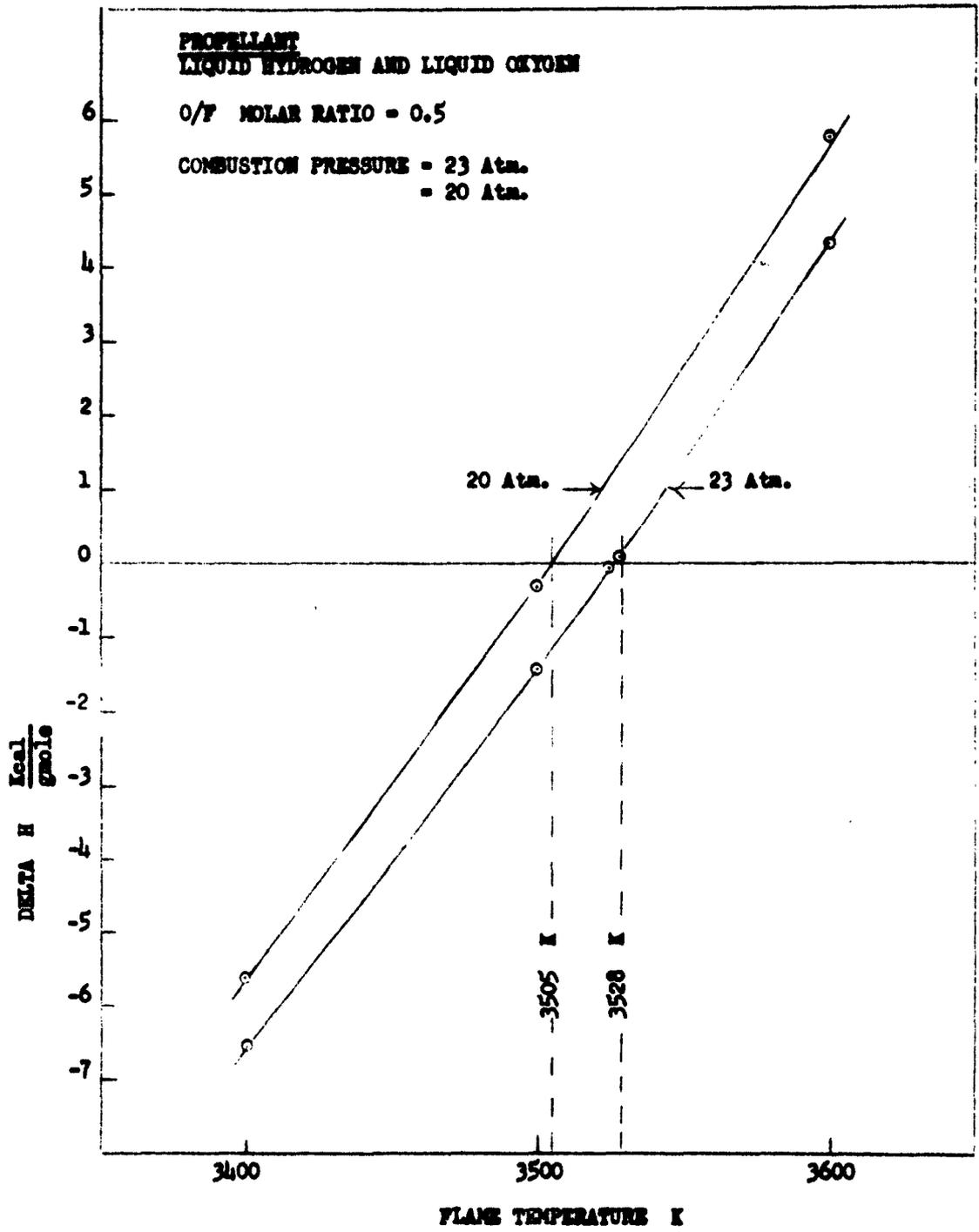


Figure 5-1. Graphical Interpolation for Combustion Flame Temperature

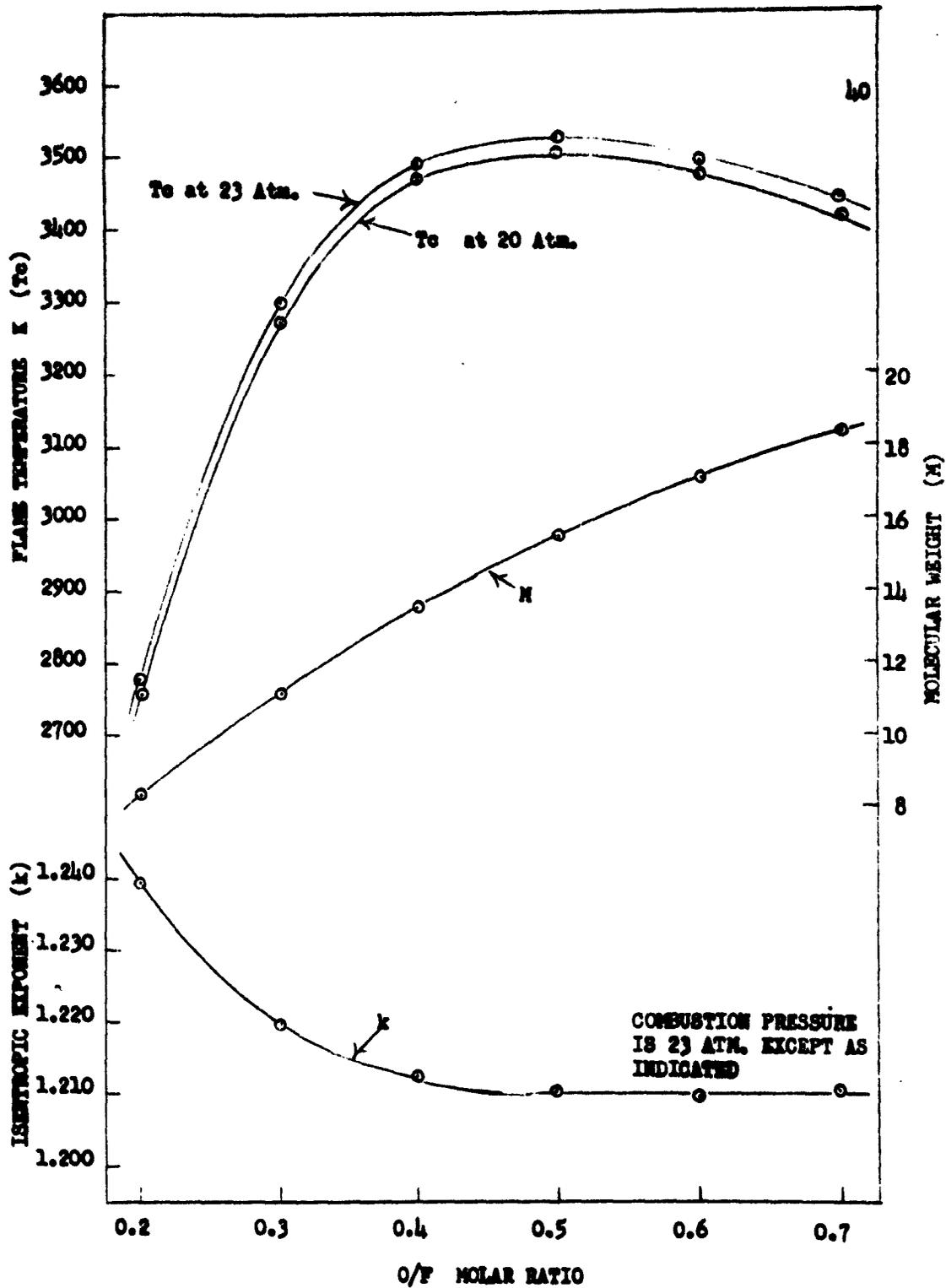


Figure 5-2. Graphical Results For Liquid Hydrogen and Liquid Oxygen

TABLE VII  
RESULTS FROM FIRST PROGRAM

-.30000000 A1  
-.10000000 A2  
.00000000 A3  
4.48435890 A4  
2.05136710 A5  
1.34662590 A6  
1.48234660 A7

The following four pages are the  
computer results from the following  
input data:

.40000000 H2  
.10000000 O2  
.40000000 H2O  
.10000000 O  
.30000000 H  
.40000000 OH  
1.70000000 G  
1.70000000 GH

Initial assumption  
for products of  
combustion.

T	3528 K
O/F	0.5
TOLER	0.00001
PS	23 Atmospheres

9.76469830

Initial convergence value

SOLUTION

-.52371340E-00 XA  
-.43600000E-00 XB  
.11604744E+01 XC  
-.11695445E+01 XD  
THE ABOVE VALUE HAS BEEN CHANGED TO -.995  
-.14979106E+01 XE  
THE ABOVE VALUE HAS BEEN CHANGED TO -.995  
-.90008880E-00 XF  
-.42074042E-00 XG

Results of initial calculations  
for the error functions.

-.15087310  
-.01745420  
.00000000  
-11.40451800  
-7.41533000  
-6.55833300  
-8.15338600

.19051464  
.05640000  
.86418976  
.00050000  
.00150000  
.03996448  
1.15306880  
.98474132

33.69989100

SOLUTION

-.18793932E-00  
 .18042300E-02  
 -.75171440E-01  
 .40532358E+01  
 .35893352E+01  
 .11329576E+01  
 -.48720557E-01

-.00000020  
 -.00000000  
 .00000000  
 -6.57387400  
 -4.11718150  
 -4.12958100  
 -4.87263250

.15470945  
 .05650175  
 .79922741  
 .00252661  
 .00688400  
 .08524254  
 1.10509170  
 1.09689070

19.69326700

SOLUTION

.34152510E-01  
 -.73875990E-01  
 -.34020070E-01  
 .24102371E+01  
 .20865257E+01  
 .34546440E-00  
 .21717281E-01

-.00000010  
 -.00000010  
 .00000000  
 -3.10104200  
 -1.91799860  
 -2.09381940  
 -2.36364870

.15999316  
 .05232763  
 .77203769  
 .00861636  
 .02124765

.11469080  
1.12891320  
1.12909120

9.47650880

3.06712780

Here Sense Switch 3 was turned on.

.44407657

.01147719

.00000870

Here Sense Switch 3 was turned off.

SOLUTION

.38571400E-06  
-.58173300E-06  
.43619820E-07  
.15603613E-05  
.49408466E-06  
-.14800950E-06  
.10245536E-06

The values of the error  
functions are now very small  
numbers.

.00000010 A1  
-.00000000 A2  
.00000000 A3  
-.00000020 A4  
-.00000010 A5  
-.00000020 A6  
-.00000020 A7

.16086923 H<sub>2</sub>  
.05080107 O<sub>2</sub>  
.75149282 H<sub>2</sub>O  
.02813721 O<sup>c</sup>  
.05650815 H  
.11876787 OH  
1.16657620 G  
1.16657620 GH

Final values for the  
products of combustion.

.00000080

Final convergence value

.71556908E+02  
.71496150E+02  
.60758000E-01

Enthalpy of products at 3528 K  
Enthalpy of reactants at 298.16 K  
 $\Delta H$

STOP

TABLE VIII

RESULTS FROM SECOND PROGRAM

THE MOLECULAR WEIGHT OF THE MIX IS 15.42976  
THE CP VALUE FOR THE MIX IS 11.44081  
THE VALUE FOR CP/CV IS 1.21020  
STOP

## BIBLIOGRAPHY

## BIBLIOGRAPHY

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**APPENDIX**

## SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

### Introduction

This program is a replica of program number (5.0.007) from the IBM 1620 General Program Library. It has been rewritten as necessary to be compatible with the present 1620 (20K) computer and the FORTRAN programming system with format statements. Although this program was tested by its author using the sample problems, no warranty, expressed or implied, is made by the author or IBM.

### Description of the Program

A knowledge of the IBM 1620 FORTRAN system is required to understand the following program.

This program solves sets of non-homogeneous simultaneous linear equations and provides either typewriter or punched card output. Up to 25 equations in 25 unknowns may be solved. The first card read for each set of equations states the number of equations following. The program automatically sizes itself for the proper matrix dimensions. Any number of sets of equations may be solved one after the other without reloading the program deck. When a solution has been obtained the word SOLUTION is typed. Under this heading the solution variables are typed one per line in the order in which they appear from left to right in the original equations. Punched card output is identical, with one card punched for each line typed.

If a set of equations is submitted which has more than one solution, a valid solution will be typed or punched, but no indication will be given that there are other solutions as well.

If the equations in the set are not all independent, a typewriter message will indicate that a diagonal element is zero. No solution is developed in this case, as there are infinite solutions to the set of equations.

Additional information regarding the characteristics of the program is contained in the discussion of the method of computation.

### Method of Computation

General Description. The Jordan method of elimination<sup>1</sup> is used to accomplish the solution. Briefly this method consists of diagonalizing the augmented coefficient matrix. After diagonalization the right hand or augmented column contains the solution values for the variables.

The reduction of the matrix takes place in the same storage locations where the original coefficients are stored. Thus at the completion of the solution the original coefficients are lost, and in

<sup>1</sup> Alston S. Householder, Principles of Numerical Analysis (New York: McGraw-Hill Book Co., Inc., 1953), pp. 68-72.

their place remain an identity matrix and the column of answers.

Division by a Zero Diagonal. In the process of diagonalization the elements of each row to the right of the diagonal and the diagonal itself are divided by the diagonal element. The diagonal elements are used in the same order in which they appear in the original matrix. No attempt is made to select these pivotal elements by magnitude. Hence a zero must not appear on the diagonal of the matrix. If such a condition exists, a message will be typed indicating which diagonal element is zero and control passes to reading the next problem.

The possibility of zero diagonal elements may be minimized by observing two rules in laying out the original matrix.

1. The upper left hand element should not be zero.
2. No diagonal element may be zero if all elements in the row to the left of it are zero.

There is a slight chance of generating a zero diagonal element in the course of calculations. Equations which are not independent (a unique solution undefined) will also generate a zero diagonal. If it is known that the coefficient matrix is non-singular, that is, that there is a unique solution, division by zero may be easily corrected and the problem submitted again. A simple rearrangement of the columns will usually suffice. In rearranging the columns the equality vector always must be kept on the right. As indicated later, rearrangement of columns may be accomplished simply by rearranging input cards. No additional punching is required.

Tolerance warning Level. When the diagonal element is very small relative to the values to its right in the row, a loss of accuracy will result from round-off errors. In this program the operator has control over this situation. When the absolute value of the divisor is less than or equal to some tolerance level selected by the operator, a warning message is typed. The operator then has the choice of continuing with the solution or proceeding to the next problem. If he should elect to continue, he does so with the knowledge that the answer may contain significant rounding errors. Of course, checking the answers will quickly show the accuracy of the solution.

#### Input Card Format

The first card of the input for each set of equations must be a card with the number of equations punched according to the FORMAT STATEMENT (I2).

The matrix of coefficients is punched column-wise beginning with the left-most column and ending with the equality column. Each column must begin with a new card. A card must contain five values punched successively according to the FORMAT STATEMENT (E14.8). It is obvious

that the five values will take up the first 70 spaces on the card. The column may be continued over as many cards as necessary. (Five cards is the maximum number, as the program is limited to 25 unknowns.) If the number of rows is not a multiple of five, dummy zero values must be punched to finish out five entries on the last card of the column. It is never necessary to punch more than four dummy zero entries for a given column. The number of cards per column will be the same for all columns within a given problem, but may vary from problem to problem. The dummy entries used to fill out the five entries on the last card of a column need not be zero. These entries are accessed during the read in, but are never accessed during calculation. Hence they must be present, but their value is immaterial.

#### Output Card and Typewriter Format

The first statement for each problem will be the word SOLUTION followed by the answers typed according to FORMAT STATEMENT (E14.8). If it is desired to have the answers punched with the same format statement, Sense Switch 1 should be turned on. The word SOLUTION will not be punched; however, the answers including the word SOLUTION will continue to be typed. The cards will contain the solution, one per card in the order in which the variables appeared in the original matrix.

#### Sense Switch Settings

##### Sense Switch

1	ON	Solution is typed and punched.
	OFF	Solution is typed.
2	ON	Next problem after tolerance stop.
	OFF	Continue after tolerance stop.
3	ON	Tolerance level entered for each problem.
	OFF	Tolerance level entered only once.
4	ON	To correct error in typing tolerance level.
	OFF	Tolerance level entered correctly.

#### Normal Loading Procedure

1. Clear Storage
2. Depress RESET
3. Depress LOAD button
4. Depress READER START when hopper is empty
5. LOAD DATA is typed by typewriter
6. Enter data cards
7. Depress COMPUTER START
8. Depress READER START

### Special Loading Instructions

At any time the program may be initialized and started by branching to 08300.

### Other Instructions and Remarks

Tolerance Level. When the program begins, the typewriter will request the operator to enter the tolerance level as a floating point number in the form (+.000000).

If the entry is typed correctly, set Sense Switch 4 OFF, press RELEASE and COMPUTER START. The data cards will then be read.

If the entry is typed incorrectly, turn Sense Switch 4 ON, press RELEASE and START. The program will immediately return control to the typewriter so the entry may be made again. If the retry is correct, follow the procedure for a correct entry.

If it is desired to enter a tolerance level for each set of equations, turn Sense Switch 3 ON. If not, turn Switch 3 OFF, and the last tolerance level entered will automatically be applied to all succeeding sets of equations.

When a tolerance warning stop occurs, directions for the use of Switch 2 are typed. Only at this time is the setting of Switch 2 interrogated.

All programed stops are accompanied by typewriter messages which are self explanatory and which indicate the required action.

## SAMPLE PROBLEMS

The following four problems were used one after the other.

$$8x_1 - 5x_2 + 7x_3 = 29$$

$$+2x_2 - 2x_3 = -2$$

$$-x_1 + 9x_2 - 6x_3 = 1$$

$$\text{Answer: } x_1 = 2, \quad x_2 = 3, \quad x_3 = 4$$

$$x_1 + 2x_2 + 3x_3 - 4x_4 + 5x_5 - 6x_6 + 7x_7 - 8x_8 = -28$$

$$7x_2 \quad \quad \quad -2x_5 \quad \quad \quad + x_7 + x_8 = 19$$

$$2x_1 + 3x_2 - 4x_3 - 5x_4 \quad \quad \quad + 6x_6 \quad \quad \quad = 12$$

$$x_1 + x_2 + x_3 + x_4 + x_5 + x_6 + x_7 + x_8 = 36$$

$$10x_1 + 3x_2 - 4x_3 \quad \quad \quad + x_5 + 2x_6 - 9x_7 \quad \quad \quad = -42$$

$$3x_1 - 3x_2 - 2x_3 + 2x_4 \quad \quad \quad + x_6 \quad \quad \quad = 5$$

$$-8x_1 \quad \quad \quad -9x_3 \quad \quad \quad + 7x_5 \quad \quad \quad + 6x_7 - 3x_8 = 18$$

$$+ 3x_7 - 5x_8 = -19$$

$$\text{Answers: } x_1 = 1, \quad x_2 = 2, \quad x_3 = 3, \quad x_4 = 4$$

$$x_5 = 5, \quad x_6 = 6, \quad x_7 = 7, \quad x_8 = 8$$

$$3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 = -20$$

$$+ 2x_2 \quad \quad \quad + x_4 + 5x_5 = 40$$

$$\quad \quad \quad + 4x_4 + 6x_5 = -18$$

$$2x_1 + 4x_2 + 7x_3 \quad \quad \quad + 9x_5 = 12$$

$$x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 = 7$$

This problem will cause diagonal 3 to be zero. It was included merely to illustrate the typewriter message.

$$\begin{aligned}
 3x_1 + 8x_2 + 6x_3 + 10x_4 + 42x_5 &= -20 \\
 +2x_2 + x_4 + 5x_5 &= 40 \\
 +.01x_3 + 4x_4 + 6x_5 &= -18 \\
 2x_1 + 4x_2 + 7x_3 + 9x_5 &= 12 \\
 x_1 + 4x_2 + 6x_3 - 2x_4 + 10x_5 &= 7
 \end{aligned}$$

This problem will make diagonal 3 go below a tolerance level of 0.1. It was included merely to illustrate this typewriter message.

COMMENTS ON THE TYPEWRITER LOG  
FOR SAMPLE PROBLEMS

On the typewriter log, which follows, several points should be noted. Sense Switch 3 was on at the beginning. Note that a tolerance level was entered for each of the first three problems. After the tolerance was entered for the third problem, Sense Switch 3 was turned off. When diagonal 3 went to zero and COMPUTER START was pressed to continue with the fourth problem, the solution began immediately without the entry of a tolerance level, as Switch 3 was off. Note the tolerance level in the warning message of the fourth problem is the last entry made--that for problem 3. When this warning message appeared, Switch 2 was turned off and calculation continued to obtain a solution.

4908300RS  
 ACCEPT TOLERANCE IN FORM +.000000 PUSH RS  
 +.000001RS

SOLUTION  
 .20000000E+01  
 .30000000E+01  
 .40000000E+01  
 ACCEPT TOLERANCE IN FORM +.000000 PUSH RS  
 +.000001RS

SOLUTION  
 .10000065E+01  
 .19999976E+01  
 .30000053E+01  
 .39999963E+01  
 .49999916E+01  
 .59999990E+01  
 .70000022E+01  
 .80000012E+01  
 ACCEPT TOLERANCE IN FORM +.000000 PUSH RS  
 +.1RS  
 DIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM  
 IS 3

DIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER  
 IS 3  
 TURN SW 2 OFF TO CONT. ON FOR NEXT PROBLEM  
 THEN PUSH START

SOLUTION  
 -.67605150E+01  
 .34405115E+02  
 -.70773320E+01  
 .59439480E+01  
 -.69508359E+01

## SOURCE PROGRAM FOR SOLUTION OF SIMULTANEOUS LINEAR EQUATIONS

ENTER SOURCE PROGRAM  
THEN PUSH START

```

    DIMENSION X(26,27)
30 FORMAT(12)
31 FORMAT(ELL.8,ELL.8,ELL.8,ELL.8,ELL.8)
32 FORMAT(//8HSOLUTION)
33 FORMAT(14HDIAGONAL THAT IS LESS THAN OR EQUAL TO TOLER)
34 FORMAT(2HIS I3)
35 FORMAT(12HTURN SW 2 OFF TO CONT, ON FOR NEXT PROBLEM)
36 FORMAT(15HTHEN PUSH START)
37 FORMAT(15HDIAGONAL IS ZERO, PUSH START FOR NEXT PROBLEM)
38 FORMAT(14HACCEPT TOLERANCE IN FORM +.000000 PUSH RS)
39 FORMAT(F8.6)
40 FORMAT(ELL.8)
10 PRINT 38
    ACCEPT 39, TOLER
1 READ 30, N
    N1 = N + 1
    DO 2 J = 1, N1
    DO 2 I = 1, N, 5
2 READ31,X(I,J), X(I+1,J), X(I+2,J), X(I+3,J), X(I+4,J)
    DO 14 I = 1, N, 1
    DIAG = X(I,I)
    IF (DIAG) 3, 20, 4
3 IF (DIAG + TOLER) 5, 19, 19
4 IF (DIAG - TOLER) 19, 19, 5
5 DO 6 J = I, N1
6 X(I,J) = X(I,J) / DIAG
    K = 1
9 IF (K-I) 11, 13, 11
11 FELMT = X(K,I)
    DO 12 J = I, N1
12 X(K,J) = X(K,J) - FELMT * X(I,J)
13 K = K + 1
    IF (K-N) 9, 9, 14
14 CONTINUE
    J=N1
    IF (SENSE SWITCH 1) 15, 17
15 TYPE 32
    DO 16 I = 1, N
    PUNCH 40, X(I,J)
16 TYPE 40, X(I,J)
    GO TO 21
17 TYPE 32
    DO 18 I=1 , N

```

```
18 TYPE 40, X(I,J)
21 IF (SENSE SWITCH 3) 10,1
19 TYPE 33
   TYPE 34,I
   TYPE 35
   TYPE 36
   PAUSE
   IF (SENSE SWITCH 2) 21,5
20 TYPE 37
   TYPE 34,I
   PAUSE
   GO TO 21
END
```

TABLE XXX—THERMODYNAMIC PROPERTIES OF H<sub>2</sub> (GAS)

(Molecular weight, 2.016)

T (°K)	C <sub>p</sub> (cal/mole °K)	H <sub>2</sub> -H <sub>0</sub> (kcal/mole)	H <sub>2</sub> (kcal/mole)	S <sub>0</sub> (cal/mole °K)	$\frac{\Delta H^{\circ}}{RT}$	$\ln\left(-\frac{\Delta H^{\circ}}{RT}\right) - \frac{-\Delta T}{100}\left(\frac{a}{T} + b\right)$		log K	$\delta \log K = \frac{-\delta T}{T} \left(\frac{c}{T} + d\right)$	
						a	b		c	d
0	.....	0	67.4169	.....	.....	.....	.....	.....	.....	.....
298.16	6.892	2.0298	69.4407	31.211	175.8297	.....	.....	71.2998	.....	.....
300	6.895	2.0365	69.4344	31.253	174.7610	.....	.....	70.7414	.....	.....
400	6.974	2.7310	70.1179	33.250	141.4165	.....	.....	51.7421	.....	.....
500	6.954	3.4255	70.8064	34.899	108.4541	.....	.....	40.3099	.....	.....
600	7.008	4.1286	71.5155	36.081	88.1261	.....	.....	32.6669	.....	.....
700	7.075	4.8415	72.2484	37.167	73.7451	.....	.....	27.1921	.....	.....
800	7.078	5.5734	72.9943	38.108	66.4582	.....	.....	23.0744	.....	.....
900	7.079	6.3240	73.7519	38.936	60.2922	.....	.....	19.8936	.....	.....
1000	7.079	6.9658	74.5227	39.709	55.4178	.....	.....	17.2883	.....	.....
1100	7.100	7.6023	75.3092	40.293	51.7111	.....	.....	.....	.....	.....
1200	7.107	8.2281	75.8150	41.045	48.7599	.....	.....	.....	.....	.....
1300	7.109	8.8479	76.3008	41.6331	46.4128	.....	.....	.....	.....	.....
1400	7.115	9.4601	77.3470	42.1908	38.5100	.....	.....	.....	.....	.....
1500	7.122	10.0669	78.1138	42.7227	36.0168	.....	.....	.....	.....	.....
1600	7.129	11.4710	78.8099	43.2343	34.8620	.....	.....	.....	.....	.....
1700	7.129	12.2613	79.6782	43.7016	34.1311	.....	.....	.....	.....	.....
1800	8.0185	13.0581	80.4783	44.1751	30.2121	.....	.....	.....	.....	.....
1900	8.0163	13.8618	81.2817	44.5941	28.6716	.....	.....	.....	.....	.....
2000	8.1749	14.6800	82.0969	45.0112	27.2829	.....	.....	.....	.....	.....
2100	8.2762	15.5036	82.9265	45.4140	26.0245	.....	.....	.....	.....	.....
2200	8.3737	16.3351	83.7520	45.7998	24.8756	.....	.....	.....	.....	.....
2300	8.4274	17.1741	84.5910	46.1728	23.8308	.....	.....	.....	.....	.....
2400	8.4977	18.0234	85.4373	46.5729	22.8887	.....	.....	.....	.....	.....
2500	8.5617	18.8835	86.2804	46.8812	21.9622	.....	.....	.....	.....	.....
2600	8.6286	19.7331	87.1500	47.2183	21.1627	.....	.....	.....	.....	.....
2700	8.6986	20.5910	88.0160	47.5154	20.4627	.....	.....	.....	.....	.....
2800	8.7479	21.4769	88.8878	47.8622	19.8699	.....	.....	.....	.....	.....
2900	8.8112	22.3915	89.7551	48.1702	19.3369	.....	.....	.....	.....	.....
3000	8.8887	23.3317	90.6186	48.4696	18.8208	.....	.....	.....	.....	.....
3100	8.9118	24.1262	91.5371	48.7609	17.8437	.....	.....	.....	.....	.....
3200	8.9536	25.0110	92.4309	49.0117	17.3017	.....	.....	.....	.....	.....
3300	9.0133	25.9129	93.3298	49.3243	16.7919	.....	.....	.....	.....	.....
3400	9.0639	26.8168	94.2337	49.5911	16.3113	.....	.....	.....	.....	.....
3500	9.1125	27.7256	95.1425	49.8545	15.8574	.....	.....	.....	.....	.....
3600	9.1692	28.6392	96.0561	50.1119	15.4283	.....	.....	.....	.....	.....
3700	9.2090	29.5576	96.9745	50.3645	15.0214	.....	.....	.....	.....	.....
3800	9.2529	30.4806	97.8975	50.6097	14.6356	.....	.....	.....	.....	.....
3900	9.2979	31.4081	98.8250	50.8506	14.2687	.....	.....	.....	.....	.....
4000	9.3421	32.3401	99.7570	51.0886	13.9197	.....	.....	.....	.....	.....
4100	9.3856	33.2765	100.6934	51.3178	13.5872	.....	.....	.....	.....	.....
4200	9.4284	34.2172	101.6341	51.5445	13.2701	.....	.....	.....	.....	.....
4300	9.4704	35.1621	102.5790	51.7698	12.9672	.....	.....	.....	.....	.....
4400	9.5118	36.1113	103.5282	51.9850	12.6785	.....	.....	.....	.....	.....
4500	9.5526	37.0645	104.4813	52.1992	12.4033	.....	.....	.....	.....	.....
4600	9.5928	38.0217	105.4389	52.4096	12.1517	.....	.....	.....	.....	.....
4700	9.6324	38.9839	106.3999	52.6164	11.9000	.....	.....	.....	.....	.....
4800	9.6711	39.9482	107.3651	52.8196	11.6555	.....	.....	.....	.....	.....
4900	9.7099	40.9173	108.3342	53.0194	11.4085	.....	.....	.....	.....	.....
5000	9.7479	41.8901	109.3070	53.2159	11.1736	.....	.....	.....	.....	.....
5100	9.7853	42.8668	110.2837	53.4093	10.9572	.....	.....	.....	.....	.....
5200	9.8222	43.8472	111.2641	53.5997	10.7477	.....	.....	.....	.....	.....
5300	9.8586	44.8312	112.2481	53.7871	10.5444	.....	.....	.....	.....	.....
5400	9.8945	45.8189	113.2358	53.9717	10.3511	.....	.....	.....	.....	.....
5500	9.9299	46.8101	114.2270	54.1536	10.1631	.....	.....	.....	.....	.....
5600	9.9649	47.8048	115.2217	54.3328	9.9816	.....	.....	.....	.....	.....
5700	9.9994	48.8031	116.2200	54.5095	9.8070	.....	.....	.....	.....	.....
5800	10.0334	49.8047	117.2210	54.6837	9.6393	.....	.....	.....	.....	.....
5900	10.0669	50.8097	118.2256	54.8555	9.4720	.....	.....	.....	.....	.....
6000	10.1001	51.8181	119.2330	55.0250	9.3129	.....	.....	.....	.....	.....

TABLE XLIV--THERMODYNAMIC PROPERTIES OF O<sub>2</sub> (GAS)

(Molecular weight, 32.0000)

T (°K)	C <sub>p</sub> (cal mole °K)	H <sub>2</sub> -H <sub>0</sub> (kcal mole)	H <sub>T</sub> (kcal mole)	S <sub>T</sub> (cal mole °K)	-ΔH° RT	(-ΔH°/RT) = -ΔT (a/T + b)		log K'	Δ log K' = -ΔT (c/T + d)		
						a	b		c	d	
0	.....	0	2.0362	.....	.....	.....	.....	.....	.....	.....	
298.16	7.021	2.0747	3.1169	49.011	192.6835	.....	.....	80.4082	.....	.....	
300	7.023	2.0826	3.1208	49.076	191.6535	.....	.....	81.0807	.....	.....	
400	7.496	2.7077	4.8339	61.088	149.2649	.....	.....	58.5109	.....	.....	
500	7.431	3.3288	6.5650	62.728	119.7043	.....	.....	45.5311	.....	.....	
600	7.070	.....	6.3263	54.105	90.9669	.....	.....	36.6260	.....	.....	
700	7.683	5.0620	7.0982	55.303	85.8310	.....	.....	30.4399	.....	.....	
800	8.063	5.8396	7.8958	56.368	78.2106	.....	.....	25.1854	.....	.....	
900	8.212	6.6737	8.7069	57.327	68.9937	.....	.....	22.3515	.....	.....	
1000	8.336	7.5012	9.5374	58.190	60.3812	.....	.....	19.4490	2001	0.01923	
1100	8.439	8.3100	10.3702	58.993	51.9651	.....	.....	17.0545	2370	0.01550	
1200	8.527	9.0884	11.2245	59.761	50.1479	.....	.....	15.0640	2173	0.01322	
1300	8.604	10.0108	12.0810	60.4220	46.6219	.....	.....	13.3777	2060	0.01200	
1400	8.674	10.9787	12.9449	61.0622	43.3096	.....	.....	11.9307	1867	0.01083	
1500	8.738	11.7793	13.8155	61.6928	40.4926	.....	.....	10.6752	1744	0.00990	
1600	8.800	12.6562	14.6924	62.2287	37.5993	.....	.....	9.5756	1637	0.00926	
1700	8.858	13.5391	15.5753	62.7610	35.7976	.....	.....	8.6044	1542	0.00873	
1800	8.916	14.4278	16.4640	63.2719	33.8787	.....	.....	7.7463	1458	0.00828	
1900	8.973	15.3223	17.3585	63.7585	32.0845	.....	.....	6.9655	1383	0.00790	
2000	9.029	16.2234	18.2586	64.2172	30.5043	.....	.....	6.2685	1314	0.00759	
2100	9.084	17.1260	19.1644	64.6500	29.0733	.....	.....	5.6384	1253	0.00735	
2200	9.139	18.0392	20.0754	65.0829	27.7711	.....	.....	5.0613	1197	0.00710	
2300	9.194	18.9658	20.9920	65.5064	26.5839	.....	.....	4.5308	1146	0.00670	
2400	9.248	19.9079	21.9141	65.8828	25.4889	.....	.....	4.0586	1099	0.00636	
2500	9.301	20.8654	22.8416	66.2614	24.4533	.....	.....	3.6187	1056	0.00605	
2600	9.354	21.7881	23.7743	66.6272	23.5510	.....	.....	3.2060	1016	0.00579	
2700	9.405	22.6761	24.7123	66.9812	22.6928	.....	.....	2.8277	980	0.00556	
2800	9.455	23.6191	25.6553	67.3241	21.8922	.....	.....	2.4786	945	0.00534	
2900	9.503	24.5670	26.6052	67.6568	21.1462	.....	.....	2.1477	913	0.00517	
3000	9.551	25.5197	27.5559	67.9797	20.4494	.....	.....	1.8415	883	0.00506	
3100	9.596	26.4770	28.5132	68.2936	19.7969	.....	.....	1.5550	855	0.00494	
3200	9.640	27.4388	29.4750	68.5990	19.1846	.....	.....	1.2862	829	0.00489	
3300	9.682	28.4049	30.4411	68.8963	18.6091	.....	.....	1.0337	804	0.00482	
3400	9.724	29.3752	31.4114	69.1859	18.0760	.....	.....	0.7960	781	0.00476	
3500	9.762	30.3494	32.3856	69.4683	17.5756	.....	.....	0.5718	759	0.00477	
3600	9.799	31.3275	33.3637	69.7439	17.0723	.....	.....	0.3600	739	0.00477	
3700	9.835	32.3092	34.3454	70.0126	16.6148	.....	.....	0.0350	719	0.00469	
3800	9.869	33.2944	35.3306	70.2756	16.1813	.....	.....	.....	700	0.00471	
3900	9.901	34.2829	36.3191	70.5323	15.7698	.....	.....	.....	682	0.00470	
4000	9.932	35.2745	37.3107	70.7834	15.3788	.....	.....	.....	665	0.00470	
4100	9.960	36.2691	38.3053	71.0290	15.0067	.....	.....	0.00107	-0.5447	649	0.00468
4200	9.987	37.2665	39.3027	71.2693	14.6524	.....	.....	.....	-0.6980	634	0.00461
4300	10.013	38.2665	40.3027	71.5046	14.3144	.....	.....	.....	-0.8179	619	0.00462
4400	10.037	39.2690	41.3052	71.7351	13.9918	.....	.....	.....	-0.9022	604	0.00458
4500	10.060	40.2738	42.3100	71.9609	13.6835	.....	.....	.....	-1.1243	592	0.00450
4600	10.081	41.2809	43.3171	72.1822	13.3887	.....	.....	-0.00089	-1.2515	579	0.00451
4700	10.102	42.2901	44.3263	72.3966	13.1084	.....	.....	.....	-1.0027	567	0.00454
4800	10.121	43.3013	45.3373	72.6122	12.8400	.....	.....	.....	-1.0162	555	0.00453
4900	10.139	44.3143	46.3505	72.8210	12.5766	.....	.....	.....	-1.0266	543	0.00450
5000	10.156	45.3290	47.3652	73.0251	12.3277	.....	.....	.....	-1.0308	533	0.00449
5100	10.172	46.3454	48.3816	73.2273	12.0886	.....	.....	-0.00232	-1.1238	522	0.00462
5200	10.187	47.3634	49.3996	73.4250	11.8588	.....	.....	.....	-0.0240	512	0.00460
5300	10.201	48.3828	50.4190	73.6192	11.6378	.....	.....	.....	-0.0248	502	0.00464
5400	10.215	49.4030	51.4398	73.8100	11.4251	.....	.....	.....	-0.0232	493	0.00456
5500	10.228	50.4257	62.4619	73.9975	11.2201	.....	.....	.....	-0.0286	484	0.00457
5600	10.239	51.4502	63.4858	74.1819	11.0226	.....	.....	-0.00238	-2.3928	475	0.00467
5700	10.250	52.4755	64.5097	74.3632	10.8322	.....	.....	.....	-2.3798	466	0.00476
5800	10.261	53.4991	65.5323	74.5416	10.6483	.....	.....	.....	-2.4379	458	0.00477
5900	10.271	64.3250	66.5618	74.7171	10.4709	.....	.....	.....	-2.8662	449	0.00486
6000	10.279	55.5331	67.5893	74.8896	10.2995	.....	.....	.....	-2.6321	.....	.....

TABLE XXXIII—THERMODYNAMIC PROPERTIES OF H<sub>2</sub>O (GAS)

[Molecular weight, 18.016]

T (°K)	C <sub>p</sub> (cal/mole °K)	H <sub>2</sub> °-H <sub>2</sub> (cal/mole)	H <sub>2</sub> (cal/mole)	S <sup>o</sup> (cal/mole °K)	-ΔH° RT	e(-ΔH°/RT) = -ΔT°/(T+)		log K	Δ log K = -ΔT°/(T+)	
						a	b		c	d
0		0	11.3411							
25	8.025	2.3677	13.4888	45.106	378.2260			181.5648		
50	8.025	2.3820	13.7181	45.151	370.5541			160.5708		
100	8.185	3.1940	14.5251	47.490	279.0556			110.2372		
200	8.415	4.0255	15.3566	49.344	223.9553			85.9209		
300	8.677	4.8822	16.2133	50.603	187.1653			69.7280		
400	8.959	5.7715	17.1026	52.269	154.8693			58.0546		
500	9.251	6.6866	18.0207	53.490	131.1213			49.3548		
600	9.559	7.6347	18.9658	54.599	115.7485			42.8361		
800	9.864	8.6280	19.9391	55.6183	118.4355	11.015	0.07316	37.0674	4875	0.02156
1000	10.145	9.6683	20.9391	56.5712	109.3187	10.019	0.06833	32.5840	4439	0.04193
1200	10.413	10.6592	21.9673	57.4654	94.9312	9.188	0.06491	28.8369	4076	0.03492
1400	10.668	11.6062	23.0213	58.3059	87.7986	8.496	0.06137	25.6655	3704	0.03157
1600	10.919	12.5101	24.1002	59.1084	80.6728	7.880	0.05866	22.8265	3395	0.03013
1800	11.141	13.3712	25.2022	59.8687	76.3045	7.366	0.05618	20.5727	3276	0.28010
2000	11.343	14.1955	26.3262	60.5939	71.7046	6.913	0.04853	18.4983	3075	0.02158
2200	11.524	14.9889	27.4700	61.2873	67.5896	6.514	0.04401	16.6852	2808	0.02580
2400	11.708	15.7610	28.6321	61.9515	63.9267	6.160	0.03950	15.0332	2741	0.01657
2600	11.865	16.4797	29.8106	62.5887	60.6450	5.843	0.03560	13.5170	2690	0.01770
2800	12.008	17.1473	31.0444	63.2010	57.6876	5.557	0.03271	12.2533	2714	0.01570
3000	12.148	17.7666	32.3117	63.7900	55.0087	5.299	0.02996	11.0505	2359	0.01423
3200	12.286	18.3403	33.5314	64.3574	52.5794	5.064	0.02846	9.9730	2255	0.01277
3400	12.424	18.8713	34.6934	64.9015	50.3418	4.849	0.02688	8.9798	2190	0.01150
3600	12.563	19.3727	35.8078	65.4328	48.2667	4.653	0.02220	8.0583	2072	0.01060
3800	12.553	19.8235	37.1546	65.9434	46.4133	4.471	0.02049	7.2289	1991	0.00863
4000	12.638	20.2831	38.4142	66.4374	44.6732	4.304	0.01893	6.4743	1916	0.00927
4200	12.715	20.7508	39.6819	66.9159	43.0405	4.149	0.01791	5.7853	1846	0.00650
4400	12.786	21.2278	40.9599	67.3796	41.5138	4.005	0.01717	5.0751	1781	0.00856
4600	12.852	21.7147	42.2388	67.8394	40.1153	3.871	0.01607	4.4334	1721	0.00813
4800	12.913	22.1990	43.5271	68.2861	38.8409	3.747	0.01529	3.8617	1666	0.00728
5000	12.968	22.6760	44.8211	68.6904	37.6808	3.630	0.01413	3.3170	1613	0.00664
5200	13.018	23.1493	46.1204	69.1029	36.6303	3.520	0.01360	2.8590	1561	0.00656
5400	13.064	23.6031	47.4245	69.5642	35.6417	3.417	0.01300	2.3555	1511	0.00612
5600	13.107	24.0420	48.7331	69.9849	34.7048	3.320	0.01253	1.8729	1463	0.00624
5800	13.147	24.4747	50.0458	70.3764	33.8473	3.228	0.01205	1.4458	1431	0.00610
6000	13.184	24.9012	51.2623	70.6663	32.5476	3.142	0.01161	1.0422	1392	0.00585
6200	13.218	25.3224	52.4821	70.9680	31.6884	3.060	0.01156	0.6591	1355	0.00572
6400	13.250	25.7477	53.6958	71.3049	30.8779	2.981	0.01184	0.2788	1320	0.00554
6600	13.280	26.1612	54.9024	71.7054	30.1087	2.907	0.01125	-0.1062	1287	0.00525
6800	13.308	26.5666	56.0917	72.0420	29.3777	2.836	0.01070	-0.3732	1255	0.00520
7000	13.334	26.9627	57.2638	72.3710	28.6822	2.769	0.00921	-0.6845	1226	0.00480
7200	13.358	27.3505	58.3281	72.6926	28.0197	2.705	0.00823	-0.9812	1198	0.00459
7400	13.381	27.7243	59.3854	73.0071	27.3875	2.643	0.00737	-1.2643	1170	0.00449
7600	13.403	28.0954	60.4363	73.3150	26.7843	2.584	0.00658	-1.5347	1144	0.00438
7800	13.424	28.4648	61.4809	73.6164	26.2079	2.528	0.00584	-1.7933	1119	0.00434
8000	13.444	28.8322	62.5182	73.9117	25.6568	2.473	0.00503	-2.0400	1095	0.00412
8200	13.461	29.1976	63.5487	74.2011	25.1281	2.421	0.00419	-2.2780	1073	0.00396
8400	13.478	29.5610	64.5821	74.4847	24.6218	2.371	0.00328	-2.5085	1051	0.00381
8600	13.502	29.9232	65.7313	74.7625	24.1361	2.323	0.00270	-2.7306	1030	0.00370
8800	13.521	30.2844	66.8825	75.0355	23.6698	2.276	0.00203	-2.9436	1010	0.00356
9000	13.540	30.6444	68.0363	75.3038	23.2217	2.232	0.00177	-3.1351	991	0.00342
9200	13.559	30.9997	69.1934	75.5669	22.7907	2.189	0.00150	-3.3091	973	0.00329
9400	13.577	31.3502	70.3542	75.8254	22.3766	2.148	0.00122	-3.4559	955	0.00316
9600	13.596	31.7048	71.5189	76.0794	21.9785	2.108	0.00103	-3.6050	938	0.00305
9800	13.614	32.0633	72.6864	76.3290	21.5961	2.070	0.00090	-3.8005	921	0.00304
10000	13.633	32.4277	73.8588	76.5745	21.2293	2.033	0.00163	-4.0370	905	0.00293
10200	13.651	32.7919	75.0330	76.8159	20.8820	1.998	0.00122	-4.1987	890	0.00285
10400	13.669	33.1579	76.2100	77.0535	20.5450	1.963	0.00108	-4.3350	875	0.00279
10600	13.687	33.5258	77.3898	77.2879	20.2186	1.930	0.00108	-4.4861	860	0.00277
10800	13.705	33.8953	78.5694	77.5176	19.8985	1.898	0.00108	-4.6428	845	0.00277

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XLIII—THERMODYNAMIC PROPERTIES OF O (GAS)

[Atomic weight, 16.0000]

T (°K)	$C_p$ ( $\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$ )	$H_2 - H_1$ ( $\frac{\text{cal}}{\text{mole}}$ )	$H_f$ ( $\frac{\text{kcal}}{\text{mole}}$ )	$S_f$ ( $\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$ )
0	.....	0	50.9011	.....
200	5.2961	1.6074	51.3115	38.4696
300	5.2538	1.6159	51.3211	38.8010
400	5.1511	2.1319	51.7490	39.9915
500	5.0802	2.6154	52.2495	41.1908
600	5.0486	3.1517	52.7528	42.0540
700	5.0281	3.6535	53.2596	42.8307
800	5.0150	4.1576	53.7617	43.5611
900	5.0055	4.6587	54.2628	44.0614
1000	4.9988	5.1588	54.7629	44.6183
1100	4.9936	5.6584	55.2625	45.0945
1200	4.9894	6.1576	55.7617	45.5286
1300	4.9864	6.6564	56.2605	45.9281
1400	4.9838	7.1549	56.7590	46.2977
1500	4.9819	7.6532	57.2573	46.6413
1600	4.9805	8.1513	57.7554	46.9626
1700	4.9792	8.6493	58.2534	47.2616
1800	4.9781	9.1471	58.7512	47.5492
1900	4.9778	9.6450	59.2491	47.8184
2000	4.9776	10.1427	59.7468	48.0737
2100	4.9778	10.6405	60.2446	48.3165
2200	4.9784	11.1383	60.7421	48.5481
2300	4.9796	11.6362	61.2393	48.7685
2400	4.9812	12.1343	61.7364	48.9684
2500	4.9834	12.6325	62.2336	49.1498
2600	4.9862	13.1310	62.7307	49.3066
2700	4.9897	13.6298	63.2279	49.4490
2800	4.9935	14.1289	63.7250	49.5791
2900	4.9986	14.6285	64.2220	49.6984
3000	5.0041	15.1287	64.7188	50.0050
3100	5.0102	15.6294	65.2155	50.2592
3200	5.0170	16.1307	65.7121	50.4618
3300	5.0245	16.6328	66.2086	50.6228
3400	5.0325	17.1357	66.7050	50.7529
3500	5.0411	17.6393	67.2014	50.8659
3600	5.0502	18.1439	67.6978	51.0111
3700	5.0599	18.6494	68.1943	51.1496
3800	5.0700	19.1559	68.6906	51.2846
3900	5.0805	19.6634	69.1870	51.4165
4000	5.0914	20.1720	69.6831	51.5452
4100	5.1026	20.6817	70.1790	51.6711
4200	5.1140	21.1925	70.6749	51.7942
4300	5.1257	21.7045	71.1706	51.9147
4400	5.1375	22.2177	71.6662	52.0322
4500	5.1495	22.7320	72.1617	52.1483
4600	5.1616	23.2476	72.6571	52.2615
4700	5.1738	23.7644	73.1525	52.3727
4800	5.1860	24.2824	73.6479	52.4817
4900	5.1981	24.8016	74.1433	52.5888
5000	5.2102	25.3220	74.6387	52.6939
5100	5.2223	25.8436	75.1341	52.7972
5200	5.2344	26.3664	75.6295	52.8988
5300	5.2464	26.8905	76.1249	52.9986
5400	5.2583	27.4157	76.6203	53.0965
5500	5.2701	27.9421	77.1157	53.1933
5600	5.2818	28.4697	77.6111	53.2884
5700	5.2935	28.9985	78.1065	53.3820
5800	5.3047	29.5284	78.6019	53.4742
5900	5.3159	30.0594	79.0973	53.5650
6000	5.3270	30.5916	79.5927	53.6544

TABLE XXIX—THERMODYNAMIC PROPERTIES OF H<sub>2</sub> (GAS)

[Atomic weight, 1.008]

T (°K)	C <sub>p</sub> ( $\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$ )	H <sub>2</sub> - H <sub>0</sub> (kcal/mole)	H <sub>2</sub> (kcal/mole)	S <sub>2</sub> ( $\frac{\text{cal}}{\text{mole} \cdot ^\circ\text{K}}$ )
0	-----	0	85.3285	-----
200	4.1680	1.4812	86.8097	27.3927
300	4.1680	1.4904	86.8153	27.4253
400	4.1680	1.4972	87.7157	28.8524
500	4.1680	2.4810	87.8125	29.0610
600	4.1680	2.4808	88.3093	30.8507
700	4.1680	3.4775	88.8061	31.0525
800	4.1680	3.4714	89.3029	32.2050
900	4.1680	4.4712	89.7997	32.8811
1000	4.1680	4.4680	90.2965	33.4045
1100	4.1680	5.4648	90.7933	33.8780
1200	4.1680	5.4616	91.2901	34.3103
1300	4.1680	6.4584	91.7869	34.7079
1400	4.1680	6.4552	92.2837	35.0761
1500	4.1680	7.4520	92.7805	35.4188
1600	4.1680	7.4488	93.2773	35.7395
1700	4.1680	8.4456	93.7741	36.0407
1800	4.1680	8.4424	94.2709	36.3246
1900	4.1680	9.4392	94.7677	36.5932
2000	4.1680	9.4360	95.2645	36.8480
2100	4.1680	10.4328	95.7613	37.0904
2200	4.1680	10.4296	96.2581	37.3215
2300	4.1680	11.4264	96.7549	37.5424
2400	4.1680	11.4232	97.2517	37.7539
2500	4.1680	12.4200	97.7485	37.9560
2600	4.1680	12.4168	98.2453	38.1515
2700	4.1680	13.4136	98.7421	38.3390
2800	4.1680	13.4104	99.2389	38.5196
2900	4.1680	14.4072	99.7357	38.6940
3000	4.1680	14.4040	100.2325	38.8624
3100	4.1680	15.4008	100.7293	39.0253
3200	4.1680	15.3976	101.2261	39.1830
3300	4.1680	16.3944	101.7229	39.3359
3400	4.1680	16.3912	102.2197	39.4842
3500	4.1680	17.3880	102.7165	39.6282
3600	4.1680	17.3848	103.2133	39.7681
3700	4.1680	18.3816	103.7101	39.9043
3800	4.1680	18.3784	104.2069	40.0368
3900	4.1680	19.3752	104.7037	40.1658
4000	4.1680	19.3720	105.2005	40.2916
4100	4.1680	20.3688	105.6973	40.4142
4200	4.1680	20.3656	106.1941	40.5340
4300	4.1680	21.3624	106.6909	40.6509
4400	4.1680	21.3592	107.1877	40.7651
4500	4.1680	22.3560	107.6845	40.8767
4600	4.1680	22.3528	108.1813	40.9859
4700	4.1680	23.3496	108.6781	41.0926
4800	4.1680	23.3464	109.1749	41.1973
4900	4.1680	24.3432	109.6717	41.2998
5000	4.1680	24.3400	110.1685	41.4002
5100	4.1680	25.3368	110.6653	41.4985
5200	4.1680	25.3336	111.1621	41.5950
5300	4.1680	26.3304	111.6589	41.6893
5400	4.1680	26.3272	112.1557	41.7823
5500	4.1680	27.3240	112.6525	41.8738
5600	4.1680	27.3208	113.1493	41.9632
5700	4.1680	28.3176	113.6461	42.0511
5800	4.1680	28.3144	114.1429	42.1376
5900	4.1680	29.3112	114.6397	42.2224
6000	4.1680	29.3080	115.1365	42.3059

GENERAL METHOD AND TABLES FOR COMPUTATION OF EQUILIBRIUM COMPOSITION AND TEMPERATURE

TABLE XLV—THERMODYNAMIC PROPERTIES OF OH (GAS)

[Molecular weight, 17.008]

T (°K)	C <sub>p</sub> (cal mole*°K)	H <sub>f</sub> -H <sub>0</sub> (kcal mole)	H <sub>f</sub> (kcal mole)	S <sub>f</sub> (cal mole*°K)	-ΔH <sup>0</sup> RT	(-ΔH <sup>0</sup> /RT) - (-ΔT/(T <sup>2</sup> +d))		ln K	log K = -ΔT/(T <sup>2</sup> +d)	
						a	b		c	d
0	7.141	0	41.7266	41.888	176.7827	.....	.....	.....	.....	.....
25	7.139	2.1225	46.8491	43.931	169.7265	.....	.....	69.3677	.....	.....
50	7.071	2.8296	47.5562	45.978	127.6916	.....	.....	59.9110	.....	.....
75	7.018	3.5357	48.2616	47.559	102.3472	.....	.....	52.4585	.....	.....
100	7.073	4.2408	48.9671	48.810	85.6393	.....	.....	46.3577	.....	.....
125	7.087	4.9459	49.6725	49.927	74.6991	.....	.....	41.2570	.....	.....
150	7.100	5.6510	50.3779	50.877	67.1888	.....	.....	36.9577	.....	.....
175	7.114	6.3574	51.1040	51.723	61.5882	.....	.....	33.2643	.....	.....
200	7.133	7.1000	51.8526	52.4910	57.1964	5931	0.02814	30.0483	.....	.....
225	7.140	7.8436	52.5712	53.1919	53.8119	4575	0.02860	27.2907	.....	.....
250	7.151	8.5872	53.3208	53.8170	51.5401	4191	0.02915	24.9113	3029	0.02157
275	7.163	9.3309	54.0815	54.4556	49.2118	3873	0.02977	22.8178	1863	0.02172
300	7.172	10.1246	54.8532	55.0278	47.4566	3599	0.03047	21.0007	1223	0.01609
325	7.185	10.9680	55.6359	55.5375	45.9292	3361	0.03127	19.5493	1008	0.01677
350	7.197	11.7611	56.4286	56.0788	44.5898	3153	0.03210	18.4213	1494	0.01535
375	8.006	12.5543	57.2299	56.5650	43.0217	2970	0.03210	17.4657	1407	0.01558
400	8.152	13.3142	58.0408	57.0285	41.3186	2808	0.0341	16.6285	1327	0.01594
425	8.283	14.1315	58.8041	57.4714	39.5813	2663	0.0360	15.8753	1255	0.01687
450	8.398	14.9665	59.5871	57.8955	37.8209	2533	0.0381	15.2027	1190	0.01608
475	8.578	15.7918	60.3214	58.3027	36.2771	2415	0.0417	14.6042	1132	0.01508
500	8.743	16.6159	61.0255	58.6899	34.8935	2308	0.0462	14.0549	1080	0.01439
525	8.894	17.4812	61.7008	59.0705	33.6452	2210	0.0516	13.5493	1032	0.01370
550	9.011	18.3905	62.3463	59.4537	32.5105	2121	0.0576	13.0792	989	0.01302
575	9.114	19.3352	63.0213	59.7842	31.4805	2038	0.0641	12.6413	949	0.01245
600	9.203	20.3151	63.7267	60.1210	30.5558	1962	0.0710	12.2303	912	0.01198
625	9.277	21.3377	64.4518	60.4585	29.7362	1892	0.0782	11.8418	878	0.01161
650	9.345	22.4016	65.1971	60.7984	28.9984	1826	0.0857	11.4804	846	0.01134
675	9.408	23.5066	65.9622	61.1371	28.3315	1765	0.0934	11.1413	817	0.01116
700	9.465	24.6534	66.7371	61.4733	27.7254	1708	0.1013	10.8213	790	0.01107
725	9.517	25.8422	67.5218	61.8058	27.1701	1655	0.1094	10.5163	764	0.01105
750	9.563	27.0737	68.3163	62.1347	26.6656	1605	0.1177	10.2213	740	0.01112
775	9.604	28.3480	69.1208	62.4596	26.2017	1558	0.1262	9.9413	718	0.01127
800	9.640	29.6652	69.9353	62.7815	25.7682	1513	0.1349	9.6713	697	0.01144
825	9.671	31.0163	70.7598	63.1000	25.3651	1471	0.1438	9.4163	677	0.01162
850	9.697	32.4016	71.5943	63.4151	24.9922	1432	0.1529	9.1713	659	0.01181
875	9.719	33.8221	72.4388	63.7266	24.6493	1395	0.1622	8.9343	641	0.01200
900	9.736	35.2776	73.2933	64.0341	24.3364	1360	0.1717	8.7013	624	0.01220
925	9.749	36.7681	74.1578	64.3376	24.0525	1325	0.1814	8.4713	608	0.01241
950	9.758	38.2836	75.0323	64.6371	23.7976	1290	0.1913	8.2443	593	0.01262
975	9.763	39.8241	75.9168	64.9326	23.5717	1255	0.2014	8.0213	579	0.01283
1000	9.765	41.3896	76.8113	65.2241	23.3748	1220	0.2117	7.8013	565	0.01304
1025	9.764	42.9801	77.7158	65.5116	23.2059	1185	0.2222	7.5843	551	0.01325
1050	9.760	44.5956	78.6303	65.7951	23.0640	1150	0.2329	7.3713	537	0.01346
1075	9.753	46.2361	79.5548	66.0746	22.9481	1115	0.2438	7.1613	523	0.01367
1100	9.743	47.8916	80.4893	66.3501	22.8572	1080	0.2549	6.9543	509	0.01388
1125	9.730	49.5621	81.4338	66.6216	22.7903	1045	0.2662	6.7513	495	0.01409
1150	9.714	51.2476	82.3883	66.8891	22.7474	1010	0.2777	6.5513	481	0.01430
1175	9.695	52.9481	83.3528	67.1526	22.7285	975	0.2894	6.3543	468	0.01451
1200	9.673	54.6636	84.3273	67.4121	22.7326	940	0.3013	6.1613	454	0.01472
1225	9.648	56.3941	85.3018	67.6676	22.7597	905	0.3134	5.9713	440	0.01493
1250	9.620	58.1396	86.2763	67.9191	22.8098	870	0.3257	5.7843	426	0.01514
1275	9.589	59.8901	87.2508	68.1666	22.8829	835	0.3382	5.6013	412	0.01535
1300	9.555	61.6456	88.2253	68.4101	22.9790	800	0.3509	5.4213	398	0.01556
1325	9.518	63.4061	89.1998	68.6496	23.0981	765	0.3638	5.2443	384	0.01577
1350	9.478	65.1716	90.1743	68.8851	23.2402	730	0.3769	5.0713	370	0.01598
1375	9.435	66.9421	91.1488	69.1166	23.4063	695	0.3902	4.9013	356	0.01619
1400	9.389	68.7176	92.1233	69.3441	23.5954	660	0.4037	4.7343	342	0.01640
1425	9.340	70.4981	93.0978	69.5676	23.8085	625	0.4174	4.5713	328	0.01661
1450	9.289	72.2836	94.0723	69.7871	24.0456	590	0.4313	4.4113	314	0.01682
1475	9.236	74.0741	95.0468	69.9926	24.3077	555	0.4454	4.2543	300	0.01703
1500	9.181	75.8696	96.0213	70.1941	24.5948	520	0.4597	4.1013	286	0.01724
1525	9.124	77.6701	96.9958	70.3916	24.9079	485	0.4742	3.9513	272	0.01745
1550	9.065	79.4756	97.9703	70.5851	25.2470	450	0.4889	3.8043	258	0.01766
1575	9.004	81.2861	98.9448	70.7746	25.6121	415	0.5038	3.6613	244	0.01787
1600	8.941	83.1016	99.9193	70.9601	26.0042	380	0.5189	3.5213	230	0.01808
1625	8.876	84.9221	100.8938	71.1426	26.4233	345	0.5342	3.3843	216	0.01829
1650	8.809	86.7476	101.8683	71.3221	26.8694	310	0.5497	3.2513	202	0.01850
1675	8.740	88.5781	102.8428	71.4986	27.3425	275	0.5654	3.1213	188	0.01871
1700	8.669	90.4136	103.8173	71.6721	27.8436	240	0.5813	2.9943	174	0.01892
1725	8.596	92.2541	104.7918	71.8426	28.3727	205	0.5974	2.8713	160	0.01913
1750	8.521	94.1096	105.7663	72.0101	28.9398	170	0.6137	2.7513	146	0.01934
1775	8.444	95.9801	106.7408	72.1746	29.5449	135	0.6302	2.6343	132	0.01955
1800	8.365	97.8656	107.7153	72.3361	30.1880	100	0.6469	2.5213	118	0.01976
1825	8.284	99.7661	108.6898	72.4946	30.8691	65	0.6638	2.4113	104	0.01997
1850	8.201	101.6816	109.6643	72.6501	31.5882	30	0.6809	2.3043	90	0.02018
1875	8.116	103.6121	110.6388	72.8026	32.3453	0	0.6982	2.2013	76	0.02039
1900	8.029	105.5676	111.6133	72.9521	33.1404	.....	0.7157	2.1013	62	0.02060
1925	7.940	107.5381	112.5878	73.0986	33.9735	.....	0.7334	2.0043	48	0.02081
1950	7.849	109.5236	113.5623	73.2421	34.8446	.....	0.7513	1.9113	34	0.02102
1975	7.756	111.5241	114.5368	73.3826	35.7537	.....	0.7694	1.8213	20	0.02123
2000	7.661	113.5396	115.5113	73.5201	36.7008	.....	0.7877	1.7343	6	0.02144