User's Guide for Vectorized Code EQUIL for Calculating Equilibrium Chemistry on Control Data STAR-100 Computer

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APRIL 1980

FOR REFERENCE

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User's Guide for Vectorized Code EQUIL for Calculating Equilibrium Chemistry on Control Data STAR-100 Computer

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SUMMARY

A vectorized code, EQUIL, is developed for calculating the equilibrium chemistry of a reacting gas mixture on the Control Data STAR-100 computer. The code provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. The code is set up for the e⁻, H, He, C, O, N system of elements. In all, 24 chemical species are included.

INTRODUCTION

This report presents a vectorized code, EQUIL, developed for the Control Data STAR-100 computer, which calculates the equilibrium chemistry of a reacting gas mixture. Only gaseous species are considered. The code (see appendix A) provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. It can be used as a subprogram to a flow-field code. The code is set up for the e⁻, H, He, C, O, N system of elements. In all, 24 species are included. The method given in references 1 and 2 is used in the present code for calculating the equilibrium composition. It uses the free-energy-minimization technique in which the method of steepest descent is utilized. Thermodynamic properties, thermal conductivity, and viscosity of each input species are evaluated by polynomial expressions. The coefficients for these polynomials are prescribed input to the code. The mixture transport properties are determined by using the semiempirical relation of Wilke (ref. 3).

The code is set up for calculating the equilibrium chemistry over 500 mesh points. The number of mesh points can be varied by suitably changing the code dimensions. The system of elements and species considered in this code can also be changed by suitably modifying the input data.

SYMBOLS

\[ a_1, a_2, \ldots, a_7 \] coefficients in approximating polynomials for \( c_p \), \( H \), and \( F \)
\[ b_1, b_2, b_3 \] coefficients in approximating polynomial for \( \mu \)
\[ c_1, c_2 \] coefficients in approximating polynomial for \( k \)
\[ c_p \] specific heat at constant pressure
\[ F \] free energy
\[ H \] enthalpy
\( k \) : thermal conductivity

\( R \) : universal gas constant

\( T \) : temperature

\( \mu \) : viscosity

**PROGRAM INPUT**

Most of the data input to the EQUIL code is by punched cards. The detailed input information is presented in the following section.

**Chemistry and Transport Model Input**

The elements and species in the mixture are input through NAMELIST THERMO, which is described in table I. Thermodynamic properties (refs. 4 to 7), thermal conductivity, and viscosity of each input species are represented by approximating polynomials. The thermodynamic data are input by cards as follows. There are eight cards for each atomic, molecular, or ionic species:

Card 1 (Format (A6, 4X, 6F5.0)): Field 1 contains the alphanumeric identifier for the \( i \)th species \( \text{SYMB}(I) \), which is right justified in columns 1 to 6. Fields 2 to 7 (columns 11 to 15, 16 to 20, etc.) contain the array \( \text{AA}(I,J) \) for \( J = 1 \) to \( NE \), which specifies the number of atoms of each element in the species (see table II). The order must correspond to the order of input of the MWEL array. For example, card 1 for species \( \text{NO}^+ \) would be:

\[
\text{NO}^+ \quad -1. \quad 0. \quad 0. \quad 0. \quad 1. \quad 1.
\]

Cards 2 and 3 (Format (5E14.6)) contain the seven constants \( a_1 \) to \( a_7 \) used in the polynomials for calculating the specific heat, enthalpy, and free energy of each species in the temperature range from 300 K to 1000 K. These polynomials are:

\[
\frac{C_P}{R} = a_1 + a_2 T + a_3 T^2 + a_4 T^3 + a_5 T^4
\]

\[
\frac{H}{RT} = a_1 + \frac{a_2}{2} + \frac{a_3}{3} T^2 + \frac{a_4}{4} T^3 + \frac{a_5}{5} T^4 + \frac{a_6}{T}
\]

\[
\frac{F}{RT} = a_1 (1 - \ln T) - \frac{a_2}{2} - \frac{a_3}{6} T^2 - \frac{a_4}{12} T^3 - \frac{a_5}{20} T^4 + \frac{a_6}{T} + a_7
\]

Columns 29 to 80 of card 2 may be used for identification purposes.
Cards 4 and 5 (Format (5E14.6)) contain constants $a_1$ to $a_7$ for the thermodynamic data in the temperature range from 1000 K to 6000 K.

Cards 6 and 7 (Format (5E14.6)) contain constants $a_1$ to $a_7$ for the thermodynamic data in the temperature range above 6000 K.

Card 8 (Format (5E14.6)) contains the constants $b_1$, $b_2$, $b_3$, $c_1$, and $c_2$ in the approximating polynomials for viscosity and thermal conductivity, which are

$$
\mu = b_1 + b_2 T + b_3 T^2
$$

$$
k = c_1 + c_2
$$

where $T$ is in K, $\mu$ is in lbm/ft-sec, and $k$ is in Btu/ft-sec-°R.*

Coefficients for the species used in this code are given in appendix B.

The elements are input in the order $e^-$, H, He, C, O, and N. The order of species input is shown in table II. The species composition is described using the AA(24,6) array in table II. For example, AA(1,2) defines the number of hydrogen atoms in species i, and AA(i,4) defines the number of carbon atoms in species i. If species i is a positive ion, then AA(i,1) is -1.

Temperature, Pressure, and Elemental Mass Fractions Input

The code is set to calculate the equilibrium chemistry at 500 mesh points. This can be varied by changing the dimensions of various variables. The temperature, pressure, and elemental mass fractions at all the mesh points are input to the code through vectors $T(500)$, $P(500)$, and $CL(500,6)$. The temperature is in kelvins and pressure is in atmospheres. The code requires that at least one element of the temperature vector be in each temperature range used to calculate the thermodynamic properties in subroutine THERMO. As an example, the present code is set to use only two temperature ranges, 1000 K < $T$ < 6000 K and $T$ > 6000 K. There is a transition range from 5500 K to 6500 K to assure smooth transition from one temperature range to another. The temperature vector should have at least one element less than 5500 K, at least one element between 5500 K and 6500 K, and at least one element above 6500 K.

The vector $CL(500,1)$ is an elemental array and, for the present setup, represents the charge balance, which is zero. However, the solution procedure does not allow zero values for an elemental array; therefore, the "electron" elemental array is set to an arbitrary small number. In this code, $CL(500,1)$ is taken as 1.0E-10 for all cases. No element should have zero mass fraction. For cases where the mixture does not include a particular element, the mass fraction for that element can be prescribed as an arbitrary small number.

*1 lbm/ft-sec = 1.488 Pa-sec; 1 Btu/ft-sec-°R = 6226.5 W/m-K.
In addition to the aforementioned input quantities, a criterion for the convergence of the calculation procedure is required. The convergence criterion is as follows:

\[ \text{CRIT} = \sum_{i=1}^{N} |X_i - Y_i| < 1.0 \times 10^{-6} \]

Here, the values of \( X_i \) are the species mole numbers for the current iteration, and the values of \( Y_i \) are the species mole numbers for the previous iteration. Thus, when the sum of the absolute values of the changes in the mole numbers for all the species is less than \( 1.0 \times 10^{-6} \) from one iteration to the next, the calculation is terminated. The value of CRIT can be changed if necessary.

**CODE STRUCTURE**

Code EQUIL has a main program in which the quantities such as temperature, pressure, and elemental mass fractions are prescribed at all the mesh points. The value of CRIT is also input here. In addition to the main program, there are six subroutines.

Subroutine READ reads the NAMELIST THERMO and thermodynamic and transport data for various species. Subroutine THERMO calculates the thermodynamic properties of various species at all the mesh points. Subroutines CHEQ, MINENG, and EQSOL use the method of steepest descent to minimize the free energy. An initial assumption is made on the mole numbers of various species, and then an iterative procedure is followed to find the set of mole numbers of various species which minimizes the free energy.

Knowing the right mole numbers of various species, the subroutine CHEQ then calculates the mixture molecular weight, mole fractions, and the enthalpy of the mixture. Subroutine TP calculates the mixture specific heat, thermal conductivity, viscosity, and Prandtl number.

Finally, the main program EQUIL converts the mixture viscosity, conductivity, and specific heat to SI units. The species mass fractions are also obtained here. The printed output includes the mole fractions of various species, and the enthalpy, specific heat, viscosity, conductivity, Prandtl number, and molecular weight of the mixture.

**LIST OF VARIABLES**

- CIS: Species mass fraction
- CL: Elemental mass fraction
- COND: Thermal conductivity of mixture
- CONDI: Thermal conductivity of individual species
CP  Specific heat of mixture
CPI  Specific heat of individual species
CRIT  Convergence criterion
FORT  Free energy of individual species
HI  Enthalpy of individual species
KTEST  A parameter equal to either zero or one
MOLEF  Mole fraction of species
MW  Molecular weight of species
MWEL  Molecular weight of element
P  Pressure
SH  Enthalpy of mixture
SIG  Prandtl number of mixture
T  Temperature
VIS  Viscosity of mixture
VISI  Viscosity of individual species
WMIX  Molecular weight of mixture
Y  Mole number of species in current iteration
YII  Mole number of species in previous iteration used to start a new iteration for KTEST = 1

SAMPLE CALCULATIONS

Two sample calculations are presented here. The first example is for a mixture consisting mainly of e^−, H, He, C, and O elements. The input temperature, pressure, and elemental mass fractions are listed below:

\[ T(1;100) = 4000. \]
\[ T(101;100) = 6000. \]
\[ T(201;300) = 12570. \]
\[ P(1;500) = 6.3549 \]
\[
\begin{align*}
CL(1,1;500) &= 1.0E-10 \\
CL(1,3;500) &= 0.1008 \\
CL(1,4;500) &= 0.4518 \\
CL(1,5;500) &= 0.02443 \\
CL(1,6;500) &= 5.0E-6 \\
CL(1,2;500) &= 1.0 & \text{(Sum of other five elemental mass fractions)}
\end{align*}
\]

The mass fraction for the sixth element, nitrogen, was prescribed as a very small number. It took 24 iterations for the solution to converge. The actual computing time on the Control Data STAR-100 computer for this example was 5.3 seconds. The output for this example is given in table III.

The second example is for air. For this example, the elemental mass fractions for H, He, and C were prescribed as small numbers. The input temperature, pressure, and elemental mass fractions are as follows:

\[
\begin{align*}
T(1;100) &= 7000. \\
T(101;100) &= 6000. \\
T(201;300) &= 3991.17 \\
P(1;500) &= 1.146 \\
CL(1,1;500) &= 1.0E-10 \\
CL(1,2;500) &= 5.0E-6 \\
CL(1,3;500) &= 5.0E-6 \\
CL(1,4;500) &= 5.0E-6 \\
CL(1,5;500) &= 0.233 \\
CL(1,6;500) &= 1.0 & \text{(Sum of other five elemental mass fractions)}
\end{align*}
\]

It took 26 iterations and 6.2 seconds actual computing time for the solution to converge. The output for this example is given in table IV.

In these examples, the input conditions for the first 100 mesh points, for the next 100 mesh points, and for the last 300 mesh points were the same; consequently, tables III and IV give the results only at mesh points 1, 101, and 201.
CONCLUDING REMARKS

The code presented in appendix A calculates the enthalpy of the mixture for given temperature, pressure, and elemental mass fractions. However, in most flow-field calculations, it is the temperature which is to be calculated for given enthalpy and pressure. To use this code for such calculations, an iterative technique can be used in which a temperature is assumed initially. For this temperature, the enthalpy of the mixture is obtained from EQUIL. The temperature is then changed using the Newton-Raphson technique until the enthalpy of the mixture is obtained within desired accuracy to the initially known value. This iterative technique can be incorporated in the main program EQUIL, and only subroutines THERMO and CHEQ are required to be put in the iterative loop.

To save significantly on time for such calculations, a parameter KTEST is used. For the initial guess of temperature, KTEST is set equal to zero and for subsequent guesses, KTEST is set equal to one. When KTEST = 0, the subroutine CHEQ starts with a very crude approximation of species mole numbers. For KTEST = 1, mole numbers calculated in the previous iteration are taken as the starting approximation and the solution converges in fewer iterations.

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February 19, 1980
APPENDIX A

PROGRAM LISTING

The computational program EQUIL is listed in this appendix in Control Data
STAR-100 FORTRAN language 1.4 (an extension of ANSI FORTRAN for the Control
Data STAR-100 computer). This program consists of one main program and six
subroutines.

PROGRAM EQUIL(INPUT,OUTPUT,TAPE5=INPUT,TAPF6=OUTPUT)
DIMENSION CIS(500,24)
COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
COMMON/E2/HI(500,24),MOLFF(500,24),CP(500,24)
COMMON/E4/MW(24),SYM(24),AA(24,6),MWIL(6),AAA(500,24,6)
COMMON/FR/NE,NS
COMMON/E14/VIS(500),COND(500),SIG(500),CP(500)
COMMON/E15/RR,CRIT,RCRIT,MNS,MME,MNF,MX
COMMON/E16/ENT(500,24),CP(500,24)
EQUIVALENCE (CIS(1,1),ENT(1,1))
REAL MW,MWIL,MOF
RR=1.987
CRIT=1.E-6
RCRIT=.1*CRIT
M1=500
C T IS IN DEGREE K AND P IS IN ATM.
T(1:100)=4000.
T(101:100)=6000.
T(201:300)=12570.
P(1:M1)=6.3549
C THE ELEMENTS ARE IN THE ORDER OF FE,H,HE,C,O AND N.
CL(1,1:M1)=1.E-10
CL(1,2:M1)=.422964999E
CL(1,3:M1)=1008
CL(1,4:M1)=.4518
CL(1,5:M1)=.02443
CL(1,6:M1)=5.E-6
CALL READ(M1)
MNS=M1*NS
MME=ME+1
MNF=MN+1
MNE=MME=M1
MX=MME=MME=M1
CALL THERMO(M1)
KTEST=0
CALL CHEQ(KTEST,M1)
CALL TP(M1)
D0 10 I=1,NS
C CIS IS THE MASS FRACTION OF SPECIE I. HI IS IN J/KG.
CW=MW(I)
CW1=4184./CW
CIS(1,1:M1)=MOF(1,1:M1)*CW/MIX(1:M1)
10 HI(1,1:M1)=HI(1,1:M1)*CW1
C HERE SH IS IN J/KG, CP IS IN J/KG K, VIS IS IN N SEC/M2, COND IS
C IN W/M K.
SH(1:M1)=SH(1:M1)*4184.

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\[ \text{CP}(1:M1) = \text{CP}(1:M1) \times 4184.4 / \text{WMIX}(1:M1) \]
\[ \text{VIS}(1:M1) = 0.1 \times \text{VIS}(1:M1) \]
\[ \text{COND}(1:M1) = 4184.4 \times \text{COND}(1:M1) \]

C SPECIES ARE IN THE ORDER OF \(\text{F}^-, \text{H}, \text{H}_2, \text{H}^+, \text{He}, \text{He}^+, \text{C}, \text{C}_2, \text{C}_3, \text{C}^+, \text{C}_2^+ \), \(\text{C}_2^2, \text{C}_3^3, \text{C}_4^4, 0, \text{O}_2, 0^+, \text{CN}, \text{CN}_2, \text{N}, \text{N}_2, \text{N}^+, \text{NO}, \text{NO}^+ \)

WRITE(6,100)
WRITE(6,130)(M,MOLEF(M,1),MOLEF(M,2),MOLEF(M,3),MOLEF(M,4),MOLEF(M,5),MOLEF(M,6),M=1,M1,100)
WRITE(6,120)
WRITE(6,130)(M,MOLEF(M,7),MOLEF(M,8),MOLEF(M,9),MOLEF(M,10),MOLEF(M,11),MOLEF(M,12),M=1,M1,100)
WRITE(6,140)
WRITE(6,130)(M,MOLEF(M,13),MOLEF(M,14),MOLEF(M,15),MOLEF(M,16),MOLEF(M,17),MOLEF(M,18),M=1,M1,100)
WRITE(6,160)
WRITE(6,130)(M,MOLEF(M,19),MOLEF(M,20),MOLEF(M,21),MOLEF(M,22),MOLEF(M,23),MOLEF(M,24),M=1,M1,100)
WRITE(6,150)
WRITE(6,130)(M,SH(M),CP(M),VIS(M),COND(M),SIG(M),WMIX(M),M=1,M1,1100)

100 FORMAT(14X,'M',11X,'SH',13X,'CP',13X,'VIS',12X,'COND',11X,'SIG',11X,WIXM\',/)
120 FORMAT(14X,'M',11X,'SH',12X,'CP',13X,'VIS',12X,'COND',11X,'SIG',11X,WIXM\',/)
130 FORMAT(2X,I4,2X,6E15.5)
140 FORMAT(14X,'M',11X,'SH',12X,'CP',13X,'VIS',12X,'COND',11X,'SIG',11X,WIXM\',/)
160 FORMAT(14X,'M',11X,'SH',12X,'CP',13X,'VIS',12X,'COND',11X,'SIG',11X,WIXM\',/)

STOP
END

SUBROUTINE READ(M1)
COMMON/F3/AI(24,3),BI(24,3),CI(24,3),DI(24,3),EI(24,3),FI(24,3),GI(24,3)
COMMON/F4/MW(24),SMB(24),AA(24,6),MWEL(6),AAA(500,24,6)
COMMON/EB/NE,NS
COMMON/XM/MW(24),XMB(24),XMC(24),XKA(24),XKB(24)
DIMENSION ILW(9),ILWP(6)
REAL MW,MWEL
DATA ILW/5H SI,5H F,5H 0,5H N,5H C,F5H HE,
15H H,5H E-,5H /
/NAMELIST/HERMO/ MW,MWEL,NE,NS
C INPUT PROBLEM NAMELISTS
20 READ(5,THRM0)
APPENDIX A

WRITE(6,THERMO)
DO 60 I=1,NS
READ(5,901) SYMB(I),(AA(I,J),J=1,NE)
DO 55 J=1,3
55 READ(5,902)AI(I,J),BI(I,J),CI(I,J),DI(I,J),EI(I,J),FI(I,J),GI(I,J)
READ(5,902)XMA(I),XMB(I),XMC(I),XKA(I),XKB(I)
60 CONTINUE

C THERMOCHEMICAL PROPERTIES
WRITE(6,919)
DO 120 I=1,NS
WRITE(6,920) SYMB(I),(AI(I,J),BI(I,J),CI(I,J),DI(I,J),EI(I,J),FI(I,J),
            GI(I,J),JI(I,J),J=1,3)
CONTINUE
122 WRITE(6,921)
DO 130 I=1,NS
WRITE(6,922) SYMB(I),XMA(I),XMB(I),XMC(I),XKA(I),XKB(I)
CONTINUE

C SPECIES/ELEMENTAL COMPOSITION MATRIX
DO 135 I=1,NE
ILWP(I)=ILW(I)
IF(MWEL(I).LT.27.) ILWP(I)=ILW(2)
IF(MWEL(I).LT.17.) ILWP(I)=ILW(3)
IF(MWEL(I).LT.15.) ILWP(I)=ILW(4)
IF(MWEL(I).LT.13.) ILWP(I)=ILW(5)
IF(MWEL(I).LT.4.1) ILWP(I)=ILW(6)
IF(MWEL(I).LT.1.1) ILWP(I)=ILW(7)
IF(MWEL(I).LT.0.1) ILWP(I)=ILW(8)
IF(MWEL(I).EQ.0.0) ILWP(I)=ILW(9)
CONTINUE
WRITE(6,923) ILWP
DO 140 I=1,NS
DO 137 J=1,NE
IF(AA(I,J).EQ.O.) AA(I,J)=O.
CONTINUE
WRITE(6,924) SYMB(I),(AA(I,J),J=1,NE)
CONTINUE

901 FORMAT(A6,4X,6F5.0)
902 FORMAT(5E14.6)
919 FORMAT(1H1,34X,'THERMOPHYSICAL PROPERTIES - CURVE FIT COEFFICIENTS
     /46X,'1) THERMODYNAMIC PROPERTIES'//4X,'SPECIES',11X,'A',14X,
     'B',14X,'C',14X,'D',14X,'E',14X,'F',14X,'G'/)
920 FORMAT(1H0,5X,A6,3X,7E15.6,' T= 300K'/15X,7F15.6,' T=1000K'/15X,
     /7E15.6,' T=6000K'/)
921 FORMAT(1H0/4X,'SPECIES',30X,'VISCOSITY',28X,1H*,12X,'CONDUCTIVITY'/)
922 FORMAT(1H ,4X,A6,4X,3E20.6,3X,1H*,E16.6,E20.6)
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923 FORMAT(1H0//49X,'ELEMENTAL PARTICLES TABLE',42X,'SPECIES ',6A5)
924 FORMAT(1H,43X,A6,1X,6F5.0)

NSNEM1=NS*N=MI
AAA(1,1,1:NSNEM1)=0.
DO 110 I=1,MI
  DO 110 J=1,NS
  DO 110 K=1,NE
110 AAA(I,J,K)=AA(J,K)
RETURN
END

SUBROUTINE THERMO(MI)
C FREE ENERGY, ENTHALPY, AND SPECIFIC HEAT BY APPROXIMATING POLYNOMIALS
DIMENSION BG(500)
COMMON/E1/T(500),P(500),WMIX(500),CL(500,6),SH(500)
COMMON/E2/H(500,24),MOLEF(500,24),CPI(500,24)
COMMON/E3/AL(24,3),BL(24,3),CL(24,3),DL(24,3),EL(24,3),FL(24,3),
1GL(24,3)
COMMON/E5/PL(500,24),Y(500,24),X(500,24),YBAR(500)
COMMON/E8/NE,NS
COMMON/E9/A(500),A10(500),A13(500),A500(500),A500(500),TV1(500),
1TV2(500)
COMMON/E15/RR,CRIT,CRIT,MNS,MMM,MNE,MNEI,MX
COMMON/E16/ENT(500,24),CPII(500,24)

C COEFFICIENTS ARE INPUT FOR THREE TEMPERATURE RANGES. (1) 300K TO
C 1000K, (2) 1000K TO 6000K, AND (3) 6000K TO 15000K. K AND L
C DENOTES THE SET OF COEFFICIENTS THAT ARE BEING USED. COMBINE TO
C ASSURE SMOOTH TRANSITION BETWEEN EACH OF THE THREE TEMPERATURE
C INTERVALS. T IS GENERALLY GREATER THAN 6500K.
C T VECTOR SHOULD CONTAIN ATLEAST ONE ELEMENT LESS THAN 5500K, ONE
C ELEMENT BETWEEN 5500S AND 6500K, AND ONE ELEMENT ABOVE 6500K.
BG(1:M1)=T(1:M1),LE.6500.
ASSIGN DA9,A9(I:M1)
DA9=08VCMPRS(T(1:M1),BG(1:M1):DA9)
L1=08SLN(DA9)
BG(1:L1)=A9(1:L1),LE.5500.
ASSIGN DA1,A10(I:M1)
DA1=08VCMPRS(A9(1:L1),BG(1:L1):DA1)
L2=08SLN(DA1)
DA1(1:L2)=DA1*DA1
AA2(1:L2)=DA1*AA1(1:L2)
AA2(1:L2)=DA1*AA1(1:L2)
AS2(1:L2)=DA1*AS1(1:L2)
AS2(1:L2)=DA1*AS1(1:L2)
TV2(1:L2)=VALOG(DA1:TV2(1:L2))
TV2(1:L2)=1.-TV2(1:L2)
APPENDIX A

DO 10 I=1,NS
  CPI(1,1:L2)=RR*(AI(I,2)+RI(I,2)+DA1+CI(I,2)*AA1(1:L2)+DI(I,2)*AA2(1:L2)+EI(I,2)*AA3(1:L2))
  FORT(1,1:L2)=AI(I,2)*TV2(1:L2)-.5*BI(I,2)*DA1-CI(I,2)*AA1(1:L2)*6.*
  1-DI(I,2)*AA2(1:L2)/12.-EI(I,2)*.05*AI3(1:L2)+FI(I,2)/DA1-GI(I,2)
  ENT(1,1:L2)=RR*DA1*(AI(I,2)+5.*RI(I,2)+DA1+CI(I,2)*AA1(1:L2)/3.+DI(I,2)*AA2(1:L2)/4.+EI(I,2)*AI3(1:L2)/5.+FI(I,2)/DA1)
  CONTINUE
10  CONTINUE

DO 20 I=1,NS
  TV1(1:L3)=RR*((6.5-.005*DA1)*(AI(I,2)+.5*BI(I,2)*DA1+CI(I,2)*AA1(1:L3)+DI(I,2)*AA2(1:L3)+EI(I,2)*A13(1:L3))
  CPI(1,1:L1)=OSVMERG(TV1(1:L3),CPI(1,1:L2),BG(1:L1);CPI(1,1:L1))
  TV1(1:L3)=(6.5-.005*DA1)*(AI(I,2)*TV2(1:L3)-.5*BI(I,2)*DA1-CI(I,2)*AA1(1:L3)+DI(I,2)*AA2(1:L3)
  +EI(I,2)*A13(1:L3))/6.-DI(I,2)*AA2(1:L3)/12.-EI(I,2)*.05*AA1(1:L3)+FI(I,2)/DA1)
  HI(1,1:L1)=OSVMERG(TV1(1:L3),FORT(1,1:L2),BG(1:L1);HI(1,1:L1))
  TV1(1:L3)=RR*(AI(I,3)+.5*BI(I,3)*DA1+CI(I,3)*AA1(1:L3)+DI(I,3)*AA2(1:L3)+EI(I,3)*A13(1:L3)/3.+DI(I,3)*AA2(1:L3)/4.+EI(I,3)*.05*AA1(1:L3)+FI(I,3)/DA1)
  MOLEF(1,1:L1)=OSVMERG(TV1(1:L3),ENT(1,1:L2),BG(1:L1);MOLEF(1,1:L1))
20 CONTINUE

DO 30 I=1,NS
  TV1(1:L2)=RR*(AI(I,3)+RI(I,3)*DA1+CI(I,3)*AA1(1:L2)+DI(I,3)*AA2(1:L2)+EI(I,3)*AA3(1:L2))
  CPI(1,1:M1)=OSVMERG(TV1(1:L2),CPI(1,1:L1),BG(1:M1);CPI(1,1:M1))
30 CONTINUE

DO 40 I=1,NS
  TV1(1:L2)=RR*(AI(I,3)+RI(I,3)*DA1+CI(I,3)*AA1(1:L2)+DI(I,3)*AA2(1:L2)+EI(I,3)*AA3(1:L2))
  CPI(1,1:M1)=OSVMERG(TV1(1:L2),CPI(1,1:L1),BG(1:M1);CPI(1,1:M1))
40 DO 10 10 10


APPENDIX A

\[
TV1(1;L2) = AI(1,3) * TV2(1;L2) - 5 * BI(1,3) * DA1 - CI(1,3) * AA1(1;L2) / 6 - DI 
1(1;L2) * AA2(1;L2) / 12 - EI(1,3) * 0.05 * AA1(1;L2) + FI(1,3) / DA1 - GI(1,3) 
\]

\[
FORT(1,1;M1) = QVMERG(TVI(1;L2), HI(1,1;L1), BG(1;MI); FORT(1,1;M1)) 
TV1(1;L2) = RR * DA1 * (AI(1,3) + 5 * BI(1,3) * DA1 + CI(1,3) * AA1(1;L2) / 3 + DI(1,3) * AA2(1;L2) / 4 + EI(1,3) * AA1(1;L2) / 5 + FI(1,3) / DA1) 
\]

ENT(1,1;M1) = QVMERG(TVI(1;L2), MOLEF(1,1;L1), BG(1;MI); ENT(1,1;M1))

30 CONTINUE

TV1(1;M1) = VALOG(P(1;M1); TV1(1;M1))
DO 50 I = 1, NS

50 FORT(I,1;M1) = FORT(I,1:M1) + TV1(I;M1)
HI(1,1;NS*M1) = ENT(1,1;NS*M1)
RETURN
END

SUBROUTINE CHEO(KTEST, M1)

C CHEMICAL EQUILIBRIUM OF MULTIPHASE SYSTEMS BASED ON THE PRINCIPLE OF MINIMIZATION OF THE FREE ENERGY OF THE MIXTURE

C THE CONDENSED SPECIES OPTION IS NOT CURRENTLY IMPLEMENTED.

COMMON/ EI/ T(500), P(500), WMIX(500), CL(500,6), SH(500)
COMMON/ E2/ HI(500,24), MOLEF(500,24), CPI(500,24)
COMMON/ E4/ MW(24), SYMB(24), AA(24,6), MWEL(6), AAA(500,24,6)
COMMON/ E5/ FORT(500,24), Y(500,24), X(500,24), YBAR(500)
COMMON/ E6/ Y1(500,24)
COMMON/ FP/ NE, NS
COMMON/ E0/ SKIP(500)
COMMON/ E11/ CONV(500), XLAMB(500), DELT(500,24), F(500,24), DEBAR(500)
COMMON/ E12/ A9(500), A10(500), A13(500), AA1(500), AA2(500), TV1(500), TV2(500)
COMMON/ E15/ RR, CRIT, RCRT, MNS, MMM, MNE, MNE1, MX
DIMENSION BIG(500), WMIX1(500)
EQUIVALENCE (WMIX1(1), A9(1))
BIT BIG
REAL MW, MWEL, MOLEF
NT = 0

C IF KTEST EQ 1 USE MOLE NUMBERS COMPUTED PREVIOUSLY FOR THIS STATION AS INITIAL GUESS.
C OTHERWISE, ESTIMATE SPECIES MOLE NUMBERS FROM ELEMENT MASS FRACTIONS.
C MASS FRACTIONS.
    IF(KTEST.EQ.1) GO TO 48
C STARTING ASSUMPTION - ATOMS ONLY, NO COMPOUNDS
    Y(1,1;MNS) = 1. E-7
    Y(1,1;M1) = CL(1,1;M1) / MWEL(1)
    Y(1,2;M1) = CL(1,2;M1) / MWEL(2)
    Y(1,5;M1) = CL(1,3;M1) / MWEL(3)
    Y(1,7;M1) = CL(1,4;M1) / MWEL(4)

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APPENDIX A

\begin{verbatim}
Y(1,15:M1)=CL(1,5:M1)/MWEL(5)
Y(1,20:M1)=CL(1,6:M1)/MWEL(6)
GO TO 50
48 CONTINUE
   DO 42 I=1,NS
42   Y(I,1:M1)=Y11(I,1:M1)
50 CONTINUE
C FREE ENERGY MINIMIZATION BY STEEPEST DESCENT
60 CONTINUE
   NT=NT+1
   CALL MINENG(NS,NE,M1)
C LAMBDA AND DIRECTIONAL DERIVATIVE (DFDL), AND CONVERGENCE TEST
   XLAMBD(1:M1)=1.
   DELT(1,1:MNS)=X(1,1:MNS)-Y(1,1:MNS)
   DO 100 M=1,M1
      IF(SKIP(M).EQ.1.)GO TO 105
      IF(NT.LE.8)GO TO 107
      IF(NT.LE.22)GO TO 107
      DO 101 I=1,NS
         IF(DELT(M,I).GE.0.)GO TO 103
         IF(Y11(M,I).LT.1.E-7)GO TO 102
         XLAM=-Y(M,I)/DELT(M,I)
         IF(XLAM.GE.XLAMBD(M))GO TO 103
         XLAMBD(M)=0.9999999*XLAM
         GO TO 101
102 DELT(M,I)=0.
101 CONTINUE
   GO TO 100
107 DO 103 I=1,NS
      IF(DELT(M,I).GE.0.)GO TO 103
      XLAM=-Y(M,I)/DELT(M,I)
      IF(XLAM.GE.XLAMBD(M))GO TO 103
      XLAMBD(M)=0.9999999*XLAM
103 CONTINUE
   GO TO 100
105 DO 106 J=1,NS
106   DELT(M,J)=0.
100 CONTINUE
C DERIVATIVE FOR GASEOUS SPECIES.
   F(I,1:MNS)=VABS(DELT(I,1:MNS):F(I,1:MNS))
   CONV(I:M1)=0.
   DEBAR(I:M1)=0.
   DO 110 I=1,NS
      CONV(I:M1)=F(I,1:M1)+CONV(I:M1)
110   DEBAR(I:M1)=DELT(I,1:M1)+DEBAR(I:M1)
   NTRIES=0
\end{verbatim}
APPENDIX A

120 CONTINUE
HALL(1:M1)=1./(YBAR(1:M1)+XLAMBO(1:M1)*DFBAR(1:M1))
NTRIES=NTRIES+1
DO 130 I=1,NS
130 F(I,I;M1)=(Y(I,I;M1)+XLAMBO(1;M1)*DELT(I,I;M1))*HALL(I;M1)
F(I,1;MNS)=VALOG(F(I,1;MNS);F(I,1;MNS))
DFDL(I;M1)=0.
DO 140 I=1,NS
F(I,1;M1)=DELT(I,1;M1)*(FORT(I,1;M1)+F(I,1;M1))
140 DFDL(I;M1)=DFDL(I;M1)+F(I,1;M1)
C IF DFDL < 0, WE ARE GOING THE RIGHT WAY ON FREE ENERGY SURFACE.
C IF NOT, REDUCE LAMBDA AND TRY AGAIN...
BIG(1;M1)=SKIP(I;M1).EQ.1.
DFDL(I;M1)=QSVCTRL(1.E-10,BIG(I;M1);DFDL(I;M1))
BIG(1;M1)=QSVCTRL(1.M1);GE.1.E-9
HALL(I;M1)=.75*XLAMBD(I;M1)
XLAMBO(1;M1)=QSVCTRL(HALL(I;M1),BIG(I;M1);XLAMBO(I;M1))
II=Q8SGE(DFDL(I;M1),1.E-9)
IF(II.EQ.1)GO TO 200
IF(NTRIES.GT.16)GO TO 600
GO TO 120
200 CONTINUE
C NEW MOLE FRACTIONS
HALL(1;M1)=VAHS(DFDL(I;M1);HALL(I;M1))
BIG(1;M1)=HALL(I;M1);LT.1.E-9
CONV(I;M1)=QSVCTRL(CRIT,BIG(I;M1);CONV(I;M1))
BIG(1;M1)=CONV(I;M1);GE.CRIT
XLAMBO(1;M1)=QSVCTRL(0.,BIG(1;M1);XLAMBO(I;M1))
SKIP(I;M1)=QSVCTRL(1.,BIG(I;M1);SKIP(I;M1))
II=Q8SGE(0.,BIG(I;M1);CRIT)
IF(II.EQ.1)GO TO 600
DO 220 I=1,NS
220 Y(I,1;M1)=Y(I,1;M1)+XLAMBO(1,1;M1)*DELT(1,1;M1)
IF(NT.LT.50)GO TO 500
WRITE(6,231)
231 FORMAT(/IX,'NO. OF ITERATIONS EXCEED 50'/)
DO 350 M=1,M1
IF(SKIP(M).EQ.1.)GO TO 350
WRITE(6,300)M,P(M),T(M),DFDL(M),CONV(M),XLAMBD(M)
350 CONTINUE
300 FORMAT(1X,'I4,5X,'P='F12.5,5X,'T='F13.5,5X,'DFDL=',
1F12.5,3X,'CONV=',F12.5,3X,'XLAMBD='F11.5)
GO TO 600
500 GO TO 60
600 CONTINUE
WRITE(6,70)NT
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70 FORMAT(/,10X,'NO. OF ITERATIONS=',I4,/) 
YII(1,1:MNS)=Y(1,1:MNS) 
SH(1:M1)=0. 
WMIX1(1:M1)=0. 
TV2(1:M1)=0. 
DO 10 I=1,NS 
   CW=MW(I) 
   WMIX1(1:M1)=WMIX1(1:M1)+YII(1,1:M1) 
10   TV2(1:M1)=TV2(1:M1)+YII(1,1:M1)*CW 
C MOLECULAR WEIGHT OF EQUILIBRIUM MIXTURE 
WMIX1(1:M1)=TV2(1:M1)/WMIX1(1:M1) 
C ENTHALPY OF EQUIL. MIXTURE IN CAL/MOL. DIVIDE BY MIXTURE MOL. WT. 
C TO GET IN CAL/GM. 
C 1 CAL/GM = 4184 J/KG. 
   DO 20 I=1,NS 
      SH(1:M1)=SH(1:M1)+HI(1,1:M1)*YII(1,1:M1) 
20   MOLFF(1,1:M1)=YII(1,1:M1)/WMIX1(1:M1) 
   SH(1:M1)=SH(1:M1)/TV2(1:M1) 
   RETURN 
END 
C SUBROUTINE MINENG(NS,NE,M1) 
C FIT N-DIMENSIONAL PARABOLA TO POINT IN FREE-ENERGY SPACE, WHERE 
C N IS NUMBER OF ELEMENTS IN SYSTEM. 
DIMENSION DELTA(500,24,6),F(500,24),DELT(500,24),BUM(500), 
   IXYBAR(500,500,7,7) 
COMMON/E4/MW(24),SYMB(24),AA(24,6),MWEL(6),AAA(500,24,6) 
COMMON/E5/FORT(500,24),Y(500,24),X(500,24),YBAR(500) 
COMMON/E6/YII(500,24) 
COMMON/E7/AA(500,7,7),BBI(500,7) 
COMMON/E10/SKIP(500) 
COMMON/E15/RR,CRT,CRT,MNS,MM,E,MNE1,MX 
COMMON/E16/ENT(500,24),CPII(500,24) 
EQUIVALENCE (F(I,I),ENT(I,I)),(DELT(I,I),CPII(I,I)) 
   YBAR(1:M1)=0. 
   DO 100 I=1,NS 
100   YBAR(1:M1)=YBAR(1:M1)+Y(1,1:M1) 
C SET UP AND SOLVE MATRIX 
   BBI(1,1:MNE1)=0. 
   DO 110 J=1,NE 
      DELTA(1,1,J:MNS)=AAA(1,1,J:MNS)*Y(1,1:MNS) 
110   DO 100 I=1,NS 
   BBI(1,1,J:M1)=DELTA(1,1,J:M1)+BBI(1,1,J:M1) 
C (1) FREE ENERGY - GASEOUS SPECIES 
   DO 170 I=1,NS 
170   YII(1,1:M1)=Y(1,1:M1)/YBAR(1:M1) 
   F(1,1:MNS)=VALOG(YII(1,1:MNS):F(1,1:MNS))
APPENDIX A

DO 180 I=1,NS
180 F(I,1:M1)=Y(I,1:M1)*(FORT(I,1:M1)+F(I,1:M1))

C INITIALIZE MATRICES
   A1(I,1,1:MX)=0.
   R1(I,1,1:MX)=0.
   A1(I,1,1:MNE)=BBI(I,1,1:MNE)
   DO 270 J=1,NE
   DO 270 K=1,J
   DELT(1,1:MNS)=AAA(1,1,J:MNS)*DELT(1,1,K:MNS)
   DO 275 I=1,NS
   R1(I,J,K:M1)=DELT(1,1:M1)+R1(I,J,K:M1)
   DO 270 J=I,NE
   K=J-1
   280 A1(I,1,J:MNE)=R1(I,1,J:K:MNE)
   DO 310 J=2,MMM
   K=J-1
   DO 320 J=1,NE
   DELT(1,1:MNS)=AAA(1,1,J:MNS)*F(1,1:MNS)
   BUM(1:M1)=0.
   DO 330 I=1,NS
   330 BUM(1:M1)=DELT(1,1:M1)+BUM(1:M1)
   320 BBI(I,J:M1)=BBI(I,J:1:M1)+BUM(1:M1)
   BUM(1:M1)=0.
   DO 340 I=1,NS
   340 BUM(1:M1)=BUM(1:M1)+F(1,1:M1)
   BBI(I,MMM:M1)=BUM(1:M1)
   CALL EQSOL(MMM,NE,M1)

C NEW MOLE FRACTIONS (X)
   XYBAR(I:M1)=BBI(I,1,1:M1)
   BBI(I,1,MNE)=BBI(I,2,MNE)
   DELT(1,1:MNS)=0.
   DO 390 J=1,NE
   DO 400 I=1,NS
   400 DELT(1,1:M1)=DELT(1,1:M1)+AAA(1,1,J:M1)*BBI(I,1,J:M1)
   390 CONTINUE
   DO 410 I=1,NS
   410 DELT(1,1:M1)=DELT(1,1:M1)+XYBAR(1:M1)
   X(I,1,MNS)=DELT(1,1:MNS)*Y(I,1,MNS)-F(1,1:MNS)
RETURN
END

SUBROUTINE EOSOL(MMM,NE,M1)
COMMON/E7/A1(500,7,7),BBI(500,7)
DIMENSION U(500,7),S(500),TK2(500),UT(500)
DO 200 K=1,NE

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APPENDIX A

\[ J = K \]
\[ S(1:M1) = 0. \]
\[ \text{DO 20 I = K, MMM} \]
\[ S(1:M1) = S(1:M1) + A(1, I, J; M1) \times A(1, I, J; M1) \]
\[ S(1:M1) = \sqrt{S(1:M1)} \times A(1, K, J; M1) \times U(1; M1) \]
\[ KPI = K + 1 \]
\[ KMI = M1 \times (MMM - K) \]
\[ U(1, K, J; M1) = A(1, K, J; M1) \times V \times S(1:M1) \times A(1, K, J; M1) \times U(1; M1) \]
\[ TK2(1, M1) = U(1, K, M1) \times S(1:M1) \]
\[ J = K + 1 \]
\[ \text{DO 70 JJ = JK, MMM} \]
\[ UT(1; M1) = 0. \]
\[ \text{DO 50 III = K, MMM} \]
\[ UT(1; M1) = UT(1; M1) + U(1, III; M1) \times A(1, III, JJ; M1) \]
\[ UT(1; M1) = UT(1; M1) / TK2(1; M1) \]
\[ \text{DO 40 III = K, MMM} \]
\[ A(1, III, JJ; M1) = A(1, III, JJ; M1) - UT(1; M1) \times UT(1; M1) \]
\[ \text{DO 200 CONTINUE} \]
\[ BB1(1, 1; M1) = BB1(1, 1; M1) / A(1, 1, 7; M1) \]
\[ BB1(1, 6; M1) = BB1(1, 6; M1) - A(1, 1, 6; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ BB1(1, 5; M1) = BB1(1, 5; M1) - A(1, 1, 5; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ BB1(1, 4; M1) = BB1(1, 4; M1) - A(1, 1, 4; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ BB1(1, 3; M1) = BB1(1, 3; M1) - A(1, 1, 3; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ BB1(1, 2; M1) = BB1(1, 2; M1) - A(1, 1, 2; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ BB1(1, 1; M1) = BB1(1, 1; M1) - A(1, 1, 1; M1) \times BB1(1, 1, 7; M1) / A(1, 1, 6; M1) \]
\[ \text{RETURN} \]
\[ \text{END} \]

SUBROUTINE TP(M1)
APPENDIX A

DIMENSION BI(500), VISI(500, 24), CONDI(500, 24)
COMMON/E1/T(500), P(500), WMIX(500), CL(500, 6), SH(500)
COMMON/E2/HT(500, 24), MOLEF(500, 24), CPI(500, 24)
COMMON/E4/MW(24), SYMB(24), AA(24, 6), MVEL(6), AAA(500, 24, 6)
COMMON/E5/FORT(500, 24), Y(500, 24), X(500, 24), YBAR(500)
COMMON/E8/NE, NS
COMMON/E9/XMA(24), XMB(24), XMC(24), XKA(24), XKB(24)
COMMON/E12/A9(500), A10(500), A13(500), AA1(500), AA2(500), TV1(500), TV2(500)
COMMON/E14/VIS(500), COND(500), SIG(500), CP(500)
COMMON/E16/ENT(500, 24), CPII(500, 24)
EQUIVALENCE (VISI(I,I), ENT(I,I)), (COND(I,I), CPII(I,I))

REAL MOLEF, MW
C HERE VISI IS THE VISCOSITY OF SPECIFIC I.
DO 200 I=1, NS
VISI(I,I;MI)=(XMA(I)+XMB(I)*T(I;MI)+XMC(I)*T(I;MI)*T(I;MI))/.0672
BI(I;MI)=VISI(I,I;MI).LE.0.
VISI(I,I;MI)=8VCTRL(I.E-10, 81(1;MI): VISI(I,I;MI))
200 CONTINUE
C CP IS SPECIFIC HEAT OF MIXTURE.
CP(I;MI)=0.
DO 210 I=1, NS
CP(I;MI)=CP(I;MI)+CPI(I,I;MI)*MOLEF(I,I;MI)
210 CONTINUE
C HERE CONDI IS THE THERMAL CONDUCTIVITY OF SPECIFIC I.
DO 220 I=1, NS
COND(I;MI)=(XKA(I)+XKB(I)*T(I;MI))/.0672
220 CONTINUE
C WILKE RELATION FOR MIXTURE VISCOSITY AND THERMAL CONDUCTIVITY.
VIS(I;MI)=0.
COND(I;MI)=0.
DO 240 I=1, NS
A13(I;MI)=0.
DO 230 J=1, NS
WJI=MW(J)/MW(I)
DENOMI=2.82*SORT(I.+1./WJI)
WJI=SORT(WJI)
WJI=SORT(WJI)
AA1(I;MI)=VISI(I,I;MI)/VISI(I,J;MI)
AA1(I;MI)=VSORT(AA1(I;MI):AA1(I;MI))
AA1(I;MI)=AA1(I;MI)*AA1(I;MI)
AA1(I;MI)=AA1(I;MI)*AA1(I;MI)
A13(I;MI)=A13(I;MI)+MOLEF(I,J;MI)*AA1(I;MI)/DENOMI
230 CONTINUE
VIS(I;MI)=MOLEF(I;MI)*VISI(I;MI)/A13(I;MI)+VIS(I;MI)
COND(I;MI)=MOLEF(I;MI)*COND(I;MI)/A13(I;MI)+COND(I;MI)
240 CONTINUE
C PRANDTL NUMBER
SIG(I;MI)=VIS(I;MI)*CP(I;MI)/COND(I;MI)/WMIX(I;MI)
RETURN
END
APPENDIX B

PROGRAM INPUT

The input for the present setup of the program EQUIL is given in this appendix.

6.THERMO
NS=24, NE=6,
MDEL(1)=5.486E-4,1.008,4.01,12.011,16.0,14.0,
MDEL(1)=5.486E-4,1.008,2.016,1.008,4.01,12.001,24.022,36.033,12.01,25.03,26.038,
37.041,49.04,
16.,32.,16.,28.011,44.01,
14.,28.,14.,26.,10.,
16.,16.,16.,16.,16.,

6.END

E-  1
-0.250000E+01 0.  0.  0.  0.  0.  F  2
-0.745375E+03-0.1173402E+02 GORDON AND MCBRIDE NASA SP-273  F  3
0.250000E+01 0.  0.  0.  0.  0.  F  4
-0.7453749E+03-0.1173402E+02 GORDON AND MCBRIDE NASA SP-273  F  5
0.2508E+01 0. -0.6332E-05 0.1364E-08 -0.1094E-12 0.2934E-17 E-  6
-0.7450E+03 -0.1208E+02 ESCH ETAL NASA CR-111989 E-  7
0.  0.  -0.5000E-07 -0.1000E-12 26.0000E-05 0.0  E-  8
H  1
0.250000E+01 0.  0.  0.  0.  0.  H  2
0.2547162E+05 0.4601176E+00 GORDON AND MCBRIDE NASA SP-273  H  3
0.250000E+01 0.  0.  0.  0.  0.  H  4
0.2547162E+05 0.4601176E+00 GORDON AND MCBRIDE NASA SP-273  H  5
2.475164E+00 7.366387E-05 -2.537593E-08 2.386674E-12 -4.551431E-17 H  6
2.523626E+04 3.749137E-01 NICOLET NASA CR-132470 H  7
0.2948E+00 0.889E-07 -0.811E-12 2.496E-05 5.1290E-08 H  8
H2  2
0.3057445E+01 0.2676520E-02-0.5809916E-05 0.5521039E-08-0.1812273E-11 H2  9
-0.9889047E+03-0.2299705E+01 GORDON AND MCBRIDE NASA SP-273 H2  10
0.3100190E+01 0.5111946E-03 0.5264421E-07-0.3490997E-10 0.3694534E-14 H2  11
-0.8773804E+03-0.1962942E+01 GORDON AND MCBRIDE NASA SP-273 H2  12
0.3363E+01 0.4656E-03 -0.5127E-07 0.2802E-11 -0.4905E-16 H2  13
-0.1018E+04 -0.3716E+01 ESCH ETAL NASA CR-111989 H2  14
-0.079E+00 -0.791E-07 -0.886E-12 3.211E-05 5.3440E-08 H2  15
H+  -1  1
0.250000E+01 0.  0.  0.  0.  0.  H+  2
0.1840334E+06 0.1153862E+01 GORDON AND MCBRIDE NASA SP-273 H+  3
0.250000E+01 0.  0.  0.  0.  0.  H+  4
0.1840334E+06 0.1153862E+01 GORDON AND MCBRIDE NASA SP-273 H+  5
0.250000E+01 0.  0.  0.  0.  0.  H+  6
0.1840334E+06 0.1153862E+01 GORDON AND MCBRIDE NASA SP-273 H+  7
0.0  0.5000E-07 -0.1000E-12 26.0000E-05 0.0  H+  8
HE  1
0.250000E+01 0.  0.  0.  0.  0.  HE  2
-0.7453749E+03 0.9153488E+00 GORDON AND MCBRIDE NASA SP-273 HE  3
0.250000E+01 0.  0.  0.  0.  0.  HE  4
APPENDIX B

-0.7453749E+03 0.9153488E+00 GORDON AND MCBRIDE NASA SP-273

0.2500000E+01 0. 0. 0. GORDON AND MCBRIDE NASA SP-273

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0.2853426E+06 0.1608404E+01 GORDON AND MCBRIDE NASA SP-273

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C 1

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C2 2

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C+ -1 1

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APPENDIX B

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0.1879490 & \times 10^{0} \quad 0.4388435 & \times 10^{1} \quad \text{GORDON AND MCBRINE NASA SP-273} \\
0.2560440 & \times 10^{0} \quad 0.1446424 & \times 10^{-6} \quad 0.1246604 & \times 10^{-7} \quad 0.6445474 & \times 10^{-11} \quad 0.6544887 & \times 10^{-15} \\
0.1879470 & \times 10^{0} \quad 0.4379470 & \times 10^{1} \quad \text{GORDON AND MCBRINE NASA SP-273} \\
0.2944 & \times 10^{0} \quad -0.4108 & \times 10^{-3} \quad 0.9156 & \times 10^{-7} \quad -0.5846 & \times 10^{-11} \quad 0.1190 & \times 10^{-15} \\
0.1879 & \times 10^{0} \quad 0.1750 & \times 10^{-1} \quad \text{ESCH ETAL. NASA CR-111989} \\
0.39 & \times 10^{0} \quad 0.0508 & \times 10^{-7} \quad -1.0000 & \times 10^{-12} \quad 0.0000 & \times 10^{-0} \\
\end{align*}
\end{array}
\]
REFERENCES


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<td>NE</td>
<td>Number of elements present in the mixture, including electrons; NE = 6</td>
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<td>MW</td>
<td>An array of molecular weights of the species present</td>
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<td>Values for AA(i,j) array using element (j) -</td>
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TABLE III.- RESULTS FOR FIRST EXAMPLE

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TABLE IV.- Concluded

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A vectorized code, EQUIL, is developed for calculating the equilibrium chemistry of a reacting gas mixture on the Control Data STAR-100 computer. The code provides species mole fractions, mass fractions, and thermodynamic and transport properties of the mixture for given temperature, pressure, and elemental mass fractions. The code is set up for the e⁻, H, He, C, O, N system of elements. In all, 24 chemical species are included.