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AN EFFICIENT NUMERICAL METHOD FOR THE CALCULATION OF CHEMICAL EQUILIBRIUM IN THE H/C/O/N/A SYSTEM

I. T. Osgerby and R. P. Rhodes

ARO, Inc.

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FOREWORD

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ABSTRACT

An efficient method is presented for calculating equilibrium chemical composition at a given pressure and stoichiometry with temperature, enthalpy, or entropy specified as the additional condition. A substantial reduction in computational time was achieved over conventional methods by employing a linearization technique and reducing the number of equations to be solved to a small number of linear algebraic equations. Examples are given for the H_2/O_2 system (six equations reduced to two) and $C/H_2/O_2/N_2/Ar$ system (eleven equations reduced to three). A computer program is presented for solving problems with fuels which involve C and H (hydrocarbon or hydrogen) or N and H (such as hydrazine) and with oxidants such as O_2, H_2O_2, and HNO_3. Extension of the method to include other systems is explained in sufficient detail to eliminate the requirement for an extensive knowledge of chemistry by potential users.

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NOMENCLATURE

a_{ji}	Matrix coefficient
a,b,c,x,y,z	Relative atom moles of nitrogen (N), argon (Ar), carbon dioxide (CO_2), carbon (C), hydrogen (H), and oxygen (O)
$b_{i,k}$	k^{th} coefficient in polynomial thermodynamic property of species i
C_p	Specific heat of mixture, cal/°K
$\overline{C}_p$	Mean specific heat, Btu/lb°R
C_{p_i}	Specific heat of species i, cal/mole°K
d_{ji}	Matrix coefficient
F	Gibbs free energy of the mixture, cal/mole°K
$F_{T,i}$	Standard Gibbs free energy of species i at 1 atm and temperature T, cal/mole°K
H	Enthalpy of the mixture, cal/gm
$\overline{H}$	Mean enthalpy, Btu/lb

h_i	Enthalpy of species i, cal/mole°K
$J(a_{ji})$	Determinant of matrix of coefficients
K	Equilibrium constant
m	Number of independent species which determines order of matrix
n	Total number of species
P	Pressure, atm
P_i	Partial pressure, atm
P_v	Vapor pressure, atm
Q_{comb}	Heat of combustion of a fuel, Btu/lb
q	Number of elements
R	Gas constant, cal/mole°K or cm^3 atm/mole°K
r	Ratio of number of atom moles of a species to that of another
S	Entropy of mixture, cal/gm°K
$S_{T,i}$	Standard entropy of species i at temperature T and 1 atm, cal/mole°K
T	Temperature, °K
XX	Dummy variables
δ	Decrement of specie i
ν'_{ij}, ν''_{ij}	Stoichiometric coefficients of species i in reaction j
ϕ	Equivalence ratio

SUPERSCRIPTS

o	Standard state
*	Specified input value
′	Current estimate of variable

SUBSCRIPTS

i,j,k,β	Dummy indices
i	Property of ith species
j	Property of jth reaction
ref	Property evaluated at reference temperature
T	Temperature

SECTION I
INTRODUCTION

There are many problems involving the performance of propulsion systems in which it is necessary to know the equilibrium properties of combustion gases. As long as combustion temperatures are relatively low ($T < 3000$ to $3500°R$) good results can be obtained by assuming no dissociation of the combustion products and including an empirical correction for dissociation as a function of temperature only. An effective isentropic exponent can be determined and fluid dynamic properties may be calculated using conventional aerodynamic functions.

When it is necessary to evaluate systems where higher temperatures occur, such as turbojets with afterburners, ramrockets, or ramjets, low temperature empirical corrections rapidly become very poor. A much more difficult equilibrium chemistry calculation must then be carried out since the complete set of nonlinear equations which describe chemical equilibrium must be solved.

Solution of the complete set of nonlinear equations is very laborious by conventional methods, even for a relatively simple system such as a laboratory flame. Computers alleviated this problem (Refs. 1 through 3). Increasing system complexity and requirements for thousands of data point calculations brought new problems directly associated with the old, time-consuming methods of calculation.

Numerical techniques for solving systems of nonlinear equations have been developed to a high degree; therefore, it is necessary to devise operations in the system of equations to effect significant reductions in the overall calculation time. The most successful operation which has been applied is that of linearization, using a truncated Taylor series expansion about the solution (Refs. 4 and 5). The method of Ref. 4 employs an expansion of the free energy of the mixture, using the method of steepest descent to minimize this quantity corresponding to chemical equilibrium. The method of Ref. 5 employs an expansion of the conservation equations and the Newton-Raphson method to solve for the equilibrium composition.

The technique described in this report is essentially that of Weinberg (Ref. 5) extended to allow temperature to be calculated simultaneously with the chemical composition and, in addition, to include a numerically stable computational technique. When temperature is to be determined, either enthalpy or entropy may be specified at a given pressure, thus allowing the temperature to be obtained from an energy balance on an engine or from the known entropy at some point along an isentropic expansion or compression.

SECTION II
CALCULATION OF EQUILIBRIUM COMPOSITION

In order to calculate the equilibrium composition of a mixture of n components (species) at a given temperature, pressure, and equivalence ratio, one needs n independent equations. For a system containing q elements from which n species are constituted, it is possible to write q conservation equations which are linear combinations of the

concentrations of species, and n-q chemical equilibrium equations which are, in general, nonlinear combinations of the species concentrations. These chemical equilibrium equations define the relative amounts of each species at a particular pressure and temperature.

In general, it is possible to choose any q species which, as a group, contain all the elements and write equilibrium equations for the remaining species. Substituting these equations into the conservation equations results in a set of q nonlinear equations in q unknowns.

Several methods have been developed for solving nonlinear equations with the Newton-Raphson method—the most frequently used. There are limitations to the use of this method, but it is a powerful tool, and convergence can usually be guaranteed. The nonlinear equations are linearized by expanding the equations in a first-order Taylor series. In order to solve the linearized set it is necessary to have approximate values of concentration for q of the species. The set of q linearized equations is then solved for corrections to the approximate values. The process is repeated to find new corrections to the previous values. Although the Newton-Raphson technique always converges to a solution, some experience is necessary to ensure that the physically realistic solution is obtained. In addition, the rate of convergence is greatly improved if experience is used to specify which of the q species should be chosen and good approximations are made for the initial values. Finally, if the number of equations can be reduced, considerable savings in computational time are obtained since, if there are q equations for q unknowns, q^2 operations are necessary to solve for the q unknowns.

The method developed in this report is essentially the application of experience to improve established methods for equilibrium calculations. The method is extremely efficient in obtaining solutions for a variety of complex systems including the simultaneous solution of the energy or entropy equations to determine temperature if it is an additional unknown.

The species are assigned partial pressures P_i and the necessary equations are (temperature is not a variable in the following derivation)

$$P_i = g(P_\beta) \qquad i = 1, n-m; \beta = 1, m \tag{1}$$

where the functions g(P) are the equilibrium equations and may include one or more of the conservation equations. The conservation equations are expressed in the form

$$a_\beta = g(P_K) \qquad K = 1, n; \beta = 1, m \tag{2}$$

where a_β is defined in such a way that it is identically equal to zero when the solution has been obtained. Expanding Eq. (2) in a Taylor series and neglecting orders higher than the first

$$a_\beta = a_\beta' + \sum_{K=1}^{n} \frac{\partial a_\beta}{\partial P_K} \delta_K \qquad \beta = 1, m \tag{3}$$

Differentiating Eq. (1) one obtains:

$$\delta_i = \sum_{\beta=1}^{m} \frac{\partial g(P_K)}{\partial P_\beta} \tag{4}$$

Note that since the equations are to be solved in finite difference form, finite difference notation is used throughout.

Substituting Eqs. (4) in Eqs. (3), evaluating the partial derivatives using Eqs. (1), and letting a_β approach 0, one obtains m equations for the m unknown δ_β. The δ_β's are the desired corrections to the initial values of P_β which are denoted by P'_β. Thus the corrected value is given by

$$P_\beta = P'_\beta + \delta_\beta \tag{5}$$

and the remaining (n - m)P_i's are obtained by substituting the P_β's in Eqs. (1). The process is repeated until the δ_β's are within acceptable limits.

Some examples of increasing complexity are given which illustrate this method of calculation and, in addition, a method is included which simultaneously solves for the temperature when enthalpy or entropy is known.

2.1 APPLICATIONS OF THE METHOD

2.1.1 Hydrogen/Oxygen (m = 2)

The following n equations completely describe the relationship between the n unknown partial pressures.

Dissociation Equilibria

$$\begin{array}{lll} j = 1 & 0.5\,H_2 \leftrightharpoons H & P_1 = K_1\sqrt{P_5} \\ j = 2 & 0.5\,O_2 \leftrightharpoons O & P_2 = K_2\sqrt{P_6} \\ j = 3 & H_2O \leftrightharpoons 0.5\,H_2 + OH & P_3 = K_3P_4/\sqrt{P_5} \\ j = 4 & H_2O \leftrightharpoons H_2 + 0.5\,O_2 & P_4 = K_4P_5\sqrt{P_6} \end{array} \tag{6}$$

Species

i =	1	2	3	4	5	6
	H	O	OH	H_2O	H_2	O_2

Element Conservation Equations

$$\begin{array}{ll} \text{H atoms:} & 2P_5 + P_1 + P_3 + 2P_4 = P_H \\ \text{O atoms:} & 2P_6 + P_2 + P_3 + P_4 = P_O \end{array} \tag{7}$$

In addition, there is the following conservation equation for species

$$\sum_{i=1}^{n} P_i = P \tag{8}$$

Let the ratio of H atoms to O atoms in the unburned mixture be denoted $r_{HO} = P_H/P_O$. The O atom conservation equation can then be substituted into the H atom conservation equation as follows:

$$2P_5 + P_1 + P_3 + 2P_4 - r_{HO}(2P_6 + P_2 + P_3 + P_4) = 0 \tag{9}$$

One thus has six equations for the six unknown partial pressures. The equilibrium constants K_j are known functions of temperature (see Appendix I). It remains to choose the two species to which the remaining four species are to be related. The two appearing in the largest concentration should be selected in order to minimize numerical problems. At low temperatures, dissociation will be almost zero. The partial pressure of atomic hydrogen and oxygen and hydroxyl radicals will be negligible. For fuel lean calculations the partial pressure of hydrogen molecules will be negligible as will be the partial pressure of oxygen molecules for fuel rich calculations. For stoichiometric calculations, all the partial pressures are small except that of water vapor. Thus, water vapor is a natural choice and hydrogen and oxygen are used for rich and lean calculations, respectively. Stoichiometric calculations are made with hydrogen as the second variable although oxygen could be used instead.

FUEL LEAN CASE

$$\begin{aligned} P_1 &= K_1 K_4^{-1/2} P_4^{1/2} P_6^{-1/4} & P_3 &= K_3 K_4^{1/2} P_4^{1/2} P_6^{1/4} \\ P_2 &= K_2 P_6^{1/2} & P_5 &= K_4^{-1} P_4 P_6^{-1/2} \end{aligned} \tag{10}$$

These equations represent those expressed as Eqs. (1). Differentiating these equations

$$\begin{aligned} \delta_1 &= 0.5 \frac{P_1}{P_4} \delta_4 - 0.25 \frac{P_1}{P_6} \delta_6 \\ \delta_2 &= 0.5 \frac{P_2}{P_6} \delta_6 \\ \delta_3 &= 0.5 \frac{P_3}{P_4} \delta_4 + 0.25 \frac{P_3}{P_6} \delta_6 \\ \delta_5 &= \frac{P_5}{P_4} \delta_4 - 0.5 \frac{P_5}{P_6} \delta_6 \end{aligned} \tag{11}$$

These equations represent those expressed as Eqs. (4).

Let

$$\alpha_1 = 2P_5 + P_1 + P_3 + 2P_4 + r_{HO}(2P_6 + P_2 + P_3 + P_4)$$

and

$$\alpha_2 = \sum_{i=1}^{6} P_i - P \tag{12}$$

These equations represent those expressed as Eqs. (2). Differentiating these equations

$$\frac{\partial \alpha_1}{\partial P_1} = 1 \qquad \frac{\partial \alpha_1}{\partial P_i} = -r_{HO} \qquad \frac{\partial \alpha_1}{\partial P_3} = 1 - r_{HO}$$

$$\frac{\partial \alpha_1}{\partial P_4} = 2 - r_{HO} \qquad \frac{\partial \alpha_1}{\partial P_5} = 2 \qquad \frac{\partial \alpha_1}{\partial P_6} = -2r_{HO} \tag{13}$$

$$\frac{\partial \alpha_2}{\partial P_i} = 1 \qquad i = 1,6$$

These expressions together with Eqs. (11) above represent those expressed as Eqs. (3).

METHOD OF SOLUTION

1. Assume values for P_4' and P_6' using the stoichiometric equation

$$P_4' = 2\phi P/(1+\phi) \qquad P_6' = P - P_4' \qquad r_{HO} = 2\phi$$

where ϕ is the prescribed equivalence ratio.

2. Compute initial values of P_k' where

$$P_1' = K_1 K_4^{-1/2} P_4'^{-1/2} P_6'^{-1/4}$$

similarly for P_2', P_3', and P_5'.

3. Compute initial values of the coefficients of the δ_k Eqs. (11) where

$$\delta_1 = 0.5 P_1'/P_4' \delta_4 - 0.25 \frac{P_1'}{P_6'} \delta_6$$

similarly for δ_2, δ_3, and δ_5.

4. Compute a_1 and a_2 using Eqs. (12).

5. Compute the $(\partial a/\partial P_k)\,\delta_k$ terms using Eqs. (13) and collect all the coefficients of δ_4 and δ_6 together to form a 2 by 2 matrix

$$-a_1 = \frac{1}{P_4'}[0.5\,P_1' + 0.5(1-r_{HO})P_3' + (2-r_{HO})P_4' + 2P_5']\,\delta_4 + \frac{1}{P_6'}[-0.25P_1' - 0.5\,r_{HO}P_2' - 0.25(1-r_{HO})P_3' + P_5' - 2r_{HO}P_6']\,\delta_6 \tag{14}$$

$$-a_2 = \frac{1}{P_4'}[0.5\,P_1' - 0.5\,P_3' + P_4' + P_5']\,\delta_4 + \frac{1}{P_6'}[-0.25P_1' + 0.5\,P_2' + 0.25P_3' - 0.5\,P_5' + P_6']\,\delta_6 \tag{15}$$

Substituting for δ_6 from Eq. (6) into Eq. (5) gives an equation for δ_4. Substitution of δ_4 into either Eq. (14) or (15) gives an equation for δ_6.

6. Compute $P_4 = P_4' + \delta_4$ and $P_6 = P_6' + \delta_6$

7. Repeat processes 2 through 6 until δ_4 and δ_6 are very small (10^{-5} is considered sufficiently small for most calculations). The resulting errors in dependent species concentrations are always less than this (see Eqs. (11)).

8. Compute final values of P_1, P_2, P_3, and P_5 to obtain the equilibrium composition.

FUEL RICH OR STOICHIOMETRIC CASES

$$\begin{aligned}
P_1 &= K_1P_5^{1/2} & \delta_1 &= 0.5\,\frac{P_1}{P_5}\,\delta_5 \\
P_2 &= K_2K_4^{-1}P_4P_5^{-1} & \delta_2 &= \frac{P_2}{P_4}\,\delta_4 - \frac{P_2}{P_5}\,\delta_5 \\
P_3 &= K_3P_4P_5^{-1/2} & \delta_3 &= \frac{P_3}{P_4}\,\delta_4 - 0.5\,\frac{P_3}{P_5}\,\delta_5 \\
P_6 &= K_4^{-2}P_4^2P_5^{-2} & \delta_6 &= 2\,\frac{P_6}{P_4}\,\delta_4 - 2\,\frac{P_6}{P_5}\,\delta_5
\end{aligned} \tag{16}$$

Thus

$$-a_1 = \frac{1}{P_4'}[-r_{HO}P_2' + (1-r_{HO})P_3' + (2-r_{HO})P_4' - 4\,r_{HO}P_6']\,\delta_6 + \frac{1}{P_5'}[0.5\,P_1' + r_{HO}P_2' + 0.5(1-r_{HO})P_3' + 2P_5' + 4r_{HO}P_6']\,\delta_5 \tag{17}$$

$$-a_2 = \frac{1}{P_4'}[P_2' + P_3' + P_4' + 2P_6']\,\delta_4 + \frac{1}{P_5'}[0.5\,P_1' - P_2' - 0.5\,P_3' + P_5' - 2P_6']\,\delta_5$$

Solve as for lean case with

$$P_5' = P - P_4' \qquad \phi > 1$$

$$P_5' = 10^{-2} \qquad \phi = 1$$

1.2 C/H/O/N/A (m = 3)

In this example, a system of equations is derived which can be used to calculate equilibrium composition for hydrogen/air or hydrocarbon/air combustion with pressure specified and either temperature, enthalpy, or entropy specified. This set has been programmed in FORTRAN IV for general use, and a copy of the listing is attached as Appendix II.

The following n dissociation equilibrium and conservation equations completely describe the relationship between the n unknown partial pressures.

j	Fuel Lean	Fuel Rich
1	$P_1 = K_1 P_8^{1/2} P_7^{1/4}$	$P_1 = K_1 P_6^{1/2}$
2	$P_2 = K_2 P_7^{1/2}$	$P_2 = K_2 P_8 P_6^{-1}$
3	$P_3 = K_3 P_8^{1/2} P_7^{1/4}$	$P_3 = K_3 P_8 P_1^{-1}$
4	$P_4 = K_4 P_{10}^{1/2} P_7^{1/2}$	$P_4 = K_4 P_8^{1/2} P_{10}^{1/2} P_6^{-1}$
5	$P_5 = K_5 P_9 P_7^{-1/2}$	$P_5 = K_5 P_9 P_6 P_8^{-1}$
6	$P_6 = K_6 P_8 P_7^{-1/2}$	$P_7 = K_6 P_8^2 P_6^{-2}$

(18)

Species

i =	1	2	3	4	5	6	7	8	9	10	Ar
	H	O	OH	H_2O	NO	CO	H_2	O_2	CO_2	N_2	A

Conservation Equations

Lean

$$P_9 = r_{CN}(2P_{10} + P_4)/(1 + K_5 P_7^{-1/2})$$

Rich

$$
\begin{aligned}
P_9 &= r_{CN}(2P_{10} + P_4)/(1 + K_5P_6/P_8) \\
P_{AR} &= r_{AN}(2P_{10} + P_4) \\
P_1 + P_3 + 2P_6 + 2P_8 + r_{HN}(2P_{10} + P_4) &= 0 \\
P_2 + P_3 + P_4 + P_5 + 2P_7 + P_8 + 2P_9 - r_{ON}(2P_{10} + P_4) &= 0 \\
\sum_1^{10} P_i - (P - P_{AR}) &= 0
\end{aligned}
\tag{19}
$$

A more sophisticated method of bookkeeping is used in order to simplify the program logic in this example. The matrix is set up as follows

$$\sum_{i=1}^{3} a_{ji}\delta_i = \alpha_j \qquad j = 1,3 \tag{20}$$

The solutions are obtained using Cramer's Rule

$$\delta_1 = \frac{\begin{vmatrix} -\alpha_1 & a_{12} & a_{13} \\ -\alpha_2 & a_{22} & a_{23} \\ -\alpha_3 & a_{32} & a_{33} \end{vmatrix}}{(a_{ji})} \tag{21}$$

and similarly for δ_2 and δ_3, where $J(a_{ji})$ is the determinant of the coefficient matrix.

$$J(a_{ij}) = \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{vmatrix} \neq 0 \tag{22}$$

For fuel lean mixtures, $\delta_1 \equiv \delta_7$. $\delta_2 \equiv \delta_8$, and $\delta_3 \equiv \delta_{10}$; for fuel rich or stoichiometric mixtures, $\delta_1 \equiv \delta_6$ with $\delta_2 \equiv \delta_8$ and $\delta_3 \equiv \delta_{10}$. The coefficients in the matrix equation are derived as in the example given in section 2.1.1.

$$
\begin{aligned}
\alpha_1 &= P_1' + P_3' + 2P_6' + 2P_8' - r_{HN}(2P_{10}' + P_4') \\
\alpha_2 &= P_2' + P_3' + P_4' + P_5' + 2P_7' + P_8' + 2P_9' - r_{ON}(2P_{10}' + P_4') \\
\alpha_3 &= \sum_{i=1}^{10} P_i' - (P - P_{AR})
\end{aligned}
\tag{23}
$$

$$a_{1i} = d_{1,i} + d_{3,i} + 2d_{6,i} + 2d_{8,i} - r_{HN}(2d_{10,i} + d_{4,i})$$

$$a_{2i} = d_{2,i} + d_{3,i} + d_{4,i} + d_{5,i} + 2d_{7,i} + d_{8,i} + d_{9,i} - r_{ON}(2d_{10,i} + d_{4,i}) \quad (23)$$

(Continued)

$$a_{3,i} = \sum_{K=1}^{10} d_{K,i} + d_{AR,i}$$

FUEL LEAN CASE

$$\left.\begin{array}{lll}
d_{1,1} = -0.25\,P_1'/P_7' & d_{1,2} = P_1'/P_8' & d_{1,3} = 0 \\
d_{2,1} = 0.5\,P_2'/P_7' & d_{2,2} = 0 & d_{2,3} = 0 \\
d_{3,1} = 0.25\,P_3'/P_7' & d_{3,2} = 0.5\,P_3'/P_8' & d_{3,3} = 0 \\
d_{4,1} = 0.5\,P_4'/P_7' & d_{4,2} = 0 & d_{4,3} = 0.5\,P_4'/P_{10}' \\
\multicolumn{3}{l}{d_{9,1} = r_{CN}[d_{4,1} - 0.5(2P_{10}' + P_4')(K_5/P_7'^{\,3/2})/(1 + K_5/P_7'^{\,1/2})]/(1 + K_5/P_7'^{\,1/2})} \\
d_{9,2} = 0 & \multicolumn{2}{l}{d_{9,3} = r_{CN}(2 + d_{4,3})/(1 + K_5/P_7'^{\,1/2})} \\
d_{5,1} = d_{9,1}\dfrac{P_5'}{P_9'} - 0.5\dfrac{P_5'}{P_7'} & d_{5,2} = 0 & d_{5,3} = d_{9,3}\dfrac{P_5'}{P_9'} \\
d_{6,1} = -0.5\,P_6'/P_7' & d_{6,2} = P_6'/P_8' & d_{6,3} = 0 \\
d_{7,1} = 1 & d_{7,2} = 0 & d_{7,3} = 0 \\
d_{8,1} = 0 & d_{8,2} = 1 & d_{8,3} = 0 \\
d_{10,1} = 0 & d_{10,2} = 0 & d_{10,3} = 1 \\
d_{AR,1} = r_{AN}\,d_{4,1} & d_{AR,2} = 0 & d_{AR,3} = r_{AN}(2 + d_{4,3})
\end{array}\right\} \quad (24)$$

FUEL RICH CASE

$$\begin{array}{lll}
d_{1,1} = 0.5\,P_1'/P_6' & d_{1,2} = 0 & d_{1,3} = 0 \\
d_{2,1} = -P_2'/P_6' & d_{2,2} = P_2'/P_8' & d_{2,3} = 0 \\
d_{3,1} = d_{1,1}P_3'/P_1' & d_{3,2} = P_3'/P_8' & d_{3,3} = 0 \\
d_{4,1} = -P_4'/P_6' & d_{4,2} = P_4'/P_8' & d_{4,3} = 0.5\,P_4'/P_{10}' \\
d_{7,1} = -2P_7'/P_6' & d_{7,2} = 2P_7'/P_8' & d_{7,3} = 0
\end{array} \quad (25)$$

$$d_{9,1} = (r_{CN}d_{4,1} - K_5P_8'P_9')(1 + K_5P_6'/P_8')$$

$$d_{9,2} = (r_{CN}d_{4,2} + K_5P_6'P_9'/P_8'^2)(1 + K_5P_6'/P_8')$$

$$d_{9,3} = r_{CN}(2 + d_{4,3})(1 + K_5P_6'/P_8')$$

$$d_{5,1} = (d_{9,1}K_5/P_8' + P_5')/P_6'$$

$$d_{5,2} = (d_{9,2}K_5P_6' - P_5')/P_8' \qquad (25)$$

$$d_{5,3} = (d_{9,3}K_5P_6')/P_8' \qquad \text{(Continued)}$$

$$d_{6,1} = 1 \qquad d_{6,2} = 0 \qquad d_{6,3} = 0$$

$$d_{8,1} = 0 \qquad d_{8,2} = 1 \qquad d_{8,3} = 0$$

$$d_{10,1} = 0 \qquad d_{10,2} = 0 \qquad d_{10,3} = 1$$

$$d_{AR,1} = r_{AN}d_{4,1} \qquad d_{AR,2} = r_{AN}d_{4,2} \qquad d_{AR,3} = r_{AN}(2 + d_{4,3})$$

METHOD OF SOLUTION

1. Assume values for P_8', P_{10}', and P_7' or P_6'; evaluate r_{AN}, r_{CN}, r_{HN}, and r_{ON} using the stoichiometric equation

$$xC + yH + zO + aN + bA$$

$$xCO_2 + \frac{y}{2}H_2O + \left(\frac{z}{2} - x - \frac{y}{4}\right)O_2 + \frac{a}{2}N_2 + bA \qquad \text{(Lean)} \qquad (26)$$

or

$$\frac{x}{2}CO + \frac{x}{2}CO_2 + (z - 1.5x)H_2O + (0.5y - z - 1.5x)H_2 + \frac{a}{2}N_2 + bA \qquad \text{(Rich)}$$

Rich Fuel Case

$$P_6' = P\left(\frac{y}{2} - z + 1.5x\right)/\left[x + 0.5(y + a)\right]$$

$$P_8' = P(z - 1.5x)/[x + 0.5(y + a)] \qquad (27)$$

$$P_{10}' = Pa/[x + 0.5(y + a)]$$

Lean Fuel Case

$$P_7' = P[z - (2x + 0.5y)]/(0.5y + z + a)$$

$$P_8' = Py/(0.5y + z + a) \qquad (28)$$

$$P_{10}' = Pa/(0.5y + z + a)$$

Atomic Ratios

$$r_{AN} = b/a \qquad r_{CN} = c/a \qquad r_{HN} = y/a \qquad r_{ON} = z/a$$

2. Compute P_i' using the dissociation equilibrium (Eqs. (18))

3. Compute d_{ji}, a_{ji}, and α_j using Eqs. (23) and (24)

4. Solve for δ_i as in Eq. (21).

5. Correct P_8', P_{10}', and either P_6' or P_7' using the δ_i ($P_i = P_i' + \delta_i$).

6. Compute new P_i', i = 1, 5, P_7', and P_6', using the dissociation equilibria.

7. Repeat cycle 3 through 6 until the δ_i are less than a specified magnitude (10^{-5} is usually adequate). If there is no carbon in the fuel, then x should be set equal to zero. If there is no carbon in the system, r_{CN} is zero and the "lean" $d_{5,1}$ and $d_{5,3}$ calculations should be bypassed.

SOOT FORMATION

If there is insufficient oxygen to burn all the carbon, then soot will be produced. This case is handled by adding the carbon formation equation

$$C_s + CO_2 \leftrightharpoons 2CO \qquad K_s = P_9/P_5^2 \tag{29}$$

The carbon vapor (saturation) pressure can be obtained using Gibb's phase rule, assuming coexistence of condensed phase and vapor phase

$$P_v = \exp[(F^{\circ}_{c,s} - F^{\circ}_{c,v})/RT] \tag{30}$$

where F_c° is the standard free energy of carbon and subscripts s and v denote solid (soot) and vapor phases, respectively. Actually, $P_v \approx 0$ for most applications; thus, only P_s (soot concentration - not a pressure) needs to be considered and it is evaluated using the carbon conservation equation (thus P_9 and P_5 are modified to include P_s). If P_v is not approximately zero ($T > 4000°C$) then it is also added to the carbon conservation equation and, in addition, is added to the sum of the partial pressures (P_s is not).

2.2 CALCULATIONS WHEN TEMPERATURE IS UNKNOWN

2.2.1 Given Static Enthalpy or Total Enthalpy and Velocity

The static (sensible plus chemical) enthalpy (H) is calculated from the current values of partial pressure and the initial or current estimate of static pressures and the initial or current estimate of static temperature (T). If the given value is denoted by H*, then the correction equation for temperature is obtained from the enthalpy equation

$$H = \frac{1}{PW} \sum_{i=1}^{n} P_i h_i \tag{31}$$

where

$$h_i = \int C_{p_i} dT + \Delta h_{form\ i} \text{ and } P_w = \sum_{i=1}^{n} P_i W_i \tag{32}$$

$$P(HdW + WdH) = \sum_{i=1}^{n} \frac{\partial H}{\partial P_i} dP_i + \frac{\partial H}{\partial T} dT \tag{33}$$

For temperatures below about 4500°R, the frozen specific heat is essentially equal to the equilibrium specific heat, i.e.,

$$\sum_{i=1}^{n} \frac{\partial H}{\partial P_i} dP_i - PWdW << \frac{\partial H}{\partial T} dT \tag{34}$$

thus Eq. (33) is approximated quite well (for calculation purposes) by

$$H^* - H = \Delta H \approx C_p \Delta T \tag{35}$$

or

$$\Delta T \approx \Delta H / C_p \tag{36}$$

The corrected temperature $T = \Delta T + T$.

Using Eq. (35) results in a considerable saving in the number of calculations which must be made and does not require an increase in the order of the matrix which must be solved. The converged solution is the same whether Eq. (34) or (35) is used for the correction equation.

2.2.2 Given Entropy

The entropy is used as a control variable in isentropic expansions in which it is desired to obtain the temperature and composition as the pressure is reduced during an expansion. The correction equation used is

$$S^* - S = \frac{C_p}{T} \Delta T \tag{37}$$

or

$$\Delta T = T'/C_p \ \Delta S \tag{38}$$

The corrected temperature $T = T + \Delta T$.

Above T = 4500°R the difference between the frozen and equilibrium values of specific heat becomes significant and difficulties are experienced in obtaining convergence of the iteration equations. Some additional logic controls were incorporated in the computer program to prevent stable oscillations. This technique has proved to be satisfactory for temperatures below 5500°R.

SECTION III
COMPUTER PROGRAM

A computer program was written for the Raytheon 520 digital computer to solve for the equilibrium composition and thermodynamic properties of a chemical system containing carbon, hydrogen, oxygen, nitrogen, and argon, specifically hydrocarbon air combustion systems. However, because of the versatility of the input, other types of problems may be solved. These include most fuel oxidizer combinations which contain at least hydrogen, oxygen, and nitrogen in the fuel and oxidizer. For example,

1. Hydrogen or hydrocarbons with oxygen-enriched or vitiated air

2. Hydrazine or methyl hydrazines with N_2O_4 or nitric acid

There have been some difficulties obtaining a solution to some types of problems. These are discussed near the end of this section. The program listing is presented in Appendix II and the results of some calculations are given in Appendix III.

The computation was divided between two subroutines which are called by a main program whose function is to input and output data. The main program will not be discussed in detail since it is assumed that any other user would choose to rewrite this section for his own specific purpose. The equilibrium calculations are made in subroutine PROP which calls on subroutine THERM for the required thermodynamic properties.

There are four optional calculations which can be made using PROP. These are controlled by the integer variable IT in the argument list, and are discussed below.

IT = 0. Given the moles of the elements carbon (CAR), hydrogen, (HYD), oxygen (OX), nitrogen (AN2) and Argon (AR), the pressure (PR) in atmospheres, and the enthalpy (H) in Btu/lb, plus an initial estimate for the temperature (TT) in °R, the subroutine returns the equilibrium temperature (TT) in °R, the entropy (S) in Btu/lb°R, the specific heat (CP) in Btu/lb°R, the molecular weight (WTM), an array of the partial pressures of the 10 species (P) in atmospheres, the partial pressure of argon (PAR) in atmospheres, and the number of iterations (NT) required to obtain the solution.

IT = 1. Given the moles of the elements, the temperature (TT), and the pressure (PR), the subroutine returns the enthalpy (H), partial pressures, and the other properties returned when IT = 0.

IT = 2. Given the moles of the elements, the entropy (S), and the pressure (PR), the subroutine returns the composition, temperature, and other thermodynamic properties returned when IT = 0.

IT = 3. Given the composition (array of P's and PAR), the entropy, and the pressure, the subroutine returns the thermodynamic properties for a frozen composition. In this case, if a series of entries to the subroutine are made at different pressures (for example, a frozen isentropic expansion to a series of known pressures) the previous composition is stored so only the initial compositions must be entered.

Normally for this case and the previous one (IT = 2) the input (S) and compositions are obtained by running a type 0 or 1 case immediately before the type 2 or 3 series. For example, in an isentropic nozzle expansion the combustion chamber conditions are first calculated from the fuel-to-air ratio, enthalpy, and pressure, then, using the entropy from this calculation, constant entropy cases (IT = 2 for equilibrium or IT = 3 for frozen expansion) may be calculated.

In summary the argument list of PROP is as follows: Inputs which are unchanged are

CAR	Relative moles of carbon
HYD	Relative moles of hydrogen atom
OX	Relative moles of oxygen atom
AN2	Relative moles of nitrogen atom
AR	Relative moles of argon
PR	System pressure in atmosphere
IT	Type of case

Variables which are both input and output are

H Enthalpy, Btu/lb. For IT = 0, H is entered as the desired mixture enthalpy and returned as the enthalpy of the mixture found by the program. For all other cases, it is an output only and is the mixture enthalpy.

TT Temperature, °R. For IT = 1, it is the desired mixture temperature and is not changed. For all other cases, it is entered as an initial estimate of mixture temperature and is returned as the converged mixture temperature.

S Entropy, Btu/lb°R. For IT = 4,S is entered as the desired mixture entropy and is returned as the calculated mixture entropy. For IT = 1 and 0, it is an output only and is the mixture entropy.

P(10) An array of species partial pressures, atm. For IT = 3, it is an input using the values from the previous calculation and is returned ratioed by the pressure in the previous calculation to that in the present one. For all other cases, it is an output only.

PAR Argon partial pressure, atm. It is used the same way as the other partial pressures.

Variables which are output only are

CP Specific heat, Btu/lb°R

WTM Molecular weight

NT Number of iterations required for convergence

A brief description of the subroutine PROP follows. In this subroutine the equations are solved as outlined in Section 2.1.2.

1. A decision is made as to whether the mixture is rich or lean and initial estimates are made of the partial pressures of the control species (H_2, H_2O, and N_2 for a rich case and O_2, H_2O , and N_2 for a lean case).

2. Inside the main iteration loop, the partial pressures (P(I)) of the remaining species are calculated from equilibrium constants calculated from free energies obtained from THERM.

3. The partial derivatives (D1(J) to DAR(J)) of the species with respect to the control species are calculated.

4. The coefficients A1(I) of the error terms DEL1, DEL2, and DEL3 and the constants SP1 and SP3 in the expanded conservation equations are determined. The matrix is solved for the three error terms which are then added to their respective estimates of partial pressure for the control species.

5. If T is known (IT = 1), these new pressures are used as estimates and the process is repeated until convergence occurs, i.e., the absolute value of DEL1, DEL2, and DEL3 is less than DELL (10^{-6} in this version).

6. For the other cases, an enthalpy or entropy is calculated using the new partial pressures and the estimated temperature by calling THERM. The temperature estimate is then corrected and the entire process repeated with the new T and control specie pressures until convergence occurs, i.e., the

absolute value of the DEL's less than DELL and the error in H or S less than the frozen value of specific heat or $\partial S/\partial T$, respectively. This control gives a maximum error in termperature of 1°K. Subroutine THERM computes the thermodynamic properties of mixtures of the eleven species using the curve fit coefficients from Ref. 6. It is called through an argument list consisting of the following terms:

Inputs not changed by the subroutine are

P	Array of partial pressures of the species
T	Temperature, °K
PR	System pressure, atm
PAR	Argon partial pressure, atm
KT	Integer variable

Outputs are

KT = 0

H = Mixture enthalpy, cal/gm

CP = Mixture specific heat, cal/gm°K

F = Array of H/RT for 10 species

WTM = System molecular weight

KT = 1

F = Array of F/RT for 10 species

H and CP and WTM are meaningless

NOTE: The only input necessary with this option is T.

KT = 2

H = Mixture entropy, cal/gm°K

CP = Mixture S/T, cal/gm°K^2

F = Array of S/R for the 10 species

WTM = System molecular weight

A sample calculation typical of that done in a main program is outlined in detail in Appendix III.

In solving a combustion problem at known enthalpy or entropy for composition and thermodynamic properties, there are four unknowns. These are the three control species compositions and the temperature. The error terms in the species equations neglect the partial derivatives of composition with respect to temperature, and the error term in the energy equation neglects the partial derivatives of enthalpy with respect to composition. This is a great simplification since the neglected partials require time-consuming computation and also add an additional term to the matrix of error terms.

In some test problems, the solution instead of converging has oscillated around the correct answer. These have been cases where the temperature was high and the uncoupling of the species and energy equations was potentially serious. No cases of nonconvergence were seen when the final temperature was below 5000°R which should include almost all problems of interest involving air as an oxidizer.

Several controls have been added to the program to increase the numerical stability for type 0, 2, and 3 problems.

1. For equivalence ratios near stoichiometric, the initial estimate of species concentration for H_2 in rich mixtures and stoichiometric or O_2 in lean mixtures is set equal to 0.01. If this is not done, the initial estimate of some of the free radicals will be abnormally high and the calculation will not converge.

2. When the error in temperature changes sign, two iterations of composition are made at the same temperature. This control has prevented the solution from oscillating in most cases.

3. The initial estimate of temperature has been left as an input. A good estimate will increase the speed of convergence. However, it is usually safer to estimate low rather than high since the equilibrium constants are set up to be large at high temperature and thus can greatly overpredict the dependent species if the temperature estimate is too high.

4. The change in temperature per iteration step is reduced below that calculated by the enthalpy equation.

SECTION IV
RESULTS OF CALCULATIONS

Some results of calculations obtained using this program are given in Appendix III. Table I is a computer printout listing the results from a number of cases where equivalence ratio, enthalpy, and pressure were specified for a C_nH_{2n} hydrocarbon burning in air. Table II lists the results of cases where equivalence ratio temperature and pressure were specified. Table III lists the results of a frozen entropic expansion, and Table IV lists the results

of an equilibrium isentropic expansion from 10 atm to a given pressure for an equilibrium gas with a given equivalence ratio and temperature. These results have been compared with those of Ref. 7 and computed results using the program of Ref. 1. For the same input conditions the temperatures agree to within 1°K, the compositions of the major species to less than 1 percent, and the minor species to a few percent.

The number of iterations required shows that problems where composition or temperature only is a variable (frozen isentropic expansions or known temperature) converge more quickly than problems where both temperature and composition are varied. It also shows that solutions are obtained more quickly at lower temperatures where dissociation is small.

The times required for the calculations shown in Table I are for the Raytheon 520 computer and would be expected to decrease if a faster machine were used (approximately a factor of five for the IBM 360).

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APPENDIXES

I. THERMODYNAMICS OF CHEMICAL EQUILIBRIUM MIXTURES OF PERFECT GASES

II. COMPUTER PROGRAM LISTINGS

III. COMPUTER PROGRAM CALCULATIONS

APPENDIX I
THERMODYNAMICS OF CHEMICAL EQUILIBRIUM MIXTURES OF PERFECT GASES

A chemical reaction is formulated generally as follows:

$$(P_{ij})^{\nu'_{ij}} = (P_{ij})^{\nu''_{ij}}$$

The free energy per mole of a mixture is given by

$$F = \sum_{i=1}^{n} \frac{P_i}{P} F_i = \sum_{i=1}^{n} \frac{P_i}{P} (F^{\circ}_{T,i} + RT \ln P_i)$$

The logarithm of the equilibrium constant for the reaction is given by

$$\ln K_j = \ln \prod_{i=1}^{n} (P_{ij})^{(\nu''_{ij} - \nu'_{ij})} = \sum_{i=1}^{n} (\nu''_{ij} - \nu'_{ij}) \ln P_{ij}$$

The change in free energy in a chemical reaction is given by

$$\Delta F_j = \sum_{i=1}^{n} (\nu''_{ij} - \nu'_{ij}) F_i$$

$$= \sum_{i=1}^{n} (\nu''_{ij} - \nu'_{ij})(F^{\circ}_{T,i} + RT \ln P_{ij})$$

$$= RT \ln K_j + \sum_{i=1}^{n} (\nu''_{ij} - \nu'_{ij}) F^{\circ}_{T,i}$$

Chemical equilibrium is readily defined as follows:

$$\Delta F_j = 0$$

$$\therefore K = \exp\left(-\frac{\Delta F^{\circ}_j}{RT}\right)$$

All enthalpies for the reference states of the elements are 0 at 77°F (298.15°K).

H_{fuel} is the molar enthalpy of the fuel at the inlet temperature. For a compound such as the fuel, or the CO_2 in the air, or an element not in the standard state, the molar enthalpy is:

$$\int_{536.67}^{T,\,^{\circ}R} C_p dT + H_{f_{536.67^{\circ}R}}$$

for example, air at 540°R

$$
\begin{aligned}
H = \; & 0.780881 \times 23.22 && = \; 18.132 \\
& +0.209495 \times 23 && = \; 4.902 \\
& +0.909324 \times 16.56 && = \; 0.154 \\
& +0.00030 \times -169263.7 && = \; \underline{-50.779} \\
& && \quad -27.590 \text{ Btu/lb mole}
\end{aligned}
$$

Heats of formation are not available for most mixed hydrocarbon fuels such as JP4. The energy content of this type of fuel is more commonly given as heat of combustion. The relation between these two properties may be derived as follows:

$$H_{reactants\,(T\ ref)} = H_{products\,(T\ products)}$$

$$= Q_{comb.\,(T\ ref)} + H_{products\,(T\ ref)}$$

The reaction for a CH_n fuel is

$$CH_n + (1 + \tfrac{n}{2})O_2 \rightarrow CO_2 + \tfrac{n}{2} H_2O$$

for a basis of 1 mole of fuel with a heat of combustion of $Q_{comb.} \times WTM_{fuel}$

$$H_{fuel\,(T\ fuel)} + CP_{fuel} \times (T_{ref} - T_{fuel}) + (1 - \tfrac{n}{2}) C_{P_{O_2}} (T - 77) = Q_{comb.(T_{ref})}$$
$$\times (12.011 + 1.008n) + H_{CO_2(T\ ref)} + \tfrac{n}{2} H_{H_2O(T\ ref)}$$

For example, a CH_2 hydrocarbon with a lower heating value of 18,000 Btu/lb at 70°F and a specific heat of 0.53 Btu would have an enthalpy at 20°F calculated as follows:

$$
\begin{aligned}
H_{fuel\,(T=20)} &= -0.5 \times 14.027(70-20) - \left(1 + \frac{2}{2}\right) \times 7.02(70-77) \\
&\quad + 18000 \times 14.027 - 169.335 - 104092 \\
&= -21410 \text{ Btu/lb mole}
\end{aligned}
$$

If this fuel is mixed with 540°R air at an equivalence ratio of 0.5, the enthalpy entered into the program is:

$$
\begin{aligned}
\overline{H} &= \frac{-27.59 + 0.5 \times -21410}{28.9666 + 0.5 \times 1.95905} \\
&= -358.4 \text{ Btu/lb}
\end{aligned}
$$

APPENDIX II
COMPUTER PROGRAM LISTINGS

NOMENCLATURE FOR MAIN PROGRAMS INPUTS

IT = 0

NPHI = Number of equivalence ratios

NP = Number of pressures

NH = Number of enthalpies

PHI = Equivalence ratio

P = Pressure, atm

H = Enthalpy, Btu/lb

IT = 1

same as IT = 0, except

NH = Number of temperatures

T = Temperature, °F

IT = 2 or 3

same as IT = 1, except

T = Stagnation temperature, °F

ITT = IT

MAIN PROGRAM FOR KNOWN ENTHALPY, IT = 0

```
C
      DIMENSION XX(14,50)
      DIMENSION PHI(10),P(10),H(10),X(10)
      READ (29,97) NPHI,NP,NH
      READ (29,96) (PHI(J),J=1,NPHI)
      READ (29,96) (P(J),J=1,NP)
      READ (29,96) (H(J),J=1,NH)
   99 FORMAT (     2F12.4,F10.1,F12.2,2F12.5,F11.3,2I6,F9.3)
   98 FORMAT (10E12.4)
   97 FORMAT (3I5)
   96 FORMAT (8E10.)
   95 FORMAT (8X,2HEQ,10X,1HP,9X,1HT,11X,1HH,11X,1HS,12X,2HCP,7X,3HMOL,
     *5X,2HNO,4X,4HTYPE,2X,4HTIME)
   94 FORMAT (8X,5HRATIO,6X,3HATM,6X,5HDEG R,7X,6HBTU/LB,5X,9HBTU/LB OR
     *,  4X,9HBTU/LB OR,4X,2HWT,5X,4HITER,3X,4HCASE,3X,3HSEC/)
   93 FORMAT (5X,2HEQ ,6X,1HP,7X,1HT,12X,25HSPECIES   MOL   FRACTIONS)
   92 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,1HH, 11X,1HO,11X,2HOH,
     *10X,2HNO,10X,2HCO/)
   91 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,2HH2,10X,2HO2,9X
     *,3HH2O,9X,
     *3HCO2,10X,2HN2,10X,1HA/)
   90 FORMAT (80H1 SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A
     * CH2 HYDROCARBON WITH AIR)
   89 FORMAT (F9.3,F7.2,F8.1,6E12.4)
   88 FORMAT (F9.3,F7.2,F8.1,5E12.4)
      C=.41959
      D=1.561762
      E=.009324
      KK=0
      WRITE (21,90)
      WRITE (21,95)
      WRITE (21,94)
      IT=0
      DO 1 J=1,NPHI
      A=.1396633*PHI(J)+.0003
      B=.279326*PHI(J)
      DO 2 JJ=1,NP
      DO 3 JJJ=1,NH
      T=4000.
      CALL PROP (A,B,C,D,E,T,P(JJ),H(JJJ),S,CP,WT,X,PAR,TIME,NT,IT)
      IF (NT.GE.50) GO TO 2
      WRITE (21,99) PHI(J), P(JJ),T,H(JJJ),S,CP,WT,NT,IT,TIME
      KK=KK+1
      RP=1./P(JJ)
      DO 4 K=4,13
    4 XX(K ,KK)=X(K-3)*RP
      XX(1 ,KK)=PHI(J)
      XX(2 ,KK)=P(JJ)
      XX(3 ,KK)=T
      XX(14,KK)=PAR*RP
    3 CONTINUE
    2 CONTINUE
    1 CONTINUE
      WRITE (21,90)
      WRITE (21,93)
      WRITE (21,92)
      WRITE (21,88) ((XX(J,K),J=1,8),K=1,KK)
      WRITE (21,90)
      WRITE (21,93)
      WRITE (21,91)
      WRITE (21,89) ((XX(J,K),J=1,3),(XX(J,K),J= 9,14),K=1,KK)
      STOP
      END
```

MAIN PROGRAM WHERE TEMPERATURE IS KNOWN, IT = 1

```
C
      DIMENSION XX(14,50)
      DIMENSION PHI(10),P(10),T(10),X(10)
      READ (29,97) NPHI,NP,NH
      READ (29,96) (PHI(J),J=1,NPHI)
      READ (29,96) (P(J),J=1,NP)
      READ (29,96) (T(J),J=1,NH)
   99 FORMAT (     2F12.4,F10.1,F12.2,2F12.5,F11.3,2I6,F9.3)
   98 FORMAT (10E12.4)
   97 FORMAT (3I5)
   96 FORMAT (8E10. )
   95 FORMAT (8X,2HEQ,10X,1HP,9X,1HT,11X,1HH,11X,1HS,12X,2HCP,7X,3HMOL,
     *5X,2HNO,4X,4HTYPE,2X,4HTIME)
   94 FORMAT (8X,5HRATIO,6X,3HATM,6X,5HDEG R,7X,6HBTU/LB,5X,9HBTU/LB OR
     *,  4X,9HBTU/LB OR,4X,2HWT,5X,4HITER,3X,4HCASE,3X,3HSEC/)
   93 FORMAT (5X,2HEQ ,6X,1HP,7X,1HT,12X,25HSPECIES   MOL   FRACTIONS)
   92 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,1HH, 11X,1HO,11X,2HOH,
     *10X,2HNO,10X,2HCO/)
   91 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,2HH2,10X,2HO2,9X
     *,3HH2O,9X,
     *3HCO2,10X,2HN2,10X,1HA/)
   90 FORMAT (83H1 SPECIFY TEMPERTUREY EQUIVALENCE RATIO AND PRESSURE FO
     *R A CH2 HYDROCARBON WITH AIR)
   89 FORMAT (F9.3,F7.2,F8.1,6E12.4)
   88 FORMAT (F9.3,F7.2,F8.1,5E12.4)
      C=.41959
      D=1.561762
      E=.009324
      KK=0
      WRITE (21,90)
      WRITE (21,95)
      WRITE (21,94)
      IT=1
      DO 1 J=1,NPHI
      A=.1396633*PHI(J)+.0003
      B=.279326*PHI(J)
      DO 2 JJ=1,NP
      DO 3 JJJ=1,NH
      CALL PROP (A,B,C,D,E,T(JJJ),P(JJ),H,S,CP,WT,X,PAR,TIME,NT,IT)
      IF (NT.GE.50) GO TO 2
      WRITE (21,99) PHI(J), P(JJ),T(JJJ),H,S,CP,WT,NT,IT,TIME
      KK=KK+1
      RP=1./P(JJ)
      DO 4 K=4,13
    4 XX(K ,KK)=X(K-3)*RP
      XX(1 ,KK)=PHI(J)
      XX(2 ,KK)=P(JJ)
      XX(3 ,KK)=T(JJJ)
      XX(14,KK)=PAR*RP
    3 CONTINUE
    2 CONTINUE
    1 CONTINUE
      WRITE (21,90)
      WRITE (21,93)
      WRITE (21,92)
      WRITE (21,88) ((XX(J,K),J=1,8),K=1,KK)
      WRITE (21,90)
      WRITE (21,93)
      WRITE (21,91)
      WRITE (21,89) ((XX(J,K),J=1,3),(XX(J,K),J= 9,14),K=1,KK)
      STOP
      END
```

MAIN PROGRAM FOR ISENTROPIC EXPANSIONS, IT = 2 OR 3

```
      DIMENSION XX(14,50)
      DIMENSION PHI(10),P(10),T(10),X(10)
  100 CONTINUE
      READ (29,97) NPHI,NP,NH,ITT
      IF  (NPHI.EQ.0) GO TO 101
      READ (29,96) (PHI(J),J=1,NPHI)
      READ (29,96) (P(J),J=1,NP)
      READ (29,96) (T(J),J=1,NH)
   99 FORMAT (     2F12.4,F10.1,F12.2,2F12.5,F11.3,2I6,F9.3)
   98 FORMAT (10E12.4)
   97 FORMAT (4I5)
   96 FORMAT (8E10.0)
   95 FORMAT (8X,2HEQ,10X,1HP,9X,1HT,11X,1HH,11X,1HS,12X,2HCP,7X,3HMOL,
     *5X,2HNO,4X,4HTYPE,2X,4HTIME)
   94 FORMAT (8X,5HRATIO,6X,3HATM,6X,5HDEG R,7X,6HBTU/LB,5X,9HBTU/LB OR
     *,  4X,9HBTU/LB OR,4X,2HWT,5X,4HITER,3X,4HCASE,3X,3HSEC/)
   93 FORMAT (5X,2HEQ ,6X,1HP,7X,1HT,12X,25HSPECIES   MOL   FRACTIONS)
   92 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,1HH, 11X,1HO,11X,2HOH,
     *10X,2HNO,10X,2HCO/)
   91 FORMAT (4X,5HRATIO,3X,3HATM,4X,5HDEG R,7X,2HH2,10X,2HO2,9X
     *,3HH2O,9X,
     *3HCO2,10X,2HN2,10X,1HA/)
   90 FORMAT (83H1 SPECIFY TEMPERTURE  EQUIVALENCE RATIO AND PRESSURE FO
     *R A CH2 HYDROCARBON WITH AIR)
   89 FORMAT (F9.3,F7.2,F8.1,6E12.4)
   88 FORMAT (F9.3,F7.2,F8.1,5E12.4)
   85 FORMAT (45H0    FROZEN ISENTROPIC EXPANSION FROM 10 ATM.)
   86 FORMAT (1H0)
   87 FORMAT (45H0EQULIBRIUM ISENTROPIC EXPANSION FROM 10 ATM.)
      C=.41959
      D=1.561762
      E=.009324
      KK=0
      WRITE (21,90)
      IF (ITT.EQ.2) WRITE (21,87)
      IF (ITT.EQ.3) WRITE (21,85)
      WRITE (21,95)
      WRITE (21,94)
      DO 1 J=1,NPHI
      A=.1396633*PHI(J)+.0003
      B=.279326*PHI(J)
      DO 2 JJJ=1,NH
      TX=T(JJJ)
      IT=1
      DO 3 JJ=1,NP
      IF (JJ-2) 10,12,12
   12 IT=ITT
      TX    = TX    *(P(JJ)/P(JJ-1))**(1.987/(CP*WT))
   10 CALL PROP (A,B,C,D,E,TX     ,P(JJ),H,S,CP,WT,X,PAR,TIME,NT,IT)
      IF (NT.GE.50) GO TO 2
      WRITE (21,99) PHI(J), P(JJ),TX     ,H,S,CP,WT,NT,IT,TIME
      KK=KK+1
      RP=1./P(JJ)
```

ISENTROPIC EXPANSIONS, IT = 2 OR 3 (Concluded)

```
      DO 4 K=4,13
    4 XX(K ,KK)=X(K-3)*RP
      XX(1 ,KK)=PHI(J)
      XX(2 ,KK)=P(JJ)
      XX(3 ,KK)=TX
      XX(14,KK)=PAR*RP
    3 CONTINUE
    2 CONTINUE
    1 CONTINUE
      WRITE (21,90)
      IF (ITT.EQ.2) WRITE (21,87)
      IF (ITT.EQ.3) WRITE (21,85)
      WRITE (21,93)
      WRITE (21,92)
      WRITE (21,88) ((XX(J,K),J=1,8),K=1,KK)
      WRITE (21,90)
      IF (ITT.EQ.3) WRITE (21,85)
      IF (ITT.EQ.2) WRITE (21,87)
      WRITE (21,93)
      WRITE (21,91)
      WRITE (21,89) ((XX(J,K),J=1,3),(XX(J,K),J= 9,14),K=1,KK)
      GO TO 100
  101 CONTINUE
      STOP
      END
```

SUBROUTINE PROP

```
      SUBROUTINE PROP(CAR,HYD,OX,AN2,AR,TT,PR,H,S,CP,WTM,P,PAR,
     *TIME,NT,IT)
C     SPECIES ARE 1-H,2-O,3-OH,4-NO,5-CO,6-H2,7-O2,8-H2O,9-CO2,10-N2
C     SUBROUTINE FOR DETERMINING EQUILIBRIUM PARTIAL PRESSURES
C     T IS TEMP. IN DEG R AND CAN BE EITHER INPUT OR OUTPUT
C     P IS PRESS IN ATMOSPHERES AND IS AN INPUT
C     H IS THE ENTHALPY IN BTU PER LBM AND IS EITHER AN INPUT OR OUTPUT
C     S IS THE ENTROPY IN BTU PER LBM-DEG R AND EITHER INPUT OR OUTPUT
C     CP IS THE SPECIFIC HEAT IN BTU PER LBM-DEG R AND IS AN OUTPUT
C     WTM IS THE MOLECULAR WT OF THE MIXTURE AN IS AND OUTPUT
C     TIME IS THE PROGRAM EXECUTION TIME IN SECONDS AND IS AN OUTPUT
C     NT IS THE NO. OF ITERATIONS TO FIND PARTIAL PRESS AND IS AN OUTPUT
C     IT IS A CONTROL CONSTANT FOR THE SUBROUTINE
C     IT=0  H AND P ARE KNOWN AND T,CP & WTM ARE FOUND
C     IT=1  T & P ARE KNOWN AND ARRAY OF PARTIAL PRESSURES ARE FOUND
C     IT=2  S & P ARE KNOWN AND T,CP, & WTM ARE FOUND
C     IT=3  T & P & PARTIAL PRESSURES ARE KNOWN - FROZEN CASE
C     IT=1 HAS BEEN MODIFIED TO ALSO CALCULATE H,S,CP,WTM
      DIMENSION     D1(3),D2(3),D4(3),D5(3),D6(3),D7(3),D8(3),D9(3),D10
     *(3),D3(3),E(6)
      DIMENSION DAR(3)
      DIMENSION  F(10),A1(3),A2(3),A3(3),P(10)
C     CHANGE UNITS OF INPUTS TO BE COMPATABLE WITH PROGRAM
      T = (5./9.)*TT
      H0= (5./9.)*H/.99931
      IF (IT.GE.2)  H0=S/.999331
C
      ICT=0
      DELTL=0.
      CALL TIMER (TT1)
      IF (IT - 3) 3,2,3
    3 CONTINUE
      DELL=.000001
      FUEL=2.*CAR+.5*HYD
C     RATIO OF ELEMENTS
      RAN = AR/AN2
      RCN= CAR/AN2
      RHN=HYD/AN2
      RON=OX/AN2
C
      DEL1=0.
      DEL2=0.
      DEL3=0.
      IF(OX.GT.FUEL) GO TO 1
      IF (CAR.LE.OX) GO TO 20
      WRITE(21,97)
      RETURN
   20 XX=1./(CAR+.5*(HYD+AN2))
C     INITIAL GUESS OF H2 H2O AND N2 PARTIAL PRESSURES
      P(6)=PR*XX*(.5*HYD-OX+1.5*CAR)
      P(8)=PR*XX*(       +OX-1.5*CAR)
      P(10)=PR*XX*AN2*.5
      L= 6
      GO TO 71
    1 CONTINUE
```

SUBROUTINE PROP (Continued)

```
C       INITIAL GUESS OF O2,H2O,N2 PARTIAL PRESSURES
        XX =.5/((.5*HYD+OX+AN2)+.5+AR)
        P(7)=PR*XX*(OX-FUEL)
        P(8)=HYD*XX*PR
        P(10)=   AN2*XX*PR
        L= 7
        GO TO 71
C
C       RESET PARTIAL PARTIAL PRESSURES FOR FROZEN CASE--IT=3
      2 CONTINUE
        PX=PR/PHOLD
        DO 72 J=1,10
     72 P(J)=P(J)*PX
        PAR=PAR*PX
C
C       ITERATION LOOP TO FIND PARTIAL PRESSURES
     71 CONTINUE
        IF (P(L).LE.(1) P(L)=.01
        DO 4  K=1,50
        KOUNT=K
C       SKIP PARTIAL PRESSURE CALCULATION FOR FROZEN CASE
        IF (IT - 3) 8,7,8
      8 CONTINUE
C       CHECK ALL INITIAL PARTIAL PRESSURES FOR NEGATIVE VALUES
        DO 41 J=1,10
     41 IF (P(J).LT.0.) P(J)=1.E-5
C       DON'T RECALCULATE FREE ENERGY RELATION FOR T KNOWN--IT=1
        IF (L.EQ.6) GO TO 42
        IF (K.GE.2.AND.IT.EQ.1) GO TO 10
        CALL THERM ( P,T,H,CP,F,PR,PAR,WTM,1)
        E(1) = 2.7182818285**(.5*F(8)-.25*F(7)-F(1))
        E(2) = 2.7182818285**(.5* F(7)-F(2))
        E(3) = 2.7182818285**(.5 *F(8)+.25*F(7)-F(3))
        E(4) = 2.7182818285**(.5*F(10)+.5*F(7)-F(4))
        E(5) = 2.7182818285**(F(9)-.5*F(7)-F(5))
        E(6) = 2.7182818285**(F(8)-.5*F(7)-F(6))
C       CALCULATE PARTIAL PRESSURES OF THE ASSUMED KNOWN SPECIES
     10 P(1)= SQRT(P(8)/SQRT(P(7)))*E(1)
        P(2)= SQRT(P(7))*E(2)
        P(3)=SQRT(P(8)*SQRT(P(7)))*E(3)
        P(4)=SQRT(P(10)*P(7))*E(4)
        XX=1./(1.+E(5)/SQRT(P(7)))
        P(9)= RCN*(2.*P(10)+P(4))*XX
        P(5)= P(9)/SQRT(P(7))*E(5)
        P(6)= P(8)/SQRT(P(7))*E(6)
        PAR = (2. * P(10) + P(4))*RAN
C
        GO TO 43
     42 CONTINUE
        IF (K.GE.2.AND.IT.EQ.1) GO TO 46
        CALL THERM ( P,T,H,CP,F,PR,PAR,WTM,1)
        E(1)= EXP(.5*F(6)-F(1))
        E(2)= EXP(F(8)-F(6)-F(2))
        E(3)=EXP(F(8)-F(1)-F(3))
        E(4)= EXP(F(8)+.5*F(10)-F(6)-F(4))
```

SUBROUTINE PROP (Continued)

```
      E(5)=EXP(F(6)+F(9)-F(5)-F(8))
      E(6)= EXP(2.*F(8)-2.*F(6)-F(7))
   46 P(1)=E(1)*SQRT(P(6))
      P(2)=E(2)*P(8)/P(6)
      P(3)=E(3)*P(8)/P(1)
      P(4)=E(4)*P(8)*SQRT(P(10))/P(6)
      P(7)=E(6)*P(8)*P(8)/(P(6)*P(6))
      YY=E(5)*P(6)/P(8)
      XX=1./(1.+YY)
      P(9)=RCN*(2.*P(10)+P(4))*XX
      P(5)=P(9)*YY
      PAR = (2. * P(10) + P(4))*RAN
   43 CONTINUE
C     DERIVATION OF RELATIONSHIP OF KNOWN SPECIES WITH RESPECT TO GUESS
      DO 11 I=1,3
      D1(I)=0.
      D2(I)=0.
      D3(I)=0.
      D4(I)=0.
      D5(I)=0.
      D6(I)=0.
      D7(I)=0.
      D8(I)=0.
      D9(I)=0.
   11 D10(I)=0.
      IF (L.EQ.6) GO TO 44
      D1(1)= -P(1)/P(7)*.25
      D1(2)=  P(1)/P(8)*.5
      D2(1)=  P(2)/P(7)*.5
      D3(1)=  P(3)/P(7)*.25
      D3(2)=  P(3)/P(8)*.5
      D4(1)=  P(4)/P(7)*.5
      D4(3)=P(4)/P(10)*.5
      IF (CAR.EQ.0.0) GO TO 441
      D9(1)= RCN*(D4(1)+(2.*P(10)+P(4))*XX*.5*E(5)/ P(7)**1.5)*XX
      D9(3)=  RCN*XX*(2.+D4(3))
      D5(1)=  P(5)/P(9)*D9(1)-P(5)/P(7)*.5
      D5(3)=  P(5)/P(9)*D9(3)
  441 CONTINUE
      D6(1)= -P(6)/P(7)*.5
      D6(2)=  P(6)/P(8)
      D7(1)=1.0
      D8(2)=1.0
      D10(3)=1.0
      DAR(1)=RAN*D4(1)
      DAR(2)=0.
      DAR(3)=RAN*(D4(3)+2.)
      GO TO 45
   44 CONTINUE
      D1(1)=P(1)/P(6)*.5
      D2(1)=-P(2)/P(6)
      D2(2)= P(2)/P(8)
      D3(1)=-P(3)/P(1)*D1(1)
      D3(2)= P(3)/P(8)
      D4(1)=-P(4)/P(6)
```

SUBROUTINE PROP (Continued)

```
      D4(2)= P(4)/P(8)
      D4(3)= P(4)/P(10)*.5
      D7(1)=-2.*P(7)/P(6)
      D7(2)= P(7)/P(8)*2.
      IF (CAR.EQ.0.0) GO TO 442
      D9(2)=XX*(RCN*D4(2)+ E(5)*P(6)*P(9)/(P(8)*P(8)))
      D9(1)=XX*(RCN*D4(1)-P(9)*E(5)/P(8))
      D9(3)=RCN*XX*(2.+D4(3))
      D5(1)=YY*D9(1)+P(5)/P(6)
      D5(2)=YY*D9(2)-P(5)/P(8)
      D5(3)=YY*D9(3)
  442 CONTINUE
      D6(1)=1.
      D8(2)=1.
      D10(3)=1.
      DAR(1)=RAN*D4(1)
      DAR(2)=RAN*D4(2)
      DAR(3)=RAN*(2.+D4(3))
   45 CONTINUE
C
C     DERIVATION OF MATRIX COEFFICIENTS
      DO12 I=1,3
      A1(I)=  D1(I)+D3(I)+2.*D6(I)+2.*D8(I)-RHN*(2.*D10(I)+D4(I))
      A2(I)=  D2(I)+D3(I)+D4(I)+D5(I)+2.*D7(I)+D8(I)+2.*D9(I)-RON*(2.
     **D10(I)+D4(I))
      A3(I)= D1(I)+D2(I)+D3(I)+D4(I)+D5(I)+D6(I)+D7(I)+D8(I)+D9(I)+D10(
     *I)+DAR(I)
   12 CONTINUE
      SP1  = P(1)+P(3)+2.*P(6)+2.*P(8)-RHN*(2.*P(10)+P(4))
      SP2  = P(2)+P(3)+P(4)+P(5)+2.*P(7)+P(8)+2.*P(9)-RON*(2.*P(10)+P(4
     *))
      SP3  =0.
      DO 13 I=1,10
   13 SP3  =SP3  +P(I)
      SP3=SP3-PR+PAR
C
C     SOLUTION OF MATRIX
      DEN=  A1(1)*(A2(2)*A3(3)-A3(2)*A2(3))-A2(1)*(A1(2)*A3(3)-A3(2)*
     *A1(3))+A3(1)*(A1(2)*A2(3)-A2(2)*A1(3))
      DEN=1./DEN
      XN1 =SP1*(A3(2)*A2(3)-A2(2)*A3(3))+SP2*(A1(2)*A3(3)-A1(3)*A3(2))+
     *SP3*(A1(3)*A2(2)-A1(2)*A2(3))
      XN2 =SP1*(A2(1)*A3(3)-A3(1)*A2(3))+SP2*(A3(1)*A1(3)-A1(1)*A3(3))+
     *SP3*(A1(1)*A2(3)-A2(1)*A1(3))
      XN3 =SP1*(A3(1)*A2(2)-A2(1)*A3(2))+SP2*(A1(1)*A3(2)-A3(1)*A1(2))+
     *SP3*(A2(1)*A1(2)-A1(1)*A2(2))
C
C     CALCULATION OF PARTIAL PRESS CORRECTION AND NEW GUESSED PART PRESS
      DEL1= XN1 *DEN
      DEL2= XN2 *DEN
      DEL3=XN3*DEN
      P(L)=P(L)+DEL1
      P(8)=P(8)+DEL2
      P(10)=P(10)+DEL3
C
```

SUBROUTINE PROP (Concluded)

```
C       FIND ENTHALPY OR ENTROPY FOR ITERATION TO FIND TEMP.
      7 CONTINUE
        IF(IT-1)18,6 ,17
     17 CALL THERM(P,T,H,CP,F,PR,PAR,WTM,2)
        GO TO 80
     18 CALL THERM (P,T,H,CP,F,PR,PAR,WTM,0)
     80 CONTINUE
        IF (ICT.GT.0) GO TO 85
        DELT=(H0-H)/CP
        IF (DELT*DELTL) 81,81,82
     82 T=T+DELT*.83
        GO TO 85
     81 T=T+DELT*.38
        ICT=2
     85 ICT=ICT-1
        DELTL=DELT
        IF (T.LE.300.) T=300.
        IF (T.GE.5000.) T=5000.
C
C       ITERATION CONTROL--TEMP.WITHIN 1 DEG OR PRESS WITHIN DELL
        IF(ABS(H0-H) - CP)6,6,4
      6 IF(IT-2) 21,21,5
     21 IF(ABS(DEL1) - DELL) 22,22,4
     22 IF (ABS(DEL2) - DELL) 23,23,4
     23 IF(ABS(DEL3) - DELL) 5,5,4
      4 CONTINUE
      5 CONTINUE
        PHOLD=PR
        S=H
C
        CALL THERM(P,T,H,CP,F,PR,PAR,WTM,2)
        S=H*.999331
C       CALCULATE ENTHALPY AND ENTROPY ETC. FOR TEMP KNOWN--IT=1
        CALL THERM(P,T,H,CP,F,PR,PAR,WTM,0)
        H=H*.999331*9./5.
        CP=CP*.999331
        WTM=WTM
        TT=T*1.8
        NT=KOUNT
        CALL TIMER (TT2)
        TIME = TT2-TT1
        RETURN
     99 FORMAT (  41H ITERATION DID NOT CONVERGE IN 50 STEPS  )
     97 FORMAT(36H THIS CASE HAS TOO LITTLE O2 TO RUN )
        END
```

SUBROUTINE THERM

```
      SUBROUTINE THERM (ALP,T,H,CP,F,PR,PAR,WTM,KT)
      DIMENSION   ALP(10),CC(6),CT(140),TT(5),F(10)
      DATA CT              /   2.5,4*0.,2.5470497E4,-4.6001096E-1,
     *2.5,4*0.,2.5470497E4,-4.6001096E-1,3.0218894,-2.1737249E-3,
     *3.7542203E-6,-2.9947200E-9,9.0777547E-13,2.9137190E4,2.6460076E0,
     *2.5372567E0,-1.8422190E-5,-8.8017921E-9,5.9643621E-12,
     *-5.5743608E-16,2.9230007E4,4.9467942E0,3.8234708E0,-1.1187229E-3,
     *1.2466819E-6,-2.1035896E-10,-5.2546551E-14,3.5852787E3,
     *5.8253029E-1,2.8895544E0,9.9835061E-4,-2.1879904E-7,1.9802785E-11,
     *-3.8452940E-16,3.8811792E3,5.5597016E0,4.1469476E0,-4.1197237E-3,
     *9.6922467E-6,-7.8633639E-9,2.2309512E-12,9.7447894E3,2.5694290E0,
     *3.1529360E0,1.4059955E-3,-5.7078462E-7,1.0628209E-10,
     *-7.3720783E-15,9.8522048E3,6.9446465E0,3.7871332E0,-2.1709526E-3,
     *5.0757337E-6,-3.4737726E-9,7.7216841E-13,-1.4363508E4,2.6335459E0,
     *2.9511519E0,1.5525567E-3,-6.1911411E-7,1.1350336E-10,
     *-7.7882732E-15,-1.4231827E4,6.5314450E0,2.8460849E0,4.1932116E-3,
     *-9.6119332E-6,9.5122662E-9,-3.3093421E-12,-9.6725372E2,
     *-1.4117850E0,3.0436897E0,6.1187110E-4,-7.3993551E-9,-2.0331907E-11
     *,2.4593791E-15,-8.5491002E2,-1.6481339E0,3.7189946E0,
     *-2.5167288E-3,8.5837353E-6,-8.2998716E-9,2.7082180E-12,
     *-1.0576706E3,3.9080704E0,3,5976129E0,7.8145603E-4,-2.2386670E-7,
     *4.2490159E-11,-3.3460204E-15,-1.1927918E3,3.7492659E0,
     *4.1565016E0,-1.7244334E-3,5.6982316E-6,-4.5930044E-9,1.4233654E-12
     *,-3.0288770E4,-6.8616246E-1,2.6707532E0,3.0317115E-3,
     *-8.5351570E-7,1.1790853E-10,-6.1973568E-15,-2.9888994E4,
     *6.8838391E0,2.1701000E0,1.0378115E-2,-1.0733938E-5,6.3459175E-9,
     *-1.6280701E-12,-4.8352602E4,1.0664388E1,4.4129266E0,3.1922896E-3,
     *-1.2978230E-6,2.4147446E-10,-1.6742986E-14,-4.8944043E4,
     *-7.2875769E-1,3.6916148E0,-1.3332552E-3,2.6503100E-6,
     *-9.7688341E-10,-9.9772234E-14,-1.0628336E3,2.2874980E0,2.8545761
     *,1.5976316E-3,-6.2566254E-7,1.1315849E-10,-7.6897070E-15,
     *-8.9017445E2,6.3902879E0/
      TTLN = ALOG(T)
      TLN = 1.-TTLN
      CP=0.
      H=0.
      RT=1.98718*T
      TT(1)=T
      DO 1      K=2,4
    1 TT(K)= TT(K-1)*T
      TT(5)=1./T
      KA=7
      IF(T.LE.1000.)  KA=0
      DO 2 K=1,10
      KK= 14*(K-1)+KA
      DO 3 J=2,6
      KKK=(KK+J)
    3 CC(J)= CT(KKK )*TT(J-1)
      CC(1)= CT(KK+1)
      IF(KT-1) 10,4,5
   10 F(K)=          CC(1)+.5*CC(2)+CC(3)/3.+.25*CC(4)+.2*CC(5)+CC(6)
      GO TO 6
    4 F(K)=(CC(1)*TLN )-.5*CC(2)-(CC(3)+.5*CC(4))/6.-.05*CC(5)+CC(6)-
     *CT(KK+7)
      GO TO 2
```

SUBROUTINE THERM (Concluded)

```
    5 IF (ALP(K).LE.0.)  GO TO 2
      F(K) = CC(1)*TTLN+CC(2)+.5*CC(3)+CC(4)/3.0 +
     *.25*CC(5) + CT(KK+7) - ALOG(ALP(K))
    6 H = H + ALP(K)*F(K)
      CPP  =        ALP(K)*(CC(1)+CC(2)+CC(3)+CC(4)+CC(5))
      CP = CP + CPP
    2 CONTINUE
      PARL=0.
      IF (PAR.GT.0.)  PARL=ALOG(PAR)
      WTM = ALP(1)*1.00797 +ALP(2)*15.9994+ALP(3)*17.0074+ALP(4)*30.0061
     1+ALP(5)*28.01055+ALP(6)*2.01594+ALP(7)*31.9988+ALP(8)*18.01534
     2+ALP(9)*44.00995+ALP(10)*28.0134+PAR*39.948
      CP=(CP+PAR*2.5)*(1.98718/WTM)
      IF(KT-1) 7,8,9
    7 H=(PAR*(2.5-(745.375/T))+H)*(RT/WTM)
      WTM=WTM/PR
      GO TO 8
    9 S= (H + PAR*(2.5*TTLN +4.3661076 -PARL       ))*(1.98718/WTM)
      DSDT =CP/T
      H=S
      CP=DSDT
      WTM=WTM/PR
    8 RETURN
      END
```

APPENDIX III
COMPUTER PROGRAM CALCULATIONS

TABLE I

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	H BTU/LB	S BTU/LB OR	CP BTU/LB OR	MOL WT	NO ITER	TYPE CASE	TIME SEC
.5000	.1	2802.4	.01	2.26695	.30941	28.932	7	0	1.452
.5000	.1	3407.5	199.64	2.33133	.31765	28.913	6	0	1.264
.5000	.1	3913.0	400.21	2.38604	.32249	28.798	8	0	1.641
.5000	.1	4274.7	600.06	2.43476	.32498	28.527	12	0	2.390
.5000	.1	4538.7	800.03	2.48009	.32637	28.145	8	0	1.640
.5000	1.0	2803.1	.01	2.10890	.30942	28.933	8	0	1.639
.5000	1.0	3418.0	199.64	2.17322	.31777	28.924	7	0	1.452
.5000	1.0	3973.8	400.13	2.22746	.32305	28.871	5	0	1.077
.5000	1.0	4423.9	600.10	2.27502	.32607	28.709	12	0	2.390
.5000	1.0	4770.3	800.03	2.31847	.32775	28.431	15	0	2.952
.5000	10.0	2803.5	.02	1.95087	.30942	28.933	9	0	1.827
.5000	10.0	3422.6	199.65	2.01515	.31783	28.929	9	0	1.828
.5000	10.0	4003.6	400.16	2.06920	.32333	28.905	3	0	.702
.5000	10.0	4518.9	600.09	2.11610	.32677	28.825	9	0	1.827
.5000	10.0	4950.4	800.10	2.15831	.32883	28.653	12	0	2.389
.9000	.1	3927.9	-.11	2.41762	.33835	28.637	11	0	2.203
.9000	.1	4214.9	199.63	2.46661	.34028	28.292	9	0	1.828
.9000	.1	4438.6	400.36	2.51297	.34140	27.877	8	0	1.640
.9000	.1	4624.2	600.27	2.55707	.34221	27.428	11	0	2.202
.9000	.1	4785.0	800.31	2.59958	.34290	26.959	19	0	3.702
.9000	1.0	4034.3	-.02	2.25834	.33952	28.765	6	0	1.266
.9000	1.0	4396.5	199.69	2.30565	.34192	28.512	12	0	2.390
.9000	1.0	4682.1	400.40	2.34983	.34323	28.172	12	0	2.390
.9000	1.0	4920.4	600.25	2.39144	.34407	27.786	8	0	1.639
.9000	1.0	5128.1	800.40	2.43127	.34469	27.371	12	0	2.388
.9000	10.0	4100.4	.00	2.09963	.34024	28.844	7	0	1.454
.9000	10.0	4540.7	199.72	2.14580	.34320	28.687	12	0	2.392
.9000	10.0	4897.5	400.38	2.18829	.34484	28.434	15	0	2.954
.9000	10.0	5196.6	600.24	2.22787	.34582	28.121	15	0	2.952
.9000	10.0	5460.1	800.44	2.26544	.34648	27.772	12	0	2.389
1.0000	.1	4035.6	.02	2.44752	.34274	28.385	10	0	2.015
1.0000	.1	4286.0	199.68	2.49546	.34425	28.006	10	0	2.014
1.0000	.1	4490.6	400.57	2.54122	.34525	27.576	11	0	2.202
1.0000	.1	4664.1	600.11	2.58479	.34601	27.124	17	0	3.327
1.0000	.1	4816.5	800.21	2.62700	.34670	26.655	25	0	4.826
1.0000	1.0	4181.8	-.02	2.28693	.34427	28.560	9	0	1.828
1.0000	1.0	4494.2	199.63	2.33292	.34606	28.296	9	0	1.827
1.0000	1.0	4753.3	400.58	2.37636	.34715	27.892	11	0	2.203
1.0000	1.0	4975.0	600.08	2.41736	.34790	27.496	10	0	2.013
1.0000	1.0	5172.1	800.38	2.45683	.34851	27.077	12	0	2.388
1.0000	10.0	4294.6	-.03	2.12721	.34542	28.693	9	0	1.827
1.0000	10.0	4672.9	199.54	2.17169	.34759	28.470	9	0	1.827
1.0000	10.0	4993.2	400.61	2.21328	.34888	28.179	12	0	2.391
1.0000	10.0	5271.3	600.04	2.25213	.34972	27.851	9	0	1.827
1.0000	10.0	5521.1	800.40	2.28925	.35034	27.493	11	0	2.202

TABLE I (Continued)

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	H BTU/LB	S BTU/LB OR	CP BTU/LB OR	MOL WT	NO ITER	TYPE CASE	TIME SEC
1.1000	.1	4073.1	.37	2.47555	.34626	28.058	20	0	3.425
1.1000	.1	4323.5	200.11	2.52307	.34785	27.688	21	0	3.586
1.1000	.1	4522.7	400.08	2.56824	.34887	27.285	21	0	3.587
1.1000	.1	4691.3	600.21	2.61166	.34968	26.815	23	0	3.915
1.1000	.1	4838.7	799.78	2.65354	.35039	26.352	29	0	4.900
1.1000	1.0	4206.4	.41	2.31307	.34759	28.214	12	0	2.113
1.1000	1.0	4536.4	200.05	2.35867	.34963	27.940	21	0	3.589
1.1000	1.0	4793.6	400.05	2.40152	.35077	27.587	21	0	3.587
1.1000	1.0	5011.5	600.19	2.44234	.35156	27.194	13	0	2.274
1.1000	1.0	5202.9	799.89	2.48143	.35220	26.779	12	0	2.110
1.1000	10.0	4283.0	.37	2.15128	.34834	28.302	10	0	1.784
1.1000	10.0	4707.7	199.95	2.19561	.35104	28.141	15	0	2.604
1.1000	10.0	5037.3	400.00	2.23664	.35248	27.874	21	0	3.589
1.1000	10.0	5315.5	600.13	2.27529	.35338	27.552	14	0	2.437
1.1000	10.0	5560.4	800.00	2.31203	.35403	27.199	17	0	2.929
1.5000	.1	3737.7	.38	2.57079	.35452	26.343	7	0	1.293
1.5000	.1	4178.9	199.88	2.62111	.35899	26.213	11	0	1.950
1.5000	.1	4482.5	399.96	2.66722	.36154	25.938	15	0	2.606
1.5000	.1	4691.3	600.31	2.71085	.36309	25.568	12	0	2.112
1.5000	.1	4852.3	800.32	2.75274	.36423	25.157	20	0	3.423
1.5000	1.0	3756.6	.38	2.39730	.35468	26.366	9	0	1.622
1.5000	1.0	4264.7	199.79	2.44702	.35959	26.313	7	0	1.291
1.5000	1.0	4677.2	400.01	2.49173	.36274	26.159	12	0	2.113
1.5000	1.0	4979.3	600.36	2.53317	.36463	25.891	18	0	3.098
1.5000	1.0	5207.8	800.34	2.57240	.36588	25.551	10	0	1.782
1.5000	10.0	3763.1	.38	2.22390	.35473	26.373	11	0	1.954
1.5000	10.0	4301.1	199.80	2.27340	.35984	26.355	11	0	1.952
1.5000	10.0	4793.4	400.02	2.31742	.36342	26.290	8	0	1.456
1.5000	10.0	5202.9	600.40	2.35747	.36580	26.141	12	0	2.113
1.5000	10.0	5525.9	800.39	2.39472	.36735	25.904	18	0	3.097
2.0000	.1	3173.9	.39	2.66156	.36186	24.369	9	0	1.623
2.0000	.1	3687.5	199.81	2.71973	.36887	24.340	7	0	1.293
2.0000	.1	4124.7	399.91	2.77090	.37373	24.233	10	0	1.785
2.0000	.1	4456.2	600.49	2.81758	.37699	24.019	12	0	2.112
2.0000	.1	4699.3	800.43	2.86120	.37925	23.726	11	0	1.947
2.0000	1.0	3176.2	.39	2.47394	.36189	24.371	11	0	1.953
2.0000	1.0	3707.1	199.81	2.53196	.36904	24.361	9	0	1.623
2.0000	1.0	4201.7	399.91	2.58257	.37423	24.317	8	0	1.457
2.0000	1.0	4626.0	600.45	2.62797	.37790	24.202	9	0	1.619
2.0000	1.0	4962.7	800.56	2.66966	.38047	24.003	12	0	2.112
2.0000	10.0	3176.9	.39	2.28632	.36190	24.372	12	0	2.120
2.0000	10.0	3714.0	199.81	2.34430	.36910	24.369	10	0	1.790
2.0000	10.0	4234.6	399.92	2.39470	.37444	24.353	10	0	1.788
2.0000	10.0	4720.7	600.46	2.43949	.37839	24.305	9	0	1.622
2.0000	10.0	5149.3	800.59	2.48002	.38130	24.202	8	0	1.456

TABLE I (Continued)

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H	O	OH	NO	CO
.500	.10	2802.4	.1743-08	.8520-05	.1578-03	.1162-02	.7481-05
.500	.10	3407.5	.2148-04	.2777-03	.1451-02	.3984-02	.3460-03
.500	.10	3913.0	.3824-03	.2228-02	.5341-02	.8236-02	.3265-02
.500	.10	4274.7	.1933-02	.7304-02	.1087-01	.1236-01	.1058-01
.500	.10	4538.7	.5174-02	.1532-01	.1633-01	.1581-01	.1978-01
.500	1.00	2803.1	.3116-07	.2705-05	.8900-04	.1163-02	.2376-05
.500	1.00	3418.0	.4101-05	.9233-04	.8446-03	.4057-02	.1159-03
.500	1.00	3973.8	.9293-04	.8740-03	.3488-02	.8894-02	.1349-02
.500	1.00	4423.9	.6481-03	.3555-02	.8259-02	.1438-01	.5874-02
.500	1.00	4770.3	.2192-02	.8695-02	.1390-01	.1941-01	.1363-01
.500	10.00	2803.5	.5559-08	.8574-06	.5013-04	.1184-02	.7531-08
.500	10.00	3422.6	.7529-08	.2986-04	.4825-03	.4091-02	.3757-04
.500	10.00	4003.8	.1922-04	.3067-03	.2111-02	.9234-02	.4840-03
.500	10.00	4518.9	.1691-03	.1456-02	.5579-02	.1575-01	.2612-02
.500	10.00	4950.4	.7309-03	.4173-02	.1054-01	.2242-01	.7691-02
.900	.10	3927.9	.7816-03	.1146-02	.5115-02	.4035-02	.1169-01
.900	.10	4214.9	.2703-02	.3315-02	.9582-02	.6238-02	.2547-01
.900	.10	4438.6	.6217-02	.6997-02	.1450-01	.8495-02	.3960-01
.900	.10	4624.2	.1144-01	.1221-01	.1936-01	.1062-01	.5196-01
.900	.10	4785.0	.1841-01	.1890-01	.2377-01	.1254-01	.6205-01
.900	1.00	4034.3	.2444-03	.4946-03	.3578-02	.4328-82	.6260-02
.900	1.00	4396.5	.1092-02	.1665-02	.7455-02	.6983-02	.1735-01
.900	1.00	4882.1	.2924-02	.3914-02	.1222-01	.9916-02	.3086-01
.900	1.00	4920.4	.5978-02	.7412-02	.1735-01	.1286-01	.4400-01
.900	1.00	5128.1	.1046-01	.1226-01	.2245-01	.1567-01	.5559-01
.900	10.00	4100.4	.6056-04	.1861-03	.2277-02	.4478-02	.2711-02
.900	10.00	4540.7	.3577-03	.7208-03	.5258-02	.7405-02	.9922-02
.900	10.00	4897.5	.1152-02	.1889-02	.9340-02	.1085-01	.2114-01
.900	10.00	5198.6	.2859-02	.3897-02	.1414-01	.1456-01	.3375-01
.900	10.00	5480.1	.5088-02	.6911-02	.1933-01	.1832-01	.4604-01
1.000	.10	4035.8	.1613-02	.1187-02	.5657-02	.3251-02	.2436-01
1.000	.10	4286.0	.4214-02	.3299-02	.1012-01	.5345-02	.3906-01
1.000	.10	4490.6	.8497-02	.6828-02	.1501-01	.7486-02	.5281-01
1.000	.10	4864.1	.1450-01	.1174-01	.1976-01	.9488-02	.6435-01
1.000	.10	4816.5	.2225-01	.1801-01	.2404-01	.1130-01	.7362-01
1.000	1.00	4181.8	.8269-03	.4909-03	.3944-02	.3133-02	.1714-01
1.000	1.00	4494.2	.1903-02	.1619-02	.7879-02	.5662-02	.3053-01
1.000	1.00	4753.3	.4282-02	.3780-02	.1268-01	.8476-02	.4448-01
1.000	1.00	4975.0	.7959-02	.7102-02	.1778-01	.1127-01	.5718-01
1.000	1.00	5172.1	.1313-01	.1187-01	.2281-01	.1393-01	.6803-01
1.000	10.00	4294.8	.2088-03	.1685-03	.2450-02	.2721-02	.1093-01
1.000	10.00	4872.9	.7366-03	.6629-03	.5476-02	.5427-02	.2176-01
1.000	10.00	4993.2	.1861-02	.1769-02	.9631-02	.8762-02	.3456-01
1.000	10.00	5271.3	.3769-02	.3659-02	.1444-01	.1231-01	.4735-01
1.000	10.00	5521.1	.6692-02	.6500-02	.1963-01	.1590-01	.5926-01

TABLE I (Continued)

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H	O	OH	NO	CO
1.100	.10	4073.1	.2475-02	.8478-03	.4977-02	.2123-02	.4143-01
1.100	.10	4323.5	.5787-02	.2840-02	.9752-02	.4231-02	.5442-01
1.100	.10	4522.7	.1082-01	.6160-02	.1475-01	.6321-02	.6669-01
1.100	.10	4691.3	.1763-01	.1080-01	.1952-01	.8266-02	.7705-01
1.100	.10	4838.7	.2610-01	.1664-01	.2375-01	.1000-01	.8525-01
1.100	1.00	4206.4	.1040-02	.2535-03	.2934-02	.1522-02	.3619-01
1.100	1.00	4536.4	.2761-02	.1244-02	.7187-02	.4005-02	.4714-01
1.100	1.00	4793.6	.5681-02	.3246-02	.1220-01	.6782-02	.5954-01
1.100	1.00	5011.5	.1001-01	.6375-02	.1742-01	.9527-02	.7102-01
1.100	1.00	5202.9	.1584-01	.1064-01	.2245-01	.1209-01	.8071-01
1.100	10.00	4283.0	.3796-03	.4644-04	.1308-02	.7605-03	.3307-01
1.100	10.00	4707.7	.1150-02	.3988-03	.4409-02	.3059-02	.4013-01
1.100	10.00	5037.3	.2603-02	.1366-02	.8798-02	.6309-02	.5096-01
1.100	10.00	5315.5	.4942-02	.3112-02	.1382-01	.9819-02	.6248-01
1.100	10.00	5560.4	.8371-02	.5754-02	.1911-01	.1332-01	.7322-01
1.500	.10	3737.7	.1959-02	.1303-04	.5090-03	.6863-04	.1189+00
1.500	.10	4178.9	.7575-02	.3066-03	.3032-02	.5882-03	.1216+00
1.500	.10	4482.5	.1665-01	.1759-02	.7924-02	.1876-02	.1245+00
1.500	.10	4691.3	.2742-01	.4706-02	.1323-01	.3479-02	.1279+00
1.500	.10	4852.3	.3932-01	.8844-02	.1791-01	.5026-02	.1311+00
1.500	1.00	3756.6	.6632-03	.1511-05	.1756-03	.2402-04	.1192+00
1.500	1.00	4264.7	.3057-02	.5345-04	.1331-02	.2730-03	.1222+00
1.500	1.00	4677.2	.8342-02	.5283-03	.4805-02	.1279-02	.1247+00
1.500	1.00	4979.3	.1586-01	.2049-02	.1003-01	.3094-02	.1278+00
1.500	1.00	5207.8	.2486-01	.4749-02	.1546-01	.5186-02	.1312+00
1.500	10.00	3763.1	.2147-03	.1590-06	.5722-04	.7861-05	.1193+00
1.500	10.00	4301.1	.1069-02	.6701-05	.4812-03	.1009-03	.1225+00
1.500	10.00	4793.4	.3405-02	.9704-04	.2181-02	.6189-03	.1248+00
1.500	10.00	5202.9	.7633-02	.5828-03	.3918-02	.2050-02	.1273+00
1.500	10.00	5525.9	.1345-01	.1848-02	.1104-01	.4312-02	.1303+00
2.000	.10	3173.9	.2984-03	.1849-07	.1071-04	.5017-06	.1791+00
2.000	.10	3687.5	.2515-02	.2476-05	.1767-03	.1407-04	.1828+00
2.000	.10	4124.7	.1012-01	.6150-04	.1096-02	.1248-03	.1841+00
2.000	.10	4456.2	.2396-01	.4615-03	.3372-02	.4878-03	.1837+00
2.000	.10	4699.3	.4113-01	.1634-02	.6656-02	.1133-02	.1826+00
2.000	1.00	3176.2	.9541-04	.1894-08	.3433-05	.1613-06	.1791+00
2.000	1.00	3707.1	.8557-03	.2896-06	.6122-04	.4947-05	.1831+00
2.000	1.00	4201.7	.4024-02	.1000-04	.4611-03	.5487-04	.1852+00
2.000	1.00	4626.0	.1159-01	.1136-03	.1818-02	.2845-03	.1858+00
2.000	1.00	4962.7	.2351-01	.5795-03	.4473-02	.8499-03	.1854+00
2.000	10.00	3176.9	.3028-04	.1909-09	.1091-05	.5127-07	.1792+00
2.000	10.00	3714.0	.2775-03	.3058-07	.1998-04	.1623-05	.1832+00
2.000	10.00	4234.6	.1400-02	.1225-05	.1643-03	.1991-04	.1857+00
2.000	10.00	4720.7	.4604-02	.1842-04	.7653-03	.1249-03	.1869+00
2.000	10.00	5149.3	.1088-01	.1305-03	.2298-02	.4680-03	.1873+00

TABLE I (Continued)

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H2	O2	H2O	CO2	N2	A
.500	.10	2802.4	.2638-05	.1006+00	.6739-01	.6775-01	.7539+00	.9009-02
.500	.10	3407.5	.8209-04	.9887-01	.6661-01	.6737-01	.7520+00	.9003-02
.500	.10	3913.0	.6272-03	.9621-01	.6367-01	.6418-01	.7469+00	.8967-02
.500	.10	4274.7	.1892-02	.9396-01	.5823-01	.5623-01	.7377+00	.8883-02
.500	.10	4538.7	.3543-02	.9175-01	.5134-01	.4616-01	.7261+00	.8764-02
.500	1.00	2803.1	.8378-06	.1006+00	.6743-01	.6776-01	.7539+00	.9009-02
.500	1.00	3418.0	.2741-04	.9897-01	.6700-01	.6763-01	.7523+00	.9006-02
.500	1.00	3973.8	.2520-03	.9606-01	.6529-01	.6627-01	.7484+00	.8990-02
.500	1.00	4423.9	.9769-03	.9298-01	.6152-01	.6137-01	.7415+00	.8940-02
.500	1.00	4770.3	.2209-02	.9039-01	.5604-01	.5295-01	.7317+00	.8853-02
.500	10.00	2803.5	.2656-06	.1006+00	.6745-01	.6776-01	.7539+00	.9009-02
.500	10.00	3422.6	.8882-05	.9904-01	.6721-01	.6772-01	.7524+00	.9008-02
.500	10.00	4003.6	.8955-04	.9611-01	.6625-01	.6721-01	.7492+00	.9001-02
.500	10.00	4518.9	.4168-03	.9239-01	.6393-01	.6490-01	.7438+00	.8976-02
.500	10.00	4950.4	.1147-02	.8890-01	.6004-01	.5942-01	.7360+00	.8922-02
.900	.10	3927.9	.2382-02	.2289-01	.1118+00	.1057+00	.7257+00	.8690-02
.900	.10	4214.9	.5162-02	.2811-01	.1044+00	.9054-01	.7159+00	.8585-02
.900	.10	4438.6	.8350-02	.3316-01	.9532-01	.7471-01	.7042+00	.8459-02
.900	.10	4624.2	.1157-01	.3707-01	.8523-01	.6050-01	.6917+00	.8323-02
.900	.10	4785.0	.1457-01	.3963-01	.7462-01	.4849-01	.6788+00	.8180-02
.900	1.00	4034.3	.1193-02	.2009-01	.1146+00	.1117+00	.7288+00	.8728-02
.900	1.00	4396.5	.3178-02	.2379-01	.1092+00	.9956-01	.7211+00	.8652-02
.900	1.00	4682.1	.5794-02	.2830-01	.1019+00	.8466-01	.7110+00	.8549-02
.900	1.00	4920.4	.8717-02	.3232-01	.9328-01	.6994-01	.6997+00	.8432-02
.900	1.00	5128.1	.1175-01	.3537-01	.8375-01	.5665-01	.6877+00	.8305-02
.900	10.00	4100.4	.4964-03	.1838-01	.1163+00	.1156+00	.7308+00	.8752-02
.900	10.00	4540.7	.1676-02	.2007-01	.1129+00	.1077+00	.7253+00	.8705-02
.900	10.00	4897.5	.3553-02	.2332-01	.1075+00	.9545-01	.7172+00	.8628-02
.900	10.00	5196.6	.5895-02	.2690-01	.1007+00	.8156-01	.7074+00	.8533-02
.900	10.00	5460.1	.8553-02	.3006-01	.9284-01	.6784-01	.6966+00	.8427-02
1.000	.10	4035.6	.5188-02	.1155-01	.1194+00	.1041+00	.7192+00	.8559-02
1.000	.10	4286.0	.8497-02	.1798-01	.1108+00	.8770-01	.7045+00	.8444-02
1.000	.10	4490.6	.1205-01	.2364-01	.1007+00	.7201-01	.6926+00	.8315-02
1.000	.10	4664.1	.1551-01	.2800-01	.8986-01	.5841-01	.6802+00	.8178-02
1.000	.10	4816.5	.1865-01	.3103-01	.7859-01	.4703-01	.6674+00	.8037-02
1.000	1.00	4181.8	.3345-02	.7600-02	.1234+00	.1121+00	.7196+00	.8611-02
1.000	1.00	4494.2	.5970-02	.1312-01	.1168+00	.9736-01	.7107+00	.8520-02
1.000	1.00	4753.3	.9063-02	.1854-01	.1084+00	.8176-01	.7001+00	.8410-02
1.000	1.00	4975.0	.1236-01	.2313-01	.9895-01	.6727-01	.6887+00	.8291-02
1.000	1.00	5172.1	.1570-01	.2664-01	.8863-01	.5452-01	.6768+00	.8164-02
1.000	10.00	4294.6	.1994-02	.4459-02	.1263+00	.1189+00	.7232+00	.8652-02
1.000	10.00	4672.9	.3864-02	.8582-02	.1216+00	.1071+00	.7162+00	.8584-02
1.000	10.00	4993.2	.6275-02	.1321-01	.1152+00	.9298-01	.7072+00	.8497-02
1.000	10.00	5271.3	.9045-02	.1754-01	.1076+00	.7871-01	.6971+00	.8398-02
1.000	10.00	5521.1	.1210-01	.2125-01	.9891-01	.6518-01	.6863+00	.8290-02

TABLE I (Concluded)

SPECIFY ENTHALPY EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H2	O2	H2O	CO2	N2	A
1.100	.10	4073.1	.9758-02	.4583-02	.1250+00	.9736-01	.7030+00	.8407-02
1.100	.10	4323.5	.1301-01	.1055-01	.1159+00	.8254-01	.6927+00	.8296-02
1.100	.10	4522.7	.1665-01	.1610-01	.1052+00	.6817-01	.6810+00	.8169-02
1.100	.10	4691.3	.2020-01	.2057-01	.9361-01	.5559-01	.6687+00	.8034-02
1.100	.10	4838.7	.2335-01	.2383-01	.8182-01	.4510-01	.6563+00	.7896-02
1.100	1.00	4206.4	.7972-02	.1725-02	.1293+00	.1034+00	.7072+00	.8453-02
1.100	1.00	4536.4	.1025-01	.6156-02	.1227+00	.9106-01	.6991+00	.8372-02
1.100	1.00	4793.6	.1342-01	.1127-01	.1138+00	.7691-01	.6889+00	.8266-02
1.100	1.00	5011.5	.1692-01	.1586-01	.1036+00	.6349-01	.6776+00	.8148-02
1.100	1.00	5202.9	.2041-01	.1951-01	.9265-01	.5175-01	.6659+00	.8024-02
1.100	10.00	4283.0	.7029-02	.3640-03	.1318+00	.1069+00	.7098+00	.8480-02
1.100	10.00	4707.7	.8053-02	.2605-02	.1281+00	.9906-01	.7046+00	.8432-02
1.100	10.00	5037.3	.1036-01	.6506-02	.1215+00	.8692-01	.6963+00	.8352-02
1.100	10.00	5315.5	.1331-01	.1066-01	.1133+00	.7381-01	.6865+00	.8255-02
1.100	10.00	5560.4	.1661-01	.1438-01	.1039+00	.6132-01	.6758+00	.8149-02
1.500	.10	3737.7	.5349-01	.1238-04	.1183+00	.5436-01	.6448+00	.7699-02
1.500	.10	4178.9	.4977-01	.3028-03	.1171+00	.5079-01	.6413+00	.7661-02
1.500	.10	4482.5	.4841-01	.1651-02	.1096+00	.4609-01	.6339+00	.7581-02
1.500	.10	4691.3	.4888-01	.3905-02	.9870-01	.4021-01	.6241+00	.7473-02
1.500	.10	4852.3	.4984-01	.6288-02	.8674-01	.3434-01	.6132+00	.7352-02
1.500	1.00	3756.6	.5373-01	.1437-05	.1190+00	.5419-01	.6453+00	.7706-02
1.500	1.00	4264.7	.5015-01	.5369-04	.1204+00	.5083-01	.6439+00	.7690-02
1.500	1.00	4677.2	.4817-01	.5278-03	.1170+00	.4732-01	.6396+00	.7645-02
1.500	1.00	4979.3	.4816-01	.1883-02	.1089+00	.4243-01	.6322+00	.7567-02
1.500	1.00	5207.8	.4942-01	.3810-02	.9821-01	.3680-01	.6228+00	.7468-02
1.500	10.00	3763.1	.5381-01	.1511-06	.1192+00	.5413-01	.6455+00	.7708-02
1.500	10.00	4301.1	.5039-01	.6770-05	.1219+00	.5081-01	.6450+00	.7703-02
1.500	10.00	4793.4	.4813-01	.1005-03	.1217+00	.4808-01	.6432+00	.7684-02
1.500	10.00	5202.9	.4733-01	.5844-03	.1175+00	.4463-01	.6388+00	.7640-02
1.500	10.00	5525.9	.4809-01	.1687-02	.1098+00	.4001-01	.6319+00	.7571-02
2.000	.10	3173.9	.1313+00	.4753-08	.7557-01	.2815-01	.5787+00	.6910-02
2.000	.10	3687.5	.1262+00	.6696-06	.7919-01	.2421-01	.5780+00	.6902-02
2.000	.10	4124.7	.1204+00	.1716-04	.7981-01	.2202-01	.5754+00	.6871-02
2.000	.10	4456.2	.1133+00	.1303-03	.7709-01	.2056-01	.5702+00	.6811-02
2.000	.10	4699.3	.1061+00	.4525-03	.7153-01	.1913-01	.5629+00	.6728-02
2.000	1.00	3176.2	.1314+00	.4868-09	.7562-01	.2812-01	.5788+00	.6911-02
2.000	1.00	3707.1	.1269+00	.7816-07	.7958-01	.2405-01	.5785+00	.6908-02
2.000	1.00	4201.7	.1230+00	.2777-05	.8136-01	.2161-01	.5774+00	.6895-02
2.000	1.00	4626.0	.1182+00	.3196-04	.8070-01	.2004-01	.5746+00	.6863-02
2.000	1.00	4962.7	.1127+00	.1616-03	.7723-01	.1872-01	.5696+00	.6806-02
2.000	10.00	3176.9	.1314+00	.4906-10	.7563-01	.2811-01	.5788+00	.6911-02
2.000	10.00	3714.0	.1271+00	.8247-08	.7971-01	.2399-01	.5787+00	.6910-02
2.000	10.00	4234.6	.1241+00	.3394-06	.8203-01	.2144-01	.5783+00	.6905-02
2.000	10.00	4720.7	.1210+00	.5170-05	.8276-01	.1977-01	.5771+00	.6892-02
2.000	10.00	5149.3	.1179+00	.3662-04	.8152-01	.1852-01	.5749+00	.6863-02

TABLE II

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	H BTU/LB	S BTU/LB OR	CP BTU/LB OR	MOL WT	NO ITER	TYPE CASE	TIME SEC
.5000	.1	3000.0	63.06	2.28869	.31243	28.930	2	1	.322
.5000	.1	4000.0	442.16	2.39664	.32316	28.754	2	1	.322
.5000	.1	5000.0	1295.10	2.58364	.32848	27.003	3	1	.373
.5000	1.0	3000.0	62.49	2.13044	.31243	28.932	2	1	.322
.5000	1.0	4000.0	410.51	2.23007	.32326	28.865	3	1	.373
.5000	1.0	5000.0	963.64	2.35194	.32862	28.141	3	1	.372
.5000	10.0	3000.0	62.21	1.97231	.31243	28.933	2	1	.322
.5000	10.0	4000.0	398.84	2.06887	.32330	28.906	3	1	.372
.5000	10.0	5000.0	825.68	2.16345	.32903	28.625	3	1	.372
.9000	.1	3000.0	-391.15	2.30552	.32718	28.906	3	1	.372
.9000	.1	4000.0	44.68	2.42892	.33890	28.568	4	1	.424
.9000	.1	5000.0	1108.12	2.66247	.34390	26.222	4	1	.423
.9000	1.0	3000.0	-391.97	2.14706	.32719	28.908	2	1	.322
.9000	1.0	4000.0	-16.42	2.25426	.33925	28.780	2	1	.322
.9000	1.0	5000.0	674.29	2.40637	.34431	27.635	4	1	.423
.9000	10.0	3000.0	-392.32	1.98878	.32719	28.910	2	1	.322
.9000	10.0	4000.0	-40.11	2.08972	.33940	28.862	3	1	.373
.9000	10.0	5000.0	465.69	2.20149	.34921	28.337	4	1	.423
1.0000	.1	3000.0	-498.27	2.30733	.33073	28.887	5	1	.474
1.0000	.1	4000.0	-24.84	2.44134	.34249	28.427	5	1	.473
1.0000	.1	5000.0	1074.16	2.68280	.34760	26.003	4	1	.423
1.0000	1.0	3000.0	-500.95	2.14817	.33075	28.897	7	1	.575
1.0000	1.0	4000.0	-98.19	2.26294	.34292	28.679	4	1	.423
1.0000	1.0	5000.0	624.31	2.42222	.34798	27.446	4	1	.423
1.0000	10.0	3000.0	-502.21	1.98953	.33075	28.901	7	1	.575
1.0000	10.0	4000.0	-133.00	2.09516	.34316	28.797	5	1	.474
1.0000	10.0	5000.0	405.11	2.21418	.34890	28.172	6	1	.524
1.1000	.1	3000.0	-454.00	2.34839	.33333	28.347	6	1	.465
1.1000	.1	4000.0	-47.40	2.46372	.34570	28.132	15	1	.849
1.1000	.1	5000.0	1047.05	2.70379	.35124	25.771	7	1	.506
1.1000	1.0	3000.0	-454.15	2.18704	.33333	28.348	4	1	.379
1.1000	1.0	4000.0	-96.05	2.28958	.34591	28.294	3	1	.335
1.1000	1.0	5000.0	589.20	2.44014	.35152	27.216	6	1	.463
1.1000	10.0	3000.0	-454.20	2.02572	.33333	28.348	4	1	.379
1.1000	10.0	4000.0	-108.37	2.12503	.34596	28.334	5	1	.421
1.1000	10.0	5000.0	375.55	2.23176	.35233	27.910	10	1	.634
1.5000	.1	3000.0	-270.86	2.49012	.34444	26.376	4	1	.379
1.5000	.1	4000.0	111.49	2.59950	.35729	26.288	4	1	.379
1.5000	.1	5000.0	1019.77	2.79728	.36527	24.688	5	1	.420
1.5000	1.0	3000.0	-271.09	2.31668	.34444	26.377	4	1	.379
1.5000	1.0	4000.0	92.56	2.42107	.35719	26.350	4	1	.379
1.5000	1.0	5000.0	616.42	2.53639	.36475	25.866	5	1	.422
1.5000	10.0	3000.0	-271.17	2.14330	.34444	26.377	4	1	.380
1.5000	10.0	4000.0	86.85	2.24618	.35716	26.369	4	1	.378
1.5000	10.0	5000.0	495.39	2.33690	.36468	26.231	5	1	.422

TABLE II (Continued)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H	O	OH	NO	CO
.500	.10	3000.0	.1036-05	.3100-04	.3599-03	.1837-02	.3108-04
.500	.10	4000.0	.5816-03	.3022-02	.6436-02	.9149-02	.4475-02
.500	.10	5000.0	.2024-01	.4484-01	.2587-01	.2178-01	.3806-01
.500	1.00	3000.0	.1843-06	.9805-05	.2025-03	.1837-02	.9831-05
.500	1.00	4000.0	.1054-03	.9566-03	.3691-02	.9176-02	.1487-02
.500	1.00	5000.0	.4409-02	.1467-01	.1844-01	.2300-01	.2083-01
.500	10.00	3000.0	.3278-07	.3101-05	.1139-03	.1838-02	.3109-05
.500	10.00	4000.0	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	10.00	5000.0	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.900	.10	3000.0	.2071-05	.1361-04	.3158-03	.7959-03	.1238-03
.900	.10	4000.0	.1090-02	.1513-02	.6041-02	.4514-02	.1458-01
.900	.10	5000.0	.3218-01	.3167-01	.2905-01	.1499-01	.7328-01
.900	1.00	3000.0	.3685-06	.4301-05	.1776-03	.7956-03	.3919-04
.900	1.00	4000.0	.2074-03	.4355-03	.3307-02	.4125-02	.5554-02
.900	1.00	5000.0	.7466-02	.9052-02	.1927-01	.1392-01	.4852-01
.900	10.00	3000.0	.6553-07	.1360-05	.9992-04	.7957-03	.1240-04
.900	10.00	4000.0	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	10.00	5000.0	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
1.000	.10	3000.0	.5502-05	.2125-05	.1310-03	.1239-03	.8697-03
1.000	.10	4000.0	.1392-02	.1012-02	.5158-02	.3003-02	.2256-01
1.000	.10	5000.0	.3535-01	.2847-01	.2869-01	.1339-01	.8288-01
1.000	1.00	3000.0	.1195-05	.4509-06	.6041-04	.8315-04	.4113-03
1.000	1.00	4000.0	.3038-03	.2222-03	.2472-02	.2095-02	.1146-01
1.000	1.00	5000.0	.8504-02	.7590-02	.1840-01	.1161-01	.5860-01
1.000	10.00	3000.0	.2609-06	.9474-07	.2770-04	.5525-04	.1961-03
1.000	10.00	4000.0	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	10.00	5000.0	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.100	.10	3000.0	.3369-04	.5657-07	.2136-04	.3257-05	.2818-01
1.100	.10	4000.0	.1919-02	.5611-03	.3944-02	.1652-02	.3856-01
1.100	.10	5000.0	.3867-01	.2535-01	.2795-01	.1184-01	.9278-01
1.100	1.00	3000.0	.1066-04	.5656-08	.6756-05	.1030-05	.2818-01
1.100	1.00	4000.0	.5511-03	.7038-04	.1420-02	.6575-03	.3276-01
1.100	1.00	5000.0	.9734-02	.6176-02	.1714-01	.9382-02	.7044-01
1.100	10.00	3000.0	.3370-05	.5656-09	.2136-05	.3257-06	.2818-01
1.100	10.00	4000.0	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	10.00	5000.0	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.500	.10	3000.0	.8366-04	.7882-08	.7390-05	.8323-06	.1116+00
1.500	.10	4000.0	.4543-02	.9352-04	.1556-02	.2630-03	.1205+00
1.500	.10	5000.0	.5354-01	.1444-01	.2205-01	.6531-02	.1338+00
1.500	1.00	3000.0	.2646-04	.7880-09	.2337-05	.1367-06	.1116+00
1.500	1.00	4000.0	.1447-02	.9357-05	.4957-03	.8333-04	.1208+00
1.500	1.00	5000.0	.1653-01	.2222-02	.1047-01	.3257-02	.1281+00
1.500	10.00	3000.0	.8367-05	.7880-10	.7390-06	.4322-07	.1116+00
1.500	10.00	4000.0	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	10.00	5000.0	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00

TABLE II (Continued)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H2	O2	H2O	CO2	N2	A
.500	.10	3000.0	.9433-05	.1002+00	.6728-01	.6773-01	.7535+00	.9008-02
.500	.10	4000.0	.8389-03	.9569-01	.6271-01	.6287-01	.7453+00	.8953-02
.500	.10	5000.0	.7229-02	.8239-01	.3269-01	.2518-01	.6933+00	.8408-02
.500	1.00	3000.0	.2986-05	.1002+00	.6737-01	.6775-01	.7536+00	.9009-02
.500	1.00	4000.0	.2753-03	.9589-01	.6514-01	.6612-01	.7482+00	.8988-02
.500	1.00	5000.0	.3432-02	.8823-01	.5077-01	.4508-01	.7224+00	.8763-02
.500	10.00	3000.0	.9450-06	.1003+00	.6742-01	.6776-01	.7536+00	.9009-02
.500	10.00	4000.0	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	10.00	5000.0	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.900	.10	3000.0	.3771-04	.1931-01	.1180+00	.1184+00	.7342+00	.8771-02
.900	.10	4000.0	.2948-02	.2399-01	.1103+00	.1026+00	.7237+00	.8669-02
.900	.10	5000.0	.1828-01	.4111-01	.5837-01	.3424-01	.6589+00	.7957-02
.900	1.00	3000.0	.1194-04	.1929-01	.1182+00	.1185+00	.7343+00	.8772-02
.900	1.00	4000.0	.1067-02	.1988-01	.1149+00	.1125+00	.7293+00	.8733-02
.900	1.00	5000.0	.9842-02	.3358-01	.8984-01	.6480-01	.6953+00	.8386-02
.900	10.00	3000.0	.3777-05	.1929-01	.1182+00	.1185+00	.7343+00	.8772-02
.900	10.00	4000.0	.3571-03	.1831-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	10.00	5000.0	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
1.000	.10	3000.0	.2662-03	.4725-03	.1301+00	.1299+00	.7294+00	.8710-02
1.000	.10	4000.0	.4807-02	.1073-01	.1203+00	.1061+00	.7164+00	.8571-02
1.000	.10	5000.0	.2207-01	.3321-01	.6335-01	.3481-01	.6499+00	.7840-02
1.000	1.00	3000.0	.1257-03	.2121-03	.1304+00	.1304+00	.7297+00	.8713-02
1.000	1.00	4000.0	.2290-02	.5173-02	.1258+00	.1183+00	.7231+00	.8647-02
1.000	1.00	5000.0	.1277-01	.2361-01	.9774-01	.6563-01	.6873+00	.8276-02
1.000	10.00	3000.0	.5985-04	.9362-04	.1305+00	.1306+00	.7298+00	.8714-02
1.000	10.00	4000.0	.1092-02	.2364-02	.1284+00	.1247+00	.7265+00	.8683-02
1.000	10.00	5000.0	.6333-02	.1331-01	.1151+00	.9266-01	.7070+00	.8494-02
1.100	.10	3000.0	.9985-02	.3337-06	.1299+00	.1120+00	.7113+00	.8493-02
1.100	.10	4000.0	.9136-02	.3299-02	.1268+00	.1006+00	.7051+00	.8429-02
1.100	.10	5000.0	.2641-01	.2633-01	.6750-01	.3470-01	.6408+00	.7721-02
1.100	1.00	3000.0	.9986-02	.3336-07	.1300+00	.1120+00	.7113+00	.8494-02
1.100	1.00	4000.0	.7533-02	.5191-03	.1312+00	.1072+00	.7097+00	.8477-02
1.100	1.00	5000.0	.1673-01	.1563-01	.1042+00	.6418-01	.6782+00	.8194-02
1.100	10.00	3000.0	.9987-02	.3336-08	.1300+00	.1120+00	.7113+00	.8494-02
1.100	10.00	4000.0	.7195-02	.5796-04	.1324+00	.1087+00	.7109+00	.8489-02
1.100	10.00	5000.0	.1004-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.500	.10	3000.0	.6155-01	.6477-08	.1116+00	.6184-01	.6456+00	.7709-02
1.500	.10	4000.0	.5118-01	.9164-04	.1184+00	.5238-01	.6433+00	.7683-02
1.500	.10	5000.0	.5061-01	.8549-02	.7371-01	.2892-01	.6010+00	.7215-02
1.500	1.00	3000.0	.6157-01	.6475-09	.1116+00	.6183-01	.6456+00	.7709-02
1.500	1.00	4000.0	.5191-01	.9174-05	.1201+00	.5252-01	.6449+00	.7701-02
1.500	1.00	5000.0	.4825-01	.2023-02	.1081+00	.4200-01	.6315+00	.7560-02
1.500	10.00	3000.0	.6158-01	.6474-10	.1116+00	.6183-01	.6456+00	.7709-02
1.500	10.00	4000.0	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	10.00	5000.0	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02

TABLE II (Concluded)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQULIBRIUM ISENTROPIC EXPANSION FROM 10 ATM.

EQ RATIO	P ATM	T DEG R	H BTU/LB	S BTU/LB OR	CP BTU/LB OR	MOL WT	NO ITER	TYPE CASE	TIME SEC
.5000	10.0000	4000.0	398.84	2.06887	.32330	28.906	3	1	.375
.5000	5.0000	3485.0	220.84	2.06887	.31852	28.927	7	2	1.637
.5000	1.0000	2463.1	-105.35	2.06885	.30335	28.934	2	2	.569
.5000	.5000	2104.4	-213.29	2.06908	.29556	28.934	2	2	.568
.5000	10.0000	5000.0	825.68	2.16345	.32903	28.625	3	1	.374
.5000	5.0000	4491.5	598.16	2.16345	.32658	28.798	9	2	2.064
.5000	1.0000	3319.7	166.72	2.16345	.31663	28.927	7	2	1.637
.5000	.5000	2865.5	19.75	2.16344	.31041	28.933	5	2	1.210
.9000	10.0000	4000.0	-40.11	2.08972	.33940	28.862	3	1	.375
.9000	5.0000	3509.6	-218.97	2.08972	.33436	28.900	7	2	1.636
.9000	1.0000	2515.4	-549.78	2.08972	.31804	28.910	5	2	1.210
.9000	.5000	2162.2	-660.95	2.08973	.30961	28.911	4	2	.997
.9000	10.0000	5000.0	465.69	2.20149	.34521	28.337	4	1	.425
.9000	5.0000	4565.2	234.48	2.20149	.34319	28.597	12	2	2.707
.9000	1.0000	3512.6	-214.91	2.20149	.33438	28.889	7	2	1.637
.9000	.5000	3061.1	-371.35	2.20149	.32816	28.907	5	2	1.210
1.0000	10.0000	4000.0	-133.00	2.09516	.34316	28.797	5	1	.476
1.0000	5.0000	3536.2	-312.83	2.09516	.33840	28.868	8	2	1.852
1.0000	1.0000	2556.4	-648.07	2.09514	.32225	28.904	4	2	.992
1.0000	.5000	2201.6	-761.17	2.09515	.31373	28.905	4	2	.994
1.0000	10.0000	5000.0	405.11	2.21418	.34890	28.172	6	1	.526
1.0000	5.0000	4577.7	172.26	2.21416	.34694	28.448	8	2	1.850
1.0000	1.0000	3590.9	-283.51	2.21416	.33898	28.832	11	2	2.492
1.0000	.5000	3159.5	-444.45	2.21416	.33328	28.885	10	2	2.276
1.1000	10.0000	4000.0	-108.37	2.12503	.34596	28.334	5	1	.423
1.1000	5.0000	3483.8	-289.92	2.12503	.34036	28.346	11	2	2.240
1.1000	1.0000	2488.1	-623.88	2.12503	.32346	28.348	11	2	2.244
1.1000	.5000	2142.2	-736.11	2.12503	.31510	28.348	9	2	1.859
1.1000	10.0000	5000.0	375.55	2.23176	.35233	27.910	10	1	.636
1.1000	5.0000	4556.8	140.84	2.23175	.35009	28.159	15	2	2.998
1.1000	1.0000	3421.7	-310.77	2.23174	.33957	28.345	8	2	1.667
1.1000	.5000	2965.6	-465.65	2.23174	.33275	28.348	9	2	1.859
1.5000	10.0000	4000.0	86.85	2.24618	.35716	26.369	4	1	.381
1.5000	5.0000	3462.0	-107.61	2.24618	.35117	26.376	12	2	2.432
1.5000	1.0000	2450.6	-462.64	2.24617	.33407	26.377	9	2	1.858
1.5000	.5000	2106.0	-581.64	2.24603	.32609	26.377	8	2	1.664
1.5000	10.0000	5000.0	495.39	2.33690	.36468	26.231	5	1	.424
1.5000	5.0000	4416.9	248.82	2.33690	.36078	26.333	11	2	2.241
1.5000	1.0000	3176.9	-208.68	2.33689	.34721	26.376	11	2	2.241
1.5000	.5000	2738.0	-362.77	2.33689	.33984	26.377	11	2	2.244

TABLE III

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQULIBRIUM ISENTROPIC EXPANSION FROM 10 ATM.

EQ RATIO	P ATM	T DEG R	SPECIES H	MOL FRACTIONS O	OH	NO	CO
.500	10.00	4000.0	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	5.00	3485.0	.1886-05	.5628-04	.6885-03	.4526-02	.7285-04
.500	1.00	2463.1	.7489-09	.1806-06	.1576-04	.4438-03	.1190-06
.500	.50	2104.4	.6822-11	.5727-08	.1647-05	.1144-03	.2477-08
.500	10.00	5000.0	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.500	5.00	4491.5	.2550-03	.1912-02	.6301-02	.1535-01	.3362-02
.500	1.00	3319.7	.2120-05	.5735-04	.6240-03	.3431-02	.6867-04
.500	.50	2865.5	.9434-07	.5858-05	.1389-03	.1353-02	.5378-05
.900	10.00	4000.0	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	5.00	3509.6	.4417-05	.2739-04	.6462-03	.2024-02	.3300-03
.900	1.00	2515.4	.2829-08	.1265-06	.1864-04	.2277-03	.7903-06
.900	.50	2162.2	.3552-10	.5083-08	.2267-05	.6392-04	.2140-07
.900	10.00	5000.0	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
.900	5.00	4565.2	.6407-03	.1130-02	.6586-02	.7860-02	.1390-01
.900	1.00	3512.6	.1500-04	.6230-04	.9751-03	.2041-02	.7429-03
.900	.50	3061.1	.1026-05	.8757-05	.2665-03	.9049-03	.8288-04
1.000	10.00	4000.0	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	5.00	3536.2	.1179-04	.6608-05	.3386-03	.4510-03	.1908-02
1.000	1.00	2556.4	.2623-07	.5899-08	.4437-05	.8481-05	.3857-04
1.000	.50	2201.6	.6913-09	.8092-10	.3202-06	.7579-06	.3864-05
1.000	10.00	5000.0	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.000	5.00	4577.7	.8638-03	.7594-03	.5661-02	.5154-02	.2261-01
1.000	1.00	3590.9	.4550-04	.2697-04	.7044-03	.7057-03	.3780-02
1.000	.50	3159.5	.5765-05	.2526-05	.1623-03	.1811-03	.1022-02
1.100	10.00	4000.0	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	5.00	3483.8	.4176-04	.2208-06	.6036-04	.1732-04	.2994-01
1.100	1.00	2488.1	.4340-06	.2341-11	.8030-07	.4838-08	.2502-01
1.100	.50	2142.2	.2983-07	.3056-14	.1734-08	.4411-10	.2147-01
1.100	10.00	5000.0	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.100	5.00	4556.8	.1148-02	.3688-03	.4032-02	.2576-02	.3911-01
1.100	1.00	3421.7	.7308-04	.6083-06	.9623-04	.2571-04	.2977-01
1.100	.50	2965.6	.1257-04	.7278-08	.7435-05	.1075-05	.2802-01
1.500	10.00	4000.0	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	5.00	3462.0	.9979-04	.2356-07	.1832-04	.1878-05	.1168+00
1.500	1.00	2450.6	.7489-06	.1749-12	.1873-07	.4290-09	.1016+00
1.500	.50	2106.0	.4448-07	.1919-15	.3520-09	.3517-11	.9166-01
1.500	10.00	5000.0	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00
1.500	5.00	4416.9	.2028-02	.2655-04	.1001-02	.2270-03	.1230+00
1.500	1.00	3176.9	.6433-04	.6367-08	.7727-05	.5710-06	.1139+00
1.500	.50	2738.0	.8160-05	.4354-10	.4225-06	.1655-07	.1075+00

TABLE III (Concluded)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

EQULIBRIUM ISENTROPIC EXPANSION FROM 10 ATM.

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H2	O2	H2O	CO2	N2	A
.500	10.00	4000.0	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	5.00	3485.0	.1669-04	.9877-01	.6710-01	.6768-01	.7521+00	.9007-02
.500	1.00	2463.1	.5815-07	.1010+00	.6747-01	.6777-01	.7543+00	.9009-02
.500	.50	2104.4	.1962-08	.1012+00	.6747-01	.6777-01	.7545+00	.9009-02
.500	10.00	5000.0	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.500	5.00	4491.5	.5420-03	.9255-01	.6334-01	.6409-01	.7433+00	.8967-02
.500	1.00	3319.7	.1711-04	.9933-01	.6713-01	.6768-01	.7526+00	.9007-02
.500	.50	2865.5	.1804-05	.1005+00	.6740-01	.6776-01	.7538+00	.9009-02
.900	10.00	4000.0	.3571-03	.1831-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	5.00	3509.6	.7512-04	.1872-01	.1178+00	.1182+00	.7334+00	.8769-02
.900	1.00	2515.4	.3654-06	.1959-01	.1183+00	.1185+00	.7346+00	.8773-02
.900	.50	2162.2	.1550-07	.1968-01	.1183+00	.1185+00	.7347+00	.8773-02
.900	10.00	5000.0	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
.900	5.00	4565.2	.2392-02	.2166-01	.1110+00	.1034+00	.7228+00	.8678-02
.900	1.00	3512.6	.1691-03	.1886-01	.1175+00	.1177+00	.7331+00	.8766-02
.900	.50	3061.1	.2423-04	.1924-01	.1181+00	.1184+00	.7342+00	.8772-02
1.000	10.00	4000.0	.1092-02	.2364-02	.1284+00	.1247+00	.7265+00	.8683-02
1.000	5.00	3536.2	.4337-03	.8603-03	.1298+00	.1288+00	.7288+00	.8704-02
1.000	1.00	2556.4	.1711-04	.2213-04	.1305+00	.1308+00	.7299+00	.8715-02
1.000	.50	2201.6	.2641-05	.2520-05	.1305+00	.1308+00	.7299+00	.8715-02
1.000	10.00	5000.0	.6333-02	.1331-01	.1151+00	.9266-01	.7070+00	.8494-02
1.000	5.00	4577.7	.4122-02	.9210-02	.1211+00	.1061+00	.7158+00	.8578-02
1.000	1.00	3590.9	.8467-03	.1782-02	.1290+00	.1267+00	.7277+00	.8693-02
1.000	.50	3159.5	.2824-03	.5209-03	.1301+00	.1297+00	.7293+00	.8709-02
1.100	10.00	4000.0	.7195-02	.5796-04	.1324+00	.1067+00	.7109+00	.8489-02
1.100	5.00	3483.8	.8259-02	.1536-05	.1316+00	.1103+00	.7113+00	.8493-02
1.100	1.00	2488.1	.1315-01	.1085-10	.1268+00	.1152+00	.7113+00	.8494-02
1.100	.50	2142.2	.1669-01	.1149-13	.1233+00	.1187+00	.7113+00	.8494-02
1.100	10.00	5000.0	.1004-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.100	5.00	4556.8	.8049-02	.2430-02	.1284+00	.1002+00	.7053+00	.8437-02
1.100	1.00	3421.7	.8440-02	.4151-05	.1314+00	.1104+00	.7113+00	.8493-02
1.100	.50	2965.6	.1015-01	.4233-07	.1298+00	.1122+00	.7113+00	.8494-02
1.500	10.00	4000.0	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	5.00	3462.0	.5632-01	.2136-07	.1168+00	.5661-01	.6456+00	.7709-02
1.500	1.00	2450.6	.7158-01	.1199-12	.1016+00	.7183-01	.6456+00	.7709-02
1.500	.50	2106.0	.8155-01	.1108-15	.9166-01	.8180-01	.6456+00	.7709-02
1.500	10.00	5000.0	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02
1.500	5.00	4416.9	.4967-01	.2703-04	.1217+00	.5012-01	.6444+00	.7696-02
1.500	1.00	3176.9	.5930-01	.5456-08	.1139+00	.5958-01	.6456+00	.7709-02
1.500	.50	2738.0	.6567-01	.3318-10	.1075+00	.6592-01	.6456+00	.7709-02

TABLE IV

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

FROZEN ISENTROPIC EXPANSION FROM 10 ATM.

EQ RATIO	P ATM	T DEG R	H BTU/LB	S BTU/LB OR	CP BTU/LB OR	MOL WT	NO ITER	TYPE CASE	TIME SEC
.5000	10.0	4000.0	398.84	2.06887	.32330	28.906	3	1	.374
.5000	5.0	3448.2	221.81	2.06887	.31609	28.906	4	3	.463
.5000	1.0	2415.4	-99.44	2.06888	.30241	28.906	5	3	.545
.5000	.5	2059.2	-205.77	2.06889	.29450	26.906	4	3	.464
.5000	10.0	5000.0	625.68	2.16345	.32903	28.625	3	1	.374
.5000	5.0	4316.7	602.06	2.16346	.32523	26.625	4	3	.463
.5000	1.0	3043.4	194.87	2.16346	.31284	28.625	5	3	.545
.5000	.5	2605.4	59.31	2.16347	.30593	28.625	4	3	.463
.9000	10.0	4000.0	-40.11	2.06972	.33940	26.662	3	1	.375
.9000	5.0	3471.8	-217.99	2.08973	.33383	28.862	4	3	.463
.9000	1.0	2471.3	-544.36	2.06974	.31703	28.862	5	3	.545
.9000	.5	2122.0	-651.74	2.08975	.30843	28.916	4	3	.464
.9000	10.0	5000.0	465.69	2.20149	.34521	28.337	4	1	.425
.9000	5.0	4340.2	239.20	2.20149	.34115	28.337	4	3	.464
.9000	1.0	3099.4	-176.88	2.20150	.32786	28.337	5	3	.545
.9000	.5	2668.2	-316.72	2.20151	.32046	26.337	4	3	.464
1.0000	10.0	4000.0	-133.00	2.09516	.34316	28.797	5	1	.475
1.0000	5.0	3476.0	-311.39	2.09517	.33750	28.797	4	3	.463
1.0000	1.0	2477.3	-631.25	2.09516	.31990	29.041	5	3	.546
1.0000	.5	2128.9	-728.91	2.09520	.31074	29.361	4	3	.464
1.0000	10.0	5000.0	405.11	2.21416	.34890	28.172	6	1	.526
1.0000	5.0	4343.2	177.23	2.21418	.34476	26.172	4	3	.464
1.0000	1.0	3106.2	-241.86	2.21419	.33123	26.172	5	3	.544
1.0000	.5	2679.7	-374.67	2.21425	.32338	28.386	1	3	.222
1.1000	10.0	4000.0	-106.37	2.12503	.34596	28.334	5	1	.423
1.1000	5.0	3472.0	-289.58	2.12503	.34013	28.334	4	3	.463
1.1000	1.0	2437.3	-631.51	2.12505	.32253	28.340	5	3	.545
1.1000	.5	1990.3	-766.96	2.12510	.31303	28.360	5	3	.545
1.1000	10.0	5000.0	375.55	2.23176	.35233	27.910	10	1	.636
1.1000	5.0	4343.4	145.51	2.23177	.34608	27.910	4	3	.463
1.1000	1.0	3106.3	-277.55	2.23178	.33425	27.910	5	3	.545
1.1000	.5	2545.3	-456.82	2.23178	.32632	27.930	6	3	.626
1.5000	10.0	4000.0	86.85	2.24618	.35716	26.369	4	1	.361
1.5000	5.0	3451.7	-107.31	2.24619	.35077	26.369	4	3	.464
1.5000	1.0	2420.9	-460.06	2.24620	.33165	26.369	5	3	.544
1.5000	.5	2063.9	-576.91	2.24621	.32241	26.369	4	3	.464
1.5000	10.0	5000.0	495.39	2.33690	.36468	26.231	5	1	.423
1.5000	5.0	4326.0	251.11	2.33690	.35994	26.231	4	3	.464
1.5000	1.0	3062.7	-195.14	2.33691	.34474	26.231	5	3	.544
1.5000	.5	2625.5	-344.11	2.33692	.33642	26.231	4	3	.463

TABLE IV (Continued)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

FROZEN ISENTROPIC EXPANSION FROM 10 ATM.

EQ RATIO	P ATM	T DEG R	SPECIES MOL FRACTIONS H	O	OH	NO	CO
.500	10.00	4000.0	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	5.00	3448.2	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	1.00	2415.4	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	.50	2059.2	.1888-04	.3029-03	.2095-02	.9194-02	.4774-03
.500	10.00	5000.0	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.500	5.00	4316.7	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.500	1.00	3043.4	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.500	.50	2605.4	.8477-03	.4647-02	.1123-01	.2324-01	.8534-02
.900	10.00	4000.0	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	5.00	3471.8	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	1.00	2471.3	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	.50	2122.0	.3795-04	.1322-03	.1837-02	.3964-02	.1895-02
.900	10.00	5000.0	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
.900	5.00	4340.2	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
.900	1.00	3099.4	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
.900	.50	2668.2	.1556-02	.2445-02	.1085-01	.1205-01	.2522-01
1.000	10.00	4000.0	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	5.00	3476.0	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	1.00	2477.3	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	.50	2128.9	.6637-04	.4750-04	.1154-02	.1420-02	.5647-02
1.000	10.00	5000.0	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.000	5.00	4343.2	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.000	1.00	3106.2	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.000	.50	2679.7	.1894-02	.1802-02	.9731-02	.8839-02	.3485-01
1.100	10.00	4000.0	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	5.00	3472.0	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	1.00	2437.3	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	.50	1990.3	.1703-03	.7437-05	.4639-03	.2199-03	.3144-01
1.100	10.00	5000.0	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.100	5.00	4343.4	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.100	1.00	3106.3	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.100	.50	2545.3	.2384-02	.1210-02	.8225-02	.5894-02	.4957-01
1.500	10.00	4000.0	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	5.00	3451.7	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	1.00	2420.9	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	.50	2063.9	.4586-03	.9351-06	.1571-03	.2634-04	.1209+00
1.500	10.00	5000.0	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00
1.500	5.00	4326.0	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00
1.500	1.00	3062.7	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00
1.500	.50	2625.5	.5189-02	.2508-03	.3711-02	.1172-02	.1259+00

TABLE IV (Concluded)

SPECIFY TEMPERTURE EQUIVALENCE RATIO AND PRESSURE FOR A CH2 HYDROCARBON WITH AIR

FROZEN ISENTROPIC EXPANSION FROM 10 ATM.

EQ. RATIO	P ATM	T DEG R	SPECIES MOL. FRACTIONS H2	O2	H2O	CO2	N2	A
.500	10.00	4000.0	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	5.00	3448.2	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	1.00	2415.4	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	.50	2059.2	.8844-04	.9613-01	.6626-01	.6722-01	.7492+00	.9001-02
.500	10.00	5000.0	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.500	5.00	4316.7	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.500	1.00	3043.4	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.500	.50	2605.4	.1269-02	.8850-01	.5945-01	.5851-01	.7349+00	.8913-02
.900	10.00	4000.0	.3571-03	.1831-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	5.00	3471.8	.3571-03	.1831-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	1.00	2471.3	.3571-03	.1831-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	.50	2122.0	.3571-03	.2000-01	.1168+00	.1165+00	.7315+00	.8758-02
.900	10.00	5000.0	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
.900	5.00	4340.2	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
.900	1.00	3099.4	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
.900	.50	2668.2	.4277-02	.2450-01	.1054+00	.9097-01	.7141+00	.8599-02
1.000	10.00	4000.0	.1092-02	.2364-02	.1284+00	.1247+00	.7265+00	.8683-02
1.000	5.00	3476.0	.1092-02	.2364-02	.1284+00	.1247+00	.7265+00	.8683-02
1.000	1.00	2477.3	.1092-02	.1000-01	.1284+00	.1247+00	.7265+00	.8683-02
1.000	.50	2128.9	.1092-02	.2000-01	.1284+00	.1247+00	.7265+00	.8683-02
1.000	10.00	5000.0	.6333-02	.1331-01	.1151+00	.9266-01	.7070+00	.8494-02
1.000	5.00	4343.2	.6333-02	.1331-01	.1151+00	.9266-01	.7070+00	.8494-02
1.000	1.00	3106.2	.6333-02	.1331-01	.1151+00	.9266-01	.7070+00	.8494-02
1.000	.50	2679.7	.6333-02	.2000-01	.1151+00	.9266-01	.7070+00	.8494-02
1.100	10.00	4000.0	.7195-02	.5796-04	.1324+00	.1087+00	.7109+00	.8489-02
1.100	5.00	3472.0	.7195-02	.5796-04	.1324+00	.1087+00	.7109+00	.8489-02
1.100	1.00	2437.3	.1000-01	.5796-04	.1324+00	.1087+00	.7109+00	.8489-02
1.100	.50	1990.3	.2000-01	.5796-04	.1324+00	.1087+00	.7109+00	.8489-02
1.100	10.00	5000.0	.1004-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.100	5.00	4343.4	.1004-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.100	1.00	3106.3	.1004-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.100	.50	2545.3	.2000-01	.6000-02	.1224+00	.8849-01	.6974+00	.8362-02
1.500	10.00	4000.0	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	5.00	3451.7	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	1.00	2420.9	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	.50	2063.9	.5217-01	.9163-06	.1207+00	.5254-01	.6454+00	.7707-02
1.500	10.00	5000.0	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02
1.500	5.00	4326.0	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02
1.500	1.00	3062.7	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02
1.500	.50	2625.5	.4754-01	.2578-03	.1203+00	.4659-01	.6415+00	.7666-02

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13. ABSTRACT

An efficient method is presented for calculating equilibrium chemical composition at a given pressure and stoichiometry with temperature, enthalpy, or entropy specified as the additional condition. A substantial reduction in computational time was achieved over conventional methods by employing a linearization technique and reducing the number of equations to be solved to a small number of linear algebraic equations. Examples are given for the H_2/O_2 system (six equations reduced to two) and $C/H_2/O_2/N_2/Ar$ system (eleven equations reduced to three). A computer program is presented for solving problems with fuels which involve C and H (hydrocarbon or hydrogen) or N and H (such as hydrazine) and with oxidants such as O_2, H_2O_2, and HNO_3. Extension of the method to include other systems is explained in sufficient detail to eliminate the requirement for an extensive knowledge of chemistry by potential users.

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