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A PROCEDURE FOR RAPID COMPUTATION OF EQUILIBRIUM CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF THE GENERALIZED ARGON-NITROGEN-OXYGEN-HYDROGEN GAS SYSTEM

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16. Abstract

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A PROCEDURE FOR RAPID COMPUTATION OF EQUILIBRIUM CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF THE GENERALIZED ARGON-NITROGEN-OXYGEN-HYDROGEN GAS SYSTEM

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SUMMARY

A procedure is described for the rapid computation of the equilibrium chemical composition and thermodynamic properties of the generalized argon-nitrogen-oxygen-hydrogen gas mixture system for nonionized conditions. The procedure employs a variation of the Newton iteration scheme to solve for chemical composition. The generalized model reduces to the hydrogen-air, hydrogen-oxygen, pure hydrogen, and equilibrium air systems. A computer program listing of the calculation procedure for this gas model is presented.

INTRODUCTION

The calculation of thermodynamic properties of combustion gas mixtures at high temperatures is complex, difficult, and time consuming. These difficulties arise primarily because of the determination of equilibrium chemical composition which requires the solution of a system of equations that are not simultaneously linear. In the past, iterative methods of solution such as those summarized in reference 1 have been used extensively. However, these methods have proved to be so time consuming as to preclude their direct use in calculations of engine performance, flow-field properties, and kinetic processes. As a result, the thermodynamic properties of combustion gases calculated by these methods have been presented in tabular form in the literature. For example, reference 2 is an elaborate treatment of the hydrogen-air system. To apply the results of reference 2 to more complicated problems requiring solutions by computer, the user is compelled to fit curves to the gas mixture thermodynamic properties; thus, this technique sacrifices generality, computer storage, and, most important, accuracy.

In reference 3, a new method was developed to calculate chemical composition. The method employs the Newton iteration scheme and is as much as two orders of magnitude faster in computational time than previous methods. A variation of the Newton iteration scheme has been applied with success to the simplified hydrocarbon-air combustion gas model of reference 4. The assumption of reference 4 is that atomic nitrogen

species form in negligible amounts in the range of operation of air-breathing propulsion engines and, therefore, have a small effect on the performance of these engines. However, the formation of atomic nitrogen species, such as ON and N, is important for hypersonic engine nozzle calculations which include the effects of chemical kinetics (ref. 5). During the study of reference 4 it was found that the atomic nitrogen species could be included within the framework of the same iteration scheme if carbon species were neglected.

The considerable improvement in speed of solution realized by the use of the Newton iteration scheme for the simplified hydrocarbon-air combustion gas model in reference 4 makes it desirable to extend the procedure to other gas models. The gas model of the present study includes the formation of the following chemical species:

$$O, N, Ar, H, O_2, N_2, H_2, ON, OH, H_2O$$

The computer program presented in appendix A is geared toward a generalized approach to the argon-nitrogen-oxygen-hydrogen system in that the initial proportions of atoms are input variables. This procedure allows the automatic reduction of the general gas model to the hydrogen-air, hydrogen-oxygen, pure oxygen, pure hydrogen, and equilibrium air systems. This feature permits the effect of secondary injection of oxygen or hydrogen peroxide to be taken into account. Thrust augmentation by secondary injection has been considered for some hypersonic engine cycles.

The computer program can be readily incorporated as a subroutine to a larger program or used alone to generate Mollier diagrams. Inputs to the program are the ratio of nitrogen atoms to oxygen atoms, the ratio of argon atoms to oxygen atoms, equivalence ratio, temperature, and pressure.

SYMBOLS

A, B coefficients of iteration functions

$C = 1 + 2r_{Ar} + r_N$

c_p specific heat at constant pressure, Btu/lbm-^oR (J/kg-^oK)

G Gibbs free energy, Btu/lbm (J/kg)

H enthalpy, Btu/lbm (J/kg)

K	equilibrium constant in terms of partial pressures; numerical subscripts indicate individual reaction
M	mean molecular weight
p	pressure, atm
R	universal gas constant, 1.98588 Btu/mole-^{o}R (8.314 J/mole-^{o}K)
r_{Ar}	ratio of argon atoms to oxygen atoms
r_{eq}	equivalence ratio
r_{N}	ratio of nitrogen atoms to oxygen atoms
S	entropy, Btu/lbm-^{o}R (J/kg-^{o}K)
T	temperature, ^{o}R (^{o}K)
X	mole fraction

Subscripts:

I	Ith temperature
J	Jth species

Superscript:

o	at reference pressure of 1 atmosphere (1.01325×10^5 N/m^2)

ANALYTICAL APPROACH

The general equations presented in this analysis for computing chemical composition and combustion gas properties make use of the following assumptions:

(1) The derived gas mixtures simulate the products of complete, constant-pressure, adiabatic combustion.

(2) The gas mixtures are in thermal and chemical equilibrium.

(3) The ideal gas equation of state is valid and only gas phases are considered.

(4) The effects of ionization are ignored.

With these general assumptions the determination of chemical composition must be accomplished in the presence or absence of dissociation. Once the chemical composition is determined and the thermodynamic properties of the pure constituent are provided, the thermodynamic properties of the gas mixture can be established.

Chemical Composition

The chemical species assumed for the gas model of this analysis are

$$O, N, Ar, H, O_2, N_2, H_2, ON, OH, H_2O$$

The solution of this system is centered about the Newton iteration scheme as suggested in reference 3. However, the inordinate amount of labor required to reduce the equations which represent this system to a single iteration equation was impractical. As a result, the equations were reduced to two equations and two unknowns. Newton's iteration scheme is then applied to the two equations simultaneously, in a manner similar to that presented in reference 4. It should be emphasized that rapid convergence is not necessarily assured when employing the Newton iteration scheme becuase of the highly nonlinear character of the equations. With this observation in mind, the governing equations for the solution of chemical composition can now be developed.

In a system of 10 chemical species and four chemical elements, there are six independent chemical reactions which can be written with the corresponding equilibrium expressions as

$2O = O_2$	(1) $X_{O_2} = pK_5X_O^2$
$2N = N_2$	(2) $X_{N_2} = pK_6X_N^2$
$2H = H_2$	(3) $X_{H_2} = pK_7X_H^2$
$O + N = ON$	(4) $X_{ON} = pK_8X_OX_N$
$O + H = OH$	(5) $X_{OH} = pK_9X_OX_H$
$O + 2H = H_2O$	(6) $X_{H_2O} = p^2K_{10}X_OX_H^2$

Application of the conservation of mass for each chemical element gives

$$(7)\quad \sum_J X_J = 1$$

$$(8)\quad X_N + 2X_{N_2} + X_{ON} = r_N\left(X_O + 2X_{O_2} + X_{ON} + X_{OH} + X_{H_2O}\right)$$

$$(9)\quad X_{Ar} = r_{Ar}\left(X_O + 2X_{O_2} + X_{ON} + X_{OH} + X_{H_2O}\right)$$

$$(10)\quad X_H + 2X_{H_2} + X_{OH} + 2X_{H_2O} = 2r_{eq}\left(X_O + 2X_{O_2} + X_{ON} + X_{OH} + X_{H_2O}\right)$$

Solving for two equations and two unknowns in X_O and X_H yields

$$\alpha = A_{40}X_O^4 + \left(A_{32}X_H^2 + A_{31}X_H + A_{30}\right)X_O^3 + \left(A_{24}X_H^4 + A_{23}X_4^3 + A_{22}X_H^2 + A_{21}X_H + A_{20}\right)X_O^2$$
$$+\left(A_{14}X_H^4 + A_{13}X_H^3 + A_{12}X_H^2 + A_{11}X_H + A_{10}\right)X_O + \left(A_{04}X_H^4 + A_{03}X_H^3 + A_{02}X_H^2 + A_{01}X_H + A_{00}\right) = 0$$

$$\beta = \left(B_{22}X_O^2 + B_{21}X_O + B_{20}\right)X_H^2 + \left(B_{12}X_O^2 + B_{11}X_O + B_{10}\right)X_H + \left(B_{02}X_O^2 + B_{01}X_O\right) = 0$$

where

$$A_{40} = C^2p^3K_5\left(4K_5K_6 - K_8^2\right)$$

$$A_{32} = Cp^4K_{10}\left[4(1 + C)K_5K_6 - \left(1 + r_{Ar}\right)K_8^2\right]$$

$$A_{31} = Cp^3K_9\left[4(1 + C)K_5K_6 - \left(1 + r_{Ar}\right)K_8^2\right]$$

$$A_{30} = Cp^2\left[4(1 + C)K_5K_6 - \left(1 + r_{Ar}\right)K_8^2 + 2\left(r_{Ar} - C\right)K_5K_8\right]$$

$$A_{24} = (1 + C)^2p^5K_6K_{10}^2$$

$$A_{23} = 2(1 + C)^2p^4K_6K_9K_{10}$$

$$A_{22} = p^3\left\{2(1 + C)^2K_6K_{10} + 8CK_5K_6K_7 + (1 + C)^2K_6K_9^2 + C\left[C - 2\left(1 + r_{Ar}\right)\right] + K_7K_8^2\right.$$
$$\left. + \left[2C\left(1 + r_{Ar}\right) - (1 + C)\left(1 + C + r_{Ar}\right)\right]K_8K_{10}\right\}$$

$$A_{21} = p^2\left\{8CK_5K_6 + 2(1 + C)^2K_6K_9 + C\left[C - 2\left(1 + r_{Ar}\right)\right]K_8^2 + \left[2C\left(1 + r_{Ar}\right) - (1 + C)\left(1 + C + r_{Ar}\right)\right]K_8K_9\right\}$$

$$A_{20} = p^2\left\{C\left[2\left(1 + r_{Ar}\right) - C\right]K_8^2 - 8CK_5K_6\right\} + p\left\{\left(1 + 2r_{Ar} - 2C\right)K_5 + (1 + C)^2K_6 + \left[2C\left(1 + r_{Ar}\right) - (1 + C)\left(1 + C + r_{Ar}\right)\right]K_8\right\}$$

$$A_{14} = 4(1 + C)p^4K_6K_7K_{10}$$

$$A_{13} = 4(1 + C)p^3K_6\left(K_{10} + K_7K_9\right)$$

$$A_{12} = p^2\left[4(1 + C)K_6K_7 + 4(1 + C)K_6K_9 + \left(r_{Ar} - C\right)K_{10} - 2\left(1 + r_{Ar}\right)K_7K_8\right] - 4p^3(1 + C)K_6K_{10}$$

$$A_{11} = p\left[4(1 + C)K_6 - 2\left(1 + r_{Ar}\right)K_8 + \left(r_{Ar} - C\right)K_9\right] - 4(1 + C)p^2K_6K_9$$

$$A_{10} = p\left[2\left(1 + r_{Ar}\right)K_8 - 4(1 + C)K_6\right] + \left(r_{Ar} - C\right)$$

$$A_{04} = 4p^3K_6K_7^2$$

$$A_{03} = 8p^2K_6K_7$$

$$A_{02} = p\left(4K_6 - K_7\right) - 8p^2K_6K_7$$

$$A_{01} = -1 - 8pK_6$$

$$A_{00} = 4pK_6 + 1$$

and

$$B_{22} = -2(r_{eq} + C)p^3K_8K_{10}$$

$$B_{21} = -2p^2\left[(2r_{eq} + C)K_7K_8 + (1 - r_{eq})K_{10}\right]$$

$$B_{20} = -2pK_7$$

$$B_{12} = -(2r_{eq} + C)p^2K_8K_9$$

$$B_{11} = -(1 - 2r_{eq})pK_9 - (4r_{eq} + C)pK_8$$

$$B_{10} = -1$$

$$B_{02} = -2r_{eq}p(K_8 - 2K_5)$$

$$B_{01} = 2r_{eq}(2pK_8 + 1)$$

$$C = 1 + 2r_{Ar} + r_N$$

Since the expression for β is second order, it can be satisfied by the quadratic formula if one unknown is assumed. The resulting pair of values (X_O, X_H) can then be tested for compliance with α within the desired accuracy. Although there may be a number of pairs of values (X_O, X_H) which satisfy $\alpha = 0$, only one pair satisfies the condition $0 \leqq X_J \leqq 1$. For $r_{eq} \leqq 1$, X_O was chosen to be the iteration variable.

Newton's iteration scheme in two variables can be written as

$$X_O(L + 1) = X_O(L) - \frac{\alpha\left[X_O(L), X_H(L)\right]}{\frac{d}{dX_O}\left\{\alpha\left[X_O(L), X_H(L)\right]\right\}}$$

where $X_O(L)$ is the Lth approximation of X_O and the derivative of $\alpha(X_O, X_H)$ with respect to X_O is

$$\frac{d}{dX_O}\left\{\alpha\left[X_O(L), X_H(L)\right]\right\} = \frac{\partial\alpha}{\partial X_O} - \frac{\partial\alpha}{\partial X_H}\left(\frac{\frac{\partial\beta}{\partial X_O}}{\frac{\partial\beta}{\partial X_H}}\right)$$

For $r_{eq} > 1$, X_H was chosen to be the iteration variable since α and β were insensitive to changes in X_O in this region.

Because of the highly nonlinear character of this system and the presence of extraneous solutions in the neighborhood of the correct solution, an arbitrary choice of an initial value for the iteration scheme was wholly inadequate. Rapid convergence by Newton's iteration scheme can be realized only when the function is nearly linear or an initial estimate is chosen in the neighborhood of the solution. As a result, considerable intelligence has been built into the selection of the initial value of the iteration to insure that it is approximately equal to the correct solution over the entire range of variables.

The choice of an initial value in the neighborhood of the solution has been made by formulating a simplified gas model for a particular region of equivalence ratio. The simplified models chosen were those which would provide a solution in a closed-form expression. For example, in the region $r_{eq} < 1$, the following simplified gas model was chosen:

$$H_2O, O_2, O, N_2, Ar$$

In general, the simplified models chosen for the initial iteration values give results nearly equal to the solution for the entire system. However, correction factors were necessary to insure convergence to the correct solution. The simplified gas models and correction factors are developed in detail in appendix B.

Below $T_{cut\text{-}off}$ $\left(T_{cut\text{-}off} = 100 \log_{10} p + 2800\right)$, the gas mixture is assumed to be nondissociating. The cut-off temperature is an arbitrarily defined temperature below which the effects of dissociation can be neglected. Below this temperature limit, the initial proportions of elements are sufficient to define the gas composition.

Chemical species assumed for the simplified gas model in the region $T \leq T_{cut\text{-}off}$ are

$$A_r, O_2, N_2, H_2, H_2O$$

and the mass conservation equations are

$$\sum_J X_J = 1$$

$$2X_{N_2} = r_N\left(2X_{O_2} + X_{H_2O}\right)$$

$$X_{Ar} = r_{Ar}\left(2X_{O_2} + X_{H_2O}\right)$$

$$2X_{H_2} + 2X_{H_2O} = 2r_{eq}\left(2X_{O_2} + X_{H_2O}\right)$$

Although there seems to be one less equation than required, in each region of equivalence ratio one or more species can be neglected. For $r_{eq} \leq 1$,

$$X_{H_2} = 0 \qquad X_{H_2O} = \frac{2r_{eq}}{C + r_{eq}}$$

For $r_{eq} > 1$,

$$X_{O_2} = 0 \qquad X_{H_2O} = \frac{2}{C + 2r_{eq} - 1}$$

At low temperatures for fuel-rich mixtures ammonia may form in substantial amounts. In the present study, the formation of ammonia is handled just as is done in reference 4, that is, the computer program indicates the formation of ammonia by an error statement. When the limiting pressure for ammonia formation is exceeded, the error statement is printed, but the program computes chemical composition as though ammonia had not formed.

Thermodynamic Properties of Pure Constituents

The standard reference states of the elements Ar, N, O, H taken from reference 2 are as follows:

Ar as Ar

N as N_2

O as O_2

H as H_2

By definition, the energy content of these elements in their standard reference states ($T = 0^{o}$ R) is zero.

The specific heat at constant pressure for each species $\left(\frac{c_{p,J}}{R}\right)$ is also taken from reference 2 and tabulated in the computer program as a function of temperature. The thermodynamic properties of the pure constituents $\left(\frac{H^{o}_{J}}{R}, \frac{S^{o}_{J}}{R}\right)$ are obtained by numerical integration in the form

$$\frac{H^{o}_{I,J}}{R} = \frac{H^{o}_{I-1,J}}{R} + \left(\frac{c_{p_{I,J}} + c_{p_{I-1,J}}}{2}\right)\left(T_I - T_{I-1}\right)$$

$$\frac{S^o_{I,J}}{R} = \frac{S^o_{I-1,J}}{R} + \left(cp_{I,J} + cp_{I-1,J}\right)\left(\frac{T_I - T_{I-1}}{T_I + T_{I+1}}\right)$$

The thermodynamic properties of the pure constituents obtained in this manner agree with those tabulated in reference 2 within four significant figures. With the thermodynamic properties of the pure constituents defined, the equilibrium constants can be formed. For a general reaction, the equilibrium expression is

$$aA + bB = cC + dD$$

and the equilibrium constant is

$$K = \exp\left(-\left[c\,\frac{G^o_C}{RT} + d\,\frac{G^o_D}{RT} - a\,\frac{G^o_A}{RT} - b\,\frac{G^o_B}{RT}\right]\right)$$

where

$$\frac{G^o_J}{RT} = \frac{H^o_J}{RT} - \frac{S^o_J}{R}$$

Thermodynamic Properties of Gas Mixtures

The foregoing equations have outlined the solution for gas mixture composition. With the chemical composition defined and the thermodynamic properties of the pure constituents provided, the thermodynamic properties of a gas mixture can be calculated by the following equations (ref. 2):

$$M = \sum_J X_J M_J$$

$$H = \frac{R}{M}\sum_J X_J \frac{H^o_J}{R}$$

$$S = \frac{R}{M}\sum_J X_J\left(\frac{S^o_J}{R} - \ln p - \ln X_J\right)$$

where $\frac{H^o_J}{R}$ and $\frac{S^o_J}{R}$ are the thermodynamic properties of the pure constituents at reference pressure (1 atm). These thermodynamic expressions inherently assume that the pure constituents obey the perfect gas law.

A listing of the computer program to calculate the composition and thermodynamic properties of the argon-nitrogen-oxygen-hydrogen gas model is presented and discussed in appendix A. Computational time for obtaining the chemical composition and thermodynamic properties with this program has been estimated at 12 000 cases/min on the Control Data 6600 computer system at the Langley Research Center.

RESULTS

The computer program for the present gas model was run over a wide range of input variables to establish its reliability. All combinations of the following variables were computed:

Variable	Range	Increment
r_N	0 to 5	1
r_{Ar}	0	0
r_{eq}	0 to 1	0.1
	1 to 9	1
T	$T_{cut\text{-}off}$ to 10 000° R (5556° K)	200° R (111° K)
p	0.001 to 100 atm	Orders of magnitude

For all these variable combinations, the iteration procedure converged to the proper solution with an over-all average of five iterations per case.

This program has been used to calculate the chemical composition and thermodynamic properties of hydrogen-air combustion. The results are presented in tables I, II, and III for equivalence ratios of 0 (air), 1, and 2.5, respectively. Ranges of temperature and pressure are also included. Results from the tabulations of reference 2 are presented for comparison. The good agreement between gas models is not surprising, since the present model assumes the same chemical species with the exception of NH and NH_3, both of which form in negligible amounts.

The values in table III for $r_{eq} = 2.5$, $T = 6000°$ R (3333° K), $p = 0.001$ atm and $r_{eq} = 2.5$, $T = 10\ 000°$ R (5556° K), $p = 100$ atm show substantial disagreement with those of reference 2. In a localized temperature range for fuel-rich mixtures at extreme pressures, the value of X_O in the quadratic expression for β is imaginary. For these cases, the radical term is deleted so that solutions can be obtained. The computer program prints an error statement to alert the user that results should be viewed with caution since they may be substantially in error.

CONCLUDING REMARKS

A rapid computational procedure has been developed to determine the equilibrium chemical composition and thermodynamic properties of the generalized argon-nitrogen-oxygen-hydrogen gas system. This system includes the formation of the following chemical species:

$$O, N, Ar, H, O_2, N_2, H_2, ON, OH, H_2O$$

Newton's iteration scheme is employed to calculate chemical composition with initial estimates being obtained from the solution of a simplified gas model. Chemical composition is determined within five significant figures with an average of five iterations being required per case.

The reliability of the computational procedure was established over a wide range of input variables. The computer program for this gas model has been used to calculate the chemical composition and thermodynamic properties of the hydrogen-air system for a range of variables. The results agree with those obtained by more comprehensive treatments.

The automatic reduction of the generalized gas model to such systems as hydrogen-air, hydrogen-oxygen, oxygen, hydrogen, and air facilitates the computation of thermodynamic processes involving the secondary ejection of additional fuel and/or oxidizers. This feature should prove useful when determining the performance of air-breathing engine cycles which employ forms of thrust augmentation.

Langley Research Center,
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APPENDIX A

COMPUTER PROGRAM FOR CALCULATING CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF THE Ar-N-O-H GAS SYSTEM

The calculation procedure described in the main body of the paper for obtaining the chemical composition and thermodynamic properties of this reacting gas mixture has been programed for high-speed digital computation. The purpose of this appendix is to provide a description of the necessary input and available output as well as a FORTRAN IV (ref. 6) listing of the source program. An example input case and the resulting output listing are included.

Description of Program

The program reads in the necessary reference enthalpy and Gibbs free energy and the specific heat at constant pressure of each chemical specie as a function of temperature. The variation of enthalpy and entropy for each specie at reference pressure (1 atm) is generated over the full temperature range by numerical integration. The program then reads the initial proportions of atoms, temperature, and pressure. With temperature known, the thermodynamic properties of the individual species are interpolated linearly. The Gibbs free energy, equilibrium constants, and the coefficients of the iteration functions are computed. The iteration for chemical composition is performed. With the chemical composition defined, the thermodynamic properties of the gas mixture are then calculated.

Program Listing

The FORTRAN listing of the source program used at the Langley Research Center on the Control Data series 6000 computer systems is as follows:

APPENDIX A

```
C     THERMODYNAMIC PROPERTIES OF ARGON-NITROGEN-OXYGEN-HYDROGEN SYSTEM
C  O     N     AR    H     O2    N2    H2    ON    OH    H2O
C X(1)  X(2)  X(3)  X(4)  X(5)  X(6)  X(7)  X(8)  X(9)  X(10)
      DIMENSION X(99),Y(99),Z(99),E(99),CP(110,10),H(110,10),HT(110,10),
     1S(110,10),ST(110,10),G(110,10),GT(110,10),TT(110),HR(10),
     2SR(10),GRT(10),MR(10)
      DATA(MR(J),J=1,10)/16.,14.008,39.944,1.008,32.,28.016,2.016,
     130.008,17.008,18.016/
      REAL K5,K6,K7,K8,K9,K10,MM,MR
      NAMELIST/NUM1/HT,GT,CP
      NAMELIST/NUM2/RN,RAR,REQ,T,P
      READ(5,NUM1)
      J=1
   43 I=1
      TT(1)=200.
      H(1,J)=HT(1,J)*200.
      G(1,J)=GT(1,J)
      S(1,J)=HT(1,J)-GT(1,J)
      ST(1,J)=S(1,J)
   41 IF(I.EQ.106)GO TO 42
      I=I+1
      TT(I)=TT(I-1)+100.
      H(I,J)=H(I-1,J)+(CP(I,J)+CP(I-1,J))/2.*(TT(I)-TT(I-1))
      S(I,J)=S(I-1,J)+(CP(I,J)+CP(I-1,J))*(TT(I)-TT(I-1))/(TT(I)+TT(I-1)
     1)
      HT(I,J)=H(I,J)/TT(I)
      ST(I,J)=S(I,J)
      GT(I,J)=HT(I,J)-ST(I,J)
      GO TO 41
   42 IF(J.EQ.10)GO TO 500
      J=J+1
      GO TO 43
  500 READ(5,NUM2)
  100 FORMAT(5E16.8)
      IF(EOF,5)400,401
  400 STOP
  401 DO 12 J=1,12
   12 X(J)=0.
      PRINT 300,RN,RAR,REQ,T,P
  300 FORMAT(8X3HRN=E15.8,4X4HRAR=E15.8,4X4HREQ=E15.8/20X2HT=E15.8,1HK,
     14X2HP=E15.8,3HATM/)
      DO 44 I=1,110
      IF(T-TT(I))45,45,44
   44 CONTINUE
   45 K=I-1
      DELH=(T-TT(K))/(TT(I)-TT(K))
      DELS=(ALOG(T/TT(K)))/(ALOG(TT(I)/TT(K)))
      DO 46 J=1,10
      HR(J)=(HT(K,J)+(HT(I,J)-HT(K,J))*DELH)*T
```

APPENDIX A

```
      SR(J)=ST(K,J)+(ST(I,J)-ST(K,J))*DELS
      GRT(J)=HR(J)/T-SR(J)
   46 CONTINUE
      C=1.+2.*RAR+RN
      IF(T.LT.(100.*ALOG10(P)+2800.))GO TO 30
      IF(REQ.EQ.0.)GO TO 1
      K7=EXP(GRT(4)*2.-GRT(7))
      K9=EXP(GRT(1)+GRT(4)-GRT(9))
      K10=EXP(GRT(4)*2.+GRT(1)-GRT(10))
      GO TO 2
    1 K7=0.
      K9=0.
      K10=0.
    2 IF(RN.EQ.0.)GO TO 3
      K6=EXP(GRT(2)*2.-GRT(6))
      K8=EXP(GRT(1)+GRT(2)-GRT(8))
      GO TO 4
    3 K6=0.
      K8=0.
      IF(REQ.GT.20.)X(4)=(SQRT(1.+4.*P**K7)-1.)/(2.*P**K7)
      IF(REQ.GT.20.)X(7)=1.-X(4)
      IF(REQ.GT.20.)GO TO 11
    4 K5=EXP(GRT(1)*2.-GRT(5))
      A40=C*C*P**3*K5*(4.*K6-K8*K8/K5)/10.**20
      A32=C*P**4*K10*(4.*(1.+C)*K6-(1.+RAR)*K8*K8/K5)/10.**20
      A31=C*P**3*K9*(4.*(1.+C)*K6-(1.+RAR)*K8*K8/K5)/10.**20
      A30=C*P**2*(4.*(1.+C)*K6-(1.+RAR)*K8*K8/K5+2.*(RAR-C)*K8)/10.**20
      A24=(1.+C)**2*P**5*K6*K10*K10/(K5*10.**20)
      A23=2.*(1.+C)**2*P**4*K6*K9*K10/(K5*10.**20)
      A22=P**3*(2.*(1.+C)**2*K6*K10/(K5*10.**20)+8.*C*K6*K7/10.**20+(1.
     1+C)**2*K6*K9*K9/(K5*10.**20)+C*(C-2.*(1.+RAR))*K7*K8*K8/(K5*10.
     2**20)+(2.*C*(1.+RAR)-(1.+C)*(1.+C+RAR))*K8*K10/(K5*10.**20))
      A21=P**2*(8.*C*K6/10.**20+2.*(1.+C)**2*K6*K9/(K5*10.**20)+C*(C-2.*
     1(1.+RAR))*K8*K8/(K5*10.**20)+(2.*C*(1.+RAR)-(1.+C)*(1.+C+RAR))*K8
     2*K9/(K5*10.**20))
      A20=(P**2*(C*(2.*(1.+RAR)-C)*K8*K8/K5-8.*C*K6)+P*((1.+2.*RAR-2.*C)
     1+(1.+C)**2*K6/K5+(2.*C*(1.+RAR)-(1.+C)*(1.+C+RAR))*K8/K5))/10.**20
      A14=4.*(1.+C)*P**4*K6*K7*K10/(K5*10.**20)
      A13=4.*(1.+C)*P**3*K6*(K10+K7*K9)/(K5*10.**20)
      A12=(P**2*(4.*(1.+C)*K6*K7/K5+4.*(1.+C)*K6*K9/K5+(RAR-C)*K10/K5-2.
     1*(1.+RAR)*K7*K8/K5)-4.*P**3*(1.+C)*K6*K10/K5)/10.**20
      A11=(P*(4.*(1.+C)*K6/K5-2.*(1.+RAR)*K8/K5+(RAR-C)*K9/K5)-4.*(1.+C)
     1*P**2*K6*K9/K5)/10.**20
      A10=(P*(2.*(1.+RAR)*K8-4.*(1.+C)*K6)+(RAR-C))/(K5*10.**20)
      A04=4.*P**3*K6*K7*K7/(K5*10.**20)
      A03=8.*P**2*K6*K7/(K5*10.**20)
      A02=(P*(4.*K6-K7)/K5-8.*P**2*K6*K7/K5)/10.**20
      A01=-1.*(1.+8.*P*K6)/(K5*10.**20)
      A00=(4.*P*K6+1.)/(K5*10.**20)
      B22=2.*(REQ+C)*P**3*K8*K10/K5
      B21=2.*P**2*((2.*REQ+C)*K7*K8/K5+(1.-REQ)*K10/K5)
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      B20=2.*P*K7/K5
      B12=(2.*REQ+C)*P**2*K8*K9/K5
      B11=P*((1.-2.*REQ)*K9+(4.*REQ+C)*K8)/K5
      B10=1./K5
      B02=2.*REQ*P*(K8/K5-2.)
      B01=-2.*REQ*(2.*P*K8+1.)/K5
      L=1
      IF(REQ-1.)6,5,13
    6 Y(1)=(SQRT((1.+C)**2+16.*P*K5*(1.-REQ)*(C+REQ))-(1.+C))
     1/(4.*P*K5*(C+REQ))*(1.1-.5E-4*T)
      GO TO 7
    5 Y(1)=1./((2.*(1.+C)*P**2*K10)**(1./3.))*(.34-.2E-4*T)
      GO TO 7
   13 Z(1)=(SQRT((4.*REQ+1.+C)**2+32.*REQ*(2.*REQ+1.+C)*P*K7)-(4.*REQ+1.
     1+C))/(4.*P*K7*(2.*REQ+1.+C))
      ICODE=0
      GO TO 16
    7 IF(Y(1).LT.(1./(1.+RN+RAR+2.*REQ)))GO TO 16
      Y(1)=1./(1.+RN+RAR+2.*REQ)
   16 IF(REQ.EQ.0.)GO TO 10
      IF(REQ.GT.1.)GO TO 15
      B=(Y(L)*(Y(L)*B12+B11)+B10)**2-4.*(Y(L)*(Y(L)*B22+B21)+B20)*(Y(L)
     1*(Y(L)*B02+B01))
      Z(L)=(+1.*SQRT(B)-1.*(Y(L)*(Y(L)*B12+B11)+B10))/((Y(L)*(Y(L)*B22
     1+B21)+B20)*2.)
      GO TO 9
   15 B=(Z(L)*(Z(L)*B21+B11)+B01)**2-4.*(Z(L)*(Z(L)*B22+B12)+B02)*(Z(L)
     1*(Z(L)*B20+B10))
      IF(B.LT.0.)GO TO 20
   22 IF(RN.EQ.0.)GO TO 21
      IF(ICODE.EQ.1)GO TO 21
      Y(L)=(-1.*SQRT(B)+1.*(Z(L)*(Z(L)*B21+B11)+B01))/((Z(L)*(Z(L)*B22+
     1B12)+B02)*(-2.))
      IF(Y(L).GT.Z(L))GO TO 21
      GO TO 9
   21 Y(L)=(+1.*SQRT(B)+1.*(Z(L)*(Z(L)*B21+B11)+B01))/((Z(L)*(Z(L)*B22+
     1B12)+B02)*(-2.))
      ICODE=1
      GO TO 9
   10 Z(L)=0.
    9 F(L)=Y(L)*(Y(L)*(Y(L)*(Y(L)*A40+Z(L)*(Z(L)*A32+A31)+A30)+Z(L)*(
     1Z(L)*(Z(L)*(Z(L)*A24+A23)+A22)+A21)+A20)+Z(L)*(Z(L)*(Z(L)*(Z(L)*
     2A14+A13)+A12)+A11)+A10)+Z(L)*(Z(L)*(Z(L)*(Z(L)*A04+A03)+A02)+A01)
     3+A00
      IF(L.EQ.50)GO TO 500
      DADY=Y(L)*(Y(L)*(Y(L)*4.*A40+3.*(Z(L)*(Z(L)*A32+A31)+A30))+2.*(
     1Z(L)*(Z(L)*(Z(L)*(Z(L)*A24+A23)+A22)+A21)+A20))+Z(L)*(Z(L)*(Z(L)*(
     2Z(L)*A14+A13)+A12)+A11)+A10
      DADZ=Y(L)*(Y(L)*(Y(L)*(2.*A32*Z(L)+A31)+Z(L)*(Z(L)*(Z(L)*4.*A24+
     1A23*3.)+2.*A22)+A21)+Z(L)*(Z(L)*(Z(L)*4.*A14+3.*A13)+2.*A12)+A11
     2)+Z(L)*(Z(L)*(Z(L)*4.*A04+A03*3.)+2.*A02)+A01
```

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      DRDY=Z(L)*(Z(L)*(2.*B22*Y(L)+B21)+2.*B12*Y(L)+B11)+2.*B02*Y(L)+B01
      DRDZ=2.*Z(L)*(Y(L)*(Y(L)*B22+B21)+B20)+Y(L)*(Y(L)*B12+B11)+B10
      IF(REQ.GT.1.)GO TO 14
      Y(L+1)=Y(L)-F(L)/(DADY-DADZ*DRDY/DRDZ)
      IF(((Y(L+1)/Y(L)).LT.1.00010).AND.((Y(L+1)/Y(L)).GT..99990))GO TO 8
      L=L+1
      GO TO 16
   14 Z(L+1)=Z(L)-F(L)/(DADZ-DADY*DRDZ/DRDY)
      IF((ICODE.EQ.0).AND.((DADZ-DADY*DRDZ/DRDY).LT.0.))GO TO 25
      IF((ICODE.EQ.1).AND.((DADZ-DADY*DRDZ/DRDY).GT.0.))GO TO 26
      IF(((Z(L+1)/Z(L)).LT.1.00010).AND.((Z(L+1)/Z(L)).GT..99990))GO TO 8
      L=L+1
      GO TO 16
   23 Y(L)=.9*Y(L)
      GO TO 16
   26 Z(L)=.9*Z(L)
      GO TO 16
   25 Z(L)=1.01*Z(L)
      GO TO 16
   20 B=.001
      PRINT 200
  200 FORMAT(20X27H*** RADICAL LESS THAN 0 ***)
      GO TO 22
   27 Z(L)=.9*Z(L)
      GO TO 16
   30 IF(REQ.GT.1.)GO TO 31
      X(10)=2.*REQ/(C+REQ)
      X(5)=(1.-REQ)/(C+REQ)
      GO TO 11
   31 IF(REQ.GT.20.)X(7)=1.
      IF(REQ.GT.20.)GO TO 11
      X(10)=2./(C+2.*REQ-1.)
      X(7)=(REQ-1.)*X(10)
      X(6)=(RN*(X(1)+2.*X(5)+X(8)+X(9)+X(10))-(X(8)+X(2)))/2.
      AMK=10.**((10114./T)-12.089)
      PLIM=.01/(SQRT(AMK*X(6)*X(7)**3))
      IF(P.LT.PLIM)GO TO 11
      PRINT 600
  600 FORMAT(10X26H*** AMMONIA HAS FORMED ***)
      GO TO 11
    8 X(1)=Y(L)
      X(4)=Z(L)
      X(10)=P**2*K10*X(1)*X(4)**2
      X(5)=P*K5*X(1)**2
      X(9)=P*K9*X(4)*X(1)
      X(7)=P*K7*X(4)**2
      IF(RN.EQ.0.)GO TO 11
      X(2)=(2.-(1.+C)*X(10)-2.*C*X(5)-2.*X(7)-(1.+C)*X(1)-(1.+C)*X(9)
     1-2.*X(4))/(C*P**K8*X(1)+1.)
   11 X(8)=P*K8*X(1)*X(2)
      X(6)=(RN*(X(1)+2.*X(5)+X(8)+X(9)+X(10))-(X(8)+X(2)))/2.
```

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      X(3)=RAR*(X(1)+2.*X(5)+X(8)+X(9)+X(10))
      DO 24 J=1,10
      IF((X(J).LT.0.).AND.(RFQ.LE.1.))GO TO 23
   24 CONTINUE
      PRINT 700,(X(J),J=1,10)
  700 FORMAT(8X2HXQ,13X2HXN,13X3HXAR,13X2HXH,13X3HXQ2/5E16.8/6X3HXM2,
     113X3HX42,13X3HXQN,13X3HXQH,13X4HXH2Q/5E16.8/)
      MM=0.
      HM=0.
      SM=0.
      DO 47 J=1,10
      IF(X(J).EQ.0.)GO TO 47
      MM=MM+X(J)*MR(J)
      HM=HM+X(J)*HR(J)
      SM=SM+X(J)*(SR(J)-ALOG(P*X(J)))
   47 CONTINUE
      HM=(1.98588/MM)*HM
      SM=(1.98588/MM)*SM
      PRINT 800,MM,HM,SM
  800 FORMAT(4X3HMM=E15.8,2X3HHM=E15.8,7HBTU/LBM,2X3HSM=E15.8,9HBTU/LBM-
     1R//)
      GO TO 500
      END
```

APPENDIX A

Input

A single case consists of the determination of the thermodynamic properties of the reacting gas mixture, or of one point on a Mollier diagram. It is necessary to input the specific heat at constant pressure of each species as a tabular function of temperature, in addition to the initial atomic proportions, temperature, and pressure. For the loading routine used in the program, any column except the first may be used on the input cards. A decimal format is used for the input quantities. A description of the required inputs and the names used by the source program are as follows:

Name	Description
$NUM1	The arbitrary name required by the loading routine to define the input data block: specific heat at constant pressure and reference thermodynamic properties of each chemical species.
HT(1,J)	Reference enthalpy array for each species, nondimensional; $\frac{H^o_{1,J}}{RT}$.
GT(1,J)	Reference Gibbs free energy array for each species, nondimensional; $\frac{G^o_{1,J}}{RT}$.
CP(I,J)	Specific heat at constant pressure array for each species, nondimensional; $\frac{(c_p)_{I,J}}{R}$.
$	Denotes end of case (column 2).
$NUM2	The arbitrary name required by the loading routine to define the input block: initial proportion of atoms, temperature, and pressure.
RN	r_n
RAR	r_{Ar}
REQ	r_{eq}
T	T, ^oR
P	p, atmospheres
$	Denotes end of case (column 2).

The system loading subroutine in the program (NAMELIST) is quite flexible in that the order of the input cards is unimportant and successive cases can be run by repeating the identification and $NUM cards followed by only the changed parameters and a $ card. An example of a set of input cards is given by the following listing of the inputs necessary to compute the thermodynamic properties of the stoichiometric hydrogen-air mixture at a temperature of 5000^o R (2778^o K) and a pressure of 1 atm.

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```
$NUM1 HT(1,1)=269.79,HT(1,2)=512.08,HT(1,3)=2.5003,HT(1,4)=236.28,
HT(1,5)=3.4898,HT(1,6)=3.4855,HT(1,7)=3.7283,HT(1,8)=100.99,HT(1,9)=45.522,
HT(1,10)=-254.66,GT(1,1)=253.12,GT(1,2)=496.10,GT(1,3)=-13.666,GT(1,4)=224.94,
GT(1,5)=-17.746,GT(1,6)=-16.120,GT(1,7)=-8.8678,GT(1,8)=79.275,GT(1,9)=27.011,
GT(1,10)=-273.44,
CP(1,1)=2.8374,
              2.7715,2.7107,2.6522,2.6120,2.5884,2.5690,2.5568,2.5471,2.5393,
2.5336,2.5288,2.5249,2.5218,2.5195,2.5174,2.5155,2.5141,2.5128,2.5116,2.5106,
2.5098,2.5090,2.5081,2.5075,2.5070,2.5068,2.5064,2.5057,2.5054,2.5055,2.5053,
2.5050,2.5049,2.5050,2.5049,2.5050,2.5053,2.5056,2.5059,2.5061,2.5064,2.5070,
2.5080,2.5084,2.5092,2.5103,2.5114,2.5125,2.5138,2.5152,2.5166,2.5180,2.5197,
2.5214,2.5234,2.5254,2.5277,2.5299,2.5322,2.5344,2.5367,2.5391,2.5417,2.5445,
2.5473,2.5501,2.5530,2.5562,2.5591,2.5618,2.5652,2.5685,2.5715,2.5747,2.5781,
2.5814,2.5848,2.5882,2.5915,2.5949,2.5982,2.6016,2.6049,2.6083,2.6116,2.6150,
2.6183,2.6217,2.6251,2.6284,2.6318,2.6351,2.6385,2.6418,2.6452,2.6484,2.6514,
2.6544,2.6576,2.6611,2.6642,2.6668,2.6698,2.6729,2.6758,
CP(1,2)=31*2.4999,
                 2.5000,2.5004,2.5005,2.5004,2.5007,2.5010,2.5013,2.5015,2.5017,
2.5023,2.5033,2.5041,2.5050,2.5060,2.5072,2.5086,2.5101,2.5117,2.5137,2.5161,
2.5185,2.5211,2.5244,2.5278,2.5313,2.5352,2.5394,2.5439,2.5487,2.5539,2.5593,
2.5650,2.5711,2.5775,2.5842,2.5911,2.5986,2.6065,2.6147,2.6232,2.6317,2.6406,
2.6501,2.6599,2.6700,2.6802,2.6905,2.7013,2.7123,2.7237,2.7352,2.7469,2.7589,
2.7712,2.7837,2.7963,2.8091,2.8220,2.8351,2.8483,2.8613,2.8747,2.8885,2.9022,
2.9158,2.9297,2.9438,2.9577,2.9717,2.9857,2.9997,3.0136,3.0276,3.0416,3.0556,
CP(1,3)=106*2.4999,
CP(1,4)=106*2.4999,
CP(1,5)=3.5001,
              3.4995,3.5077,3.5223,3.5568,3.6099,3.6698,
       3.7393,3.8077,3.8721,3.9329,3.9883,4.0386,4.0841,4.1246,4.1616,4.1947,
4.2244,4.2518,
              4.2767,4.2999,4.3213,4.3417,4.3610,4.3795,4.3970,4.4146,4.4315,
4.4477,4.4639,4.4801,4.4962,4.5121,4.5278,4.5434,4.5588,4.5742,4.5896,4.6049,
4.6204,4.6356,4.6506,4.6656,4.6803,4.6953,4.7099,4.7241,4.7383,4.7523,4.7660,
4.7793,4.7927,4.8061,4.8188,4.8312,4.8436,4.8557,4.8674,4.8790,4.8904,4.9015,
4.9123,4.9227,4.9329,4.9431,4.9529,4.9624,4.9716,4.9805,4.9892,4.9978,5.0057,
5.0135,5.0210,5.0285,5.0358,5.0427,5.0494,5.0559,5.0622,5.0681,5.0740,5.0804,
5.0861,5.0909,5.0960,5.1010,5.1059,5.1106,5.1151,5.1195,5.1237,5.1278,5.1316,
5.1355,5.1395,5.1432,5.1468,5.1499,5.1529,5.1560,5.1591,5.1622,5.1650,5.1674,
5.1699,
CP(1,6)=3.5003,
              3.5005,3.5011,3.5012,3.5064,3.5150,3.5325,3.5577,3.5911,3.6290,
3.6727,3.7169,3.7627,3.8072,3.8511,3.8928,3.9326,3.9698,4.0048,4.0373,4.0678,
4.0964,4.1227,4.1468,4.1695,4.1907,4.2102,4.2285,4.2454,4.2613,4.2761,4.2900,
4.3029,4.3151,4.3266,4.3374,4.3477,4.3573,4.3663,4.3746,4.3827,4.3905,4.3978,
4.4046,4.4110,4.4174,4.4236,4.4295,4.4351,4.4404,4.4454,4.4500,4.4544,4.4590,
4.4633,4.4671,4.4711,4.4754,4.4793,4.4829,4.4863,4.4896,4.4930,4.4963,4.4998,
4.5029,4.5055,4.5085,4.5117,4.5145,4.5173,4.5205,4.5233,4.5254,4.5278,4.5304,
4.5329,4.5354,4.5377,4.5399,4.5421,4.5444,4.5471,4.5493,4.5512,4.5532,4.5551,
4.5572,4.5595,4.5665,4.5714,4.5737,4.5761,4.5782,4.5806,4.5832,4.5857,4.5882,
```

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```
4.5907,4.5933,4.5962,4.5988,4.6013,4.6039,4.6068,4.6096,
CP(1,7)=2.7955,
              3.1331,3.3547,3.4404,3.4995,3.5064,3.5173,
      3.5189,3.5224,3.5277,3.5346,3.5442,3.5561,3.5709,3.5885,3.6091,3.6326,
3.6577,3.6837,3.7107,3.7384,3.7670,3.7961,3.8260,3.8555,3.8847,3.9137,3.9422,
3.9703,3.9978,4.0247,4.0506,4.0756,4.1000,4.1238,4.1466,4.1690,4.1910,4.2122,
4.2324,4.2525,4.2724,4.2915,4.3100,4.3280,4.3456,4.3628,4.3795,4.3956,4.4115,
4.4271,4.4426,4.4579,4.4728,4.4875,4.5021,4.5164,4.5303,4.5445,4.5583,4.5721,
4.5857,4.5989,4.6120,4.6252,4.6382,4.6511,4.6638,4.6763,4.6887,4.7009,4.7134,
4.7255,4.7372,4.7489,4.7607,4.7724,4.7842,4.7957,4.8071,4.8184,4.8295,4.8403,
4.8512,4.8621,4.8730,4.8840,4.8947,4.9052,4.9156,4.9259,4.9363,4.9466,4.9570,
4.9672,4.9772,4.9871,4.9968,5.0067,5.0164,5.0258,5.0354,5.0453,5.0543,5.0639,
5.0731,
CP(1,8)=3.8505,
              3.7195,3.6342,3.6006,3.5865,3.5991,3.6252,3.6679,3.7173,3.7682,
3.8216,3.8728,3.9227,3.9691,4.0124,4.0522,4.0885,4.1217,4.1523,4.1801,4.2057,
4.2291,4.2507,4.2705,4.2886,4.3049,4.3222,4.3375,4.3503,4.3626,4.3745,4.3848,
4.3932,4.4022,4.4111,4.4197,4.4278,4.4354,4.4426,4.4492,4.4558,4.4622,4.4683,
4.4740,4.4794,4.4846,4.4896,4.4946,4.4997,4.5045,4.5089,4.5131,4.5173,4.5215,
4.5256,4.5295,4.5334,4.5374,4.5411,4.5447,4.5484,4.5520,4.5554,4.5587,4.5621,
4.5654,4.5688,4.5721,4.5755,4.5787,4.5817,4.5851,4.5884,4.5914,4.5945,4.5976,
4.6006,4.6037,4.6068,4.6099,4.6126,4.6155,4.6186,4.6217,4.6248,4.6277,4.6304,
4.6334,4.6365,4.6393,4.6421,4.6449,4.6477,4.6505,4.6534,4.6566,4.6595,4.6622,
4.6647,4.6673,4.6701,4.6729,4.6757,4.6784,4.6808,4.6835,
CP(1,9)=3.7042,
              3.6653,3.6321,3.6051,3.5823,3.5640,3.5526,
      3.5476,3.5469,3.5507,3.5591,3.5719,3.5895,3.6103,3.6346,3.6609,3.6895,
3.7194,3.7500,3.7815,3.8127,3.8438,3.8743,3.9045,3.9338,3.9622,3.9909,4.0168,
4.0428,4.0677,4.0917,4.1150,4.1375,4.1590,4.1796,4.1995,4.2186,4.2368,4.2546,
4.2720,4.2886,4.3043,4.3197,4.3346,4.3490,4.3631,4.3769,4.3902,4.4030,4.4156,
4.4278,4.4397,4.4514,4.4629,4.4742,4.4851,4.4959,4.5065,4.5170,4.5273,4.5375,
4.5475,4.5573,4.5670,4.5769,4.5865,4.5960,4.6055,4.6150,4.6245,4.6340,4.6436,
4.6530,4.6621,4.6715,4.6810,4.6905,4.7001,4.7096,4.7191,4.7286,4.7381,4.7476,
4.7571,4.7665,4.7762,4.7861,4.7957,4.8051,4.7960,4.7943,4.8029,4.8099,4.8165,
4.8232,4.8300,4.8363,4.8423,4.8483,4.8541,4.8597,4.8651,4.8705,4.8755,4.8802,
4.8847,
CP(1,10)=4.0048,
              4.0059,4.0143,4.0279,4.0598,4.1086,4.1662,
      4.2345,4.3064,4.3809,4.4583,4.5377,4.6192,4.7021,4.7867,4.8714,4.9566,
5.0412,5.1246,5.2071,5.2873,5.3654,5.4409,5.5139,5.5844,5.6525,5.7176,5.7800,
5.8394,5.8964,5.9509,6.0031,6.0529,6.1005,6.1456,6.1889,6.2303,6.2697,6.3075,
6.3435,6.3780,6.4110,6.4424,6.4722,6.5012,6.5290,6.5554,6.5810,6.6056,6.6291,
6.6515,6.6732,6.6941,6.7143,6.7337,6.7522,6.7703,6.7880,6.8048,6.8208,6.8365,
6.8516,6.8663,6.8807,6.8948,6.9083,6.9210,6.9337,6.9464,6.9580,6.9689,6.9806,
6.9917,7.0019,7.0123,7.0228,7.0325,7.0415,7.0509,7.0605,7.0687,7.0773,7.0860,
7.0949,7.1022,7.1100,7.1183,7.1257,7.1324,7.1377,7.1431,7.1484,7.1536,7.1586,
7.1637,7.1691,7.1743,7.1792,7.1846,7.1898,7.1948,7.1999,7.2049,7.2099,7.2150,
7.2200$
$NUM2 RN=3.727445,RAR=.02296952,REQ=1.0,T=5000.0,P=.001$^
```

It should be noted that the input data in block $NUM1 were obtained from reference 2 and need not be changed from case to case unless fewer points are desired. The present coverage includes temperatures from 200° R to 10 000° R (111° K to 5556° K) in 100° R (56° K) increments.

Output

The output names used in the source program and the corresponding quantities from the main body of the report are as follows:

Program name	Quantity
XO	X_O
XN	X_N
XAR	X_{Ar}
XH	X_H
XO2	X_{O_2}
XN2	X_{N_2}
XH2	X_{H_2}
XON	X_{ON}
XOH	X_{OH}
XH2O	X_{H_2O}
MM	M
HM	H
SM	S

APPENDIX A

An output listing for the example input is as follows:

RN=3.72744500E+00 RAR=2.29695200E-02 REQ=1.00000000E+00

T=5.00000000E+03R P=1.00000000E+00ATM

XO	XN	XAR	XH	XO2
5.70327244E-03	2.31249727E-06	7.60417436E-03	1.61297775E-02	1.34353754E-02

XN2	XH2	XON	XOH	XH2O
6.12842267E-01	4.58018477E-02	8.30244316E-03	2.59805399E-02	2.64197990E-01

MM=2.35537499E+01 HM=7.96227455E+02BTU/LBM SM=2.76587239E+00BTU/LBM-R

APPENDIX B

FORMULATION OF INITIAL VALUES FOR THE NEWTON ITERATION SCHEME

The purpose of this appendix is to present the simplified gas models which were used to estimate the desired solution over a wide range of variables. To make certain that the simplified gas model gave results nearly equal to the entire solution, different gas models were chosen in separate regions of equivalence ratio.

For $r_{eq} < 1$:

Gas model chosen

H_2O, O_2, O, N_2, Ar

Conservation of mass equations

$$X_{H_2O} + X_{O_2} + X_O + X_{N_2} + X_{Ar} = 1$$

$$2X_{N_2} = r_N\left(X_{H_2O} + 2X_{O_2} + X_O\right)$$

$$X_{Ar} = r_{Ar}\left(X_{H_2O} + 2X_{O_2} + X_O\right)$$

$$2X_{H_2O} = 2r_{eq}\left(X_{H_2O} + 2X_{O_2} + X_O\right)$$

Equilibrium expression

$$X_{O_2} = pK_5X_O^2$$

Solving for X_O gives

$$X_O = \frac{\sqrt{(1 + C)^2 + 16\left(1 - r_{eq}\right)\left(C + r_{eq}\right)pK_5} - (1 + C)}{4\left(C + r_{eq}\right)pK_5}$$

The presence of an extraneous solution to the entire problem made it necessary to establish a correction factor which would insure convergence to the proper solution. The correction factor was determined by comparing beforehand the result of the simplified gas model with the entire solution over the range of variables. The correction factor chosen for $r_{eq} < 1$ is

$$\frac{X_O(1)}{X_O} = 1.1 - \left(0.5 \times 10^{-4}\right)T$$

The initial estimate for the iteration becomes

$$X_O(1) = \left[\frac{\sqrt{(1 + C)^2 + 16(1 - r_{eq})(C + r_{eq})pK_5} - (1 + C)}{4(C + r_{eq})pK_5}\right] \times \left[1.1 - (0.5 \times 10^{-4})T\right]$$

For $r_{eq} = 1$:

Gas model chosen

H_2O, O, H, N_2, Ar

Conservation of mass equations

$$X_{H_2O} + X_O + X_H + X_{N_2} + X_{Ar} = 1$$

$$2X_{N_2} = r_N(X_O + X_{H_2O})$$

$$X_{Ar} = r_{Ar}(X_O + X_{H_2O})$$

$$X_H + 2X_{H_2O} = 2r_{eq}(X_O + X_{H_2O})$$

Equilibrium expression

$$X_{H_2O} = p^2K_{10}X_OX_N^2$$

Solving for X_O yields

$$X_O \approx \left[2(1 + C)p^2K_{10}\right]^{-1/3}$$

The correction factor chosen for $r_{eq} = 1$ is

$$\frac{X_O(1)}{X_O} = 0.34 - (0.2 \times 10^{-4})T$$

The initial estimate for the iteration becomes

$$X_O(1) = \frac{\left[0.34 - (0.2 \times 10^{-4})T\right]}{\left[2(1 + C)p^2K_{10}\right]^{1/3}}$$

APPENDIX B

For $r_{eq} > 1$:

Gas model chosen

H_2, H, O, N_2, Ar

Conservation of mass equations

$$X_{H_2} + X_H + X_O + X_{N_2} + X_{Ar} = 1$$

$$2X_{N_2} = r_N X_O$$

$$X_{Ar} = r_{Ar} X_O$$

$$2X_{H_2} + X_H = 2r_{eq} X_O$$

Equilibrium expression

$$X_{H_2} = pK_7 X_H^2$$

Solving for X_H and determining that no correction factor was required for this case yields the following initial estimate:

$$X_H(1) = \frac{\sqrt{(4r_{eq} + 1 + C)^2 + 32r_{eq}pK_7(2r_{eq} + 1 + C)} - (4r_{eq} + 1 + C)}{4(2r_{eq} + 1 + C)pK_7}$$

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TABLE I.- CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF AIR ($r_{eq} = 0$)

[First value of paired numbers, present method; second value, ref. 2]

	T = 2000° R (1111° K)			T = 6000° R (3333° K)			T = 10 000° R (5556° K)		
	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm
X_O	0 4.4792×10^{-8}	0 1.5018×10^{-9}	0 0	0.34007 .34011	0.10807 .10836	1.2953×10^{-2} 1.2995×10^{-2}	0.22018 .22014	0.32149 .32154	0.22343 .22437
X_N	0 0	0 0	0 0	2.436×10^{-3} 2.439×10^{-3}	8.1153×10^{-5} 8.1193×10^{-5}	8.2882×10^{-6} 8.2971×10^{-6}	0.72846 .72869	8.1383×10^{-2} 8.1557×10^{-2}	8.5891×10^{-3} 8.6055×10^{-3}
X_{Ar}	9.624×10^{-3} 9.624×10^{-3}	9.624×10^{-3} 9.624×10^{-3}	9.624×10^{-3} 9.624×10^{-3}	7.9758×10^{-3} 7.9757×10^{-3}	9.1036×10^{-3} 9.1022×10^{-3}	9.5616×10^{-3} 9.5614×10^{-3}	0.50591×10^{-2} $.50583 \times 10^{-2}$	7.6853×10^{-3} 7.6843×10^{-3}	8.5075×10^{-3} 8.5029×10^{-3}
X_H	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
X_{O_2}	0.20949 .20944	0.20949 .20944	0.20949 .20944	1.1752×10^{-3} 1.1684×10^{-3}	0.1186 .1186	1.7049×10^{-1} 1.7056×10^{-2}	0.291429×10^{-6} $.28385 \times 10^{-6}$	6.2133×10^{-4} 6.0554×10^{-4}	3.0010×10^{-2} 2.9485×10^{-2}
X_{N_2}	0.78088 .78083	0.78088 .78083	0.78088 .78083	0.64353 .64353	0.71315 .71314	0.74464 .74472	4.6227×10^{-2} $.6047 \times 10^{-2}$	0.57696 .57682	0.64253 .64219
X_{H_2}	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
X_{ON}	0 1.0302×10^{-4}	0 1.0302×10^{-4}	0 1.0302×10^{-4}	4.8120×10^{-3} 4.7821×10^{-3}	5.0931×10^{-2} 5.0719×10^{-2}	6.2348×10^{-2} 6.2156×10^{-2}	0.72654×10^{-4} $.72157 \times 10^{-4}$	1.1851×10^{-2} 1.1796×10^{-2}	8.6929×10^{-2} 8.6848×10^{-2}
X_{OH}	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
X_{H_2O}	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0	0 0
X_{NH}	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0
X_{NH_3}	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0	--- 0
M	28.965 28.965	28.965 28.965	28.965 28.965	24.005 24.004	27.399 27.395	28.777 28.777	15.227 15.224	23.130 23.128	25.605 25.591
H, $\frac{Btu}{lbm}$	504.7 504.8	504.7 504.8	504.7 504.8	3296.1 3296.3	2210.2 2211.2	1835.5 1835.5	14 687.4 14 692.4	5275.8 5278.6	4135.6 4141.2
H, $\frac{J}{kg}$	1.1731×10^6 1.1734×10^6	1.1731×10^6 1.1734×10^6	1.1731×10^6 1.1734×10^6	7.6615×10^6 7.6619×10^6	5.1374×10^6 5.1397×10^6	4.2664×10^6 4.2664×10^6	34.139×10^6 34.151×10^6	12.263×10^6 12.270×10^6	9.6128×10^6 9.6258×10^6
S, $\frac{Btu}{lbm\text{-}^oR}$	2.4444 2.4445	1.9708 1.9709	1.6551 1.6552	3.1206 3.1208	2.3941 2.3944	2.0084 2.0084	4.4489 4.4497	2.7886 2.7890	2.2974 2.2979
S, $\frac{J}{kg\text{-}^oK}$	10 227 10 228	8245.8 8246.2	6924.9 6925.4	13 057 13 057	10 017 10 018	8403.1 8403.1	18 614 18 618	11 668 11 669	9612.3 9614.4

TABLE II.- CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF HYDROGEN-AIR COMBUSTION FOR $r_{eq} = 1$

[First value of paired numbers, present method; second value, ref. 2]

	T = 2000° R (1111° K)			T = 6000° R (3333° K)			T = 10 000° R (5556° K)		
	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm
X_O	0	0	0	0.20125	4.8479×10^{-2}	2.8052×10^{-3}	0.15156	0.19233	0.12007
	0	0	0	.20126	4.8651×10^{-2}	2.8201×10^{-3}	.15156	.19238	.12064
X_N	0	0	0	1.8725×10^{-3}	6.9610×10^{-5}	7.5493×10^{-6}	0.51841	6.2263×10^{-2}	6.9426×10^{-3}
	0	0	0	1.8750×10^{-3}	6.9635×10^{-5}	7.5595×10^{-6}	.51843	6.239×10^{-2}	6.9498×10^{-3}
X_{Ar}	7.9570×10^{-3}	7.9570×10^{-3}	7.9570×10^{-3}	4.7123×10^{-3}	6.5887×10^{-3}	7.6958×10^{-3}	3.4821×10^{-3}	4.5792×10^{-3}	5.4487×10^{-3}
	7.9570×10^{-3}	7.9570×10^{-3}	7.9570×10^{-3}	4.7123×10^{-3}	6.5859×10^{-3}	7.6948×10^{-3}	3.4821×10^{-3}	4.5793×10^{-3}	5.4478×10^{-3}
X_H	0	0	0	0.40729	0.11748	7.8295×10^{-3}	0.30319	0.39507	0.27773
	3.1673×10^{-9}	0	0	.40729	.11768	7.8495×10^{-3}	.30319	.39487	.27709
X_{O_2}	0	0	0	4.1154×10^{-4}	2.3883×10^{-2}	7.9961×10^{-3}	1.3808×10^{-7}	2.2237×10^{-4}	8.6659×10^{-3}
	4.2358×10^{-6}	3.9609×10^{-7}	7.6624×10^{-8}	4.0914×10^{-4}	2.3907×10^{-2}	8.0326×10^{-3}	1.3457×10^{-7}	2.1677×10^{-4}	8.5250×10^{-3}
X_{N_2}	0.64562	0.64563	0.64563	0.38032	0.52477	0.61827	2.3315×10^{-2}	0.33771	0.41975
	.64562	.64563	.64563	.38032	.52456	.61819	2.3307×10^{-2}	.33756	.41886
X_{H_2}	0	0	0	1.0593×10^{-3}	8.8132×10^{-2}	3.9147×10^{-2}	7.3389×10^{-7}	1.2460×10^{-3}	6.1580×10^{-2}
	9.1818×10^{-6}	9.4953×10^{-7}	2.1589×10^{-7}	1.0573×10^{-3}	8.8271×10^{-2}	3.9272×10^{-2}	7.3418×10^{-7}	1.2453×10^{-3}	6.1322×10^{-2}
X_{ON}	0	0	0	2.1885×10^{-3}	1.9599×10^{-2}	1.2299×10^{-2}	3.5591×10^{-5}	5.424×10^{-3}	3.7759×10^{-2}
	4.2126×10^{-7}	1.2882×10^{-7}	5.6659×10^{-8}	2.1755×10^{-3}	1.9530×10^{-2}	1.2290×10^{-2}	3.5343×10^{-5}	5.3989×10^{-3}	3.7715×10^{-2}
X_{OH}	0	0	0	8.9308×10^{-4}	6.205×10^{-2}	2.3931×10^{-2}	6.9703×10^{-7}	1.1525×10^{-3}	5.0582×10^{-2}
	5.8048×10^{-7}	5.7083×10^{-8}	1.1971×10^{-8}	8.9124×10^{-4}	6.224×10^{-2}	2.4067×10^{-2}	6.9554×10^{-7}	1.1498×10^{-3}	5.0599×10^{-2}
X_{H_2O}	0.34642	0.34642	0.34642	5.4362×10^{-6}	0.10895	0.28002	1.7262×10^{-12}	3.7192×10^{-6}	1.1474×10^{-2}
	.34641	.34642	.34642	5.3754×10^{-6}	.10848	.27976	0	3.6164×10^{-6}	1.1168×10^{-2}
X_{NH}	---	---	---	---	---	---	---	---	---
	0	0	0	1.9938×10^{-6}	2.1395×10^{-5}	1.5492×10^{-5}	1.3726×10^{-6}	2.1514×10^{-4}	1.6817×10^{-3}
X_{NH_3}	---	---	---	---	---	---	---	---	---
	0	0	0	0	9.5618×10^{-8}	3.0803×10^{-6}	0	0	0
M	24.647	24.647	24.647	14.596	20.408	23.837	10.785	14.184	16.877
	24.647	24.647	24.647	14.596	20.400	23.834	10.786	14.184	16.874
H, $\frac{Btu}{lbm}$	-814.9	-814.9	-814.9	6637.4	2650.5	1115.9	18 610.5	9314.3	6651.4
	-814.8	-814.9	-814.9	6637.6	2655.3	1117.3	18 611.1	9317.9	6667.9
H, $\frac{J}{kg}$	-1.8942×10^6	-1.8942×10^6	-1.8942×10^6	15.428×10^6	6.1608×10^6	2.5938×10^6	43.258×10^6	21.650×10^6	15.461×10^6
	-1.8939×10^6	-1.8942×10^6	-1.8942×10^6	15.428×10^6	6.1720×10^6	2.5971×10^6	43.260×10^6	21.659×10^6	15.499×10^6
S, $\frac{Btu}{lbm\text{-}^oR}$	2.8702	2.3136	1.9425	4.6147	3.0999	2.4381	6.0321	3.9998	3.1268
	2.8701	2.3135	1.9424	4.6147	3.1008	2.4383	6.0325	4.0004	3.1287
S, $\frac{J}{kg\text{-}^oK}$	12 009	9680.1	8127.4	19 308	12 970	10 201	25 238	16 735	13 083
	12 008	9679.7	8127.0	19 308	12 974	10 202	25 240	16 738	13 090

TABLE III.- CHEMICAL COMPOSITION AND THERMODYNAMIC PROPERTIES OF HYDROGEN-AIR COMBUSTION FOR $r_{eq} = 2.5$

[First value of paired numbers, present method; second value, ref. 2]

	T = 2000° R (1111° K)			T = 6000° R (3333° K)			T = 10 000° R (5556° K)		
	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm	p = 0.001 atm	p = 1.0 atm	p = 100 atm
X_O	0	0	0	0.11621	1.9146×10^{-2}	2.577×10^{-4}	0.10372	0.12046	3.1192×10^{-2}
	0	0	0	.12498	1.9260×10^{-2}	2.6015×10^{-4}	.10372	.12049	7.1178×10^{-2}
X_N	0	0	0	1.2330×10^{-3}	5.7712×10^{-5}	6.2398×10^{-6}	0.36368	4.8672×10^{-2}	6.4016×10^{-2}
	0	0	0	1.4765×10^{-3}	5.7675×10^{-5}	6.2149×10^{-6}	.36372	4.8747×10^{-2}	5.6495×10^{-3}
X_{Ar}	5.2362×10^{-3}	5.2362×10^{-3}	5.2362×10^{-3}	2.7139×10^{-3}	4.4766×10^{-3}	5.1558×10^{-3}	2.3829×10^{-3}	2.8578×10^{-3}	3.4546×10^{-3}
	5.2362×10^{-3}	5.2364×10^{-3}	5.2566×10^{-3}	2.9222×10^{-3}	4.4749×10^{-3}	5.1559×10^{-3}	2.3828×10^{-3}	2.8580×10^{-3}	3.5702×10^{-3}
X_H	0	0	0	0.65611	0.19685	2.2727×10^{-2}	0.51869	0.61491	0.43121
	6.1123×10^{-7}	1.9327×10^{-8}	1.9201×10^{-9}	.63017	.19705	2.2746×10^{-2}	.51869	.61470	.41915
X_{O_2}	0	0	0	1.3723×10^{-4}	3.7249×10^{-3}	6.7485×10^{-5}	6.4672×10^{-8}	8.722×10^{-5}	5.8487×10^{-4}
	0	0	0	1.5776×10^{-4}	3.7467×10^{-3}	6.8360×10^{-5}	6.3018×10^{-8}	8.5033×10^{-5}	2.9673×10^{-3}
X_{N_2}	0.42486	0.42486	0.42486	0.21917	0.35999	0.41786	1.1492×10^{-2}	0.20621	0.20307
	.42486	.42486	.42457	.23583	.35984	.41783	1.1472×10^{-2}	.20607	.27676
X_{H_2}	0.34194	0.34190	0.34194	2.7491×10^{-3}	0.24745	0.32985	2.1479×10^{-6}	3.0186×10^{-3}	0.14844
	.34194	.34190	.33744	2.5311×10^{-3}	.24748	.32977	2.1487×10^{-6}	3.0179×10^{-3}	.14032
X_{ON}	0	0	0	8.3215×10^{-4}	6.4171×10^{-3}	9.3387×10^{-4}	1.7087×10^{-5}	2.6557×10^{-3}	9.0449×10^{-2}
	0	0	0	1.0638×10^{-3}	6.4037×10^{-3}	9.3207×10^{-4}	1.6970×10^{-5}	2.6420×10^{-3}	1.8088×10^{-2}
X_{OH}	0	0	0	8.3077×10^{-4}	4.1065×10^{-2}	6.3816×10^{-3}	8.1607×10^{-7}	1.1235×10^{-3}	2.0402×10^{-2}
	1.9795×10^{-9}	0	0	8.5629×10^{-4}	4.1262×10^{-2}	6.4338×10^{-3}	8.1431×10^{-7}	1.1211×10^{-3}	4.5157×10^{-2}
X_{H_2O}	0.22796	0.22796	0.22796	8.1463×10^{-6}	0.12081	0.21675	3.457×10^{-12}	5.6430×10^{-6}	7.1857×10^{-2}
	.22796	.22797	.22885	7.9908×10^{-6}	.12041	.21671	0	5.4891×10^{-6}	1.5077×10^{-2}
X_{NH}	---	---	---	---	---	---	---	---	---
	0	0	0	2.4292×10^{-6}	2.9671×10^{-5}	3.6907×10^{-5}	1.6475×10^{-6}	2.6168×10^{-4}	2.0679×10^{-3}
X_{NH_3}	---	---	---	---	---	---	---	---	---
	3.9734×10^{-8}	3.9726×10^{-5}	3.8938×10^{-3}	0	3.7177×10^{-7}	6.1621×10^{-5}	0	0	0
M	16.908	16.908	16.908	8.836	14.455	16.649	7.695	9.228	11.166
	16.908	16.909	16.974	9.436	14.450	16.649	7.695	9.229	11.529
H, $\frac{Btu}{lbm}$	-498.9	-498.9	-498.9	12 183.9	3820.2	1900.3	23 860.8	14 872.7	11 308.5
	-498.9	-498.9	-504.4	11 292.9	3826.2	1901.3	23 862.0	14 876.6	10 050.5
H, $\frac{J}{kg}$	-1.1596×10^6	-1.1596×10^6	-1.1596×10^6	28.320×10^6	8.8797×10^6	4.4171×10^6	55.462×10^6	34.570×10^6	26.285×10^6
	-1.1596×10^6	-1.1596×10^6	-1.1724×10^6	26.249×10^6	8.8936×10^6	4.4194×10^6	55.465×10^6	34.579×10^6	23.361×10^6
S, $\frac{Btu}{lbm\text{-}^oR}$	3.9238	3.1124	2.5716	6.9995	4.0983	3.2028	8.1296	5.6014	4.3023
	3.9238	3.1124	2.5693	6.6182	4.0995	3.2030	8.1302	5.6021	4.1976
S, $\frac{J}{kg\text{-}^oK}$	16 417	13 022	10 760	29 286	17 147	13 401	34 014	23 436	18 001
	16 417	13 022	10 750	27 691	17 152	13 401	34 017	23 439	17 563

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