NBSIR 81-2253

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by

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1. Introduction

This report has been prepared to provide computational details and computer programs for the evaluation of the thermodynamic properties of water and steam. It is based on an extensive correlation of thermodynamic properties.[1] Included herein are the basic equations for the description of the thermodynamic properties of water and detailed listings of computer programs based on these equations. With this information, thermodynamic properties can be calculated from the freezing point to ~2500 K in temperature and from the dilute gas to well in excess of 1 GPa (10,000 bars) in pressure for liquid and gaseous states for undissociated water.

In reducing the data the molecular weight of ordinary water has been taken as 18.0152 g mol^{-1},[2] the universal gas constant as 8.31441 J mol^{-1} K^{-1}, and hence the specific gas constant as 0.461522 J g^{-1} K^{-1}.[3] Absolute temperatures on the International Practical Temperature Scale of 1968 have been used as the realization of the thermodynamic scale.

This report contains five sections and 2 appendices: A brief discussion of the structure of the thermodynamic surface for water is given in section 2, and in section 3 are the equations, parameters and constants that define the surface. Section 4 contains the thermodynamic relations used in the computer program. It also contains a discussion

of the general organization and structure of the computer program. Section 5 contains statements regarding the accuracy and range of validity of our surface. In Appendix A are the computer listings and a quide to their use, and, lastly, in appendix B, is a printout of calculations obtained with the program, so that the user can check his results.

2. Structure of the thermodynamic surface

The thermodynamic surface is composed of three parts: (1) The first, referred to as the base function, is obtained from a theoretical equation of state.[4-12] It properly describes the low-density vapor, the high temperature behavior at all densities, and the dense fluid at all temperatures. Except for a large region around the critical point, the base function yields results that are at least in semi-quantitative accord with data. (2) The second, referred to as the residual function, yields corrections to the base function. These corrections are small in regions where the base function is in good accord with data, and in regions beyond the range of the data. The contributions to the pressure from the base function and the residual function are readily integrable in closed form to yield their respective contributions to the Helmholtz function. (3) The third includes the thermodynamic properties for the ideal gas state. These have been reported recently by Woolley[13] as part of a detailed analysis of the rotation-vibration structure of the water molecule.

A major part of the work was given to the derivation of the 40 terms that form the residual function. The first 36 terms were used in a global, least squares fit to data. Each of these terms yields important contributions over wide ranges of the independent variables. Following this, small improvements were made by adding 3 terms that contribute

only in the immediate neighborhood of the critical point, and a single term that contributes only in the region of high pressures and low temperatures. Except in these very limited regions, the residual function is given by the first 36 terms. A discussion of the thermodynamic surface obtained with the residual function so restricted (terms 1-36) is given in reference [12].

The three parts are combined to obtain the expression for the Helmholtz function for fluid water,

$$A(\rho,T) = A_{base}(\rho,T) + A_{residual}(\rho,T) + A_{ideal\ gas}(T) , \qquad (1)$$

where the independent variables are density (ρ) and temperature (T). Eq. (1) is what we mean when we refer to the thermodynamic surface for water.

3. The Helmholtz function

Presented in this section are the equations that define the Helmholtz function Eq (1). The units used for the independent variables are $\rho(g/cm^3)$ and T(K), and R ($J\ g^{-1}\ K^{-1}$) for the specific gas constant, so that $A(\rho,T)$ is given in joules/g.

The base function:

$$A_{base}(\rho,T) = RT\left\{-\ell n(1-y) - \frac{\beta-1}{1-y} + \frac{\alpha+\beta+1}{2(1-y)^2} + 4y\left(\frac{B}{b} - \gamma\right)\right.$$
$$\left. - \frac{\alpha-\beta+3}{2} + \ell n\,\frac{\rho RT}{P_o}\right\}, \qquad (2)$$

where α, β, and γ are geometric constants 11, 133/3 and 7/2; y is a dimenionless density, given by $y = b\rho/4$, and $P_o = .101325$ MPa ≡ 1 atmosphere.

The parameter b is a temperature dependent hard sphere volume, and B is related to the second virial coefficient,

$$b = b_1 \ln \frac{T}{T_o} + \sum_{0,3,5}^{i} b_i \left(\frac{T_o}{T}\right)^i , \qquad (3)$$

$$B = \sum_{0,1,2,4}^{i} B_i \left(\frac{T_o}{T}\right)^i , \qquad (4)$$

where T_o = 647.073 K and the coefficients b_i and B_i are listed in table 1.

Table 1

b_i (cm^3 g^{-1})	i	B_i (cm^3 g^{-1})
.7478629	0	1.1278334
-.3540782	1	- .5944001
0	2	-5.010996
.007159876	3	0
0	4	.63684256
-.00352836	5	0

The residual function:

$$A_{residual}(\rho,T) = \sum_{1}^{36} \frac{g_i}{k(i)} \left(\frac{T_o}{T}\right)^{\ell(i)} (1-e^{-a\rho})^{k(i)}$$

$$+ \sum_{37}^{40} g_i \, \delta_i^{\ell(i)} \exp\left[-\alpha_i \, \delta_i^{k(i)} - \beta_i \, \tau_i^2\right], \qquad (5)$$

where $a = 1\ cm^3/g$, and the g_i are coefficients determined by fits to data. The quantities δ_i and τ_i are reduced densities and temperatures, respectively, given by

$$\delta_i = \frac{\rho - \rho_i}{\rho_i}, \quad \tau_i = \frac{T - T_i}{T_i},$$

and ρ_i, T_i are specified density and temperature values. The k(i) and ℓ(i) are integers. Values for the constants and parameters for the residual function are listed in table 2.

Table 2

i	k(i)	l(i)	g(i) ($J\ g^{-1}$)	i	k(i)	l(i)	g(i) ($J\ g^{-1}$)
1	1	1	-.530629685290+03	19	5	4	-.138025771779+07
2	1	2	.227449014244+04	20	5	6	-.251099143690+06
3	1	4	.787793330207+03	21	6	1	.465618261156+07
4	1	6	-.698305273750+02	22	6	2	-.727527732754+07
5	2	1	.178638328754+05	23	6	4	.417742461483+06
6	2	2	-.395147315633+05	24	6	6	.140163582446+07
7	2	4	.338038842808+05	25	7	1	-.315552313921+07
8	2	6	-.138550502027+05	26	7	2	.479296663846+07
9	3	1	-.256374366133+06	27	7	4	.409126647812+06
10	3	2	.482125759814+06	28	7	6	-.136263693884+07
11	3	4	-.341830169697+06	39	9	1	.696252208627+06
12	3	6	.122231564174+06	30	9	2	-.108349000964+07
13	4	1	.117974336558+07	31	9	4	-.227228274017+06
14	4	2	-.217348101104+07	32	9	6	.383654860007+06
15	4	4	.108299521686+07	33	3	0	.688332579443+04
16	4	6	-.254419980640+06	34	3	3	.217572455226+05
17	5	1	-.313777749478+07	35	1	3	-.266279448298+04
18	5	2	.529119107577+07	36	5	3	-.707304180821+05

i	k(i)	ℓ(i)	ρ_i(g/cm^{-3})	T_i(K)	α_i	β_i	g_i($J\ g^{-1}$)
37	2	0	.319	640.	34	20000	-.225
38	2	2	.319	640.	40	20000	-1.68
39	2	0	.319	641.6	30	40000	.055
40	4	0	1.55	270.	1050	25	-93.0

The ideal gas function:

$$A_{\text{ideal gas}}(T) = -RT\left\{1 + \left(\frac{C_1}{T_R} + C_2\right) \ln T_R + \sum_{i=3}^{18} C_i T_R^{i-6}\right\} , \quad (6)$$

where $T_R = T/100$ K.

The coefficients C_i are given in table 3.

Table 3

i	C_i
1	.197302710180+02
2	.209662681977+02
3	-.483429455355+06
4	.605743189245+05
5	.225602388500+02
6	-.987532442000+01
7	-.431355385532-01
8	.458155781927-04
9	-.477549017624-07
10	.412384608402-10
11	-.279290527404-13
12	.144816952031-16
13	-.564736589529-20
14	.162004460052-23
15	-.330382277656-27
16	.451916066716-31
17	-.370734122641-35
18	.137546067535-39

The Eqs 1 thru 6 and the values for the coefficients and parameters included in this section contain the complete thermodynamic description for water. Since $A(\rho,T)$ is everywhere analytic, it is straightforward to evaluate appropriate derivatives and to obtain closed-form expressions

for all thermodynamic properties over the entire fluid range. In the next section is a discussion of how this is done.

4. Method of calculation and the computer program

The thermodynamic quantities are calculated from $A(\rho,T)$ using the following relations:

$$P = \rho RTZ = \rho^2 \partial A/\partial\rho \quad \text{(Pressure)} \tag{7}$$

$$\frac{\partial P}{\partial \rho} = \frac{2}{\rho} P + \rho^2 \frac{\partial^2 A}{\partial \rho^2} \tag{8}$$

$$\frac{\partial P}{\partial T} = \rho^2 \frac{\partial^2 A}{\partial \rho \partial T} \tag{9}$$

$$S = -\frac{\partial A}{\partial T} \quad \text{(entropy)} \tag{10}$$

$$U = A + TS \quad \text{(internal energy)} \tag{11}$$

$$H = U + P/\rho \quad \text{(enthalpy)} \tag{12}$$

$$C_v = -T \frac{\partial^2 A}{\partial T^2} \quad \text{(isochoric heat capacity)} \tag{13}$$

$$G = A + P/\rho \quad \text{(Gibbs functions)} \tag{18}$$

$$C_p = C_v + \frac{T}{\rho^2} \frac{(\partial P/\partial T)^2}{\partial P/\partial \rho} \quad \text{(isobaric heat capacity)} \tag{19}$$

$$\omega = \left(C_p/C_v \frac{\partial P}{\partial p} \right)^{1/2} \quad \text{(speed of sound)} \tag{20}$$

$$B_{II} = \frac{1}{2RT} \left(\frac{\partial^2 P}{\partial \rho^2} \right)_{\rho=0} \quad \text{(2nd virial coef.)} \tag{21}$$

$$\frac{dB_{II}}{dT} \tag{22}$$

$$\delta_T \equiv \left(\frac{\partial H}{\partial P} \right)_T = \frac{1}{\rho} - \frac{T}{\rho^2} \frac{\partial P/\partial T}{\partial P/\partial \rho} \quad \text{(isothermal J-T coef.)} \tag{23}$$

$$\delta_H \equiv \left(\frac{\partial T}{\partial P} \right)_H = \frac{\delta_T}{C_p} \quad \text{(Joule-Thomson coef.),} \tag{24}$$

where except as indicated otherwise all dependent variables are functions of ρ and T. Since Eqs 7 thru 18 are linear in $A(\rho,T)$ each can be represented as the sum of contributions from its three parts.

The computer print-out in appendix A is the FORTRAN 77 program for calculating thermodynamic properties based on the equations contained in this report. All calculations related to the same part of $A(\rho,T)$ are included in the same sub-routine. Thus the sub-routine "BASE" includes Eqs (2-4) for the contribution from the base function to the Helmholtz function, plus each of the contributions therefrom to Eqs 7 thru 18. Similarly the sub-routine "QQ" includes all such contributions from the residual function, and sub-routine "IDEAL" contains the contributions from the ideal gas. Because the detailed equations are easily "read" from the respective sub-routines they are not reproduced here.

The contributions to the various thermodynamics properties Eqs 7-24 are summed in sub-routine "THERM". Also included are routines for properties associated with liquid-vapor coexistence. All calculations are referred to the liquid at the triple point, for which state the internal energy and entropy are zero. Though the units for the calculations are $\rho(g/cm^3)$, T(K) and joules, routine "UNIT" is included which allows use of other units. Lastly, the iteration sub-routine "DFIND" allows access with independent variables P and T.

All equations, including parameters and constants listed in sections 2 thru 4 are included in the program listing in Appendix A. Should any inconsistencies be found between the text and Appendix A, it is likely that the errors are in the text. Please let us know if you discover any.

5. Discussion

The data selected for the derivation of the thermodynamic surface were primarily $P\rho T$ data. These cover the range from $0° \leq t \leq 1000°C$ and $0 \leq P \leq 1000$ MPa. Other kinds of data used include values for the enthalpy of the saturated liquid and for the isothermal compressibility of the liquid below 100°C. No mathemtaical constraints were used to impose exact accord with pre-assigned values. The surface yields values consistent with all input data within reasonable estimates of their tolerance. It has been further validated by extensive comparison with high quality thermodynamic data, including other than $P\rho T$ that had not been used in the derivation of the surface.

At very high pressure and at very high temperatures thermodynamic values calculated with the surface are in accord with those given by the (theoretical) base function, so that the surface should yield useful estimates well beyond the range of the data used in its derivation. Thus, except very close to the melting curve, the surface should remain quantitative at pressures equal to 2000 MPa and at least semi-quantitative to 4000 MPa, for temperatures in the range $250 \leq t \leq 2500$ K for undissociated fluid water. Lastly, because the surface is analytic, it yields some results at the critical point and its immediate neighborhood which are at variance with what modern theory predicts. Though we have not found significant departure from any reliable critical region data, we caution that the surface may not conform to all theoretical expectations in the region defined by

$$T = T_c \pm 0.5 \text{ K}$$

$$\rho = \rho_c \, (1 \pm .2) \quad ,$$

where T_c and ρ_c are values at the critical point.

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APPENDIX A

This appendix contains the FORTRAN 77 programs which yield values for thermodynamic properties for liquid and gaseous states for water. The independent variables are temperature (T) and density (D). The programs should yield useful results in the range

$$250 \leq T(K) \leq 2500$$
$$10^{-8} \leq D(g/cm^3) \leq D(Pmax),$$

where Pmax is the lesser of the pressure of melting ice or 4000 MPa. For values of density less than or equal to 10^{-8} g/cm^3, the program sets the density of 10^{-8} g/cm^3.

Outlined below are the procedures for use of the subroutines which follow. In this outline, the symbol used for pressure is "P", for density is "D", and for temperature is "T". Calculations are made in the internal units of the program which are MPa, g/cm3 and deg K respectively. See III below for conversions to other units. Examples of the use of these routines are given in three main programs in Appendix B, with samples of the output which can be used for checking the implementation of the programs.

I. For Density and Temperature as independent variables, the sequence

```
CALL BB(T)
CALL BASE(D,T)
CALL QQ(T,D)
```

will place quantities in COMMON from which

P = D*GASCON*T*ZB + QØ

dP/dD = GASCON*T*(ZB+Y*DZB) + Q5

To obtain the other thermodynamic properties:

```
CALL THERM(D,T)
```

will place in COMMON "AD" (=A/RT), "GD" (=G/RT), "SD" (=S/R), "UD" (=U/RT), "HD" (=H/RT), "CVD" (=Cv/R), "CPD" (=Cp/R), "DPDT" (=dP/dT, MPa/K), "DVDT" (=dV/dT, cm3/gK), "CJTT" (isothermal joule-thompson coeff, cm3/g) and "CJTH" (adiabatic joule-thompson coeff, K/MPa). These properties in the desired units can then be obtained by R or RT as appropriate in the desired units.

II. Pressure and Temperature as independent variables

```
CALL DFIND(DOUT,P,DGUESS,T,DPDD)
```

This will return the density corresponding to the input P and T as DOUT from which the procedures in I can be used for further calculations. This routine requires an initial approximate guess for the density for use to begin the Newton iteration. dP/dD is also returned as a byproduct.

III. Use of other systems of units.

A group of three subroutines is included which facilitate the use of a system of units chosen by the user:

```
CALL UNIT
```

will query the user as to which units are desired for temperature, pressure, density and energy, and set up the necessary parameters for converting from the desired units to the internal units and back again for the output. The names of the units in alphanumeric characters are also placed in COMMON for use in labeling.

```
FUNCTION TTT(Texternal), and
FUNCTION TTI(Tinternal)
```

will convert from external T to deg K, and from deg K to the external T respectively.

```
      BLOCK DATA
      implicit double precision(a-h,o-z)
      real p,q
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      COMMON /NCONST/ G(40),II(40),JJ(40),NC
      COMMON /ELLCON/ G1,G2,GF,B1,B2,B1T,B2T,B1TT,B2TT
      COMMON /BCONST/ P(10),Q(10)
      COMMON /ADDCON/ ATZ(4),ADZ(4),AAT(4),AAD(4)
C  THIS BLOCKDATA SUBROUTINE SUPPLIES MOST OF THE FIXED PARAMETERS
C    USED IN THE REST OF THE ROUTINES. P IS THE b(i) of TABLE I,
C    Q IS THE B(i) OF TABLE I, G1,G2 AND GF ARE THE ALPHA, BETA
C    AND GAMMA OF EQ 2, AND G,II,JJ ARE THE g(i), k(i) AND
C    l(i) of EQ 5.
      DATA ATZ/2*64.D1,641.6D0,27.D1/,ADZ/3*.319D0,1.55D0/,AAT/2*2.D4
     1,4.D4,25.D0/,AAD/34.D0,4.D1,3.D1,1.05D3/
      DATA WM/18.0152D0/,GASCON/.461522D0/,TZ/647.073D0/,AA/1.D0/,NC/36/
      DATA UREF,SREF/-4328.455039D0,7.6180802D0/
      DATA G1,G2,GF/11.d0,44.333333333333d0,3.5d0/
      DATA P/.7478629,-.3540782,2*0.,.007159876,0.,-.003528426,3*0./
      DATA Q/1.1278334,0.,-.5944001,-5.010996,0.,.63684256,4*0./
      DATA G/-.530629685290 23D3,.227449014244 08D4,.787793330 20687D3
     1,-.698305273749 94D2,.178638328754 22D5,-.395147315633 38D5
     2,.338038842807 53D5,-.138550502027 03D5,-.256374366132 60D6
     3,.482125759814 15D6,-.341830169696 60D6, .122231564174 48D6
     4,.117974336558 32D7,-.217348101103 73D7, .108295216862 0D7
     5,-.254419980640 49D6,-.313777749477 67D7,.529119107577 04D7
     6,-.138025771778 77D7,-.251099143690 01D6, .465618261156 08D7
     7,-.727527732753 87D7,.417742461482 94D6,.140163582446 14D7
     8,-.315552313921 27D7,.479296663845 84D7,.409126647812 09D6
     9,-.136263693883 86D7, .696252208626 64D6,-.108349000964 47D7
     A,-.227228274016 88D6,.383654860006 60D6,.688332579443 32D4
     B,.217572455226 44D5,-.266279448297 70D4,-.707304180820 74D5
     C,-.225D0,-1.68D0,.055D0,-93.0D0/
      DATA II/4*0,4*1,4*2,4*3,4*4,4*5,4*6,4*8,2*2,0,4,3*2,4/
      DATA JJ/2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7,2,3,5,7
     1,2,3,5,7,1,3*4,0,2,0,0/
      END
```

```
C
      SUBROUTINE BB(T)
C  THIS SUBROUTINE CALCULATES THE B'S OF EQS. 3.4 USING COEFFICIENTS
C    FROM BLOCKDATA, CALCULATING ALSO THE FIRST AND SECOND DERIVS
C    W.R.TO TEMP.  THE B'S CALCULATED HERE ARE IN CM3/G.
      implicit double precision(a-h,o-z)
      real p,q
      COMMON /ELLCON/ G1,G2,GF,B1,B2,B1T,B2T,B1TT,B2TT
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      COMMON /BCONST/ P(10),Q(10)
      DIMENSION V(10)
      V(1)=1.
      DO 2 I=2,10
    2 V(I)=V(I-1)*TZ/T
      B1=P(1)+P(2)*ALOG(1./V(2))
      B2=Q(1)
      B1T=P(2)*V(2)/TZ
      B2T=0.
      B1TT=0.
      B2TT=0.
      DO 4 I=3,10
      B1=B1+P(I)*V(I-1)
      B2=B2+Q(I)*V(I-1)
      B1T=B1T-(I-2)*P(I)*V(I-1)/T
      B2T=B2T-(I-2)*Q(I)*V(I-1)/T
      B1TT=B1TT+P(I)*(I-2)**2*V(I-1)/T/T
    4 B2TT=B2TT+Q(I)*(I-2)**2*V(I-1)/T/T
      B1TT=B1TT-B1T/T
      B2TT=B2TT-B2T/T
      RETURN
      END
```

```
C
      SUBROUTINE BASE(D,T)
C This function calculates Z [=Pbase/(DRT) ] ,
C   and also Abase,Gbase,Sbase,Ubase,Hbase,CVbase, AND 1/(DRT) * DP/DT
C   for the base fct (called DPDTB)
C The AB,GB,SB,UB,HB and CVB are calculated in dimensionless units:
C   AB/RT, GB/RT, SB/R, etc.
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /ELLCON/ G1,G2,GF,B1,B2,B1T,B2T,B1TT,B2TT
C  G1,G2 AND GF ARE THE ALPHA, BETA AND GAMMA OF EQ 2, WHICH ARE
C    SUPPLIED BY THE BLOCKDATA ROUTINE.  B1 AND B2 ARE THE "EXCLUDED
C    VOLUME" AND "2ND VIRIAL" (EQS 3 AND 4) SUPPLIED BY THE SUBROUTINE
C    BB(T), WHICH ALSO SUPPLIES THE 1ST AND 2ND DERIVATIVES WITH
C    RESPECT TO T (B1T,B2T,B1TT,B2TT).
      COMMON /BASEF/ AB,GB,SB,UB,HB,CVB,DPDTB
      COMMON /ACONST/ WM,GASCON,TZ,A,Z,DZ,Y,UREF,SREF
      Y=.25*B1*D
      X=1.-Y
      Z0=(1.+G1*Y+G2*Y*Y)/X**3
      Z=Z0+4.*Y*(B2/B1-GF)
      DZ0=(G1+2.*G2*Y)/X**3 + 3.*(1.+G1*Y+G2*Y*Y)/X**4
      DZ=DZ0+4.*(B2/B1-GF)
      AB = -DLOG(X)-(G2-1.)/X+28.16666667D0/X/X+4.*Y*(B2/B1-GF)
     1  +15.166666667D0 + DLOG(D*T*4.55483D0)
      GB = AB + Z
      BB2TT=T*T*B2TT
      UB= -T*B1T*(Z-1.-D*B2)/B1-D*T*B2T
      HB=Z+UB
      CVB=2.*UB+(Z0-1.)*((T*B1T/B1)**2-T*T*B1TT/B1)
     1 - D*(BB2TT - GF*B1TT*T*T) -(T*B1T/B1)**2*Y*DZ0
      DPDTB=Z/T + D*(DZ*B1T/4.+B2T-B2/B1*B1T)
      SB = UB - AB
      RETURN
      END
C
```

```
C
      SUBROUTINE QQ(T,D)
C THIS ROUTINE CALCULATES, FOR A GIVEN T(K) AND D(G/CM3), THE RESIDUAL
C    CONTRIBUTIONS TO: PRESSURE (Q), HELMHOLTZ FCT (AR), DP/DRHO (Q5),
C    AND ALSO TO THE GIBBS FUNCTION, ENTROPY,INTERNAL ENERGY, ENTHALPY,
C    ISOCHORIC HEAT CAPACITY AND DPDT. (EQ 5)
C TERMS 37 THRU 39 ARE THE ADDITIONAL TERMS AFFECTING ONLY THE
C  IMMEDIATE VICINITY OF THE CRITICAL POINT, AND TERM 40 IS THE
C  ADDITIONAL TERM IMPROVING THE LOW T, HIGH P REGION.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /RESF/ AR,GR,SR,UR,HR,CVR,DPDTR
      COMMON /QQQQ/ Q,Q5
      DIMENSION QR(11),QT(10),QZR(9),QZT(9)
      EQUIVALENCE (QR(3),QZR(1)),(QT(2),QZT(1))
      COMMON /NCONST/ G(40),II(40),JJ(40),N
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      COMMON /ADDCON/ ATZ(4),ADZ(4),AAT(4),AAD(4)
      RT=GASCON*T
      QR(1)=0.
      Q5=0.
      Q=0.D0
      AR=0.D0
      DADT=0.
      CVR=0.
      DPDTR=0.
      E=DEXP(-AA*D)
      Q10=D*D*E
      Q20=1.D0-E
      QR(2)=Q10
      V=TZ/T
      QT(1)=T/TZ
      DO 4 I=2,10
      QR(I+1)=QR(I)*Q20
    4 QT(I)=QT(I-1)*V
      DO 10 I=1,N
      K=II(I)+1
      L=JJ(I)
      ZZ=K
      QP=G(I)*AA*QZR(K-1)*QZT(L)
      Q=Q+QP
      Q5 = Q5 + AA*(2./D-AA*(1.-E*(K-1)/Q20))*QP
      AR=AR+G(I)*QZR(K)*QZT(L)/Q10/ZZ/RT
      DFDT=Q20**K*(1-L)*QZT(L+1)/TZ/K
      D2F=L*DFDT
      DPT=DFDT*Q10*AA*K/Q20
      DADT=DADT+G(I)*DFDT
      DPDTR=DPDTR+G(I)*DPT
   10 CVR=CVR+G(I)*D2F/GASCON
      QP=0.
      Q2A=0.
```

```
C
      DO 20 J=37,40
      IF(G(J).EQ.0.D0) GO TO 20
      K=II(J)
      KM=JJ(J)
      DDZ = ADZ(J-36)
      DEL = D/DDZ - 1.
      IF(DABS(DEL).LT.1.D-10) DEL=1.D-10
      DD = DEL*DEL
      EX1 = -AAD(J-36)*DEL**K
       DEX=DEXP(EX1)*DEL**KM
      ATT = AAT(J-36)
      TX = ATZ(J-36)
      TAU = T/TX-1.
      EX2 = -ATT*TAU*TAU
      TEX = DEXP(EX2)
      Q10 = DEX*TEX
      QM = KM/DEL - K*AAD(J-36)*DEL**(K-1)
      FCT=QM*D**2*Q10/DDZ
      Q5T = FCT*(2./D+QM/DDZ)-(D/DDZ)**2*Q10*(KM/DEL/DEL+
     1  K*(K-1)*AAD(J-36)*DEL**(K-2))
      Q5 = Q5 + Q5T*G(J)
      QP = QP + G(J)*FCT
      DADT = DADT - 2.*G(J)*ATT*TAU*Q10/TX
      DPDTR = DPDTR - 2.*G(J)*ATT*TAU*FCT/TX
      Q2A = Q2A + T*G(J)*(4.*ATT*EX2+2.*ATT)*Q10/TX/TX
      AR = AR + Q10*G(J)/RT
   20 CONTINUE
      SR=-DADT/GASCON
      UR=AR+SR
      CVR=CVR+Q2A/GASCON
      Q=Q+QP
      RETURN
      END
C
```

```
C
      SUBROUTINE DFIND(DOUT,P,D,T,DPD)
C  ROUTINE TO FIND DENSITY CORRESPONDING TO INPUT PRESSURE P(MPA), AND
C    TEMPERATURE T(K), USING INITIAL GUESS DENSITY D(G/CM3). THE OUTPUT
C    DENSITY IS IN G/CM3, ALSO, AS A BYPRODUCT, DP/DRHO IS CALCULATED
C    ('DPD', MPA CM3/G)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /QQQQ/ Q0,Q5
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      DD=D
      RT=GASCON*T
      IF(DD.LE.0.) DD=1.D-8
      IF(DD.GT.1.9) DD=1.9
      L=0
    9 L=L+1
   11 IF(DD.LE.0.) DD=1.D-8
      IF(DD.GT.1.9) DD=1.9
      CALL BASE(DD,T)
      CALL QQ(T,DD)
      PP = RT*DD*Z + Q0
      DPD=RT*(Z+Y*DZ)+Q5
C  THE FOLLOWING 3 LINES CHECK FOR NEGATIVE DP/DRHO, AND IF SO ASSUME
C    GUESS TO BE IN 2-PHASE REGION, AND CORRECT GUESS ACCORDINGLY.
      IF(DPD.GT.0.D0) GO TO 13
      IF(D.GE..2967D0) DD=DD*1.02D0
      IF(D.LT..2967D0) DD=DD*.98D0
      IF(L.LE.10) GO TO 9
   13 DPDX=DPD*1.1
      IF(DPDX.LT..1) DPDX=.1
      DP=DABS(1.-PP/P)
      IF(DP.LT.1.D-8) GO TO 20
      IF(D.GT..3 .AND. DP.LT.1.D-7) GO TO 20
      IF(D.GT..7 .AND. DP.LT.1.D-6) GO TO 20
      X=(P-PP)/DPDX
      IF(DABS(X).GT..1) X=X*.1/DABS(X)
      DD=DD+X
      IF(DD.LE.0.) DD=1.D-8
   19 IF(L.LE.30) GO TO 9
   20 CONTINUE
      DOUT=DD
      RETURN
      END
C
```

```
C
      SUBROUTINE THERM(D,T)
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,Y,UREF,SREF
      COMMON /QQQQ/ QP,QDP
      COMMON /BASEF/AB,GB,SB,UB,HB,CVB,DPDTB
      COMMON /RESF/AR,GR,SR,UR,HR,CVR,DPDTR
      COMMON /IDF/ AI,GI,SI,UI,HI,CVI,CPI
      COMMON /FCTS/AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJTH
C   THIS SUBROUTINE CALCULATES THE THERMODYNAMIC FUNCTIONS IN
C     DIMENSIONLESS UNITS (AD=A/RT, GD=G/RT, SD=S/R, UD=U/RT,
C     HD=H/RT, CVD=CV/R, AND CPD=CP/R)
      CALL IDEAL(T)
      RT = GASCON*T
      Z = ZB + QP/RT/D
      DPDD = RT*(ZB+Y*DZB) + QDP
      AD = AB + AR + AI - UREF/T + SREF
      GD = AD + Z
      UD = UB + UR + UI - UREF/T
      DPDT = RT*D*DPDTB + DPDTR
      CVD = CVB + CVR + CVI
      CPD = CVD + T*DPDT**2/(D*D*DPDD*GASCON)
      HD = UD + Z
      SD = SB + SR + SI - SREF
      DVDT=DPDT/DPDD/D/D
      CJTT=1./D-T*DVDT
      CJTH=-CJTT/CPD/GASCON
       RETURN
       END
C
      FUNCTION PS(T)
C This function calculates an approximation to the vapor pressure, PS,
C   as a function of the input temperature. The vapor pressure
C   calculated agrees with the vapor pressure predicted by the surface
C   to within .02% to within a degree or so of the critical temperature,
C   and can serve as an initial guess for further refinement by
C   imposing the condition that Gl=Gv.
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(8)/-7.8889166D0,2.5514255D0,-6.716169D0
     1,33.239495D0,-105.38479D0,174.35319D0,-148.39348D0
     2,48.631602D0/
      IF(T.GT.314.D0) GO TO 2
      PL=6.3573118D0-8858.843D0/T+607.56335D0*T**(-.6)
      PS=.1*DEXP(PL)
      RETURN
    2 V=T/647.25D0
      W=DABS(1.D0-V)
      B=0.D0
      DO 4 I=1,8
      Z=I
    4 B=B+A(I)*W**((Z+1.)/2.)
      Q=B/V
      PS=22.093D0*DEXP(Q)
      RETURN
      END
```

```
C
      FUNCTION TSAT(P)
C This function calculates the saturation temperature for a given
C   pressure, by an iterative process using PSAT and TDPSDT.
      REAL*8 P , PS , TG, TSAT,TDPSDT
      TSAT=0.
      IF(P.GT.22.05) RETURN
      K=0
      PL=2.302585*DLOG(P)
C  PL=LOGE(10)*LOGE(P) TO CONVERT EQUATION FROM BARS TO MPa
      TG=372.83+PL*(27.7589+PL*(2.3819+PL*(.24834+PL*.0193855)))
    1 IF(TG.LT.273.15) TG=273.15
      IF(TG.GT.647.) TG=647.
      IF(K.LT.8) GO TO 2
      WRITE(6,3) K,P,PP,TG
    3 FORMAT()
      GO TO 8
    2 K=K+1
      PP=PS(TG)
      DP=TDPSDT(TG)
      IF(ABS(1.-PP/P).LT..00001) GO TO 8
      TG = TG*(1.+(P-PP)/DP)
      GO TO 1
    8 TSAT=TG
      RETURN
      END
C
      FUNCTION TDPSDT(T)
C This function calculates T*(dPs/dT), and is used by the function TSAT.
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION A(8)/-7.8889166D0,2.5514255D0,-6.716169D0
     1,33.239495D0,-105.38479D0,174.35319D0,-148.39348D0
     2,48.631602D0/
      V=T/647.25
      W=1.-V
      B=0.
      C=0.
      DO 4 I=1,8
      Z=I
      Y=A(I)*W**((Z+1.)/2.)
      C=C+Y/W*(.5-.5*Z-1./V)
    4 B=B+Y
      Q=B/V
      TDPSDT=22.093*DEXP(Q)*C
      RETURN
      END
```

```
C
      SUBROUTINE IDEAL(T)
C   THIS SUBROUTINE CALCULATES THE THERMODYNAMIC PROPERTIES FOR
C    WATER IN THE IDEAL GAS STATE OF H.W. WOOLLEY
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /IDF/ AI,GI,SI,UI,HI,CVI,CPI
      DIMENSION C(18)/.1973027101 8D2,.209662681977D2,-.483429455355D0
     1,.605743189245D1,22.56023885D0,-9.87532442D0,-.43135538513D1
     2,.458155781D0,-.47754901883D-1,.41238460633D-2,-.27929052852D-3
     3,.14481695261D-4,-.56473658748D-6,.16200446D-7,-.3303822796D-9
     4,.451916067368D-11,-.370734122708D-13,.137546068238D-15/
C  NOTE THAT THE TEMPERATURES ARE SCALED BY A FACTOR OF 100 HERE SO THAT
C    THE EXPONENT OF THE COEFFICIENT OF THE LAST TERM WILL BE WITHIN
C    RANGE FOR MOST COMPUTERS.
      TT=T/1.D2
      TL=DLOG(TT)
      GI=-(C(1)/TT+C(2))*TL
      HI=(C(2)+C(1)*(1.D0-TL)/TT)
      CPI=C(2)-C(1)/TT
      DO 8 I=3,18
      GI=GI-C(I)*TT**(I-6)
      HI=HI+C(I)*(I-6)*TT**(I-6)
   8  CPI=CPI+C(I)*(I-6)*(I-5)*TT**(I-6)
      AI=GI-1.
      UI=HI-1.
      CVI=CPI-1.
      SI=UI-AI
      RETURN
      END
C
      SUBROUTINE SECVIR(T,VIR)
C THIS SUBROUTINE CALCULATES THE SECOND VIRIAL IN CM3/G
C   AT TEMPERATURE T IN K.
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON /NCONST/ G(40),II(40),JJ(40),NC
      COMMON /ELLCON/ G1,G2,GF,BB1,BB2,B1T,B2T,B1TT,B2TT
      COMMON /QQQQ/ Q0,Q5
      COMMON /ACONST/ WM,GASCON,TC,AA.Z,DZ,Y,UREF,SREF
      CALL BB(T)
      V=TC/T
      VIR=BB2
      DO 3 J=1,NC
      IF(II(J).NE.0) GO TO 3
      L=JJ(J)
      VIR=VIR+G(J)*V**(L-1)/T/GASCON
   3  CONTINUE
      RETURN
      END
```

```
C
      SUBROUTINE CORR(T,P,DL,DV,DELG)
C SUBROUTINE CORR WILL CALCULATE, FOR AN INPUT T AND P AT OR
C  VAPOR PRESSURE, THE CORRESPONDING LIQUID AND VAPOR DENSIT
C  DELG = (GL-GV)/RT FOR USE IN CALCULATING THE CORRECTION T
C  PRESSURE FOR DELG = Ø.
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      COMMON /QQQQ/ QØØ,Q11
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJ
      DLIQ=DL
      IF(DL.LE.Ø.) DLIQ=1.11-.ØØØ4*T
      CALL BB(T)
      RT=GASCON*T
      CALL DFIND(DL,P,DLIQ,T,DQ)
      CALL THERM(DL,T)
      GL=GD
      DVAP=DV
      IF(DV.LE.Ø.) DVAP=P/GASCON/T
      CALL DFIND(DV,P,DVAP,T,DQ)
      IF(DV.LT.5.D-7) DV=5.D-7
      CALL THERM(DV,T)
      GV=GD
      DELG = GL-GV
      RETURN
      END
CC
      SUBROUTINE PCORR(T,P,DL,DV)
C SUBROUTINE PCORR WILL CALCULATE THE VAPOR PRESSURE P AND T
C  VAPOR DENSITIES CORRESPONDING TO THE INPUT T, CORRECTED S
C  GL-GV=Ø.  THE FUNCTION PS IS REQUIRED WHICH WILL GIVE A R
C  GOOD APPROXIMATION TO THE VAPOR PRESSURE TO BE USED AS TH
C  POINT FOR THE ITERATION.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,URFF,SREF
      P = PS(T)
   2  CALL CORR(T,P,DL,DV,DELG)
      DP=DELG*GASCON*T/(1./DV-1./DL)
      P = P+DP
      IF(DABS(DELG).LT.1.D-4) RETURN
      GOTO 2
      END
CC
      SUBROUTINE TCORR(T,P,DL,DV)
C SUBROUTINE TCORR IS SIMILAR TO "PCORR" EXCEPT THAT THE TEM
C  CORRESPONDING TO THE INPUT VAPOR PRESSURE IS FOUND. FUNCT
C  ARE TSAT AND TDPSDT WHICH GIVE AN APPROXIMATION TO T(SAT)
C  T*DP(SAT)/DT.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB,UREF,SREF
      T = TSAT(P)
   2  CALL CORR(T,P,DL,DV,DELG)
      DP=DELG*GASCON*T/(1./DV-1./DL)
      T = T*(1.-DP/TDPSDT(T))
      IF(DABS(DELG).LT.1.D-4) RETURN
      GO TO 2
      END
```

```
C
c The following 3 subroutines form a package allowing the us
c   operate in a system of units of his choice.
      SUBROUTINE UNIT
C THIS SUBROUTINE QUERIES THE USER AS TO HIS CHOICE OF UNITS
C  INTERNAL PARAMETERS APPROPRIATELY.  THE INTERNAL UNITS OF
C  TEMPERATURES IN K, DENSITIES IN G/CM3, ALL OTHER QUANTITI
C  IN DIMENSIONLESS UNITS AND DIMENSIONED AT OUTPUT TIME.
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DOUBLE PRECISION NT,ND,NP,NH,NNT,NND,NNP,NNH
      COMMON /UNITS/ IT,ID,IP,IH,NT,ND.NP,NH,FT,FD,FP,FH
      DIMENSION FFD(4),FFP(5),FFH(6),NNT(4),NND(4),NNP(5),NN
      DATA FFD/1.D-3,1.D0,.0180152D0,.016018D0/
      DATA FFP/1.D0,10.D0,9.869232667D0,145.038D0,10.1971D0/
      DATA FFH/2*1.D0,18.0152D0,.23884590D0,4.30285666D0,.42
      DATA NNT/1HK,1HC,1HR,1HF/
      DATA NND/6Hkg/m3 ,6Hg/cm3 ,6Hmol/L ,6Hlb/ft3/
      DATA NNP/6H MPa  ,6H Bar  ,6H Atm  ,6H PSI  ,6Hkg/cm2/
      DATA NNH/6hkJ/kg ,6H J/g  ,6HJ/mol ,6Hcal/g ,7Hcal/mol
      DATA A1,A2,A3,A4/8HTEMPERAT,7HDENSITY
     1,8HPRESSURE, 8HENERGY   /
      WRITE(6,11) A1
   30 WRITE(6,12)
      READ(5,10,END=99) IT
      IF(IT.EQ.0) STOP
      IF(IT.GT.4) GOTO 30
      NT=NNT(IT)
      WRITE(6,11) A2
   31 WRITE(6,13)
      READ(5,10,END=99) ID
      IF(ID.GT.4 .OR. ID.LT.1) GOTO 31
      ND=NND(ID)
      FD=FFD(ID)
      WRITE(6,11) A3
   32 WRITE(6,14)
      READ(5,10,END=99) IP
      IF(IP.GT.5 .OR. IP.LT.1) GOTO 32
      NP=NNP(IP)
      FP=FFP(IP)
      WRITE(6,11) A4
   33 WRITE(6,15)
      READ(5,10,END=99) IH
      IF(IH.GT.6 .OR. IH.LT.1) GOTO 33
      NH=NNH(IH)
      FH=FFH(IH)
      RETURN
   99 STOP
   10 FORMAT()
   11 FORMAT(' ENTER UNITS CHOSEN FOR ',A8)
   12 FORMAT(' CHOOSE FROM 1=DEG K, 2=DEG C, 3=DEG R, 4=DEG
   13 FORMAT(' CHOOSE FROM 1=KG/M3, 2=G/CM3, 3=MOL/L, 4=LB/F
   14 FORMAT(' CHOOSE FROM 1=MPA, 2=BAR, 3=ATM, 4=PSIA, 5=KG
   15 FORMAT(' CHOOSE FROM 1=KJ/KG, 2=J/G, 3=J/MOL, 4=CALORI
     1RIES/MOL, 6=BTU/LB')
      END
```

```
C
      FUNCTION TTT(T)
C FUNCTION TO CONVERT INPUT TEMPERATURES IN EXTERNAL UNITS T
      DOUBLE PRECISION T,TTT,FT,FD,FP,FH,NT,ND,NP,NH
      COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
      GO TO (1,2,3,4),IT
    1 TTT=T
      FT=1.
      RETURN
    2 TTT=T+273.15D0
      FT=1.
      RETURN
    3 TTT=T/1.8D0
      FT=.5555555555556D0
      RETURN
    4 TTT=(T+459.67D0)/1.8D0
      FT=.5555555555556D0
      RETURN
      END
      FUNCTION TTI(T)
C FUNCTION TO CONVERT INTERNAL TEMPERATURES IN DEG K TO EXTE
      DOUBLE PRECISION T,TTI,FT,FD,FP,FH,NT,ND,NP,NH
      COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
      GO TO (5,6,7,8),IT
    5 TTI=T
      RETURN
    6 TTI=T-273.15D0
      RETURN
    7 TTI=T*1.8D0
      RETURN
    8 TTI=T*1.8D0-459.67D0
      RETURN
      END
```

APPENDIX B

This appendix contains sample calculations to help the user test his program. Also listed are the main programs used to print out numerical values.

```
C THIS IS A MAIN PROGRAM FOR THE CALCULATION OF TABLES OF PROPERTIES
C    USING A CHOICE OF UNITS, AND AT A CHOICE OF CONSTANT TEMPERATURE,
C    PRESSURE OR DENSITY.  THE USER IS QUERIED AS TO HIS CHOICES OF
C    UNITS AND VARIABLES AT EXECUTION TIME.
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      DOUBLE PRECISION NT,ND,NP,NH
      COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
      COMMON /QQQQ/ Q0,Q5
      COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT
      COMMON /ACONST/ WM,GASCON,TC,AA,Z,DZ,Y,UREF,SREF
      COMMON /NCONST/ G(40),II(40),JJ(40),NC
      DATA NS1,NS2/2H m,2Hft/
      CALL UNIT
      NS=NS1
      IF(ID.EQ.4) NS=NS2
   15 WRITE(6,11)
      READ(5,*,END=9) IOPT,XISO
      IF(IOPT.EQ.0) GO TO 9
      GO TO (101,201,301),IOPT
  101 WRITE(6,102)
  102 FORMAT(' ENTER OTHER INDEPENDENT VARIABLE (2 FOR P, 3 FOR DENS'/
     1' FOLLOWED BY INITIAL, FINAL AND INCREMENTAL VALUES OF THIS VAR.')
      READ(5,*,END=9) JOPT,Y1,Y2,YI
      IF(JOPT-1) 15,101,103
  103 TT=XISO
      T=TTT(TT)
      WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
      IF(JOPT.EQ.2) DGSS=Y1/FP/T/.4
      IZ=0
      CALL BB(T)
      PSS=20000.
      DVV=0.
      IF(T.LT.TC) CALL PCORR(T,PSS,DLL,DVV)
      DGSS=DVV
      IF(DGSS.EQ.0.) DGSS=1.11-.0004*T
      PSAT=PSS*FP
      IF(JOPT.EQ.2 .AND. Y1.GT.PSAT) IZ=3
      IF(Y1.GT.PSAT) DGSS=DLL
      IF(JOPT.GE.3) IZ=3
      PIN=Y1-YI
      DIN=PIN
      PINC=YI/FP
      DINC=YI*FD
   22 IF(JOPT.EQ.2) PIN=PIN+YI
      IF(JOPT.EQ.3) DIN=DIN+YI
      IF(JOPT.EQ.2 .AND. PIN.GT.Y2) GO TO 101
      IF(JOPT.EQ.3 .AND. DIN.GT.Y2) GO TO 101
      IF(JOPT.EQ.2) PRES=PIN/FP
      IF(JOPT.EQ.3) D=DIN/FD
   24 CONTINUE
```

```
      IF(JOPT.EQ.3 .OR. (JOPT.EQ.2 .AND. PIN.LT.PSAT)) GO TO 26
      IF(JOPT.EQ.1 .AND. T.LT.TS) GO TO 26
      TSAVE=TT-YI
      IF(JOPT.EQ.1 .AND. IOPT.EQ.2 .AND. IZ.LE.2) TT=TTI(TS)
      PSAVE=PIN-YI
      IF(JOPT.EQ.2 .AND. PRES.GT.PSAT/FP .AND. IZ.GE.2) GO TO 26
      IF(JOPT.EQ.1 .AND. T.GT.TS .AND. IZ.GE.2) GO TO 26
   23 IZ=IZ+1
      IF(JOPT.EQ.2) PRES=PSAT/FP
      IF(JOPT.EQ.1) T=TS
      IF(IZ.EQ.1 .AND. JOPT.EQ.1) DGSS=DLL
      IF(IZ.EQ.1 .AND. JOPT.EQ.2) DGSS=DVV
      IF(IZ.EQ.2 .AND. JOPT.EQ.2) DGSS=DLL
      IF(IZ.EQ.2 .AND. JOPT.EQ.1) DGSS=DVV
      CALL BB(T)
   26 IF(IOPT.NE.3 .AND. JOPT.NE.3) CALL DFIND(D,PRES,DGSS,T,DQ)
   27 CALL QQ(T,D)
      CALL BASE(D,T)
      RT=GASCON*T
      PDUM = D*RT*Z + QØ
      IF(JOPT.EQ.3 .OR. IOPT.EQ.3) PRES=PDUM
      IF(IOPT.EQ.3 .OR. JOPT.EQ.3) DQ=RT*(Z+Y*DZ)+Q5
      DGSS=D + PINC/DQ
      CALL THERM(D,T)
      U = UD*T*GASCON*FH
      C=DSQRT(DABS(CPD*DQ*1.D3/CVD))
      IF(ID.EQ.4) C=C*3.280833
      H = HD*T*GASCON*FH
      S = SD*GASCON*FH*FT
      dpdtx=dpdt*fp*ft
      dpdd=dq*fp*fd
      COMP = 1.E3/D/DQ/FP
      DDDTL=1.D3*DPDT/D/DQ
      CP=CPD*GASCON*FH*FT
      CV=CVD*GASCON*FH*FT
      VL=fd/D
      DOUT=1./VL
      POUT=PRES*FP
      WRITE(6,21) TT,POUT,DOUT,DPDTX,DPDD,CV,CP,S,H,U,C
   21 FORMAT(F9.3,F12.5,F12.7,F11.5,F11.3,5F12.4,F11.3)
  444 FORMAT(5X,1HT,12X,1HP,10X,1HD,8X,5HdP/dT,5X,5HdP/dD,10X,2HCv
     1,10X,2HCp,11X,1HS,9X,1HH,11X,1HU,7X,7HVel Snd/3X,4Hdeg ,A1,7X,A8
     2,4X,A6,5X,A3,1H/,A1,4X,7H       ,15X,4H- - ,A6,A1,4H - -
     3,13X,4H- - ,A6,4H - -,8X,A2,4H/sec/)
   11 FORMAT( ´ DO YOU WISH TO CALCULATE AN ISOTHERM (ENTER 1), AN ISOBA
     1R (ENTER 2) OR AN ISOCHORE? (ENTER 3)´/´ FOLLOWED BY VALUE OF ISO.
     2   (ENTER Ø TO DISCONTINUE)´)
      IF(IZ.EQ.1) WRITE(6,12)
   12 FORMAT(´  ----------------------------------------------------
     1-----------------------------------------´)
```

```
      IF(IZ.EQ.1) GO TO 23
      IF(IZ.EQ.2 .AND. JOPT.EQ.2) PIN=PSAVE
      IF(IZ.EQ.2 .AND. JOPT.EQ.1) TT=TSAVE
      IF(IZ.EQ.2) IZ = 3
      GO TO (22,204,304),IOPT
  201 JOPT=1
      PRES = XISO/FP
  202 WRITE(6,203)
  203 FORMAT(' ENTER FIRST LAST AND INCREMENT OF T')
      READ(5,*,END=9) T1,T2,YI
      IF(T1.EQ.0.) GO TO 15
      WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
      TT=T1-YI
      T=TTT(TT)
      CALL TCORR(TS,PRES,DLL,DVV)
      D = DLL
      IF((T+YI*FT).GT.TS) D=DVV
      IZ=3
      IF((T+YI*FT).LT.TS)IZ=0
  204 TT=TT+YI
      T=TTT(TT)
      IF(TT.GT.T2) GO TO 202
      CALL BB(T)
      DGSS=D
      GO TO 24
  301 JOPT=1
      D=XISO
  302 WRITE(6,203)
      READ(5,*,END=9) T1,T2,YI
      IF(T1.LE.0.) GO TO 15
      WRITE(6,444) NT,NP,ND,NP,NT,NH,NT,NH,NS
      TT=T1-YI
      IZ=3
      T=TTT(TT)
  304 TT=TT+YI
      T=TTT(TT)
      IF(TT.GT.T2) GO TO 302
      CALL BB(T)
      GO TO 27
    9       STOP
      END
```

```
C THE FOLLOWING IS A MAIN PROGRAM FOR CALCULATING THE PROPERTIES
C    ALONG THE SATURATION CURVE UP TO 646.3 K.  THE INPUTS ARE: INITIAL T,
C    FINAL T AND THE T INCREMENT (ALL IN K).  THE VAPOR PRESSURE IS FIRST
C    CALCULATED USING "PS" AND ADJUSTED FROM THERE SO THAT
C    GL-GV=0. ALSO IN THE INPUT ARE AN INITIAL GUESS FOR THE LIQUID AND
C    VAPOR DENSITIES.  IF NOT GIVEN, THEY WILL BE INTERNALLY CHOSEN.
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON /ACONST/ WM,GASCON,TZ,AA,ZB,DZB,YB
      COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT
    3 READ(5,4,END=99) TI,TF,TD,DL,DG
    4 FORMAT()
      WRITE(6,22)
      T=TI-TD
    6 T=T+TD
      IF(T.GT.TF) GO TO 3
      IF(T.GT.646.3D0) GO TO 3
      IJK=0
      CALL BB(T)
      P=PS(T)+IJK*PT
C  THE FOLLOWING TWO LINES CALCULATE AN INITIAL GUESS FOR THE DENSITIES
C     IF GUESSES NOT SUPPLIED IN THE INPUT.
      IF(DL.LE.0.) DL=1.11-.0004*T
      IF(DG.LE.0.) DG=P/GASCON/T
    5 P=P+IJK*PT
      RT=GASCON*T
      CALL DFIND(RL,P,DL,T,DPDL)
      DL=RL
      CALL THERM(RL,T)
      SL=SD*GASCON
      HL = HD*GASCON*T
      VL=1./DL
      GL=GD
      CALL DFIND(RG,P,DG,T,DPDG)
      DG=RG
      IF(RG.LT.5.D-7) RG=5.D-7
      CALL THERM(RG,T)
      SG=SD*GASCON
      HG = HD*GASCON*T
      VG=1./DG
      GV=GD
      HEAT=HG-HL
      DELG=GL-GV
      IF(DABS(DELG).LT.2.D-6) GOTO 15
      PT = DELG*GASCON*T/(VG-VL)
      IF(T.GT.640.D0) PT=.1*PT
      IJK=IJK+1
      IF(IJK.EQ.1 .OR. (T.GT.64.D1 .AND. IJK.LE.10)) GO TO 5
   15 HEAT=HG-HL
      WRITE(6,21) T,P,RL,RG,HL,HG,HEAT,SL,SG,VL,VG
   21 FORMAT(F9.3,F13.6,F9.6,F9.7,3F9.2,2F9.4,F9.5,F11.3)
   22 FORMAT('     T,K          P,MPA     DL,G/CC  DV,G/CC  HL,J/G   HV,J/G
     1 LAT HT   SL,J/GK  SV,J/GK      VL       VG'/)
      GO TO 6
   99 STOP
      END
```

```
C THIS IS A SAMPLE MAIN PROGRAM WHICH WILL SERVE AS AN EXAMPLE FOR
C   THE USE OF THE SUBROUTINES AND FUNCTIONS GIVEN ABOVE, AND WHICH
C   WILL PRINT OUT VALUES OF VARIOUS PROPERTIES CALCULATED FOR A
C   GIVEN INPUT POINT TO A LARGE NUMBER OF SIGNIFICANT FIGURES,
C   SUITABLE FOR USE AS A CHECK ON THE OPERATION OF THE PROGRAM.
C THE USER IS QUERIED AS TO THE UNITS DESIRED.
      IMPLICIT DOUBLE PRECISION(A-H,O-Z)
      DOUBLE PRECISION NT,ND,NP,NH
      COMMON /UNITS/ IT,ID,IP,IH,NT,ND,NP,NH,FT,FD,FP,FH
      COMMON /QQQQ/ Q0,Q5
      COMMON /FCTS/ AD,GD,SD,UD,HD,CVD,CPD,DPDT,DVDT,CJTT,CJTH
      COMMON /ACONST/ WM,GASCON,TZ,AA,Z,DZ,Y,UREF,SREF
      COMMON /NCONST/ G(40),II(40),JJ(40),NC
      DATA NSS1,NSS2/2H m,2Hft/
      CALL UNIT
      NS=NSS1
      IF(ID.EQ.4) NS=NSS2
   15 WRITE(6,11)
  100 READ(5,*,END=9) IOPT,X,TT
      T=TTT(TT)
      RT=GASCON*T
      CALL BB(T)
      IF(IOPT.LE.0) GOTO 9
      GOTO (101,102,100,100,100),IOPT
  101 DD=X
      D=DD*FD
      CALL QQ(T,D)
      CALL BASE(D,T)
      PRES = FP*(RT*D*Z + Q0)
      DQ=RT*(Z+Y*DZ)+Q5
      GOTO 111
  102 PRES=X
      P=PRES/FP
      DGSS=P/T/.4
      PSAT=20000.
      IF(T.LT.TZ) CALL PCORR(T,PSAT,DLL,DGSS)
      IF(P.GT.PSAT) DGSS=DLL
      IF(P.GE.PSAT .AND. T.LT.523.15) DGSS=1.11-.0004*T
      CALL DFIND(D,P,DGSS,T,DQ)
      DD=D/FD
  111 CALL THERM(D,T)
      U = UD*T*GASCON*FH
      C=DSQRT(DABS(CPD*DQ*1.D3/CVD))
      IF(ID.EQ.4) C=C*3.280833
      H = HD*T*GASCON*FH
      S = SD*GASCON*FH*FT
      CP=CPD*GASCON*FH*FT
      CV=CVD*GASCON*FH*FT
      VL=1./D
      DPDD = DQ*FD*FP
      DPDT1=DPDT*FP*FT
      WRITE(6,20) TT,NT,PRES,NP,DD,ND
```

```
      WRITE(6,21) DPDT1,DPDD,CV,NH,NT,CP,S,H,NH,U,C,NS,CJTT,CJTH,DVDT
   20 FORMAT(' T =',F12.4,' deg ',A1,5X,'P =',F13.6,1X,A6,5X,'D ='
     1,F14.10,1X,A8)
   21 FORMAT( ' DP/DT =',F16.9,6X,'DP/DD =',F16.5/
     2 ' CV =',F12.6,1X,A6,A1,5X,'CP =',F12.6,6X,'S =',F12.6/
     3 ' H =',F14.6,1X,A6,5X,'U =',F14.6,6X,'VEL SND =',F14.6,A2,'/sec'/
     4 ' JT(T) =',F11.5,5X,'JT(H) =',F11.5,5X,'DV/DT =',F12.6/)
   11  FORMAT(' ENTER OPTION, X, AND T, WHERE FOR OPTION=1, X=DENSITY'/
     1'   AND FOR OPTION=2, X=PRESSURE (ENTER 0 TO QUIT)')
       GO TO 100
    9        STOP
       END
```

```
/@XQT POINT
ENTER UNITS CHOSEN FOR TEMPERAT
CHOOSE FROM 1=DEG K, 2=DEG C, 3=DEG R, 4=DEG F
>1
ENTER UNITS CHOSEN FOR DENSITY
CHOOSE FROM 1=KG/M3, 2=G/CM3, 3=MOL/L, 4=LB/FT3
>2
ENTER UNITS CHOSEN FOR PRESSURE
CHOOSE FROM 1=MPA, 2=BAR, 3=ATM, 4=PSIA, 5=KG/CM2
>2
ENTER UNITS CHOSEN FOR ENERGY
CHOOSE FROM 1=KJ/KG, 2=J/G, 3=J/MOL, 4=CALORIES/G, 5=CALORIES/MOL, 6=BTU/LB
>2
ENTER OPTION, X, AND T, WHERE FOR OPTION=1, X=DENSITY
  AND FOR OPTION=2, X=PRESSURE (ENTER 0 TO QUIT)
>1, .9, 873.15
T =     873.1500 deg K      P =   7110.805028  Bar        D =    .9000000000 g/cm3
DP/DT =     14.491600834       DP/DD =     28719.49752
CV =     2.827220  J/g  K     CP =     3.615462       S =     4.064690
H =    2779.151751  J/g        U =    1989.062303       VEL SND =    1916.419293 m/sec
JT(T) =      .56718     JT(H) =     -.15688     DV/DT =      .000623

>2, 225., 648.15
T =     648.1500 deg K      P =    225.000000  Bar        D =    .4103745556 g/cm3
DP/DT =      3.447886683       DP/DD =         63.95378
CV =     3.743787  J/g  K     CP =    75.284775       S =     4.221788
H =    1965.692198  J/g        U =    1910.864237       VEL SND =     358.617190 m/sec
JT(T) = -205.05536     JT(H) =     2.72373     DV/DT =      .320130

>2, .00617,  273.16
T =     273.1600 deg K      P =       .006170  Bar        D =    .9997782189 g/cm3
DP/DT =     -1.576872063       DP/DD =     19608.40085
CV =     4.225225  J/g  K     CP =     4.228690       S =      .000000
H =        .000617  J/g        U =       -.000000       VEL SND =    1400.874132 m/sec
JT(T) =     1.02220     JT(H) =     -.24173     DV/DT =     -.000080

>
```

T deg C	P MPa	D g/cm3	V cm3/g
50.000	.0100	.000067	14869.238335
50.000	.0123	.000083	12036.663719
50.000	.0123	.987991	1.012155
50.000	.1000	.988030	1.012116
50.000	1.0000	.988422	1.011713
50.000	10.0000	.992305	1.007754
50.000	20.0000	.996526	1.003486
50.000	30.0000	1.000656	.999344
50.000	40.0000	1.004700	.995322
50.000	50.0000	1.008663	.991411
50.000	60.0000	1.012550	.987605
50.000	70.0000	1.016365	.983899
50.000	80.0000	1.020109	.980287
50.000	90.0000	1.023788	.976765
50.000	100.0000	1.027403	.973328
50.000	200.0000	1.060447	.942999
50.000	300.0000	1.088794	.918448
50.000	400.0000	1.113570	.898013
50.000	500.0000	1.135810	.880429
50.000	600.0000	1.156346	.864793
50.000	700.0000	1.175655	.850590
50.000	800.0000	1.193766	.837685
50.000	900.0000	1.210356	.826203
50.000	1000.0000	1.225100	.816260

T deg C	P MPa	D g/cm3	V cm3/g
250.000	.0100	.000041	24136.161956
250.000	.1000	.000416	2406.053164
250.000	1.0000	.004298	232.644926
250.000	3.9736	.019956	50.110581
250.000	3.9736	.799072	1.251452
250.000	10.0000	.805899	1.240850
250.000	20.0000	.816284	1.225064
250.000	30.0000	.825733	1.211046
250.000	40.0000	.834438	1.198411
250.000	50.0000	.842537	1.186892
250.000	60.0000	.850128	1.176293
250.000	70.0000	.857288	1.166469
250.000	80.0000	.864075	1.157307
250.000	90.0000	.870537	1.148717
250.000	100.0000	.876711	1.140627
250.000	200.0000	.927623	1.078024
250.000	300.0000	.966827	1.034311
250.000	400.0000	.999498	1.000502
250.000	500.0000	1.027884	.972872
250.000	600.0000	1.053194	.949493
250.000	700.0000	1.076161	.929229
250.000	800.0000	1.097271	.911352
250.000	900.0000	1.116861	.895367
250.000	1000.0000	1.135179	.880918

T deg C	P MPa	D g/cm3	V cm3/g
375.000	.0100	.000033	29909.055417
375.000	.1000	.000335	2986.855135
375.000	1.0000	.003395	294.567937
375.000	10.0000	.040763	24.532263
375.000	20.0000	.130420	7.667535
375.000	22.3292	.320009	3.124909
375.000	30.0000	.558254	1.791298
375.000	40.0000	.609556	1.640537
375.000	50.0000	.641323	1.559276
375.000	60.0000	.665164	1.503388
375.000	70.0000	.684567	1.460777
375.000	80.0000	.701090	1.426350
375.000	90.0000	.715576	1.397475
375.000	100.0000	.728535	1.372617
375.000	200.0000	.816920	1.224110
375.000	300.0000	.873641	1.144634
375.000	400.0000	.917244	1.090222
375.000	500.0000	.953396	1.048882
375.000	600.0000	.984657	1.015582
375.000	700.0000	1.012420	.987732
375.000	800.0000	1.037537	.963821
375.000	900.0000	1.060570	.942889
375.000	1000.0000	1.081910	.924291

T deg C	P MPa	D g/cm3	V cm3/g
500.000	.0100	.000028	35679.867768
500.000	.1000	.000280	3565.549685
500.000	1.0000	.002824	354.099874
500.000	10.0000	.030503	32.783626
500.000	20.0000	.067711	14.768678
500.000	30.0000	.115259	8.676122
500.000	40.0000	.177974	5.618801
500.000	50.0000	.256947	3.891860
500.000	60.0000	.338443	2.954707
500.000	70.0000	.405762	2.464496
500.000	80.0000	.456993	2.188216
500.000	90.0000	.496532	2.013967
500.000	100.0000	.528211	1.893181
500.000	200.0000	.691177	1.446808
500.000	300.0000	.772885	1.293853
500.000	400.0000	.830456	1.204158
500.000	500.0000	.876029	1.141515
500.000	600.0000	.914303	1.093730
500.000	700.0000	.947615	1.055281
500.000	800.0000	.977308	1.023219
500.000	900.0000	1.004227	.995791
500.000	1000.0000	1.028941	.971873

T deg C	P MPa	D g/cm3	V cm3/g
750.000	.0100	.000021	47219.519942
750.000	.1000	.000212	4720.958893
750.000	1.0000	.002123	471.103828
750.000	10.0000	.021679	46.127641
750.000	20.0000	.044390	22.527645
750.000	30.0000	.068163	14.670731
750.000	40.0000	.092985	10.754408
750.000	50.0000	.118770	8.419621
750.000	60.0000	.145340	6.880435
750.000	70.0000	.172425	5.799609
750.000	80.0000	.199697	5.007588
750.000	90.0000	.226804	4.409089
750.000	100.0000	.253421	3.946003
750.000	200.0000	.462110	2.163988
750.000	300.0000	.584047	1.712190
750.000	400.0000	.665974	1.501561
750.000	500.0000	.728216	1.373220
750.000	600.0000	.779010	1.283680
750.000	700.0000	.822326	1.216062
750.000	800.0000	.860356	1.162309
750.000	900.0000	.894435	1.118025
750.000	1000.0000	.925435	1.080573

T deg C	P MPa	D g/cm3	V cm3/g
1000.000	.0100	.000017	58758.280969
1000.000	.1000	.000170	5875.475023
1000.000	1.0000	.001703	587.198410
1000.000	10.0000	.017122	58.404407
1000.000	20.0000	.034420	29.052786
1000.000	30.0000	.051866	19.280576
1000.000	40.0000	.069439	14.401171
1000.000	50.0000	.087117	11.478860
1000.000	60.0000	.104867	9.535858
1000.000	70.0000	.122648	8.153425
1000.000	80.0000	.140405	7.122229
1000.000	90.0000	.158081	6.325872
1000.000	100.0000	.175613	5.694349
1000.000	200.0000	.333285	3.000438
1000.000	300.0000	.451565	2.214522
1000.000	400.0000	.539879	1.852267
1000.000	500.0000	.609226	1.641426
1000.000	600.0000	.666407	1.500584
1000.000	700.0000	.715338	1.397941
1000.000	800.0000	.758357	1.318641
1000.000	900.0000	.796939	1.254801
1000.000	1000.0000	.832065	1.201830

T deg C	P MPa	D g/cm3	dP/dT MPa/C	dP/dD	Cv	Cp J/g C	S	H J/g	U	Vel Snd m/sec
50.000	.01000	.000067	.000031	148.242	1.43653	1.91016	8.17313	2591.753	2443.061	443.980
50.000	.01234	.000083	.000039	148.028	1.44287	1.91942	8.07451	2591.191	2442.604	443.756
50.000	.01234	.987891	1.033431	2287.759	4.22713	4.18167	.70374	209.327	209.315	1541.283
50.000	.10000	.988230	1.033659	2288.246	4.02690	4.18147	.70370	209.403	209.301	1541.453
50.000	1.00000	.988422	1.036005	2293.242	4.02461	4.17942	.70328	210.179	209.167	1543.195
50.000	10.00000	.992305	1.059519	2342.418	4.00224	4.15952	.69914	217.926	207.849	1560.278
50.000	20.00000	.996526	1.085811	2395.576	3.97843	4.13858	.69456	226.503	206.433	1578.610
50.000	30.00000	1.000656	1.112335	2447.431	3.95566	4.11882	.69001	235.046	205.066	1596.263
50.000	40.00000	1.004700	1.139128	2498.218	3.93387	4.10015	.68548	243.556	203.743	1613.634
50.000	50.00000	1.008663	1.166209	2548.145	3.91300	4.08253	.68097	252.033	202.462	1630.503
50.000	60.00000	1.012550	1.193580	2597.395	3.89300	4.06588	.67648	260.477	201.221	1647.039
50.000	70.00000	1.016365	1.221230	2646.133	3.87383	4.05014	.67201	268.889	200.015	1663.301
50.000	80.00000	1.020109	1.249140	2694.503	3.85545	4.03527	.66754	277.268	198.845	1679.339
50.000	90.00000	1.023788	1.277278	2742.633	3.83782	4.02121	.66310	285.615	197.706	1695.197
50.000	100.00000	1.027403	1.305609	2790.636	3.82091	4.00791	.65866	293.931	196.599	1710.910
50.000	200.00000	1.060447	1.589278	3279.014	3.68512	3.90648	.61490	375.549	186.950	1864.396
50.000	300.00000	1.088794	1.847577	3790.663	3.59236	3.83763	.57274	454.958	179.424	2012.383
50.000	400.00000	1.113570	2.083891	4283.281	3.52296	3.78717	.53264	532.794	173.599	2145.812
50.000	500.00000	1.135810	2.357987	4700.461	3.46653	3.76283	.49375	609.131	168.917	2258.617
50.000	600.00000	1.156346	2.754523	5030.355	3.42196	3.78648	.45405	683.546	164.672	2359.282
50.000	700.00000	1.175655	3.333416	5335.256	3.39432	3.88125	.41110	755.428	160.016	2469.944
50.000	800.00000	1.193766	4.073188	5741.012	3.38910	4.04441	.36352	824.454	154.306	2617.457
50.000	900.00000	1.210356	4.847013	6369.168	3.40483	4.21850	.31236	891.103	147.520	2809.132
50.000	1000.00000	1.225100	5.486680	7255.468	3.43073	4.32406	.26089	956.583	140.323	3024.027

T deg C	P MPa	D g/cm3	dP/dT MPa/C	dP/dD	Cv	Cp J/g C	S	H J/g	U	Vel Snd m/sec
375.000	.01000	.000033	.000015	299.046	1.58608	2.04800	9.52964	3228.005	2929.914	621.400
375.000	.10000	.000335	.000155	298.235	1.58945	2.05495	8.46516	3226.443	2927.758	620.951
375.000	1.00000	.003395	.001612	289.996	1.62439	2.12805	7.38423	3210.541	2915.973	616.370
375.000	10.00000	.040763	.025471	193.978	2.13161	3.43629	6.09816	3014.740	2769.418	559.201
375.000	20.00000	.130420	.113375	50.977	3.37089	12.97913	5.22456	2600.962	2447.611	443.036
375.000	22.32920	.320009	.268390	.402	6.17375	1140.34081	4.42460	2096.698	2026.922	272.487
375.000	30.00000	.558254	.614226	136.776	3.03118	8.76783	3.93035	1791.439	1737.700	628.991
375.000	40.00000	.609556	.751154	262.569	2.92898	6.67753	3.82799	1742.153	1676.531	773.697
375.000	50.00000	.641323	.845596	371.264	2.88606	5.92110	3.76322	1716.143	1639.179	872.752
375.000	60.00000	.665164	.920369	472.193	2.86293	5.50209	3.71391	1699.482	1609.276	950.597
375.000	70.00000	.684567	.983196	562.359	2.84926	5.22670	3.67338	1688.019	1585.765	1015.674
375.000	80.00000	.701090	1.037796	649.394	2.84092	5.02790	3.63960	1679.908	1565.800	1072.056
375.000	90.00000	.715576	1.086300	732.320	2.83589	4.87557	3.60794	1674.151	1548.378	1122.066
375.000	100.00000	.728535	1.130058	811.835	2.83305	4.75396	3.58039	1670.146	1532.884	1167.172
375.000	200.00000	.816920	1.428529	1490.843	2.84678	4.17620	3.39116	1676.307	1431.485	1478.869
375.000	300.00000	.873641	1.609018	2051.027	2.87736	3.94928	3.27052	1716.251	1372.860	1677.826
375.000	400.00000	.917244	1.735453	2544.669	2.90860	3.82040	3.17953	1768.875	1332.786	1826.218
375.000	500.00000	.953396	1.829497	2993.314	2.93853	3.73566	3.10583	1827.979	1303.538	1950.772
375.000	600.00000	.984657	1.901525	3408.714	2.96697	3.67609	3.04369	1890.877	1281.527	2055.094
375.000	700.00000	1.012420	1.957411	3798.243	2.99404	3.63191	2.98995	1956.169	1264.756	2146.497
375.000	800.00000	1.037537	2.000840	4166.933	3.01990	3.59836	2.94261	2023.039	1251.982	2228.253
375.000	900.00000	1.060570	2.034292	4519.434	3.04469	3.57244	2.90037	2090.975	1242.374	2302.531
375.000	1000.00000	1.081910	2.059520	4855.498	3.06850	3.55222	2.86230	2159.638	1235.346	2370.847

NBS-114A (REV. 2-8C)

U.S. DEPT. OF COMM. BIBLIOGRAPHIC DATA SHEET (See instructions)	1. PUBLICATION OR REPORT NO. NBSIR 81-2253	2. Performing Organ. Report No.	3. Publication Date 1981

4. TITLE AND SUBTITLE

A Thermodynamic Surface for Water: The Formulation and Computer Programs

5. AUTHOR(S)

Lester Haar, John S. Gallagher and George S. Kell

6. PERFORMING ORGANIZATION (If joint or other than NBS, see instructions)

NATIONAL BUREAU OF STANDARDS
DEPARTMENT OF COMMERCE
WASHINGTON, D.C. 20234

7. Contract/Grant No.

8. Type of Report & Period Covered

9. SPONSORING ORGANIZATION NAME AND COMPLETE ADDRESS (Street, City, State, ZIP)

10. SUPPLEMENTARY NOTES

☒ Document describes a computer program; SF-185, FIPS Software Summary, is attached.

11. ABSTRACT (A 200-word or less factual summary of most significant information. If document includes a significant bibliography or literature survey, mention it here)

A FORTRAN 77 program is given with which thermodynamic properties for liquid and gaseous states for water can be calculated for the temperature and pressure range, $250 \leq T(K) \leq 4000$ and $0 < P < P_{max}$, where P_{max} is the lesser of the pressure of melting ice or 4 G Pa (40,000 bar). The program yields values for enthalpy, entropy, heat capacity, speed of sound, Joule-Thomson Coef., second virial coef., isothermal compressibility coef., coef. of thermal expansion, and PρT relations that are everywhere in accord with accurate data for water. Included is a brief outline of the derivation of the equations.

12. KEY WORDS (Six to twelve entries; alphabetical order; capitalize only proper names; and separate key words by semicolons)

Enthalpy, entropy; equation of state; heat capacity; Hehnholtz function; internal energy; Joule-Thomson coef., second virial coef., speed of sound; the critical region; thermodynamic surface; water.

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14. NO. OF PRINTED PAGES 35

15. Price

USCOMM-DC 6043-P80