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DENSITY, HEAT CAPACITY, VISCOSITY, AND THERMAL CONDUCTIVITY OF MIXTURES OF CO_2, HE, H_2, H_2O, N_2, AND O_2

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TECHNICAL REVIEW AND APPROVAL

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The experiments reported herein were conducted according to the principles set forth in the current edition of the "Guide for the Care and Use of Laboratory Animals," Institute of Laboratory Animal Resources, National Research Council.

This technical report has been reviewed by the NMRI scientific and public affairs staff and is approved for publication. It is releasable to the National Technical Information Service where it will be available to the general public, including foreign nations.

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The thermodynamic properties of gas mixtures are not always well approximated by the average properties of pure gases weighted by the fractional composition. In order to improve our calculations we have turned to the literature to find formulas said to be useful for calculating the properties of mixtures in the range of temperatures and pressures encountered in human diving. Very little has been published on experimental determinations of properties of mixtures, so we have sought principally to verify that the formulas for mixtures give a good match to data on pure gases. In order to match data on pure gases, the values for the critical temperature (TC) and the critical pressure (PC) for H_2 and He were modified. In addition, ad-hoc adjustments have been made to the critical volumes (VC) to make viscosity at low pressures match tables for these two gases. Omega, the acentric factor in the formulas, is taken as zero for all gases. The properties for which we have subroutines are thermal conductivity in watts·meter^{-1}·degree K^{-1}, viscosity in μpoise, density in moles·cm^{-3}, heat capacity in Joules·mole^{-1}·degree K^{-1}, and the vapor pressure of water in torr.

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INTRODUCTION

The thermodynamic properties of gas mixtures are not always well approximated by the average properties of pure gases weighted by the fractional composition. In order to improve our calculations we have turned to a book by Reid, Prausnitz, and Poling (1987). This book provides formulas said to be useful for calculating the properties of mixtures in the range of temperatures and pressures encountered in human diving. Very little has been published on experimental determinations of properties of mixtures, so we have sought principally to verify that the formulas in question give a good match to data on pure gases and have trusted to the formulas for the interpolations for mixtures. In order to match data on pure gases, the values for the critical temperature (TC) and the critical pressure (PC) for H_2 and He were changed as suggested by Gunn, Chueh, and Prausnitz (1966). In addition, ad-hoc adjustments have been made to the critical volumes (VC) to make viscosity at low pressures match published values for these two gases. At the suggestion of one of the authors of the book (Poling), omega, the acentric factor in the formulas, is taken as zero for all gases. The properties for which we have subroutines are thermal conductivity in watts·meter^{-1}·°K^{-1}, viscosity in μpoise, density in moles·cm^{-3}, heat capacity in Joules·mole^{-1}·°K^{-1}, and the vapor pressure of water in torr.

Thermodynamic properties of pure gases are shown in Tables 1-4 at 300 °K. Pressure is given in bars rather than atmospheres, because the reference sources most commonly report in bars (1 bar= 1.01325 atmospheres). References cited are as follows: a) Weast, R.C., CRC Handbook of Chemistry, 49th edition, Chemical Rubber Co., Cleveland, OH, 1968; b) McCarty, R.D. et al., Selected Properties of Hydrogen (Engineering Design Data, National Bureau of Standards Monograph 168, U.S. Department of Commerce, Washington, DC, 1981; c) Lide, D.R. (editor), CRC Handbook of Chemistry and Physics, 73rd edition, CRC Press, 1992; d) McCarty, R.D., Thermophysical Properties of Helium-4 from 2 to 1500 °K with Pressures to 1000 Atmospheres, National Bureau of Standards Technical Note 36, U.S Department of Commerce, Washington, DC, 1972; e) Chung, T.-H., et al., "Applications of kinetic gas theories and multiparameter correlation for prediction of dilute gas viscosity and thermal conductivity," Industrial and Engineering Chemistry Fundamentals, Vol. 23, 1984; f) Lange, N.A. (editor), Handbook of Chemistry, Handbook Publishers, Inc., Sandusky, OH, 1946.

THERMAL CONDUCTIVITY

*REAL*8 FUNCTION TK(Y,TIN,PIN)*

Inputs to the function are the vector of mol fractions of CO_2, H_2, H_2O, He, N_2, O_2 in the gas mixture (Y), temperature (TIN, °C), and pressure (PIN, atmospheres). Output is the mixture thermal conductivity (TK, $W \cdot m^{-1} \cdot {}^{\circ}K^{-1}$). Formulas are from Reid, Prausnitz, and Poling, Chapter 10, "Thermal Conductivity" (1987).

TABLE 1
Thermal conductivities($W \cdot m^{-1} \cdot {}^{\circ}K^{-1}$) of pure gases at 300°K.

GAS	Pressure Bars	Program	Reference
CO_2	1	0.01724	0.0187,c 0.0166,a
H_2	1	0.1821	0.1869,c 0.1869,a 0.187,b
	10	0.1822	0.1872,b
	100	0.1926	0.1899,b
H_2O	1	0.02121	0.0178,a 0.0181,a
He	1	0.1556	0.1567,c 0.1499,a 0.1474,a 0.155,d
	10	0.1557	0.155,d
	100	0.1624	0.160,d
N_2	1	0.02646	0.026,c,a
	10	0.02652	0.0263,c
	100	0.03093	0.0319,c
O_2	1	0.02674	0.0263,c
	10	0.02678	0.0263,c
	100	0.03043	0.0316,c

VISCOSITY

*REAL*8 FUNCTION VISC(Y,TIN,PIN)*

Inputs to the function are the vector of mol fractions of CO_2, H_2, H_2O, He, N_2, O_2 in the gas mixture (Y), temperature (TIN, °C), and pressure (PIN, atmospheres). Output is the mixture viscosity (VISC, μpoise). Formula from Chapter 9, "Viscosity", and from constants in Appendix A of Reid, Prausnitz, and Poling (1987).

TABLE 2
Viscosity in μpoise of pure gases at 300°K.

GAS	Pressure Bars	Program	Reference
CO_2	1	158.7	151-219,e 152,a
H_2	1	88.6	89.53,b 89.2,a
	10	88.81	90.7,b
	100	91.83	91.7,b
H_2O	1	95.7	100,f
He	1	199.6	199.,d 197.,a
	10	199.9	200.,d
	100	203.3	203.,d
N_2	1	179.4	180,c 178.1,a
	10	180.3	181,c
	100	204.5	201,c
O_2	1	207.	206,c 208,a
	10	207.8	207,c
	100	232.2	229,c

DENSITY

*REAL*8 FUNCTION RHO(Y,TIN,PIN)*

Inputs to the functions are the vector of mol fractions of CO_2, H_2, H_2O, He, N_2, O_2 in the gas mixture (Y), temperature (TIN, °C), and pressure (PIN, atmospheres). The subroutine returns the gas density (RHO, $mol \cdot cm^{-3}$). Formula for viral equations from Reid, Prausnitz, and Poling (1987).

TABLE 3
Density ($mol \cdot L^{-1}$) of pure gases at 300°K.

GAS	Pressure Bars	Program	Reference
CO_2	1	0.0403	
H_2	1	0.0401	0.0401,b
	10	0.398	0.399,b
	100	3.78	3.78,b
H_2O	1	..	..
He	1	0.0401	0.0406,d
	10	0.399	0.404,d
	100	3.83	3.88,d
N_2	1	0.0401	0.04,c
	10	0.402	0.402,c
	100	4.07	3.989,c
O_2	1	0.0407	0.04,c
	10	0.401	0.403,c
	100	4.03	4.205,c

HEAT CAPACITY

*REAL*8 FUNCTION CP(Y,TIN)*

Inputs to the function are the vector of mol fractions of CO_2, H_2, H_2O, He, N_2, O_2 in the gas mixture (Y), temperature (TIN, °C), and pressure (PIN, atmospheres). Output is the mixture isobaric heat capacity (CP, $J{\cdot}mol^{-1}{\cdot}{}^{\circ}K^{-1}$). Formula and constants in Appendix A of Reid, Prausnitz, and Poling (1987).

TABLE 4
Heat capacity at constant pressure ($J{\cdot}mol^{-1}{\cdot}{}^{\circ}K^{-1}$) and 300°K.

GAS	Pressure Bars	Program	Reference
CO_2	1	37.25	36.6,f
H_2	1	28.89	29.9,c
	10	28.89	30.0,c
	100	28.89	30.4,c
H_2O	1	33.67	..
He	1	20.8	20.8,c
	10	20.8	20.8,c
	100	20.8	20.8,c
N_2	1	29.18	29.2,c
	10	29.18	29.6,c
	100	29.18	33.4,c
O_2	1	29.39	29.4,c
	10	29.39	29.9,c
	100	29.30	29.4,c

VAPOR PRESSURE OF WATER

*REAL*8 FUNCTION VPH2O(T,P)*

Input temperature (T,°C), pressure (P, atmospheres) returns vapor pressure of water (VPH20, torr). Formula is Equation 1 from Appendix A of Reid, Prausnitz, and Poling (1987). Pressure correction is from Glasstone (1946). Verified by comparison with Weast (1968). Maximum error <0.25%

WHY USE MIXTURE FORMULAS?

The question naturally arises: Why not calculate mixture properties from an average of the pure gas properties weighted by the fractional composition of the mixture? The answer: This does not always give the correct value, although sometimes the approximation is reasonable. For example, the fractional weighting for density and heat capacity give the same answer as the formulas to within a few percent, and represent a reasonable alternative. Indeed one could use published programs for pure gas properties of N_2 and O_2 (Younglove, 1982), and probably achieve better accuracy than with the present program over some ranges of pressure for some gases. Values for mixed-gas viscosity and thermal conductivity, however, appear very different when the calculations from mixture formulas are compared to the values obtained by fractional weighting.

TABLE 5
Comparison of mixture formulas (F) with fractional weighting (W), for viscosity (μpoise), and thermal conductivity ($W \cdot m^{-1} \cdot {}^\circ K^{-1}$) at 300°K

He	N_2	O_2	Atm	Viscosity		Thermal Conductivity	
Fractional Composition				F	W	F	W
0.8	0	0.2	1	259	201.1	0.08382	0.1299
0.8	0	0.2	6	259.2	201.3	0.08383	0.1299
0	0.79	0.21	1	185	185.6	0.0265	0.0265
0	0.79	0.21	6	185.5	185.6	0.0265	0.0265
0	0.96	0.04	10	214.4	200.2	0.1362	0.1505
0	0.2	0.8	1	201.3	201.4	0.0267	0.0267

Major differences appear only where He is present. The largest difference shown is for 80% He and 20% O_2 where about 30% discrepancies occur. Unfortunately, little empirical evidence is available to help us decide which values are in fact most reliable. Mixtures with H_2 also have higher viscosities and lower thermal conductivities predicted by the mixture formulas than by fractional weighting.

Another approximation that may frequently be considered is to ignore the presence of water vapor and CO_2. Differences in heat capacity and density are relatively small.

TABLE 6

Comparison of mixtures without water (D) with mixtures with 0.05 atmospheres of water vapor and 0.05 atmospheres of carbon dioxide (W). Viscosity (μpoise), and thermal conductivity ($W \cdot m^{-1} \cdot {}^\circ K^{-1}$) are shown. Temperature is 300°K, pressure 1 atmosphere. Other gases were each reduced by 0.05 atmospheres when water vapor and CO_2 were present.

He	N_2	O_2	Viscosity		Thermal Conductivity	
Fractional Composition			D	W	D	W
0.8	0	0.2	259	252.7	0.08382	0.0683
0	0.79	0.21	185	177.8	0.0265	0.0260
0	0.2	0.8	201	191.8	0.0267	0.0262

The effects of omitting water vapor at 1 atmosphere are modest (less than 15%). At higher pressures, CO_2 and water vapor become smaller fractions of the whole, and corrections become even smaller.

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8. Reid, R.C., Prausnitz, J.M., and Poling, B.E., The Properties of Gases and Liquids, 4th edition, McGraw-Hill Publishers, 1987.

9. Younglove, B.A., Interactive Fortran Program to Calculate Thermophysical Properties of Six Fluids. National Bureau of Standards Technical Note 1048, U.S. Department of Commerce, Washington, DC, 1982.

10. Weast, R.C., CRC Handbook of Chemistry and Physics, 49th edition, Chemical Rubber Co., Cleveland, Ohio, 1968.

APPENDIX: FORTRAN LANGUAGE SUBROUTINE

G2CON.FOR .. include file for the gas subroutines in G2.FOR

```
C..
        IMPLICIT REAL*8(A-H,M,O-Z)
        PARAMETER(NGAS=6)
        DIMENSION Y(NGAS),VC(NGAS),TC(NGAS),MW(NGAS),OMEGA(NGAS),PC(NGAS)
C..     DATA PARAMETER/CO2,H2,H2O,HE,N2,O2/99-75-77-48-56-59
        DATA VC/93.9D0,64.3D0,57.1D0,57.4D0,89.8D0,73.4D0/
C       DATA TC/304.1D0,33.D0,647.3D0,5.19D0,126.2D0,154.6D0/
C       DATA PC/73.8D0,12.9D0,221.2D0,2.27D0,33.9D0,50.4D0/
C..H2/He changed Gunn etal AICHE J 12,937(1966)
        DATA TC/304.1D0,42.D0,647.3D0,10.3D0,126.2D0,154.6D0/
        DATA PC/73.8D0,18.8D0,221.2D0,5.8D0,33.9D0,50.4D0/
C..
        DATA MW/44.01D0,2.016D0,18.015,4.003D0,28.013D0,31.999D0/
C       DATA OMEGA/.239D0,-.216D0,.344D0,-.365D0,.039,.025/
        DATA OMEGA/6*0./
        DATA R/8.3144/
C..
```

G2.FOR subroutines for calculating mixed gas thermal properties

```
C..
        REAL*8 FUNCTION TK(Y,TIN,PIN)
C..
C.. Input is the vector of mol fractions of CO2,H2,H2O,He,N2,O2 in the
C.. gas mixture, Y. Temperature, TIN, degrees C, pressure PIN, atmospheres.
C.. Output is the mixture thermal conductivity in W/(m-K)
C.. Formula from pages 491-576, chapter on thermal conductivity
C.. and mixing formulas 9-5.24 to 9-5.44,10-3.17 and 10-6.1 to 10-6.5
```

```
C.. and constants in appendix A of Reid, Robert C, John M Prausnitz,
C.. Bruce E Poling; The properties of gases and liquids, 4th edition
C.. McGraw-Hill NY,NY ,1987.
C..
C.. TC, and PC for H2 and He are changed as suggested by Gunn etal
C.. AICHE J 12,937(1966), in addition ad-hoc adjustments have been made to
C.. VC to make viscosity at low pressures match tables for these 2 gases
C.. omega is taken as zero for all gases
C..
      INCLUDE 'g2con.for'
C..
      DIMENSION AI(7),B(7)
      DATA AI/2.4166D0,-5.0924E-1,6.6107D0,1.4543D1,7.9274D-1
     &      ,-5.8634D0,9.1089D1/
C..
C.. Convert T to Kelvin, P to bars
      T=TIN+273.16
      P=PIN*1.01325D0
C.. Get mean values equations 9-5.25 to 9-5.30
      SM3=0.
      EKM=0.
      MWM=0.
      DO 2 I=1,NGAS
      DO 1 J=1,NGAS
C.. equations 9-5.32 TO 9-5.40
C.. kappa is 0 for these gases, mu also
       IF(I.EQ.J)THEN
        SIJ=.809*(VC(I)**(1.D0/3.D0))
        EKIJ=TC(I)/1.2593D0
        MIJ=MW(I)
       ELSE
```

```
          SIJ=.809D0*SQRT((VC(I)**(1.D0/3.D0))*(VC(J)**(1.D0/3.D0)))
          EKIJ=SQRT(TC(I)*TC(J))/1.2593D0
          MIJ=2.D0*MW(I)*MW(J)/(MW(I)+MW(J))
         END IF
        SM3=SM3+SIJ*SIJ*SIJ*Y(I)*Y(J)
        EKM=EKM+Y(I)*Y(J)*EKIJ*SIJ*SIJ*SIJ
        MWM=MWM+Y(I)*Y(J)*EKIJ*SIJ*SIJ*SQRT(MIJ)
1       CONTINUE
C.. rhom must be in mol/cm3 for use in calculating yy below
C.. subroutine returns in gm/cm3
2       CONTINUE
        RHOM=RHO(Y,TIN,PIN)
        EKM=EKM/SM3
        TSM=T/EKM
        MWM=MWM*MWM/(EKM*EKM*(SM3**(4.D0/3.D0)))
C.. equations 9-5.41 to 9-5.44 with omissions for mu=kappa=omega=0
        TCM=1.2593D0*EKM
        VCM=SM3/(.809*.809*.809)
        FCM=1.D0
        CVM=CP(Y,TIN)-R
        ETA0=VISC(Y,TIN,.01D0)*1.D-7
C..low pressure viscosity must be in N-s/m2 rather then uP
C..
C.. Use these mean values in equations 10-5.5 to 10-5.6 and 10-6.6
C.. as recommended on page 539
        ALPHA=(CVM/R)-1.5D0
        TR=T/TCM
        BETA=.7862
        Z=2.D0+10.5D0*TR*TR
C.. Upsilon equation 10-3.17
        UPS=1.D0+ALPHA*((.215D0+.28288D0*ALPHA-1.061D0*BETA+.26665D0*Z)/
```

```
     &      (.6366D0+BETA*Z+1.061D0*ALPHA*BETA))
            MPRIME=MWM/1000.D0
            Q=3.586D-3*SQRT(TCM/MPRIME)/(VCM**(2.D0/3.D0))
            DO 3 I=1,7
            B(I)=AI(I)
3           CONTINUE
            YY=VCM*RHO(Y,TIN,PIN)/6.D0
            G1=(1.D0-.5D0*YY)/((1.D0-YY)**3.D0)
            G2=(B(1)/YY)*(1.D0-DEXP(-B(4)*YY))
            G2=G2+B(2)*G1*DEXP(B(5)*YY)+B(3)*G1
            G2=G2/((B(1)*B(4))+B(2)+B(3))
            TK=31.2D0*ETA0*UPS*((1.D0/G2)+B(6)*YY)
            TK=TK/MPRIME
            TK=TK+Q*B(7)*YY*YY*G2*SQRT(TR)
            RETURN
            END
C..
            REAL*8 FUNCTION VISC(Y,TIN,PIN)
C..
C.. Input is the vector of mol fractions of CO2,H2,H2O,He,N2,O2 in the
C.. gas mixture, Y. Temperature, TIN, degrees C, pressure PIN, atmospheres.
C.. Output is the mixture viscosity in micro Poise.
C.. Formula from pages 388-490, chapter on viscosity and
C.. from constants in appendix A of Reid, Robert C, John M Prausnitz,
C.. Bruce E Poling; The properties of gases and liquids, 4th edition
C.. McGraw-Hill NY,NY ,1987.
C..
C.. TC, and PC for H2 and He are changed as suggested by Gunn etal
C.. AICHE J 12,937(1966), in addition ad-hoc adjustments have been made to
C.. VC to make viscosity at low pressures match tables for these 2 gases
C.. omega is taken as zero for all gases
```

```
C..
      INCLUDE 'g2con.for'
C..
      DIMENSION A(10),E(10)
      DATA A/6.324D0,1.21D-3,5.283D0,6.623D0,19.745D0,-1.9D0,
     & 24.275D0,.7972D0,-.2382D0,.06863D0/
C.. Convert T to Kelvin, P to bars
      T=TIN+273.16
      P=PIN*1.01325D0
C.. Get mean values equations 9-5.25 to 9-5.30
      SM3=0.
      EKM=0.
      MWM=0.
      DO 2 I=1,NGAS
      DO 1 J=1,NGAS
C.. equations 9-5.32 TO 9-5.40
C.. kappa is 0 for these gases, mu also
       IF(I.EQ.J)THEN
        SIJ=.809*(VC(I)**(1.D0/3.D0))
C..Ad hoc adjustments for He and H2
        IF(I.EQ.2)SIJ=SIJ/1.09D0
        IF(I.EQ.4)SIJ=SIJ/1.195D0
        EKIJ=TC(I)/1.2593D0
        MIJ=MW(I)
       ELSE
        SIJ=.809D0*SQRT((VC(I)**(1.D0/3.D0))*(VC(J)**(1.D0/3.D0)))
C..Ad hoc adjustments for He and H2
        IF((I.EQ.2).OR.(J.EQ.2))SIJ=SIJ/1.09D0
        IF((I.EQ.4).OR.(J.EQ.4))SIJ=SIJ/1.195D0
C..
        EKIJ=SQRT(TC(I)*TC(J))/1.2593D0
```

```
              MIJ=2.D0*MW(I)*MW(J)/(MW(I)+MW(J))
             END IF
            SM3=SM3+SIJ*SIJ*SIJ*Y(I)*Y(J)
            EKM=EKM+Y(I)*Y(J)*EKIJ*SIJ*SIJ*SIJ
            MWM=MWM+Y(I)*Y(J)*EKIJ*SIJ*SIJ*SQRT(MIJ)
1           CONTINUE
C.. rhom must be in mol/cm3 for use in calculating yy below
2           CONTINUE
            RHOM=RHO(Y,TIN,PIN)
            EKM=EKM/SM3
            TSM=T/EKM
            MWM=MWM*MWM/(EKM*EKM*(SM3**(4.D0/3.D0)))
C.. equations 9-5.41 to 9-5.44 with omissions for mu=kappa=0
            TCM=1.2593D0*EKM
            VCM=SM3/(.809*.809*.809)
            FCM=1.D0
C.. Use these mean values in equations 9-6.16 to 9-6.21 as recommended
C.. on page 432
            DO 3 I= 1 ,10
            E(I)=A(I)
C.. E(i) has more terms if kappa and mu are not 0
3           CONTINUE
            YY=RHOM*VCM/6.D0
            G1=(1.D0-.5D0*YY)/((1.D0-YY)**3.D0)
            G2=E(1)*(1.D0-DEXP(-E(4)*YY))/YY
            G2=G2+E(2)*G1*DEXP(E(5)*YY)
            G2=G2+E(3)*G1
            G2=G2/(E(1)*E(4)+E(2)+E(3))
            ETASS=E(7)*YY*YY*G2*DEXP(E(8)+(E(9)/TSM)+(E(10)/(TSM*TSM)))
            OMEGAV=1.16145D0*(TSM**(-.14874D0))+.52487*DEXP(-.77320*TSM)
            OMEGAV=OMEGAV+2.16178*DEXP(-2.43787D0*TSM)
```

```
      ETAS=ETASS+((SQRT(TSM)*FCM*((1.D0/G2)+E(6)*YY))/OMEGAV)
      ETA=ETAS*36.344D0*SQRT(MWM*TCM)/(VCM**(2.D0/3.D0))
      VISC=ETA
      RETURN
      END
C..
      REAL*8 FUNCTION RHO(Y,TIN,PIN)
C..
      INCLUDE 'g2con.for'
C..
C.. Input T, temperature degrees C, pressure in atmospheres,
C.. returns gas density in mol/cm3
C.. Formula for virial equations from page 37 of Reid, Robert C,
C.. John M Prausnitz,
C.. Bruce E Poling; The properties of gases and liquids, 4th edition
C.. McGraw-Hill NY,NY ,1987.
C.. Coefficients from CRC handbook of chemistry and physics 73rd edition
C.. 1992 taken from JH Dymond and EB Smithe, The virial coefficients of
C.. pure gases and mixtures, a critical compilation, Oxford U press,
C.. Oxford,1980
C..
      DIMENSION A(5,NGAS)
      DATA A/-127.D0,-288.D0,-118.D0,0.,0.,
     &  15.4D0,-9.D0,-.2D0,0.,0.,
     &  -1158.D0,-5157.D0,-10301.D0,-10597.D0,-4415.D0,
     &  12.D0,-1.D0,0.,0.,0.,
     &  -4.D0,-56.D0,-12.D0,0.,0.,
     &  -16.D0,-62.D0,-8.D0,-3.D0,0./
C..
      T=TIN+273.16
      P=1.01325*PIN
```

```
C..P in atmospheres, convert to bars
      R=83.144
C..R bar-cm3/(mol-K)
      RHOM=0.
      T0=(298.15/T)-1.D0
      DO 1 J=1,NGAS
      B=A(1,J)+T0*(A(2,J)+T0*(A(3,J)*T0*(A(4,J)+T0*A(5,J))))
      Z=1.D0+(B*P/(R*T))
      V0=R*T*Z/P
      RHOM=RHOM+(Y(J)/V0)
1     CONTINUE
      RHO=RHOM
      RETURN
      END
C..
      REAL*8 FUNCTION CP(Y,TIN)
C..
C.. Input is the vector of mol fractions of CO2,H2,H2O,He,N2,O2 in the
C.. gas mixture, Y. Temperature, TIN, degrees C, PIN in atmospheres.
C.. Output is the mixture isobaric heat capacity in J/(mol-K),
C.. Formula and constants in appendix A of Reid, Robert C, John M Prausnitz,
C.. Bruce E Poling; The properties of gases and liquids, 4th edition
C.. McGraw-Hill NY,NY ,1987.
C..
      INCLUDE 'g2con.for'
C..
      DIMENSION CPVAPA(NGAS),CPVAPB(NGAS),CPVAPC(NGAS),CPVAPD(NGAS)
C..   DATA PARAMETER/CO2,H2,H2O,HE,N2,O2/99-75-77-48-56-59
      DATA CPVAPA/19.8D0,27.14D0,32.24D0,20.8D0,31.15D0,28.11D0 /
      DATA CPVAPB/.07344D0,9.274D-3,1.924D-3,0.,-1.357D-2,-3.68D-6 /
      DATA CPVAPC/-5.602D-5,-1.381D-5,1.055D-5,0.,2.68D-5,1.746D-5 /
```

```
        DATA CPVAPD/1.715D-8,7.645D-9,-3.596D-9,0.,-1.168D-8,-1.065D-8 /
C.. Convert T to Kelvin, P to bars
        P=PIN*1.01325
        T=TIN+273.16
        CPM=0.
        DO 1 J=1,NGAS
        CPJ=CPVAPA(J)+T*(CPVAPB(J)+T*(CPVAPC(J)+T*CPVAPD(J)))
        CPM=CPM+Y(J)*CPJ
1       CONTINUE
        CP=CPM
        RETURN
        END
C..
        REAL*8 FUNCTION VPH2O(T,nP)
        IMPLICIT REAL*8(A-H,O-Z)
C.. Input T, temperature degrees C, P in atmospheres
C.. returns vapor pressure of water
C.. in torr. Formula from appendix A of Reid, Robert C, John M Prausnitz,
C.. Bruce E Poling; The properties of gases and liquids, 4th edition
C.. McGraw-Hill NY,NY ,1987 verified by comparison with
C.. Handbook Chemistry and Physics,page D-109,49th edition,
C.. Robert C Weast(editor) Chemical Rubber Co., Cleveland,Ohio,1968
C.. Maximum error <.25%
        TC=647.3
        PC=221.2
        VPA=-7.76451
        VPB=1.45838
        VPC=-2.77580
        VPD=-1.23303
        X=1.-((T+273.16)/TC)
        X3=X*X*X
```

```
      FX=VPA*X+VPB*(X**1.5)+X3*(VPC+X3*VPD)
      FX=FX/(1.D0-X)
      PVP=PC*DEXP(FX)
C..PVP is in bars, convert to torr
      VPH2O=PVP/.00133322368421
C..Correction for depth Glasstone,Samuel; Textbook of Physical Chemistry
C..2nd edition, fifth printing, 1946;D Van Nostrand Co Inc pp 446
      TA=T+273.16
      PB=P*1.01325
      VW=18.0686834
      R=83.144
C..R In bar-cm3/mol-K
      CF=DEXP(VW*(PB-PVP)/(R*TA))
      VPH2O=VPH2O*CF
      RETURN
      END
C..
```