A UNIVERSITY OF UTAH
DIRECT CONTACT GEOTHERMAL POWER
PROJECT REPORT

A Computer Program
for Determining the Thermodynamic
Properties of Light Hydrocarbons

NOTICE

PORTIONS OF THIS REPORT ARE ILLEGIBLE. It
has been reproduced from the best available
copy to permit the broadest possible avail-
ability.

Prepared for the
Energy Research and Development Administration
Under

CONTRACT NO. AT (10-1) 1523
Grant No. AER 75-01039

by

David H. Riemer
Harold R. Jacobs
Robert F. Boehm
Donald S. Cook

NOTICE
This report was prepared as an account of work
sponsored by the United States Government. Neither
the United States nor the United States Energy
Research and Development Administration, nor any of
their employees, nor any of their contractors,
subcontractors, or their employees, makes any
warranty, express or implied, or assumes any legal
liability or responsibility for the accuracy, completeness
or usefulness of any information, apparatus, product or
process disclosed, or represents that its use would not
infringe privately owned rights.

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

ACKNOWLEDGEMENT

This work was prepared as a part of ERDA Grant No. AER-75-01039 which was originally funded as a National Science Foundation RANN Grant entitled, " Feasibility Study of the Application of Direct Contact Heat Exchangers to Power Cycles Utilizing Geothermal Brines." The work was conducted in the Mechanical and Industrial Engineering Department at the University of Utah under the direction of Drs. Harold R. Jacobs and Robert F. Boehm.

Appreciation for supplemental funding and encouragement is given to Dr. J. Kunze of Aerojet Nuclear Company, Idaho Falls, Idaho, for ERDA support under contract AT(10-1)1523.

NOMENCLATURE

a	constant in SBWR equation					
A_0	constant in SBWR equation					
b	"	"	"	"		
B_0	"	"	"	"		
c	"	"	"	"		
C_0	"	"	"	"		
C_{h1}	constant in ideal gas enthalpy equation					
C_{h2}	"	"	"	"	"	"
C_{h3}	"	"	"	"	"	"
C_{h4}	"	"	"	"	"	"
C_{h5}	"	"	"	"	"	"
C_{h5}	"	"	"	"	"	"
C_{h6}	"	"	"	"	"	"
C_{s1}	constant in ideal gas entropy equation					
C_{s2}	"	"	"	"	"	"
C_{s3}	"	"	"	"	"	"
C_{s4}	"	"	"	"	"	"
C_{s5}	"	"	"	"	"	"
C_{s6}	"	"	"	"	"	"
d	constant in SBWR equation					
D_0	"	"	"	"		
E_0	"	"	"	"		
f	fugacity					
h	enthalpy (BTU/lbmole)					
P	pressure (psia)					
S	entropy (BTU/lbmole)					

T temperature ($^{\circ}\text{R}$)
 α constant in SBWR equation
 γ constant in SBWR equation
 ϕ conversion factor = 0.185057
 ρ density (lbmole/ft^3)

ABSTRACT

This program was written to be used as a subroutine. The program determines the thermodynamics of light hydrocarbons. The following light hydrocarbons can be analyzed: Butane, Ethane, Ethylene, Heptane, Hexane, Isobutane, Isopentane, Methane, Octane, Pentane, Propane and Propylene. The subroutine can evaluate a thermodynamic state for the light hydrocarbons given any of the following pairs of state quantities: pressure and quality, pressure and enthalpy, pressure and entropy, temperature and pressure, temperature and quality and temperature and specific volume. These six pairs of knowns allow the user to analyze any thermodynamic cycle utilizing a light hydrocarbon as the working fluid. The Starling-Benedict-Webb-Rubin equation of state was used. This report contains a brief description, flowchart, listing and required equations for each subroutine.

INTRODUCTION

This subroutine computes the thermodynamic properties of light hydrocarbons. The subroutine was developed to allow for a wide range of applications such that it may be used to determine the properties of light hydrocarbons in any thermodynamic cycle including, as the authors developed it, evaluating binary fluid cycles. This routine can be treated as a "black box" by the user with a limited background in programming or the program may be modified to meet the users requirements. This manual was written to assist the user in whichever manner he intends to use this program.

DEVELOPMENT OF PROPERTIES

The basic equation used is the Starling-Benedict-Webb-Rubb equation of state, which is a pressure explicit equation of the form:

$$P = \rho RT + (B_0 RT - A_0 - C_0/T^2 + D_0/T^3 - E_0/T^4)\rho^2 + (bRT - a - d/T)\rho^3 + \alpha(a + d/T)\rho^6 + C\rho^3/T^2(1 + \gamma\rho^2) e^{-\gamma\rho^2}$$

$$h = \phi(B_0 RT - 2A_0 - 4C_0/T^2 + 5D_0/T^3 - 6E_0/T^4)\rho + \phi/2(2bRT - 3a - 4d/T)\rho^2 + \alpha\phi/5(6a + 7d/T)\rho^5 + C\phi/(\gamma T^2)(3 - (3 + \gamma\rho^2/2 - \gamma^2\rho^4)e^{-\gamma\rho^2}) + C_{h1} + C_{h2}T + C_{h3}T^2 + C_{h4}T^3 + C_{h5}T^4 + C_{h6}T^5$$

$$s = \phi R \ln(\rho RT) - \phi(B_0 R + 2C_0/T^3 - 3D_0/T^4 + 4E_0/T^5)\rho - \phi/2(bR + d/T)\rho^2 + \alpha\phi d\rho^5/(5T^2) + 2\phi C/(\gamma T^3)(1 - (1 + \gamma\rho^2/2)e^{-\gamma\rho^2}) + C_{s1} + C_{s2}T + C_{s3}T^2 + C_{s4}T^3 + C_{s5}T^4 + C_{s6}T^5$$

$$\ln f = \ln(\rho RT) + 2/(RT)(B_0 RT - A_0 - C_0/T^2 + D_0/T^3 - E_0/T^4)\rho + 3/(2RT)(bRT - a - d/T)\rho^2 + 6\alpha/(5RT)(a - d/T)\rho^5 + C/(\gamma RT^3)(1 - (1 + \gamma\rho^2/2 - \gamma^2\rho^4)e^{-\gamma\rho^2})$$

Recall that a thermodynamic state requires that two properties be known and for saturation states pressure and temperature are dependent. For evaluating an ideal power cycle the following processes are employed, constant entropy (turbine, compressor and pump), constant enthalpy (expansion valve), constant pressure (heat exchanger). In order to determine properties for these processes, properties must be determined with one of the following pairs of knowns: temperature and pressure, temperature and quality, pressure and quality, pressure and enthalpy, and pressure and entropy. Since pressure is a function of density and temperature, when pressure and temperature are known a search technique must be used to find the density. Once the density is known the remaining properties may be calculated. Saturation states are defined by the equality of pressure and fugacity at the same temperature and both saturated liquid and vapor densities. When the saturation pressure is known, a three variable search on temperature and saturated liquid and vapor densities is required. When the saturation temperature is known a two variable search is required on the saturated liquid and vapor densities. Having completed either of these searches, the remaining properties may be computed by using the saturated liquid and vapor densities. The cases of pressure and entropy or enthalpy as knowns require a two variable search since both pressure and entropy or enthalpy are functions of temperature and density. This search is used only in the compressed liquid or superheated regions. The Newton-Raphson iteration technique is used for searches in CARBON because of its generally rapid convergence.

PROGRAM DEVELOPMENT

Subroutine CARBON was written in FORTRAN V for the UNIVAC 1108 series computer but should be easily adapted to any similar FORTRAN compiler.

The subroutine allows the user to use the program at two levels, first as a "black box" (the main text describes the use and general development of the program), second the program may be modified to best suit the users needs (the remaining text contains a more complete description of each subroutine). Subroutines were used throughout to allow for each modification and as a means of tracing any possible problems. This report contains variable description tables, flowcharts, equations and a brief description of all subroutines.

USE OF CARBON

In order to use CARBON the user must supply to the program the following information:

1. The process for which properties are to be determined (CYCLE)

The allowable values of CYCLE are the following pairs of knowns:

TP - temperature and pressure

TX - temperature and quality

TV - temperature and density

PH - pressure and enthalpy

PS - pressure and entropy

PX - pressure and quality

These are the only allowable values of CYCLE and the order is important, i.e., PT or SP, etc., are illegal and will generate an error termination of CARBON.

2. The value of the first known specified by the value of CYCLE (FGIVEN).
3. The value of the second known specified by the value of CYCLE (SGIVEN).

4. Light hydrocarbon type. Acceptable values of LFTYPE are ISOB, ISOP, BUT, PENT, METH, ETH, ETHYL, PROP, HEX, HEPT, OCT and PROPYL.
5. Print selector - if NPRIN = 0, then do not print out results, otherwise print results.

CARBON will return the following information:

1. Enthalpy (Btu/lbm)
2. Entropy (BTU/lbm°R)
3. Quality - applies to saturation states, if greater than one then superheated vapor region and if less than one then compressed liquid region.
4. Specific volume (ft^3/lbm)
5. Temperature (°F)
6. Pressure (psia)
7. Saturated liquid enthalpy (Btu/lbm)
8. Saturated liquid entropy (Btu/lbm°R)
9. Saturated liquid specific volume (ft^3/lbm)
10. Saturated vapor enthalpy (Btu/lbm)
11. Saturated vapor entropy (Btu/lbm°R)
12. Saturated vapor specific volume (ft^3/lbm)

A typical call on CARBON would look like

```
CALL CARBON ('TP', TEMP, PRESS, 'ISOB', H,S,V,T,P,NPRIN,SL,HL,VL,SV,  
HV,W, QUAL)
```

This call on CARBON evaluates properties for Isobutane given temperature, (TEMP) and pressure (PRESS). Subroutine CARBON was written so as to be independent of the calling program except for the passage of the above parameters, therefore, no external variables need be placed in common.

CARBON

Description

CARBON is the main routine for determining the thermodynamic properties of light hydrocarbons. The routine selects the appropriate coefficients for the particular light hydrocarbon to be evaluated. CARBON then determines if the two state quantities specified according to the value of CYCLE are legitimate quantities. An example of an illegal quantity would be qualities greater than one or less than zero for values of CYCLE equal to TX or PX. Once these tests are satisfied CARBON then determines the region to which the point corresponds, i.e., compressed liquid, saturated liquid-vapor equilibrium or superheated vapor. Having determined the region, CARBON selects the proper subroutines to determine the remaining thermodynamic state properties.

VARIABLE SYMBOL TABLE

ABST	absolute temperature difference between °F and °R = 459.6
BTOLER	lower tolerance on saturation and convergence tests
BUT	1-dimensional array containing the required coefficients for Butane
C	1-dimensional array containing the coefficients to the Starling-Benedict-Webb-Rubin equation of state for the light hydrocarbon to be evaluated
CH	1-dimensional array containing the coefficients to the ideal gas enthalpy
CONVR	conversion factor = $0.185057 \text{ Btu in}^2/\text{lb-ft}^3$
CS	1-dimensional array containing the coefficients to the ideal gas entropy

CYCLE	Type of calculation to be made, CYCLE has the following possible pairs of knowns: <ol style="list-style-type: none"> 1. temperature and pressure = TP 2. temperature and quality = TX 3. temperature and specific volume = TV 4. pressure and quality = PX 5. pressure and entropy = PS 6. pressure and enthalpy = PH
D	density (lbmole/ft ³)
DCRIT	critical density (lbmole/ft ³)
DHDD	$\partial h(\rho, T) / \partial \rho$
DHDT	$\partial h(\rho, T) / \partial T$
DL	saturated liquid density (lbmole/ft ³)
DPDD	$\partial P(\rho, T) / \partial \rho$
DPDT	$\partial P(\rho, T) / \partial T$
DSDD	$\partial S(\rho, T) / \partial \rho$
DSDT	$\partial S(\rho, T) / \partial T$
DV	saturated vapor density (lbmole/ft ³)
ETA	1-dimensional array containing the required coefficients for Ethane
EHTYL	1-dimensional array containing the required coefficients for Ethylene
FGIVEN	First known passed to CARBON, i.e., temperature for values of CYCLE of TP, TX and TV and pressure for values of CYCLE of PX, PS and PH
H	enthalpy (BTU/lbm)
HEPT	1-dimensional array containing the required coefficients for Heptane

HEX 1-dimensional array containing the required coefficients for Hexane
HL saturated liquid enthalpy (Btu/lbm)
HV saturated vapor enthalpy (Btu/lbm)
LFTYPE the light hydrocarbon to be evaluated

accepted values are:

BUT - Butane
ETHYL - Ethylene
HEPT - Heptane
HEX - Hexane
ISOB - Isobutane
ISOP - Isopentane
METH - Methane
OCT - Octane
PENT - Pentane
PROP - Propane
PROPYL- Propylene

LIMIT maximum number of iterations allowed in any one search

M2 unit number for printer

NPPIN print selector - no printout if NPRIN = 0 else print out is generated

OCT 1-dimensional array containing the required coefficients for Octane

P pressure (psia)

PCRIT critical pressure (psia)

PENT 1-dimensional array containing the required coefficients for Pentane

PROP 1-dimensional array containing the required coefficients for Propane

PROPYL 1-dimensional array containing the required coefficients for Propylene

PSAT saturation pressure (psia)

QUAL quality
 R universal gas constant 10.7335 psia-ft³/lbmole
 S entropy (BTU/lbm°R)
 SGIVEN second known passed to CARBON, i.e., quality for values of CYCLE
 of TX and PX, pressure for CYCLE = TP, specific volume for
 CYCLE = TV, enthalpy for CYCLE = PH and entropy for CYCLE = PS
 SL saturated liquid entropy (BTU/lbm °R)
 SV saturated vapor entropy (Btu/lbm°R)
 T temperature (°F)
 TCRIT critical temperature (°F)
 TR temperature (°R)
 TTOLER upper tolerance on saturation and convergence tests
 V specific volume (ft³/lbm)
 VL saturated liquid specific volume (ft³/lbm)
 VV saturated vapor specific volume (ft³/lbm)
 MW molecular weight
 XISOB 1-dimensional array containing the required coefficient for
 isobutane
 XISOP 1-dimensional array containing the required coefficients for
 isopentane
 XMETH 1-dimensional array containing the required coefficients for methane

```

1      C      *****
2      C      *
3      C      *
4      C      *
5      C      *
6      C      *
7      C      *
8      C      *
9      C      *
10     C      *
11     C      *
12     C      *
13     C      *
14     C      *
15     C      *
16     C      *
17     C      *
18     C      *
19     C      *
20     C      *
21     C      *
22     C      *
23     C      *
24     C      *
25     C      *
26     C      *
27     C      *
28     C      *
29     C      *
30     C      *
31     C      *
32     C      *
33     C      *
34     C      *

```

 C A R B O N

 THIS SUBROUTINE CALCULATES THE THERMODYNAMIC PROPERTIES FOR
 *LIGHT HYDROCARBONS BY USING K.E. STARLINGS MODIFICATION TO THE
 *BENEDICT-WEBB RUBIN EQUATION OF STATE. GIVEN THE FOLLOWING
 *PAIRS OF KNOWNS THE PROGRAM WILL CALCULATE THE REMAINING STATE
 *PROPERTIES:
 * 1) TEMPERATURE-PRESSURE
 * 2) TEMPERATURE-QUALITY
 * 3) TEMPERATURE-SPECIFIC VOLUME
 * 4) PRESSURE-QUALITY
 * 5) PRESSURE-ENTROPY
 * 6) PRESSURE-ENTHALPY
 *
 *THIS PROGRAM WAS WRITTEN BY DAVID H. RILMER.
 *

 SUBROUTINE CARBON(CYCLE,FGIVEN,SGIVEN,LFTYPE,H,S,V,TR,P,NPRIN,
 1 SL,HL,VL,SV,HV,VV,QUAL)
 COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
 PARAMETER M2=6
 DIMENSION XISOB(27),XISOP(27),XMETH(27),ETH(27),PROP(27),
 IPENT(27),HEX(27),BUT(27),HEPT(27),OCT(27),ETHYL(27),PROPYL(27)
 DATA ABST,TTOLER,BTOLER,LIMIT,R/459.67,1.005,0.995,50,10.7335/
 DATA CONVR/0.185057/
 DATA (XISOB(I),I=1,27)/479907.0E-01,37264.0,8.58663,1.87890,
 1406763.0E05,101413.0E05,216863.0E02,853176.0E06,840860.0E08,
 24.23987,7.11486,0.86401,9.079E-04,-2.073E-07,0.885E-10,-0.241E-13,
 30.0,-776.11,6.872E-02,3.071E-04,0.0,0.0,0.0,529.06,274.96,0.2373,
 458.12/
 DATA (IPENT(I),I=1,27)/162185.0,51108.2,16.6070,2.44417,135286.0E06,
 1223931.0E05,388521.0E02,101769.0E07,390860.0E08,7.06702,11.8593,

35 20.9179,1.511E-04,14.048E-07,-13.785E-10,4.560E-13,0.0,-688.09,
 36 322.267E-02,-0.89E-04,5.018E-07,-5.048E-10,0.641E-13,489.51,585.42,
 37 40.2007,72.146/
 38 DATA(PROP(1),I=1,27)/40066.4,18634.7,5.46248,0.964762,274461.0E05,
 39 1796178.0E04,150520.0E02,453708.0E06,256053.0E08,2.01402,4.56182,
 40 20.9353,26.158E-04,-56.476E-07,85.177E-10,-63.595E-13,18.451E-16,
 41 3-804.84,25.477E-02,-1.602E-04,5.160E-07,-2.110E-10,0.0,617.400,
 42 4206.13,0.3121,44.094/
 43 DATA(XMEIH(1),I=1,27)/2574.89,7520.29,0.925404,0.723251,
 44 1437222.0E03,271092.0E03,47489.1,107737.0E05,301122.0E05,0.468826,
 45 21.48640,1.7491,66.131E-04,-167.165E-07,244.251E-10,-180.176E-13,
 46 352.320E-16,-1798.16,53.978E-02,-1.345E-04,0.676E-07,1.966E-10,
 47 4-1.037E-13,673.1,-116.43,0.6274,16.042/
 48 DATA(ETH(1),I=1,27)/22404.5,13439.3,3.11206,0.826059,681826.0E04,
 49 1295195.0E04,702169.5,257477.0E06,146619.0E08,0.90681,2.99656,
 50 21.3021,23.761E-04,-32.627E-07,28.695E-10,-9.485E-13,0.0,-993.32,
 51 330.668E-02,-1.427E-04,4.203E-07,-1.567E-10,0.0,709.8,90.03,
 52 40.4218,30.068/
 53 DATA(FROPYL(1),I=1,27)/81880.4,6051.36,7.64114,0.114457,
 54 1294141.0E05,974762.0E04,54193.5E02,705921.0E06,341250.0E08,
 55 21.36532,4.07919,1.2501,7.946E-04,-1.155E-07,-0.025E-10,0.054E-13,
 56 30.0,376.86,9.868E-02,2.347E-04,0.295E-07,-0.196E-10,0.0,670.27,
 57 4197.4,0.3449,42.08/
 58 DATA(HEX(1),I=1,27)/434517.0,45333.1,29.4983,2.66233,318412.0E06,
 59 1526067.0E05,327460.0E02,552158.0E07,626433.0E09,9.70230,14.6720,
 60 21.3746,-17.514,35.568,-21.907,4.769,0.0,-618.38,0.240,4.148,-0.614
 61 3,0.0,0.0,439.4,453.45,0.1696,86.172/
 62 DATA(XISOP(1),I=1,27)/204344.0,35742.0,19.8384,1.27752,129063.0E06
 63 1,228430.0E05,349220.0E02,142115.0E07,241326.0E08,6.16154,11.7384,
 64 20.7737,9.412,-3.298,2.306,-0.953,0.129,-709.28,7.482,2.545,0.857,
 65 3-0.464,0.0,483.5,369.0,0.2027,72.146/
 66 DATA(BUT(1),I=1,27)/71181.8,32544.7,9.14066,1.56588,700044.0E05
 67 1,137436.0E05,364236.0E02,333159.0E06,230902.0E07,4.00985,7.54122,
 68 20.9008,10.06E-04,-3.006E-07,0.846E-10,0.0,0.0,-739.77,22.389E-02,
 69 3-0.661E-04,3.93E-07,-1.594E-10,0.0,551.1,305.67,0.2448,58.12/

```

70      DATA(HEPI(1),I=1,27)/359087.0,77826.9,27.4415,3.60493,374876.0E06,
71      1615662.0E05,8351150.0,777123.0E07,636251.0E07,21.8782,24.7604,
72      21.3170,-17.863E-04,36.047E-07,-22.278E-10,4.856E-13,0.0,-596.40,
73      30.549E-02,3.989E-04,-0.587E-07,0.0,0.0,396.3,512.85,0.1465,100.198
74      4/
75      DATA(OCT(1),I=1,27)/131646.0,81690.6,10.5907,4.86965,642053.0E06,
76      1996546.0E05,185906.0E03,790575.0E07,346419.0E08,34.5124,21.9888,
77      1.2641,-17.734E-04,35.827E-07,-22.131E-10,4.823E-13,0.0,-577.59,
78      30.612E-02,4.094E-04,-0.605E-07,0.0,0.0,364.4,563.79,0.1284,114.224
79      4/
80      DATA(ETHYL(I),I=1,27)/15978.1,12133.9,2.62914,0.747945,409725.0E04
81      1,163203.0E04,903550.0,517563.0E05,161706.0E05,0.589158,2.27971,
82      21.3962,23.551E-04,-34.266E-07,30.347E-10,-10.071E-13,0.0,928.25,
83      352.949E-02,-2.477E-04,4.768E-07,-1.711E-10,0.0,742.0,49.62,0.5035,
84      428.05/
85      IF(LFTYPE.EQ.'ISOB') GO TO 10
86      IF(LFTYPE.EQ.'PENT') GO TO 20
87      IF(LFTYPE.EQ.'ISOP') GO TO 30
88      IF(LFTYPE.EQ.'METH') GO TO 40
89      IF(LFTYPE.EQ.'ETH') GO TO 50
90      IF(LFTYPE.EQ.'PROP') GO TO 60
91      IF(LFTYPE.EQ.'HEX') GO TO 70
92      IF(LFTYPE.EQ.'BUT') GO TO 80
93      IF(LFTYPE.EQ.'HEPI') GO TO 90
94      IF(LFTYPE.EQ.'OCT') GO TO 100
95      IF(LFTYPE.EQ.'ETHYL') GO TO 110
96      IF(LFTYPE.EQ.'PROPYL') GO TO 120
97      WRITE(M2,9050)
98      RETURN
99      10 CALL SETUP(XISOB,PCRIT,TCRIT,DCRIT)
100      GO TO 180
101      20 CALL SETUP(PENT,PCRIT,TCRIT,DCRIT)
102      GO TO 180
103      30 CALL SETUP(XISOP,PCRIT,TCRIT,DCRIT)
104      GO TO 180

```



```

105      40 CALL SETUP(XMETH,PCRIT,TCRIT,DCRIT)
106      GO TO 180
107      50 CALL SETUP(ETH,PCRIT,TCRIT,DCRIT)
108      GO TO 180
109      60 CALL SETUP(PROP,PCRIT,TCRIT,DCRIT)
110      GO TO 180
111      70 CALL SETUP(HEX,PCRIT,TCRIT,DCRIT)
112      GO TO 180
113      80 CALL SETUP(BUT,PCRIT,TCRIT,DCRIT)
114      GO TO 180
115      90 CALL SETUP(HEPT,PCRIT,TCRIT,DCRIT)
116      GO TO 180
117      100 CALL SETUP(OCT,PCRIT,TCRIT,DCRIT)
118      GO TO 180
119      110 CALL SETUP(ETHYL,PCRIT,TCRIT,DCRIT)
120      GO TO 180
121      120 CALL SETUP(PROPYL,PCRIT,TCRIT,DCRIT)
122      180 IF(CYCLE.EQ.'TP') GO TO 200
123      IF(CYCLE.EQ.'TX') GO TO 400
124      IF(CYCLE.EQ.'PX') GO TO 600
125      IF(CYCLE.EQ.'PS') GO TO 800
126      IF(CYCLE.EQ.'PH') GO TO 1000
127      IF(CYCLE.EQ.'TV') GO TO 1200
128      WRITE(M2,9000)CYCLE
129      RETURN
130      200 T=FGIVEN
131      P=SGIVEN
132      TR=T+ABS(P)
133      IF(T.GE.TCRIT) GO TO 220
134      CALL PRESAT(TR,PSAT,DL,DV,DCRIT)
135      IF(P/PSAT.GT.TTOLER.OR.P/PSAT.LT.BTOLER) GO TO 210
136      WRITE(M2,9010)T,P
137      RETURN
138      210 IF(P/PSAT.GT.TTOLER) GO TO 240
139      220 QUAL=2.0

```

```

140      D=1.0E-06
141      GO TO 260
142 240  D=0.88589
143      QUAL=-2.0
144 260  CALL VFIND(TR,P,D)
145      CALL ENTR(TR,D,H,DHDT,DHDD)
146      CALL ENTR(TR,D,S,DSDT,DSLDD)
147      V=1.0/(D*WM)
148      CALL PRINTC(TR,P,H,S,V,QUAL,0.0,0.0,0.0,0.0,0.0,0.0,LFTYPE,NPRIN)
149      RETURN
150 400  T=FGIVEN
151      QUAL=SGIVEN
152      TR=T+ABS I
153      IF(QUAL.LE.1.0.AND.QUAL.GE.0.0) GO TO 410
154      WRITE(M2,9020)QUAL
155      RETURN
156 410  IF(T.LE.TCRIT) GO TO 420
157      WRITE(M2,9030)
158      RETURN
159 420  CALL PRESAT(TR,P,DL,DV,DCRIT)
160      CALL SATC(TR,DL,DV,HL,SL,HV,SV)
161      S=SV*QUAL+SL*(1.0-QUAL)
162      H=HV*QUAL+HL*(1.0-QUAL)
163      VV=1.0/(DV*WM)
164      VL=1.0/(DL*WM)
165      V=VV*QUAL+VL*(1.0-QUAL)
166      CALL PRINTC(TR,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
167      RETURN
168 600  P=FGIVEN
169      QUAL=SGIVEN
170      IF(QUAL.LE.1.0.AND.QUAL.GE.0.0) GO TO 610
171      WRITE(M2,9020)QUAL
172      RETURN
173 610  IF(P.LE.PCRIT) GO TO 620
174      WRITE(M2,9040)

```

```

175      RETURN
176 620 CALL TEMSAT(P,TR,DL,DV,TCRIT,DCRIT)
177      CALL SATC(TR,DL,DV,HL,SL,HV,SV)
178      S=SV*QUAL+SL*(1.0-QUAL)
179      H=HV*QUAL+HL*(1.0-QUAL)
180      VL=1.0/(DL*WM)
181      VV=1.0/(DV*WM)
182      V=VV*QUAL+VL*(1.0-QUAL)
183      CALL PRINTC(TR,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
184      RETURN
185 600 P=PGIVEN
186      S=SGIVEN
187      IF(P.LT.PCRIT) GO TO 820
188      TR=TCRIT*1.1
189      DV=1.01*DCRIT
190      GO TO 840
191 820 CALL TEMSAT(P,TR,DL,DV,TCRIT,DCRIT)
192      CALL SATC(TR,DL,DV,HL,SL,HV,SV)
193      IF(S.LT.0.0)GO TO 830
194      IF(S/SV.GT.TTOLER) GO TO 840
195      IF(S/SL.LT.BTOLER) GO TO 860
196      GO TO 835
197 830 IF(S/SV.LT.BTOLER)GO TO 840
198      IF(S/SL.GT.TTOLER)GO TO 860
199 835 QUAL=(S-SL)/(SV-SL)
200      H=HV*QUAL+HL*(1.0-QUAL)
201      VL=1.0/(DL*WM)
202      VV=1.0/(DV*WM)
203      V=VV*QUAL+VL*(1.0-QUAL)
204      CALL PRINTC(TR,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
205      RETURN
206 840 QUAL=2.0
207      DV=0.01
208      CALL PSKNOW(P,S,TR,DV)
209      D=DV

```

```

210      GO TO 880
211      880 QUAL=-2.0
212      DL=0.55
213      CALL PSKNOW(P,S,TR,DL)
214      D=DL
215      880 CALL ENTH(TR,D,H,DHDT,DHDD)
216      V=1.0/(D*WM)
217      CALL PRINTC(TR,P,H,S,V,QUAL,0.0,0.0,0.0,0.0,0.0,0.0,LFTYPE,NPRIN)
218      RETURN
219      1000 P=PGIVEN
220      H=SGIVEN
221      IF(P.LT.PCRIT) GO TO 1020
222      TR=TCRIT*1.1
223      DV=1.01*DCRIT
224      GO TO 1040
225      1020 CALL TEMSAT(P,TR,DL,DV,TCRIT,DCRIT)
226      CALL SATC(TR,DL,DV,HL,SL,HV,SV)
227      IF(H.LE.0.0) GO TO 1030
228      IF(H/HV.GT.TTOLER) GO TO 1040
229      IF(H/HL.LT.BTOLER) GO TO 1060
230      GO TO 1035
231      1030 IF(H/HV.LT.BTOLER) GO TO 1040
232      IF(H/HL.GT.TTOLER) GO TO 1060
233      1035 QUAL=(H-HL)/(HV-HL)
234      S=SV*QUAL+SL*(1.0-QUAL)
235      VL=1.0/(DL*WM)
236      VV=1.0/(DV*WM)
237      V=VV*QUAL+VL*(1.0-QUAL)
238      CALL PRINTC(TR,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
239      RETURN
240      1040 QUAL=2.0
241      DV=0.01
242      CALL PHKNOW(P,H,TR,DV)
243      D=DV
244      GO TO 1080

```

```

245      1060 QUAL=-2.0
246          DL=0.55
247          CALL PHKNOW(P,H,TR,DL)
248          D=DL
249      1080 CALL ENTR(TR,D,S,DSLT,DSDD)
250          V=1.0/(D*M)
251          CALL PRINTC(TR,P,H,S,V,QUAL,0.0,0.0,0.0,0.0,0.0,0.0,LFTYPE,NPRIN)
252          RETURN
253      1200 T=FGIVEN
254          TR=FGIVEN+ABST
255          V=SGIVEN
256          D=1.0/(V*M)
257          IF(T.GE.TCRIT) GO TO 1240
258          CALL PRESAT(TR,P,DL,DV,DCRIT)
259          IF(D/DL.LT.BTOLER) GO TO 1260
260          IF(D/DV.GT.TTOLER) GO TO 1240
261          CALL SATC(TR,DL,DV,HL,SL,HV,SV)
262          QUAL=(D-DL)/(DV-DL)
263          VL=1.0/(DL*WM)
264          VV=1.0/(DV*WM)
265          H=HV*QUAL+HL*(1.0-QUAL)
266          S=SV*QUAL+SL*(1.0-QUAL)
267          CALL PRINTC(TR,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
268          RETURN
269      1240 QUAL=2.0
270          GO TO 1280
271      1260 QUAL=-2.0
272      1280 CALL PRES(TR,D,P,DPT,DPDD)
273          CALL ENTH(TR,D,H,DH,T,DHDD)
274          CALL ENTR(TR,D,S,DSLT,DSDD)
275          CALL PRINTC(TR,P,H,S,V,QUAL,0.0,0.0,0.0,0.0,0.0,0.0,LFTYPE,NPRIN)
276          RETURN
277      9050 FORMAT(1H,4X,'***ERROR IN CARBON, THE FLUID',A6,'CANNOT BE
278              1EVALUATED, CARBON TERMINATED')
279      9010 FORMAT(1H,4X,'***ERROR IN CARBON, THE TEMPERATURE',F10.2,'AND THE

```

```

280      1PRESSURE',F10.4,'DEFINE A SATURATION STATE, CARBON TERMINATED')
281      9020 FORMAT(1H,4X,'***ERROR IN CARBON, A QUALITY OF,'F8.2,'IS
282      1MEANINGLESS')
283      9030 FORMAT(1H,4X,'*** ERROR IN CARBON, A SATURATION STATE DOES NOT
284      1EXIST FOR TEMPERATURES GREATER THAN THE CRITICAL TEMPERATURE')
285      9040 FORMAT(1H,4X,'***ERROR IN CARBON, A SATURATION STATE DOES NOT
286      1EXIST FOR PRESSURES GREATER THAN THE CRITICAL PRESSURE')
287      9000 FORMAT(1H,4X,'*** ERROR IN CARBON, THE CYCLE',A6,'CANNOT BE
288      1EVALUATED')
289      END

```

ENTH

Description

ENTH calculates the enthalpy and its derivatives with respect to density and temperature given temperature and density. The enthalpy is calculated by computing the ideal gas enthalpy and the enthalpy departure from the ideal gas enthalpy by using the Starling-Benedict-Webb-Rubin equation of state.

EQUATIONS

$$h(\rho, T) = (\text{CONVR}/\text{WM}) \left((B_0 R T - 2 A_0 - 4 C_0 / T^2 + 5 D_0 / T^3 - 6 E_0 / T^4) \rho + 1/2 (2 b R T - 3 a - 4 d / T) \rho^2 + \alpha / 5 (6 a + 7 d / T) \rho^5 + c (\gamma T^2) (3 - (3 + \gamma \rho^2 / 2 - \gamma^2 \rho^4) \exp(-\gamma \rho^2)) \right) + C_{h1} + C_{h2} T + C_{h3} T^2 + C_{h4} T^3 + C_{h5} T^4 + C_{h6} T^5$$

$$\frac{\partial h(\rho, T)}{\partial T} = (\text{CONVR}/\text{WM}) (B_0 R + 8 C_0 / T^3 - 15 D_0 / T^4 + 24 E_0 / T^5) \rho + 1/2 (2 b R + 4 d / T^2) \rho^2 - 7 \alpha d \rho^5 / 5 T^2 - 2 c / (\gamma T^3) (3 - (3 + 1/2 \gamma \rho^2) - \gamma^2 \rho^4) \exp(-\gamma \rho^2) + C_{h2} + 2 C_{h3} T + 3 C_{h4} T^2 + 4 C_{h5} T^3 + 5 C_{h6} T^4$$

$$\frac{\partial h(\rho, T)}{\partial \rho} = (\text{CONVR}/\text{WM}) (B_0 R T - 2 A_0 - 4 C_0 / T^2 + 5 D_0 / T^3 - 6 E_0 / T^4 + (2 b R T - 3 a - 4 d / T) \rho + \alpha (6 a + 7 d / T) \rho^4 + c / (\gamma T^2) (5 \gamma \rho + 5 \gamma^2 \rho^3 - 2 \gamma^3 \rho^5) \exp(-\gamma \rho^2))$$

VARIABLE SYMBOL TABLE

C	1-dimensional array containing the coefficients to the SBWR equation of state
CH	1-dimensional array containing the coefficients for the ideal gas enthalpy
CONVR	conversion factor = 0.185057 Btu-in ² /lb-ft ³

D	density (lbmole/ft ³)
DHDD	$\frac{\partial h(\rho, T)}{\partial \rho}$
DHDT	$\frac{\partial h(\rho, T)}{\partial T}$
H	enthalpy Btu/lbm)
T	temperature (°R)
TERM1	intermediate value
TERM2	intermediate value
TERM3	intermediate value
TERM4	intermediate value
WM	molecular weight

START

```
TER11 = C(4)*R*T - 2.0*C(2) - 4.0*C(6)/T**2 + 5.0*C(8)/
T**3 - 6.0*C(9)/T**4
TER12 = 2.0*C(3)*R*T - 3.0*C(1) - 4.0*C(7)/T
TER13 = C(10)*(6.0*C(1) + 7.0*C(7)/T)
TER14 = C(5)*(3.0 - (3.0 + 0.5*C(11)*D**2 - C(11)**2*D**4)*
EXP(-C(11)*D**2))/C(11)
H = TER11*D + TER12*D**2/2.0 + TERM3*D**5/5.0 + TERM4/
T**2
DHDD = TER11 + TER12*D + TERM3*D**4 + C(5)/(C(11)*T**2)*
(5.0*C(11)*D + 5.0*C(11)**2*D**3 - 2.0*C(11)**3*
D**5)*EXP(-C(11)*D**2)
TER11 = (C(4)*R + 8.0*C(6)/T**3 - 15.0*C(8)/T**4 + 24.0*
C(9)/T**5)*D
TER12 = 0.5*(2.0*C(3)*R + 4.0*C(7)/T**2)*D**2
TER13 = -C(10)*D**5*7.0*C(7)/(T**2*5.0)
TER14 = -2.0*TER14/T**3
H = H*CONVR/WM + CH(1) + CH(2)*T + CH(3)*T**2 + CH(4)*
T**3 + CH(5)*T**4 + CH(6)*T**5
DHDD = DHDD*CONVR/WM
DHDT = (TER11 + TER12 + TERM3 + TERM4)*CONVR/WM + CH(2)
+ 2.0*CH(3)*T + 3.0*CH(4)*T**2 + CH(5)*T**3*4.0
+ 5.0*CH(6)*T**4
```

RETURN

```

1      C      *****
2      C      *
3      C      *
4      C      *
5      C      *
6      C      *
7      C      *
8      C      *
9      C      *
10     C      SUBROUTINE ENTH(T,D,H,DHDT,DHDD)
11     C      COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
12     C      TERM1=(C(4)*R*T-2.0*C(2)-4.0*C(6)/T**2+5.0*C(8)/T**3-6.0*C(9)
13     C      1/T**4)
14     C      TERM2=(2.0*C(3)*R*T-3.0*C(1)-4.0*C(7)/T)
15     C      TERM3=C(10)*(6.0*C(1)+7.0*C(7)/T)
16     C      TERM4=C(5)*(3.0-(3.0+0.5*C(11)*D**2-C(11)**2*D**4)*EXP(-C(11)*
17     C      1D**2))/C(11)
18     C      H=TERM1*D+TERM2*D**2/2.0+TERM3*D**5/5.0+TERM4/T**2
19     C      DHDD=TERM1+TERM2*D+TERM3*D**4+C(5)/(C(11)*T**2)*(5.0*C(11)*D+5.0*
20     C      1C(11)**2*D**3-2.0*C(11)**3*D**5)*EXP(-C(11)*D**2)
21     C      TERM1=(C(4)*R+8.0*C(6)/T**3-15.0*C(8)/T**4+24.0*C(9)/T**5)*D
22     C      TERM2=0.5*(2.0*C(3)*R+4.0*C(7)/T**2)*D**2
23     C      TERM3=-C(10)*D**5*7.0*C(7)/(T**2*5.0)
24     C      TERM4=-2.0*TERM4/T**3
25     C      H=H*CONVR/WM+CH(1)+CH(2)*T+CH(3)*T**2+CH(4)*T**3+CH(5)*T**4+CH(6)
26     C      1*T**5
27     C      DHDD=DHDD*CONVR/WM
28     C      DHDT=(TERM1+TERM2+TERM3+TERM4)*CONVR/WM+CH(2)+2.0*CH(3)*T+3.0
29     C      1*CH(4)*T**2+CH(5)*T**3*4.0+5.0*CH(6)*T**4
30     C      RETURN
31     C      END

```

ENTR

DESCRIPTION

ENTR calculates the entropy and its derivatives with respect to temperature and density given density and temperature. The entropy is calculated by computing the ideal gas entropy and the entropy departure from the ideal gas entropy by using the Starling-Benedict-Webb-Rubin equation of state.

EQUATIONS

$$S(\rho, T) = (\text{CONVR}/\text{WM}) (-R \ln(\rho R T) - (B_0 R + 2 C_0 T^3 - 3 D_0 / T^4 + 4 E_0 / T^5) \rho - 1/2 (b R + d / T^2) \rho^2 + \alpha D \rho^5 / (5 T^2) + 2 C / (\gamma T^3) (1 - (1 + 1/2 \gamma \rho^2) \exp(-\gamma \rho^2))) + C_{s1} + C_{s2} T + C_{s3} T^2 + C_{s4} T^3 + C_{s5} T^4 + C_{s6} T^5$$

$$\frac{\partial S(\rho, T)}{\partial T} = (\text{CONVR}/\text{WM}) (-R/T - (-6 C_0 / T^4 + 12 D_0 T^5 - 20 E_0 / T^6) \rho + d \rho^2 / T^3 - 2 \alpha \rho^5 / (5 T^3) - 6 C / (\gamma T^4) (1 - (1 + 1/2 \gamma \rho^2) \exp(-\gamma \rho^2))) + C_{s2} + 2 C_{s3} T + 3 C_{s4} T^2 + 4 C_{s5} T^3 + 5 C_{s6} T^4$$

$$\frac{\partial S(\rho, T)}{\partial \rho} = (\text{CONVR}/\text{WM}) (-R/\rho - (B_0 R + 2 C_0 / T^3 - 3 D_0 / T^4 + 4 E_0 / T^5) - (b R + d / T^2) \rho + \alpha d \rho^4 / T^4 + 2 C / T^3 (\rho + \gamma \rho^3) \exp(-\gamma \rho^2))$$

VARIABLE SYMBOL TABLE

C	1-dimensional array containing the coefficients to the SBWR equation of state
CONV	conversion factor = 0.185037 Btu-in ² /lbm-ft ³
CS	1-dimensional array containing the coefficient for the ideal gas entropy
D	density (lbmole/ft ³)
DSDD	$\frac{\partial S(\rho, T)}{\partial \rho}$

DSDT $\frac{\partial S(\rho, T)}{\partial T}$

T temperature (°R)

TERM1 intermediate value

TERM2 intermediate value

TERM3 intermediate value

S entropy (Btu/lbm°R)

WM molecular weight

START

```
TERM1 = C(4)*R + 2.0*C(6)/T**3 - 3.0*C(8)/T**4 + 4.0*C(9)/
T**5
TERM2 = C(3)*R + C(7)/T**2
TERM3 = 1.0 - (1.0 + 0.5*C(11)*D**2)*EXP(-C(11)*D**2)
S = CONVR*(-R*LOG(D*R*T) - TERM1*D - 0.5*TERM2*D**2
+ C(10)*C(7)*D**5/(5.0*T**2) + 2.0*C(5)*TERM3/
(C(11)*T**3))/WM + CS(1) + CS(2)*T + CS(3)*T**2
+ CS(4)*T**3 + CS(5)*T**4 + CS(6)*T**5
DSDT = CONVR*(-R/T - (-6.0*C(6)/T**4 + 12.0*C(8)/T**5
- 20.0*C(9)/T**6)*D + C(7)*D**2/T**3 - 0.4*C(10)*
C(7)*D**5/T**3 - 6.0*C(5)*TERM3/(C(11)*T**4))/WM
+ CS(2) + 2.0*CS(3)*T + 3.0*CS(4)*T**2 + 4.0*CS(5)*
T**3 + 5.0*CS(6)*T**4
TERM11 = -(C(4)*R + 2.0*C(6)/T**3 - 3.0*C(8)/T**4 + 4.0*C(9)/
T**5)
TERM12 = -(C(3)*R + C(7)/T**2)*D
DSDD = (-R/D + TERM1 + TERM2 + C(10)*C(7)*D**4/T**2 + 2.0*
C(5)*(D + C(11)*D**3)*EXP(-C(11)*D**2)/T**3)*CONVR/
WM
```

RETURN

```

1      C      *****
2      C      *
3      C      *
4      C      *
5      C      *   THIS SUBROUTINE CALCULATES THE ENTROPY GIVEN DENSITY AND
6      C      *   TEMPERATURE
7      C      *
8      C      *****
9      SUBROUTINE ENTR(T,D,S,DSDT,DSDD)
10     COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
11     TERM1=C(4)*R+2.0*C(6)/T**3-3.0*C(8)/T**4+4.0*C(9)/T**5
12     TERM2=C(3)*R+C(7)/T**2
13     TERM3=1.0-(1.0+0.5*C(11)*D**2)*EXP(-C(11)*D**2)
14     S=CONVR*(-R*LOG(D*R*T)-TERM1*D-0.5*TERM2*D**2
15     1+C(10)*C(7)*D**5/(5.0*T**2)+2.0*C(5)*TERM3/(C(11)*T**3))/WM+CS(1)
16     2+CS(2)*T+CS(3)*T**2+CS(4)*T**3+CS(5)*T**4+CS(6)*T**5
17     DSDT=CONVR*(-R/T-(-6.0*C(6)/T**4+12.0*C(8)/T**5-20.0*C(9)/T**6)*D
18     1+C(7)*D**2/T**3-0.4*C(10)*C(7)*D**5/T**3-6.0*C(5)*TERM3/
19     2(C(11)*T**4))/WM+CS(2)+2.0*CS(3)*T+3.0*CS(4)*T**2+4.0*CS(5)*T**3
20     3+5.0*CS(6)*T**4
21     TERM1=-(C(4)*R+2.0*C(6)/T**3-3.0*C(8)/T**4+4.0*C(9)/T**5)
22     TERM2=-(C(3)*R+C(7)/T**2)*D
23     DSDD=(-R/D+TERM1+TERM2+C(10)*C(7)*D**4/T**2+2.0*C(5)*
24     1(D+C(11)*D**3)*EXP(-C(11)*D**2)/T**3)*CONVR/WM
25     RETURN
26     END

```

FUGAC

FUGAC calculates the fugacity and its derivatives with respect to temperature and density given temperature and density. The fugacity is computed using the Starling-Benedict-Webb-Rubin equation of state.

EQUATION

$$\ln f(\rho, T) = \ln(\rho R T) + 2/(R T) (B_0 R T - A_0 - C_0/T^2 + D_0/T^3 - E_0/T^4) \rho \\ + 3/(2 R T) (b R T - a - d/T) \rho^2 \\ + 6 \alpha / (5 R T) (a + d/T) \rho^5 + C (\gamma R T^3) (1 - (1 + \gamma \rho^2 / 2 - \gamma^2 \rho^4) \exp(-\gamma \rho^2))$$

$$\frac{\partial f(\rho, T)}{\partial \rho} = f(\rho, T) * (1/\rho + 2 (R T) (B_0 R T - A_0 - C_0/T^2 + D_0/T^3 - E_0/T^4) \rho \\ + 3/(R T) (b R T - a - d/T) \rho + 6 \alpha / (R T) (a + d/T) \rho^4 \\ + C/(R T^3) * \gamma (3 \gamma \rho + 3 \gamma^2 \rho^3 - 2 \gamma^3 \rho^5) \exp(-\gamma \rho^2))$$

$$\frac{\partial f(\rho, T)}{\partial T} = f(\rho, T) * (1/T + 2/(R T^2) (A_0 + 3 C_0/T^2 - 4 D_0/T^4) \rho + 3/(2 R T^2) (a + 2 d/T) \rho^2 \\ - 6 \alpha / (5 R T^2) (a + 2 d/T) \rho^5 - 3 C / (\gamma R T^4) (1 - (1 - \gamma \rho^2 / 2 - \gamma^2 \rho^4) \exp(-\gamma \rho^2))$$

VARIABLE SYMBOL TABLE

C 1-dimensional array containing the coefficients to the Starling-Benedict-Webb-Rubin equation of state

D density (lbmole/ft³)

DFDD $\frac{\partial f(\rho, T)}{\partial \rho}$

DFDT $\frac{\partial f(\rho, T)}{\partial T}$

F fugacity

R universal gas constant = 10.7355 psia-ft³/lbmole°R

T temperature (°R)

TERM1 intermediate value

TERM2 intermediate value

TERM3 intermediate value

TERM4 intermediate value

START

TERM 1 = $C(4) \cdot R \cdot T - C(2) - C(6) / T^{**2} + C(8) / T^{**3} - C(9) / T^{**4}$
TERM 2 = $C(3) \cdot R \cdot T - C(1) - C(7) / T$
TERM 3 = $C(1) + C(7) / T$
TERM 4 = $1.0 - (1.0 - 0.5 \cdot C(11) \cdot D^{**2} - C(11) \cdot D^{**4}) \cdot \text{EXP}(-3(11) \cdot D^{**2})$
 $F = \text{LOG}(D \cdot R \cdot T) + 2.0 \cdot \text{TERM 1} \cdot D / (C \cdot R \cdot T) + 3.0 \cdot D^{**2} \cdot \text{TERM 2} / (2.0 \cdot R \cdot T) + 6.0 \cdot C(10) \cdot \text{TERM 3} \cdot D^{**5} / (5.0 \cdot R \cdot T) + C(5) \cdot \text{TERM 4} / (C(11) \cdot R \cdot T^{**3})$
 $F = \text{EXP}(F)$
DFDD = $F \cdot (1.0 / D + 2.0 \cdot \text{TERM 1} / (R \cdot T) + 3.0 \cdot \text{TERM 2} \cdot D / (C \cdot R \cdot T) + 6.0 \cdot C(10) \cdot D^{**4} \cdot \text{TERM 3} / (R \cdot T) + C(5) / (R \cdot C(11) \cdot T^{**3}) \cdot (3.0 \cdot C(11) \cdot D + 3.0 \cdot C(11) \cdot D^{**2} \cdot D^{**3} - 2.0 \cdot D^{**5} \cdot C(11) \cdot D^{**3}) \cdot \text{EXP}(-C(11) \cdot D^{**2}))$
TERM 1 = $C(2) + 3.0 \cdot C(6) / T^{**2} - 4.0 \cdot C(8) / T^{**3} + 5.0 \cdot C(9) / T^{**4}$
TERM 2 = $C(1) + 2.0 \cdot C(7) / T$
DFDT = $F \cdot (1.0 / T + 2.0 \cdot \text{TERM 1} \cdot D / (T^{**2} \cdot R) + 3.0 \cdot \text{TERM 2} \cdot D^{**2} / (2.0 \cdot R \cdot T^{**2}) - 6.0 \cdot C(10) \cdot \text{TERM 2} \cdot 2 \cdot D^{**5} / (5.0 \cdot R \cdot T^{**2}) - 3.0 \cdot C(5) \cdot \text{TERM 4} / (C(11) \cdot R \cdot T^{**4}))$

RETURN

```

1      C      *****
2      C      *
3      C      *
4      C      *           F U G A C
5      C      *
6      C      *   THIS SUBROUTINE CALCULATES THE FUGACITY GIVEN DENSITY AND
7      C      *   TEMPERATURE
8      C      *
9      C      *****
10     SUBROUTINE FUGAC(T,D,F,DFDT,DFDD)
11     COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
12     TERM1=C(4)*R*T-C(2)-C(6)/T**2+C(8)/T**3-C(9)/T**4
13     TERM2=C(3)*R*T-C(1)-C(7)/T
14     TERM3=C(1)+C(7)/T
15     TERM4=1.0-(1.0-0.5*C(11)*D**2-C(11)**2*D**4)*EXP(-C(11)*D**2)
16     F=LOG(D*R*T)+2.0*TERM1*D/(R*T)+3.0*D**2*TERM2/(2.0*R*T)+6.0*C(10)
17     1*TERM3*D**5/(5.0*R*T)+C(5)*TERM4/(C(11)*R*T**3)
18     F=EXP(F)
19     DFDD=F*(1.0/D+2.0*TERM1/(R*T)+3.0*TERM2*D/(R*T)+6.0*C(10)*D**4
20     1*TERM3/(R*T)+C(5)/(R*C(11)*T**3)*(3.0*C(11)*D+3.0*C(11)**2*D**3
21     2-2.0*D**5*C(11)**3)*EXP(-C(11)*D**2))
22     TERM1=C(2)+3.0*C(6)/T**2-4.0*C(8)/T**3+5.0*C(9)/T**4
23     TERM2=C(1)+2.0*C(7)/T
24     DFDT=F*(1.0/T+2.0*TERM1*D/(T**2*R)+3.0*TERM2*D**2/(2.0*R*T**2)
25     1-6.0*C(10)*TERM2*D**5/(5.0*R*T**2)-3.0*C(5)*TERM4/(C(11)*R*T**4))
26     RETURN
      END

```

INVERT

DESCRIPTION

INVERT solves a system of three equations in three unknowns by Gaussian elimination. INVERT is used in the three variable search in TEMSAT.

VARIABLE SYMBOL TABLE

C	intermediate value
DX(1)	$\Delta\rho_L$ to be solved for
DX(2)	$\Delta\rho_V$ to be solved for
DX(3)	ΔT to be solved for
F(1)	F_1 value of first equation
F(2)	F_2 value of second equation
F(3)	F_3 value of third equation
I	index
J	index
K	index
L	index
M	index
N	index
W	working array containing the coefficient matrix and the function vector
XJACOB	coefficient matrix

```

1      C *****
2      C *
3      C *
4      C *
5      C *   THIS SUBROUTINE SOLVES THREE SIMULTANEOUS EQUATIONS BY
6      C *   *GUASSIAN ELIMINATION
7      C *
8      C *****
9      SUBROUTINE INVERT(XJACOB,F,DX)
10     DIMENSION XJACOB(3,3),DX(3),F(3),W(3,4)
11     DO 5 I=1,3
12     DO 5 J=1,4
13     IF(J=4)2,3,5
14     2 W(I,J)=XJACOB(I,J)
15     GO TO 5
16     3 W(I,J)=F(I)
17     5 CONTINUE
18     N=0
19     DO 100 K=1,2
20     N=N+1
21     DO 95 L=2,3
22     IF(K=L)10,90,90
23     10 C=-W(L,N)/W(K,N)
24     DO 80 M=1,4
25     W(L,M)=W(L,M)+C*W(K,M)
26     80 CONTINUE
27     90 CONTINUE
28     95 CONTINUE
29     100 CONTINUE
30     DX(3)=W(3,4)/W(3,3)
31     DX(2)=(W(2,4)-DX(3)*W(2,3))/W(2,2)
32     DX(1)=(W(1,4)-DX(3)*W(1,3)-DX(2)*W(1,2))/W(1,1)
33     RETURN
34     END

```

PHKNOW

DESCRIPTION

PHKNOW uses a two variable Newton-Raphson iteration technique to find the density and temperature given pressure and enthalpy in the superheated vapor or compressed liquid regions.

EQUATIONS

$$P(\rho, T) - P_{\text{known}} = 0$$

$$h(\rho, T) - h_{\text{known}} = 0$$

$$\text{Jacobian} = \left(\frac{\partial P(\rho, T)}{\partial \rho} \right) \left(\frac{\partial h(\rho, T)}{\partial T} \right) - \left(\frac{\partial P(\rho, T)}{\partial T} \right) \left(\frac{\partial h(\rho, T)}{\partial \rho} \right)$$

$$\rho_{i+1} = \rho_i - \left[\frac{(P(\rho, T) - P_{\text{known}}) \frac{\partial h(\rho, T)}{\partial T} - (h(\rho, T) - h_{\text{known}}) \frac{\partial P(\rho, T)}{\partial T}}{\text{Jacobian}} \right]_i$$

$$T_{i+1} = T_i - \left[\frac{(h(\rho, T) - h_{\text{known}}) \frac{\partial P(\rho, T)}{\partial \rho} - (P(\rho, T) - P_{\text{known}}) \frac{\partial h(\rho, T)}{\partial \rho}}{\text{Jacobian}} \right]_i$$

VARIABLE SYMBOL TABLE

BTOLER	lower tolerance on saturation and convergence tests
D	density (lbmole/ft ³)
DHDD	$\frac{\partial h(\rho, T)}{\partial \rho}$
DHDT	$\frac{\partial h(\rho, T)}{\partial T}$
DLAST	last density calculated, to be used in next iteration
DPDD	$\frac{\partial P(\rho, T)}{\partial \rho}$
DPDT	$\frac{\partial P(\rho, T)}{\partial T}$
H	known enthalpy (BTU/lbm)
HCAL	calculated enthalpy (BTU/lbm)

I	index
LIMIT	maximum number of iterations allowed in any one search
P	known pressure (psia)
PCAL	calculated pressure (psia)
T	temperature ($^{\circ}$ R)
TLAST	last temperature calculated, to be used in next iteration
TTOLER	upper tolerance on saturation and convergence tests
XJACOB	Jacobian of pressure and enthalpy

```

1      C      *****
2      C      *
3      C      *
4      C      *           P H K N O W
5      C      *
6      C      *   THIS SUBROUTINE FINDS THE DENSITY AND TEMPERATURE GIVEN
7      C      *   *PRESSURE AND ENTHALPY FOR COMPRESSED LIQUID AND SUPERHEATED VAPO*
8      C      *   *STATES
9      C      *
10     C      *****
11     C      SUBROUTINE PHKNOW(P,H,T,D)
12     C      COMMON/CA1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
13     C      PARAMETER M2=6
14     C      DLAST=D
15     C      TLAST=T
16     C      CALL PRES(T,D,PCAL,DPDT,DPDD)
17     C      CALL ENTH(T,D,HCAL,DHDT,DHDD)
18     C      DO 1000 I=1,LIMIT
19     C      XJACOB=DPDD*DHDT-DPDT*DHDD
20     C      D=DLAST-((PCAL-P)*DHDT-(HCAL-H)*DPDT)/XJACOB
21     C      T=TLAST-((HCAL-H)*DPDD-(PCAL-P)*DHDD)/XJACOB
22     C      IF(D.LE.0.0) D=DLAST/10.0
23     C      IF(T.LE.0.0) T=TLAST/10.0
24     C      CALL PRES(T,D,PCAL,DPDT,DPDD)
25     C      CALL ENTH(T,D,HCAL,DHDT,DHDD)
26     C      IF(PCAL/P.LT.TTOLER.AND.PCAL/P.GT.BTOLER.AND.HCAL/H.LT.TTOLER.
27     C      1AND.HCAL/H.GT.BTOLER)RETURN
28     C      DLAST=D
29     C      TLAST=T
30     C      1000 CONTINUE
31     C      WRITE(M2,9000)LIMIT
32     C      9000 FORMAT(1H,4X,'***PHKNOW FAILED TO CONVERGE IN',I6,'ITERATIONS')
33     C      RETURN
34     C      END

```

PRES

DESCRIPTION

PRES calculates the pressure and its derivatives with respect to temperature and density given the temperature and density. The pressure is computed using the Starling-Benedict-Webb-Rubin equation of state.

EQUATIONS

$$P(\rho, T) = \rho * R * T + (B_0 * R * T - A_0 - C_0 / T^2 + D_0 / T^3 - E_0 / T^4) \rho^2 + (6 * R * T - a - d / T) \rho^3 + \alpha (a + d / T) \rho^6 + c * \rho^3 / T^2 (1 + \gamma \rho^2) \exp(-\gamma * \rho^2)$$

$$\frac{\partial P(\rho, T)}{\partial T} = \rho * R + (B_0 * R + 2 * C_0 / T^3 - 3 * D_0 / T^4 + 4 * E_0 / T^5) \rho^2 + (b * R + d / T^2) \rho^3 - \alpha * d * \rho^6 / T^2 - 2 * C * \rho^3 / T^3 (1 + \gamma * \rho^2) \exp(-\gamma * \rho^2)$$

$$\frac{\partial P(\rho, T)}{\partial \rho} = R * T + 2 * (B_0 * R * T - A_0 - C_0 / T^2 + D_0 / T^3 - E_0 / T^4) \rho + 3 * (b * R * T - a - d / T) \rho^2 + 6 * \alpha (a + d / T) \rho^5 + 3 * C * \rho^2 / T^2 (1 + \gamma * \rho^2) \exp(-\gamma * \rho^2) - 2 * \gamma^2 * \rho^6 * C / T^2 \exp(-\gamma * \rho^2)$$

VARIABLE SYMBOL TABLE

C	1-dimensional array containing the coefficients to the SBWR equation of state
D	density (lbmole/ft ³)
DPDD	$\frac{\partial P(\rho, T)}{\partial \rho}$
DPDT	$\frac{\partial P(\rho, T)}{\partial T}$
P	pressure (psia)
R	universal gas constant = 10.7335 psia-ft ³ /lbmole°R
T	temperature (°R)
TERM1	intermediate value
TERM2	intermediate value

TERM3 intermediate value

TERM4 intermediate value

START

TERM 1 = $C(4)*R*T - C(2) - C(6)/T^{**2} + C(8)/T^{**3} - C(9)/T^{**4}$
TERM 2 = $C(3)*R*T - C(1) - C(7)/T$
TERM 3 = $C(1) + C(7)/T$
TERM 4 = $1.0 + C(11)*D^{**2}$
P = $D*R*T + TERM 1*D^{**2} + TERM 2*D^{**3} + C(10)*TERM 3*D^{**6} + C(5)*D^{**3}*TERM 4*EXP(-C(11)*D^{**2})/T^{**2}$
DPDD = $R*T + 2.0*TERM 1*D + 3.0*TERM 2*D^{**2} + 6.0*C(10)*TERM 3*D^{**5} + 3.00*C(5)*D^{**2}*TERM 4*EXP(-C(11)*D^{**2})/T^{**2} - 2.0*C(11)*D^{**2}*D^{**6} + C(5)*EXP(-C(11)*D^{**2})/T^{**2}$
DPDT = $D*R + D^{**2}*(C(4)*R + 2.0*C(6)/T^{**3} - 3.0*C(8)/T^{**4} + 4.0 + C(9)/T^{**5}) + D^{**3}*(C(3)*R + C(7)/T^{**2}) - D^{**6}*C(10)*C(7)/T^{**2} - 2.0*C(5)*D^{**3}*TERM 4*EXP(-C(11)*D^{**2})/T^{**3}$

RETURN

```

1      C      *****
2      C      *
3      C      *
4      C      *
5      C      *   THIS SUBROUTINE CALCULATES THE PRESSURE GIVEN DENSITY AND
6      C      * TEMPERATURE
7      C      *
8      C      *****
9      SUBROUTINE PRES(T,D,P,DPDT,DPDD)
10     COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
11     TERM1=C(4)*R*T-C(2)-C(6)/T**2+C(8)/T**3-C(9)/T**4
12     TERM2=C(5)*R*T-C(1)-C(7)/T
13     TERM3=C(1)+C(7)/T
14     TERM4=1.0+C(11)*D**2
15     P=D*R*T+TERM1*D**2+TERM2*D**3+C(10)*TERM3*D**6+C(5)*D**3*TERM4*
16     1EXP(-C(11)*D**2)/T**2
17     DPDD=R*T+2.0*TERM1*D+3.0*TERM2*D**2+6.0*C(10)*TERM3*D**5
18     1+3.00*C(5)*D**2*TERM4*EXP(-C(11)*D**2)/T**2-2.0*C(11)**2*D**6
19     2*C(5)*EXP(-C(11)*D**2)/T**2
20     DPDT=D*R+D**2*(C(4)*R+2.0*C(6)/T**3-3.0*C(8)/T**4+4.0+C(9)/T**5)
21     1+D**3*(C(3)*R+C(7)/T**2)-D**6*C(10)*C(7)/T**2-2.0*C(5)*D**3*TERM4*
22     2EXP(-C(11)*D**2)/T**3
23     RETURN
24     END

```

PRESAT

DESCRIPTION

PRESAT uses a two variable Newton-Raphson iteration technique to find the saturation pressure and the saturated liquid and vapor densities given temperature. At equilibrium the pressure and fugacity of the liquid and vapor phases must be equal.

EQUATIONS

$$P(\rho_L, T) - P(\rho_V, T) = 0$$

$$f(\rho_L, T) - f(\rho_V, T) = 0$$

$$\text{Jacobian} = \left(\frac{-\partial P(\rho_V, T)}{\partial \rho} \right) \left(\frac{\partial f(\rho_L, T)}{\partial \rho} \right) - \left(\frac{\partial P(\rho_L, T)}{\partial \rho} \right) \left(\frac{\partial f(\rho_V, T)}{\partial \rho} \right)$$

$$\rho_{Vi+1} = \rho_{Vi} - \left[\frac{(P(\rho_L, T) - P(\rho_V, T)) \frac{\partial f(\rho_L, T)}{\partial \rho} - (f(\rho_L, T) - f(\rho_V, T)) \frac{\partial P(\rho_L, T)}{\partial \rho}}{\text{Jacobian}} \right]_i$$

$$\rho_{Li+1} = \rho_{Li} - \left[\frac{(f(\rho_L, T) - f(\rho_V, T)) \frac{\partial P(\rho_V, T)}{\partial \rho} - (P(\rho_L, T) - P(\rho_V, T)) \frac{\partial f(\rho_V, T)}{\partial \rho}}{\text{Jacobian}} \right]_i$$

VARIABLE SYMBOL TABLE

BTOLER lower tolerance on saturation and convergence tests

DFDDL $\frac{\partial f(\rho_L, T)}{\partial \rho}$

DFDDV $-\frac{\partial f(\rho_V, T)}{\partial \rho}$

DFLDDL $\frac{\partial f(\rho_L, T)}{\partial \rho}$

DFLDT	$\frac{\partial f(\rho_L, T)}{\partial T}$
DFPDDL	$\frac{\partial P(\rho_L, T)}{\partial \rho}$
DFPDDV	$\frac{-\partial P(\rho_V, T)}{\partial \rho}$
DFVDDV	$\frac{\partial f(\rho_V, T)}{\partial \rho}$
DL	saturated liquid density (lbmole/ft ³)
DLLAST	last liquid density calculated, to be used in next iteration
DPLDDL	$\frac{\partial P(\rho_L, T)}{\partial \rho}$
DPLDT	$\frac{\partial P(\rho_L, T)}{\partial \rho}$
DPVDDV	$\frac{\partial P(\rho_V, T)}{\partial \rho}$
DPVDT	$\frac{\partial P(\rho_V, T)}{\partial T}$
DV	saturated vapor density (lbmole/ft ³)
DVLAST	last vapor density calculated, to be used in next iteration
FF	difference in fugacities - $f(\rho_L, T) - f(\rho_V, T)$
FL	liquid fugacity $f(\rho_L, T)$
FP	difference in pressures $P(\rho_L, T) - P(\rho_V, T)$
I	index
LIMIT	maximum number of iterations allowed in any one search
M2	unit number for printed
P	pressure (psia)
PL	liquid pressure $P(\rho_L, T)$ (psia)
PV	vapor pressure $P(\rho_V, T)$ (psia)

T temperature ($^{\circ}$ R)

TTOLER upper tolerance on saturation and convergence tests

XJACOB Jacobian

```

1      C      *****
2      C      *
3      C      *
4      C      *
5      C      *   THIS SUBROUTINE FINDS THE SATURATION PRESSURE AND SATURATED
6      C      * LIQUID AND VAPOR DENSITIES GIVEN TEMPERATURE
7      C      *
8      C      *****
9      SUBROUTINE PRESAT(T,P,DL,DV,DCRIT)
10     COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
11     PARAMETER M2=6
12     DL=DCRIT*2.5
13     DV=DCRIT/20.0
14     CALL FUGAC(T,DL,FL,DFLDT,DFLDDL)
15     CALL FUGAC(T,DV,FV,DFVDT,DFVDDV)
16     CALL PRES(T,DL,PL,DPLDT,DPLDDL)
17     CALL PRES(T,DV,PV,DPVDT,DPVDDV)
18     DVLAST=DV
19     DLLAST=DL
20     DO 1000 I=1,LIMIT
21     FP=PL-PV
22     FF=FL-FV
23     DFPDDV=-DPVDDV
24     DFPDDL=DPLDDL
25     DFFDDV=-DFVDDV
26     DFFDDL=DFLDDL
27     XJACOB=DFPDDV*DFFDDL-DFFDDL*DFPDDV
28     DV=DVLAST-(FP*DFFDDL-FF*DFPDDL)/XJACOB
29     DL=DLLAST-(FF*DFPDDV-FP*DFFDDV)/XJACOB
30     IF(DV.LE.0.0)DV=DVLAST/10.0
31     IF(DL.LE.0.0)DL=DLLAST/10.0
32     CALL FUGAC(T,DL,FL,DFLDT,DFLDDL)
33     CALL FUGAC(T,DV,FV,DFVDT,DFVDDV)
34     CALL PRES(T,DL,PL,DPLDT,DPLDDL)

```

```

35      CALL PRES(T,DV,PV,DPVDT,DPVDDV)
36      P=(PV+PL)/2.0
37      IF (FL/FV.LT.TTOLER.AND.FL/FV.GT.BTOLER.AND.PL/PV.LT.TTOLER.
38      1AND.PL/PV.GT.BTOLER) RETURN
39      DLLAST=DL
40      DVLAST=DV
41      1000 CONTINUE
42      WRITE(M2,9000)LIMIT
43      9000 FORMAT(1H,4X,'***PRESAT FAILED TO CONVERGE IN',I6,'ITERATIONS')
44      RETURN
45      END

```

PRINTC

DESCRIPTION

PRINTC prints the results of CARBON if NPRIN does not equal zero.

VARIABLE SYMBOL TABLE

ABST	absolute temperature difference °F to °R = 459.6
H	enthalpy (BTU/lbm)
HL	saturated liquid enthalpy (BTU/lbm)
HV	saturated vapor enthalpy (BTU/lbm)
LFTYPE	the type of light hydrocarbon to be evaluated
M2	unit number for printer
NPRIN	print selector if NPRIN = 0 then no print else print out results of CARBON
P	pressure (psia)
QUAL	quality
S	entropy (Btu/lbm°R)
SL	saturated liquid entropy (Btu/lbm°R)
SV	saturated vapor entropy (Btu/lbm°R)
T	temperature (°R)
V	specific volume (ft ³ /lbm)
VL	saturated liquid specific volume (ft ³ /lbm)
VV	saturated vapor specific volume (ft ³ /lbm)

```

1 C *****
2 C *
3 C *
4 C *
5 C *   THIS SUBROUTINE PRINTS OUT THE RESULTS OF SUBROUTINE CARBON *
6 C *
7 C *****
8 SUBROUTINE PRINTC(T,P,H,S,V,QUAL,HL,SL,VL,HV,SV,VV,LFTYPE,NPRIN)
9 PARAMETER M2=6
10 COMMON/CARL/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
11 T=T-ABST
12 IF(NPRIN.EQ.0) RETURN
13 WRITE(M2,9000)LFTYPE
14 WRITE(M2,9010)T,P
15 IF(QUAL.LE.1.0.AND.QUAL.GE.0.0) GO TO 3280
16 IF(QUAL.GT.1.0) WRITE(M2,9020)
17 IF(QUAL.LT.0.0) WRITE(M2,9030)
18 GO TO 3370
19 3280 WRITE(M2,9040) QUAL
20      WRITE(M2,9050)
21      WRITE(M2,9070) HV,HL
22      WRITE(M2,9080) SV,SL
23      WRITE(M2,9060) VV,VL
24 3370 WRITE(M2,9090)
25      WRITE(M2,9070) H
26      WRITE(M2,9080) S
27      WRITE(M2,9060) V
28 9000 FORMAT(1H1,4X,'***THERMODYNAMIC PROPERTIES OF ',A4,' USING
29      1STARLING-BWR EQUATION OF STATE**')
30 9010 FORMAT(1H ,4X,'TEMPERATURE = ',F7.1,'DEG.F',/,5X,'PRESSURE   = ',
31      1 F10.5,'PSIA')
32 9020 FORMAT(1H ,4X,'SUPERHEATED VAPOR',////////)
33 9030 FORMAT(1H ,4X,'COMPRESSED LIQUID',////////)
34 9040 FORMAT(1H ,4X,'SATURATED LIQUID-VAPOR EQUILIBRIUM',/,5X,'QUALITY =

```

```

35      1 ',F8.4)
36 9050 FORMAT(1H ,//,35X,'SATURATED',8X,'SATURATED',/,35X,'VAPOR',12X,
37      1 'LIQUID',/,5X,69('H'))
38 9060 FORMAT(1H ,4X,'SPECIFIC VOLUME (CU.FT/LBM)',5X,F9.4,8X,F9.4,////
39      1 /)
40 9070 FORMAT(1H ,4X,'ENTHALPY',8X,'(BTU/LBM)',5X,F9.3,8X,F9.3)
41 9080 FORMAT(1H ,4X,'ENTROPY',9X,'(BTU/LBM-R)',5X,F9.6,8X,F9.6)
42 9090 FORMAT(1H ,////////)
43      RETURN
44      END

```

PSKNOW

DESCRIPTION

PSKNOW uses a two variable Newton-Raphson iteration technique to find the density and temperature given pressure and entropy in the superheated vapor or compressed liquid region.

EQUATIONS

$$P(\rho, T) - P_{\text{known}} = 0$$

$$S(\rho, T) - S_{\text{known}} = 0$$

$$\text{Jacobian} = \left(\frac{\partial P(\rho, T)}{\partial \rho} \right) \left(\frac{\partial S(\rho, T)}{\partial T} \right) - \left(\frac{\partial P(\rho, T)}{\partial T} \right) \left(\frac{\partial S(\rho, T)}{\partial \rho} \right)$$

$$\rho_{i+1} = \rho_i - \left[\frac{(P(\rho, T) - P_{\text{known}}) \frac{\partial S(\rho, T)}{\partial T} - (S(\rho, T) - S_{\text{known}}) \frac{\partial P(\rho, T)}{\partial T}}{\text{Jacobian}} \right]_i$$

$$T_{i+1} = T_i - \left[\frac{(S(\rho, T) - S_{\text{known}}) \frac{\partial P(\rho, T)}{\partial \rho} - (P(\rho, T) - P_{\text{known}}) \frac{\partial S(\rho, T)}{\partial \rho}}{\text{Jacobian}} \right]_i$$

VARIABLE SYMBOL TABLE

BTOLER	lower tolerance on saturation and convergence tests
D	density (lbmole/ft ³)
DLAST	last density calculated to be used in next iteration
DPDD	$\frac{\partial P(\rho, T)}{\partial \rho}$
DPDT	$\frac{\partial P(\rho, T)}{\partial T}$
DSDD	$\frac{\partial S(\rho, T)}{\partial \rho}$
DSDT	$\frac{\partial S(\rho, T)}{\partial T}$
I	index

LIMIT	maximum number of iterations to be allowed in any one search
M2	unit number for printer
P	known pressure (psia)
PCAL	calculated pressure (psia)
S	known entropy (Btu/lbm°R)
SCAL	calculated entropy (Btu/lbm°R)
T	temperature (°R)
TLAST	last temperature calculated to be used in next iteration
TTOLER	upper tolerance on saturation and convergence tests
XJACOB	Jacobian of pressure and entropy

```

1 C *****
2 C *
3 C * P S K N O W *
4 C *
5 C * THIS SUBROUTINE FINDS THE DENSITY AND TEMPERATURE GIVEN *
6 C *PRESSURE AND ENTROPY FOR COMPRESSED LIQUID AND SUPERHEATED VAPOR*
7 C *STATES *
8 C *
9 C *****
10 C SUBROUTINE PSKNOW(P,S,T,D)
11 C COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
12 C PARAMETER M2=6
13 C DLAST=D
14 C TLAST=T
15 C CALL PRES(T,D,PCAL,DPDT,DPDD)
16 C CALL ENTR(T,D,SCAL,DSDT,DSDD)
17 C DO 1000 I=1,LIMIT
18 C XJACOB=DPDD*DSDT-DPDT*DSDD
19 C D=DLAST-((PCAL-P)*DSDT-(SCAL-S)*DPDT)/XJACOB
20 C T=TLAST-((SCAL-S)*DPDD-(PCAL-P)*DSDD)/XJACOB
21 C IF(T.LE.0.0) T=TLAST/10.0
22 C IF(D.LE.0.0) D=DLAST/10.0
23 C CALL PRES(T,D,PCAL,DPDT,DPDD)
24 C CALL ENTR(T,D,SCAL,DSDT,DSDD)
25 C IF(PCAL/P.LT.TTOLER.AND.PCAL/P.GT.BTOLER.AND.SCAL/S.LT.TTOLER.
26 C AND.SCAL/S.GT.BTOLER)RETURN
27 C DLAST=D
28 C TLAST=T
29 C 1000 CONTINUE
30 C WRITE(M2,9000)LIMIT
31 C 9000 FORMAT(1H,4X,'***PSKNOW FAILED TO CONVERGE IN',I6,'ITERATIONS')
32 C RETURN
33 C END

```

SATC

DESCRIPTION

SATC calls ENTH and ENTR to compute the saturated liquid and vapor properties given temperature and the saturated liquid and vapor densities

VARIABLE SYMBOL

$$\text{DHLDD} \quad \frac{\partial h(\rho, T)}{\partial \rho}$$

$$\text{DHLDT} \quad \frac{\partial h(\rho, T)}{\partial T}$$

$$\text{DHVDD} \quad \frac{\partial h(\rho_v, T)}{\partial \rho}$$

$$\text{DHVDT} \quad \frac{\partial h(\rho_v, T)}{\partial T}$$

DL saturated liquid density (lbmole/ft³)

$$\text{DSLDD} \quad \frac{\partial S(\rho_L, T)}{\partial \rho}$$

$$\text{DSLDT} \quad \frac{\partial S(\rho_L, T)}{\partial T}$$

$$\text{DSVDD} \quad \frac{\partial S(\rho_v, T)}{\partial \rho}$$

$$\text{DSVDT} \quad \frac{\partial S(\rho_v, T)}{\partial T}$$

DV saturated vapor density (lbmole/ft³)

HL saturated liquid enthalpy (Btu/lbm)

HV saturated vapor enthalpy (Btu/lbm)

SL saturated liquid entropy (Btu/lbm°R)

SV saturated vapor entropy (Btu/lbm°R)

T temperature (°R)

```

1 C *****
2 C *
3 C *
4 C *
5 C * THIS SUBROUTINE DETERMINES SATURATED LIQUID AND VAPOR
6 C * PROPERTIES
7 C *
8 C *****
9 SUBROUTINE SATC(T,DL,DV,HL,SL,HV,SV)
10 CALL ENTR(T,DL,HL,DHLEDT,DHLEDD)
11 CALL ENTR(T,DL,SL,DSELEDT,DSELEDD)
12 CALL ENTR(T,DV,HV,DHVEDT,DHVEDD)
13 CALL ENTR(T,DV,SV,DSEVEDT,DSEVEDD)
14 RETURN
15 END

```

SETUP

DESCRIPTION

SETUP stores the values for the light hydrocarbon to be evaluated in the coefficient arrays, C, CS and CH. PCRIT, DCRIT, WM and TCRIT are also assigned their values.

VARIABLE SYMBOL TABLE

C	1-dimensional array containing the coefficients for the Starling-Benedict-Webb-Rubin equation of state
C(1)	a
C(2)	A_0
C(3)	b
C(4)	B_0
C(5)	C
C(6)	C_0
C(7)	d
C(8)	D_0
C(9)	E_0
C(10)	α
C(11)	γ
CS	1-dimensional array containing the coefficients for the ideal gas entropy
CH	1-dimensional array containing the coefficients for the ideal gas enthalpy
DCRIT	critical density (lbmole/ft^3)
GIVEN	1-dimensional array containing the coefficients for the hydrocarbon to be evaluated

GIVEN (1)	C(1)
GIVEN (2)	C(2)
GIVEN (3)	C(3)
GIVEN (4)	C(4)
GIVEN (5)	C(5)
GIVEN (6)	C(6)
GIVEN (7)	C(7)
GIVEN (8)	C(8)
GIVEN (9)	C(9)
GIVEN (10)	C(10)
GIVEN (11)	C(11)
GIVEN (12)	CS(1)
GIVEN (13)	CS (2)
GIVEN (14)	CS (3)
GIVEN (15)	CS (4)
GIVEN (16)	CS (5)
GIVEN (17)	CS (6)
GIVEN (18)	CH (1)
GIVEN (19)	CH (2)
GIVEN (20)	CH (3)
GIVEN (21)	CH (4)
GIVEN (22)	CH (5)
GIVEN (23)	CH (6)
GIVEN (24)	PCRIT
GIVEN (25)	TRCIT
GIVEN (26)	DCRIT
GIVEN (27)	WM

I index
PCRIT critical pressure (psia)
TRCIT critical temperature (°R)
WM molecular weight

The following arrays have the same format as GIVEN: BUT, ETH, ETHYL,
HEPT, HEX, OCT, PENT, PROP, PROPYL, XISOB, XISOP, XMETH.

```

1 C *****
2 C *
3 C *
4 C *
5 C *   THIS SUBROUTINE SETS UP THE REQUIRED COEFFICIENTS FOR THE
6 C *PARTICULAR FLUID TO BE ANALYZED.
7 C *
8 C *****
9 SUBROUTINE SETUP(GIVEN,PCRIT,TCRIT,DCRIT)
10 COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
11 DIMENSION GIVEN(27)
12 DO 100 I=1,11
13 C(I)=GIVEN(I)
14 100 CONTINUE
15 DO 200 I=1,6
16 CS(I)=GIVEN(1+11)
17 CH(I)=GIVEN(1+17)
18 200 CONTINUE
19 PCRIT=GIVEN(24)
20 TCRIT=GIVEN(25)
21 DCRIT=GIVEN(26)
22 WM=GIVEN(27)
23 RETURN
24 END

```

TEMSAT

DESCRIPTION

TEMSAT uses a three variable Newton-Raphson iteration technique to find the saturation temperature and the saturated liquid and vapor densities given pressure. The conditions at equilibrium are, the pressure calculated with either the liquid or vapor density must equal the known pressure and the fugacities of both the liquid and vapor phases must also be equal.

EQUATIONS

$$P(\rho_L, T) - P_{\text{known}} = F_1$$

$$P(\rho_V, T) - P_{\text{known}} = F_2$$

$$f(\rho_V, T) - f(\rho_L, T) = F_3$$

expanding F_1 , F_2 and F_3 in a Taylor series

$$-F_1 = \frac{\partial F_1}{\partial \rho_L} \Delta \rho_L + \frac{\partial F_1}{\partial \rho_V} \Delta \rho_V + \frac{\partial F_1}{\partial T} \Delta T$$

$$-F_2 = \frac{\partial F_2}{\partial \rho_L} \Delta \rho_L + \frac{\partial F_2}{\partial \rho_V} \Delta \rho_V + \frac{\partial F_2}{\partial T} \Delta T$$

$$-F_3 = \frac{\partial F_3}{\partial \rho_L} \Delta \rho_L + \frac{\partial F_3}{\partial \rho_V} \Delta \rho_V + \frac{\partial F_3}{\partial T} \Delta T$$

solving for $\Delta \rho_L$, $\Delta \rho_V$ and ΔT and substituting in for F_1 , F_2 and F_3

$$\begin{vmatrix} \Delta \rho_L \\ \Delta \rho_V \\ \Delta T \end{vmatrix} = - \begin{vmatrix} \frac{\partial P(\rho_L, T)}{\partial \rho} & 0 & \frac{\partial P(\rho_L, T)}{\partial T} \\ 0 & \frac{\partial P(\rho_V, T)}{\partial \rho} & \frac{\partial P(\rho_V, T)}{\partial T} \\ \frac{\partial f(\rho_L, T)}{\partial \rho} & \frac{\partial f(\rho_V, T)}{\partial \rho} & \frac{\partial f(\rho_V, T)}{\partial T} - \frac{\partial f(\rho_L, T)}{\partial T} \end{vmatrix}^{-1} \begin{vmatrix} F_1 \\ F_2 \\ F_3 \end{vmatrix}$$

$$\rho_{Li+1} = \rho_{Li} + \Delta\rho_L$$

$$\rho_{Vi+1} = \rho_{Vi} + \Delta\rho_V$$

$$T_{i+1} = T_i + \Delta T$$

VARIABLE SYMBOL TABLE

BTOLER	lower tolerance on convergence and saturation tests
DCRIT	critical density (lbmole/ft ³)
DFLDDL	$\frac{\partial f(\rho_L, T)}{\partial \rho}$
DFLDT	$\frac{\partial f(\rho_L, T)}{\partial T}$
DFVDDV	$\frac{\partial f(\rho_V, T)}{\partial \rho}$
DPVDT	$\frac{\partial f(\rho_V, T)}{\partial T}$
DL	saturated liquid density (lbmole/ft ³)
DLLAST	last liquid density calculated, to be used in next iteration
DPLDDL	$\frac{\partial P(\rho_L, T)}{\partial \rho}$
DPLDT	$\frac{\partial P(\rho_L, T)}{\partial T}$
DPVDDV	$\frac{\partial P(\rho_V, T)}{\partial \rho}$
DPVDT	$\frac{\partial P(\rho_V, T)}{\partial T}$

DV	saturated vapor density (lbmole/ft ³)
DVLAST	last vapor density calculated, to be used in next iteration
DX(1)	$\Delta\rho_L$
DX(2)	$\Delta\rho_V$
DX(3)	ΔT
F(1)	F_1
F(2)	F_2
F(3)	F_3
FL	$f(\rho_L, T)$
FV	$f(\rho_V, T)$
I	index
LIMIT	maximum number of iterations allowed in any one search
M2	unit number of printer
P	known pressure (psia)
PL	$P(\rho_L, T)$
PV	$P(\rho_V, T)$
T	saturation temperature (°R)
TLAST	last temperature calculated, to be used in next iteration
XJACOB	2-dimensional array containing the Jacobian of ρ_L , ρ_V and T.

```

1      C      ****
2      C      *
3      C      *
4      C      *
5      C      *
6      C      *
7      C      *
8      C      *
9      C      *
10     C      *
11     C      *
12     C      *
13     C      *
14     C      *
15     C      *
16     C      *
17     C      *
18     C      *
19     C      *
20     C      *
21     C      *
22     C      *
23     C      *
24     C      *
25     C      *
26     C      *
27     C      *
28     C      *
29     C      *
30     C      *
31     C      *
32     C      *
33     C      *
34     C      *

```

T E M S A T

THIS SUBROUTINE FINDS THE SATURATION TEMPERATURE AND
SATURATED LIQUID AND VAPOR DENSITIES GIVEN PRESSURE

SUBROUTINE TEMSAT(P,T,DL,DV,TCRIT,DCRIT)
COMMON/CAR1/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER
DIMENSION XJACOB(3,3),F(3),DX(3)
PARAMETER M2=6
TCRITR=TCRIT+ABS1
T=640.0
DV=DCRIT/20.0
DL=DCRIT*2.5
TLAST=T
DVLAST=DV
DLLAST=DL
CALL PRES(T,DL,PL,DFLDT,DPLDDL)
CALL PRES(T,DV,PV,DPVDT,DPVDDV)
CALL FUGAC(T,DL,FL,DFLDT,DFLDDL)
CALL FUGAC(T,DV,FV,DFVDT,DFVDDV)
DO 1000 I=1,LIMIT
F(1)=PL-P
F(2)=PV-P
F(3)=FV-FL
XJACOB(1,1)=DPLDDL
XJACOB(1,2)=0.0
XJACOB(1,3)=DPLDI
XJACOB(2,1)=0.0
XJACOB(2,2)=DPVDDV
XJACOB(2,3)=DPVDI
XJACOB(3,1)=-DFLDDL

```

35      XJACOB(3,2)=DFVDDV
36      XJACOB(3,3)=DFVDI-DFLDT
37      CALL INVERT(XJACOB,F,DX)
38      DL=DLLAST-DX(1)
39      DV=DVLAST-DX(2)
40      T=TLAST-DX(3)
41      750 IF(T.LE.0.0) T=TLAST/10.0
42      IF(DL.LE.0.0) DL=DLLAST/10.0
43      IF(DV.LE.0.0) DV=DVLAST/10.0
44      IF(DV.GE.0.55) DV=DVLAST*2.0
45      IF(DL.GE.1.0) DL=DLLAST*2.0
46      IF(T.GT.TCRITR) T=TCRITR
47      CALL PRES(T,DL,PL,DPLDT,DPLDDL)
48      CALL PRES(T,DV,PV,DPVDT,DPVDDV)
49      CALL FUGAC(T,DL,FL,DFLDT,DFLDDL)
50      CALL FUGAC(T,DV,FV,DFVDT,DFVDDV)
51      IF(PL/P.LT.TTOLER.AND.PL/P.GT.BTOLER.AND.PV/P.LT.TTOLER.
52      1AND.PV/P.GT.BTOLER.AND.FL/FV.LT.TTOLER.AND.FL/FV.GT.BTOLER) RETURN
53      DLLAST=DL
54      DVLAST=DV
55      TLAST=T
56      1000 CONTINUE
57      WRITE(M2,9000)LIMIT
58      9000 FORMAT(1H ,4X,'***TEMPSAT FAILED TO CONVERGE IN',I6,'ITERATIONS')
59      RETURN
60      END

```

VFIND

DESCRIPTION

VFIND uses a Newton-Raphson iteration technique to find the density given pressure and temperature for the compressed liquid or superheated vapor regions

EQUATIONS

$$P(\rho, T) - P_{\text{known}} = 0$$

$$\rho_{i+1} = \rho_i - \left[\frac{P(\rho, T) - P_{\text{known}}}{\frac{\partial P(\rho, T)}{\partial \rho}} \right]_i$$

VARIABLE SYMBOL TABLE

BOTLER	lower tolerance on saturation and convergence tests
D	density (lbmole/ft ³)
DLAST	last density calculated, to be used in next iteration
DPDD	$\frac{\partial P(\rho, T)}{\partial \rho}$
DPDT	$\frac{\partial P(\rho, T)}{\partial T}$
I	index
LIMIT	maximum number of iterations allowed in any one search
M2	unit number of printer
P	known pressure (psia)
PCAL	calculated pressure (psia)
T	known temperature (°R)
TTOLER	upper tolerance on saturation and convergence tests

```
C  
C  
C  
C  
C  
C  
C  
  
*****  
*  
*  
*  
V F I N D  
* THIS SUBROUTINE FINDS THE DENSITY GIVEN TEMPERATURE AND  
* PRESSURE FOR COMPRESSED LIQUID AND SUPERHEATED VAPOR STATES  
*  
*****  
SUBROUTINE VFIND(T,D)  
COMMON/CARL/C(11),CS(6),CH(6),WM,R,CONVR,LIMIT,ABST,TTOLER,BTOLER  
PARAMETER M2=6  
DLAST=D  
CALL PRES(T,D,PCAL,CPUT,CPOD)  
DO 100 I=1,LIMIT  
D=(DLAST-PCAL)/CPOD  
IF(D.LE.0.0)D=DLAST/10.0  
CALL PRES(T,D,PCAL,CPUT,CPOD)  
IF(PCAL/P.GT.BTOLER.AND.PCAL/P.LT.TTOLER) RETURN  
DLAST=D  
100 CONTINUE  
WRITE(M2,9000) LIMIT  
9000 FORMAT(IH,4X,'***VFIND FAILED TO CONVERGE IN',I6,'ITERATIONS')  
RETURN  
END
```

References

1. Mechtly, E. A., The International System of Units, Physical Constants and Conversion Factors, 2nd Revision, NASA, Washington, D. C., 1973
2. Starling, Kenneth E., Fluid Thermodynamic Properties for Light Petroleum Systems, Gulf Publishing Company, Houston, 1973
3. Starling, K. E., Fish, L. W., and Yieh, D., HSGC, A Mixture Thermodynamic Properties Computer Program, ORO-4944-2, University of Oklahoma, 1975