EQUILIBRIUM CALCULATIONS
VIA THE
BENEDICT-WEBB-RUBIN EQUATION OF STATE

BY

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ABSTRACT

The performance of various vapor-liquid equilibrium calculations requires phase equilibrium data. One of the most versatile sources of this data is an equation of state, relating the pressure, temperature, and phase compositions ir a single expression. The equation under study herewith is the eight constant Benedict-Webb-Rubin Equation of State.

This paper provides a computer program which evaluates the following types of phase equilibria: bubble-points, dew-points, and two phase flash calculations. Also included in this paper is the theoretical backround of the Benedict-Webb-Rubin Equation of State, calculational techniques, and the data used in the program.

APPROVAL OF THESIS

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APPROVED: _____

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SECTION I

INTRODUCTION

The state of equilibrium is a very important concept in Chemical Engineering. By definition, equilibrium is the condition whereby opposing forces are balanced. The chemical industry has several different types of equilibria. The form of equilibrium that is the concern of this paper is vapor-liquid equilibrium. This situation occurs when the composition of both phases remains constant.

Phase equilibrium calculations can be found in the design of distillation towers, refrigeration plants, reactors, as well as many other areas within the industry. There are several types of equilibrium computations that can be made. The first is a bubble-point calculation, which is the temperature and pressure of a liquid mixture when it just begins to boil. A second type is the dew-point calculation, which exists when a gaseous mixture just starts to condense. Both of these calculations can be used to determine the saturation point of a mixture. If we have a mixture in the two-phase region, that is, between the dew-point and bubble-point, then a flash calculation can be executed to determine conditions, phase compositions, and the amount of each species in each phase. A variation in the flash calculation is to specify

the liquid-to-vapor ratio and determine the conditions and phase compositions. This can be used when only partial vaporization or condensation is required. Another variation is to specify the enthalpy of the mixture and determine the conditions, phase compositions, and moles per phase. An example of this variation is to determine the data on the downstream side of an expansion valve. A third variation would be to select a component from the mixture and specify its mole fraction in the liquid state along with either the temperature or pressure. An example of this is determining conditions at the top or bottom of a column.

This paper will present a computer approach in performing all six of the above computations. The method used will be to calculate the equilibrium constants via fugacity coefficients. The fugacities are obtained from the Benedict-Webb-Rubin Equation of State. The derivation of the equations can be found in Section II,Theory.

The program was developed on a CDC 6600 computer. It can be modified to run on the RCA Spectra 70 and the IBM 360 computers by changing the 11-8-4 punch on all the format statements using Hollerith format to a 5-8 punch.

SECTION II

THEORY

The equation of state that will be used in this paper may be regarded as a modification of the Beattie-Bridgeman equation.[2] This modification allows the new equation to represent more accurately the properties of fluids at high densities. The van der Waals assumption of the continuity in the liquid and vapor phases, which states that only one equation is necessary to represent both phases, is retained.

The theoretical derivation for this eight constant equation of state can be found in the literature.[3,4] However, in order to give a backround on the equation, a very brief summary of its derivation will be included. The basis for the equation of state is the concept of residual work, which is defined, for mixtures, as the difference between the actual work content* A of one mole of mixture to the work content of one mole of mixture in the ideal gas state at the same temperature, density, and composition. The residual work, $\tilde{A}$, may be expressed as:

2-1 $$\tilde{A} = A - RT \ln \rho - \lim_{\rho \to 0}(A - RT \ln \rho)$$

* Also known as the Helmholtz free energy or the Gibbs ψ-function.

The pressure is related to the residual work through the following relationship:[3]

$$P = RT\rho + \rho^2 \, (\partial\tilde{A}/\partial\rho)_{T,X} \tag{2-2}$$

By utilizing equation 2-1 and equation 2-2, performing the differentiation, simplifying and combining terms, we get the final form of the BWR Equation of State, which is:

$$\begin{aligned} P = {} & RT\rho + (B_oRT - A_o - C_o/T^2)\rho^2 \\ & + (bRT - a)\rho^3 + a\alpha\rho^6 \\ & + (c\rho^2/T^2)[(1 + \gamma\rho^2)\exp(-\gamma\rho^2)] \end{aligned} \tag{2-3}$$

where:

a, A_o, b, B_o, c, C_o, α, γ = BWR constants (see Appendix C)

P = pressure (psia)

T = temperature (°R)

ρ = molal density (lb. mol/cu. ft.)

R = universal gas constant

The BWR constants for the individual components are independent of temperature and pressure, and apply to both the liquid and vapor phases. The equation treats a mixture as a single component, whereby the BWR constants for the mixture are a function of the componential BWR constants in the

mixtures. The mixture constants (in this paper) are calculated from the following mixing rules:[5]

2-4 $$a = [\sum_N x_i (a_i)^{1/3}]^3$$

2-5 $$A_o = [\sum_N x_i (A_{o_i})^{1/2}]^2$$

2-6 $$b = [\sum_N x_i (b_i)^{1/3}]^3$$

2-7 $$B_o = [\sum_N x_i B_{o_i}]$$

2-8 $$c = [\sum_N x_i (c_i)^{1/3}]^3$$

2-9 $$C_o = [\sum_N x_i (C_{o_i})^{1/2}]^2$$

2-10 $$\alpha = [\sum_N x_i (\alpha_i)^{1/3}]^3$$

2-11 $$\gamma = [\sum_N x_i (\gamma_i)^{1/2}]^2$$

The equations apply independently for both phases. Using the above mixing rules and the appropriate phase compositions, the mixture constants can be obtained from pure component data only.

The use of a single equation to summarize the thermodynamic properties of mixtures has many practical advantages. First, it provides a compact summary of experimental data which covers a wide variety of conditions. With the advent of high speed digital computers, calculation of fugacity, partial volume, or partial enthalpy can be accomplished with greater ease by the use of an equation as opposed to graphical means. The ability of the equation to be used for the liquid and vapor states permits treatment in the critical region, where satisfactory representation by conventional means is difficult. Finally, the equation can give reliable prediction of the thermodynamic properties of mixtures under most conditions, which is of great practical value due to the difficulty of experimentally determining the properties of every mixture of interest.

Now that the main equation of state is established, equations are required for the other thermodynamic functions which are to be used in the paper. The basis for this is the work content, A, sometimes known as the Helmholtz free energy. Statistical mechanics establish that the fundamental equation for the work content can be obtained from an equation of state by the following relationship:

2-12
$$A = \sum_{N} x_i[RT \ln (\rho RTx_i) + E_i^\circ - TS_i^\circ] + \int_0^\rho [(P - RT\rho)/\rho^2]\, d\rho$$

The fugacity is related to the work content through the following expression:

2-13
$$RT \ln f_i = [\partial(NA)/\partial n_i] - (E_i^\circ - TS_i^\circ + RT)$$

To evaluate the componential fugacity, we apply the BWR Equation of State in equation 2-12, use that result in equation 2-13, and, after simplification, the final expression for the fugacity of the ith component becomes:

2-14
$$\begin{aligned} RT \ln (f_i^L/x_i) &= RT \ln (\rho RT) \\ &+ [(B_o + B_{o_i})RT - 2(A_oA_{o_i})^{1/2} - 2(C_oC_{o_i})^{1/2}/T^2]\rho \\ &+ 3/2[RT(b^2b_i)^{1/3} - (a^2a_i)^{1/3}]\rho^2 \\ &+ 3/5[a(\alpha^2\alpha_i)^{1/3} + \alpha(a^2a_i)^{1/3}]\rho^5 \\ &+ [(3\rho^2/T^2)(c^2c_i)^{1/3}]\{[1 - \exp(-\gamma\rho^2)]/\gamma\rho^2 - 0.50\exp(-\gamma\rho^2)\} \\ &- [(2c\rho^2/T^2)(\gamma_i/\gamma)^{1/2}]\{[1 - \exp(-\gamma\rho^2)]/\gamma\rho^2 \\ &\qquad - (0.50\gamma\rho^2 + 1)\exp(-\gamma\rho^2)\} \end{aligned}$$

The BWR constants without the subscript i refer to the mixture constants (equation 2-4 - equation 2-11). The above equation applies to the liquid state. For the vapor phase,

substitute f_i^V for f_i^L, y_i for x_i, and use vapor compositions for the mixture BWR constants. Also, use the vapor density rather than the liquid density.

The equilibrium constant for each component can be found from its definition:

2-15 $$K_i = (f_i^L/x_i)/(f_i^V/y_i)$$

An added feature of the program is the calculation of the liquid and vapor enthalpies. We utilize two basic thermodynamic expressions, which are:

2-16 $$E = A + TS$$
$$H = E + P/\rho$$

By combining the BWR Equation of State with equation 2-12 for P, and utilizing equation 2-16, we find that the expression for the enthalpy of a mixture is:

2-17 $$(1/0.1850)\ H^L = \sum_N x_i H_i^\circ + (B_oRT - 2A_o - 4C_o/T^2)\rho + (2bRT - 3a)\rho^2/2 + 1.20a\alpha\rho^5 + c\rho^2/T^2\{3[1 - \exp(-\gamma\rho^2)]/\gamma\rho^2 - (0.50 - \gamma\rho^2)\exp(-\gamma\rho^2)\}$$

units = BTU/lb. mol

The equation, as shown, is for the liquid phase; the BWR constants used here utilized liquid fractions in the mixing

rules. In the equation for the vapor phase, substitute H^V for H^L, y_i for x_i, and use the vapor mole fractions to evaluate the mixture constants. When the equation for enthalpy is being used for the liquid state, the liquid density should be used; on the other hand, use the vapor density when applying these equations to the vapor state. Values of H_i° as a function of temperature can be found in the literature.[11]

The equations derived in this section are extremely accurate under normal conditions and fairly reliable under extreme conditions. However, due to the limited amount of P-V-T data available, the BWR constants are not available for all hydrocarbons and some nonhydrocarbons. After a great deal of work, a reduced form of the BWR Equation of State has been derived. According to the theory of corresponding states, every component will have the same BWR constant. From this reduced equation we can relate the reduced constant, denoted by a prime, to the constants in equation 2-3 as follows:[9]

2-18 $$a' = aP_c^2/R^3T_c^3$$

2-19 $$A_o' = A_oP_c/R^2T_c^2$$

2-20 $$b' = bP_c^2/R^2T_c^2$$

2-21 $$B_o' = B_oP_c/RT_c$$

2-22 $$c' = cP_c^2/R^3T_c^5$$

2-23 $$C_o' = C_oP_c/R^2T_c^4$$

2-24 $$\alpha' = \alpha P_c^3/R^3T_c^3$$

2-25 $$\gamma' = \gamma P_c^2/R^2T_c^2$$

Therefore, the BWR constants for any component can be found by knowing its critical properties as well as the reduced constants. The values for the constants are listed in Appendix D.

SECTION III

CALCULATIONAL PROCEDURES

This section describes the various convergence methods used in each one of the equilibrium calculations. In some cases, several methods were available. The method chosen was the one best suited for BWR calculations, that is, the technique that gave the most reliable results for this complicated equation. Some of the subroutines converge very slowly. Although more computer time is required, it allows each subroutine to properly converge on the correct solution. Otherwise, each successive trial may oscillate around the solution, and therefore, may never converge.

The program can do six different equilibrium calculations. These routines, along with associated options, are as follows:

TYPE	OPTIONS
Bubble-Point	2 - constant T; constant P
Dew-Point	2 - constant T; constant P
Flash, conditions known	1 - known T and P, L/F unknown

TYPE	OPTIONS
Flash, liquid fraction specified	2 - constant T; constant P
Flash, liquid fraction for one component specified	2 - constant T; constant P
Flash, enthalpy specified	2 - constant T; constant P

In order to perform these calculations, initial estimates of the liquid and vapor phases are required. The K-values are obtained through the following relation ship:

3-1 $$\ln K_i = 2.303[(f/p)^0 + \omega(f/p)^1]$$

where:

ω = Pitzers' Accentric Factor

3-2 $$(f/p)^0 = A_o + A_1/T_r + A_2T_r + A_3T_r^2 + A_4T_r^3 + (A_5 + A_6T_r + A_7T_r^2)P_r + (A_8 + A_9T_r)P_r^2 - \log P_r$$

3-3 $$(f/p)^1 = A_{10} + A_{11}T_r + A_{12}T_r^2 + A_{13}T_r^3 + A_{14}(P_r - 0.60)$$

T_r and P_r are the reduced conditions. The accentric factor may be obtained from tables or calculated as follows:[7]

3-4 $$\omega = \{(3/7)\log(P_r)/[(T_c/B_p) - 1.0]\} - 1.0$$

B_p is the boiling point of the component. Constants for equation 3-2 and equation 3-3 are found in Appendix E. Once the initial compositions are established, all K-values are found using the BWR Equation of State.

BUBBLE-POINT - After the initial compositions are set and tested, new conditions are found using the following selection rules:[10]

3-5 $$T_{n+1} = T_n/R_b$$
$$P_{n+1} = P_n R_b$$

where:

3-6 $$R_b = 1.0 + (\sum_N y_i - 1.0)/S$$

3-7 $$S = \begin{cases} 45(\sum_N y_i - 1.0) + 0.25/(\sum_N y_i - 1.0) & |\sum_N y_i - 1.0| \geq 0.04 \\ 4.0 & |\sum_N y_i - 1.0| < 0.04 \end{cases}$$

The value for S is always greater than one. This is the technique that is used to slow down the convergence. It should be noted that the constants in equation 3-7 were determined empirically.

DEW-POINT - This routine is almost identical to the bubble-point calculations. The only difference is that the selection rules, equation 3-5, become the following:

3-8
$$T_{n+1} = T_n R_b$$
$$P_{n+1} = P_n / R_b$$

FLASH CALCULATION (L/F variable) - In this subroutine, a feed of known composition, temperature, and pressure is examined. The program will then determine the composition of both phases as well as the number of moles in each phase. The equilibrium relationships used are as follows:

3-9
$$y_i = F_i / \{1.0 - (L/F)[1.0 - (1.0/K_i)]\}$$

3-10
$$x_i = y_i / K_i$$

In the above equation, F_i is the feed composition for component i, while L/F is the liquid fraction. After initially setting L/F = 1.0, all successive trials are calculated through these equations:[8]

3-11
$$(L/F)_{n+1} = (L/F)_n - (\sum_N y_i - 1.0) / [\sum_N dy_i / d(L/F)]$$

3-12
$$\frac{dy_i}{d(L/F)} = \frac{F_i[1 - (1/K_i)]}{\{1 - (L/F)[1 - (1/K_i)]\}^2}$$

This technique will normally converge on a solution after ten iterations, although the program allows for a maximum of 75 iterations. This routine was put through many test problems and was found to be better than 95% reliable.

It should be noted that before any part of this procedure occurs, the input data is tested as to the existence of two phases. This is accomplished by calculating constant pressure dew-point and bubble-point temperatures. If the given temperature falls within these calculated results, the L/F ratio is then determined. Otherwise, the trial will be stopped and a comment will appear as output, stating the situation.

FLASH CALCULATION (constant enthalpy) - The input data, as above, is first tested for the existence of two phases. If two phases exist, the program continues. The initial trial is predicated on the assumption that a linear relationship exists for enthalpy with temperature or pressure within this region. Successive iterations use the following equation:

3-13 $$P_{n+1} = P_n[1.0 + (H_n - H_s)/(\ |H_n| + |H_s|\ )]$$

for constant T

The equation is the same for constant pressure, except that P in equation 3-13 is replaced with T.

Several techniques were used in seven test probelms to obtain the best convergence. Of those tested, the one used (equation 3-13) was the only one that had reliable answers in all of the test cases. The answer occurs when :

$$|H_n - H_s| \leq 0.0001|H_s|$$

Fifty iterations are allotted to obtain an answer. In general, less than ten iterations were used with this technique.

FLASH CALCULATION (L/F specified) - This routine is initiated with a bubble-point calculation, where L/F = 1.0. Assuming constant temperature, each succeeding pressure is found through the following empirical relationship:

3-14 $$P_{n+1} = P_n\{1.0 + [(L/F)_s - (L/F)_n]/D\}$$

$$D = \begin{cases} 55|(L/F)_s - (L/F)_n| & |(L/F)_s - (L/F)_n| \geq 0.04 \\ 1.5 & |(L/F)_s - (L/F)_n| < 0.04 \end{cases}$$

Under the new conditions, a constant T, constant P flash calculation is accomplished. This gives a new liquid fraction ratio. Equation 3-14 is then applied and the cycle continues until:

$$|(L/F)_s - (L/F)_n| \leq 0.0001$$

Due to its slow convergence, this subroutine is extremely reliable.

<u>FLASH CALCULATION</u> (L/F specified for one component) - A semi-random search technique is used to perform this flash calculation. Due to the excessive amount of computer time required for this routine, only two trials were performed. In both cases, the actual mole fraction for the specified was within $2x10^{-4}$, and the actual temperature or pressure was exact.

SECTION IV

INPUT - OUTPUT

For most programs, four input cards define the problem. A fifth card is required for the flash calculation with the liquid fraction specified for a single component. The four (or five) cards, in order, will contain the following data:

CARD	COLUMN	FORMAT	DATA
1	1-76	19A4	Statement of problem
2	1-2(RJ)*	I2	Number of new components
	4-5(RJ)	I2	Total number of components
	9-10(RJ)	I2	Type calculation (see Appendix F)
	14-15(RJ)	I2	Unit code (see Appendix G)
	20	I1	Use "2" if L/F or H to be specified is from the previous problem. Otherwise, use "1".
	21-28	F8.2	Temperature
	29-36	F8.2	Pressure
	37-50	F14.2	Specified enthalpy
	51-60	F10.4	Specified liquid fraction

* RJ indicates that the data is to be right justified.

CARD	COLUMN	FORMAT	DATA
3	1-3(RJ)	I3	First component number (see Appendix B)
	4-6(RJ)	I3	Second component number
	7-9(RJ)	I3	Third component number
	. . .		
	73-75(RJ)	I3	Twenty-fifth component number
4	1-10	F10.4	Feed rate first component
	11-20	F10.4	Feed rate second component
	. . .		
	71-80	F10.4	Feed rate eighth component
5	3-4(RJ)	I2	Specified component (use a "1" if it's the first component on card 3, etc.)
	6-14	F9.4	Specified liquid fraction

Remember that card 5 is only used with the option of L/F specified for one component.

Due to space allocation, there is a maximum of 25 components allowed. If there are more than eight components in

the system, a second card for feed rates (card 4) may be used. All problems will have a temperature and pressure as input. In general, however, one will be the given condition, while the other will be the initial trial.

The program has a built-in check as to when all of the data has been read. The last card to be run, behind all of the data, will be an end-of-file card. This card will have a one (1) in column 77. This will terminate the program.

As mentioned before, the program can generate data for components not included in Appendix B. To do this, the program requires an additional data card for each new component. This set of data cards is inserted after card 2. The format of this card is as follows:

COLUMN	FORMAT	DATA
1-20	5A4	Name of component
21	I1	If the component is a non-hydrocarbon use "1". Leave blank for hydrocarbons.
22-28	F7.3	Molecular weight
29-35	F7.4	Specific gravity
36-45	F10.3	Boiling point (°R)
46-55	F10.3	Critical temperature (°R)

COLUMN	FORMAT	DATA
56-65	F10.3	Critical pressure (psia)
66-72	F7.4	Critical compressibility factor

The number of cards inserted here will be the same number that appears on columns 1-2, card 2. After these cards are read in, card 3 follows. These new components will be numbered consecutively and begin with 41. These numbers are required on card 3. Figures 1 and 2 give an example of the data input. Figure 3 contains a listing that shows the several forms of data that may be used.

Figure 4 gives a sample of the output for each problem. The first line is a machine created statement as to the type of calculation. The second line is a problem statement and the data printed here is found on card 1. Next comes the temperature and pressure of the final result, each of which is in four units. Equilibrium data follows, and some of the more important physical properties are next. On flash calculations, the liquid to vapor and the liquid to feed ratios are included. It should be noted that the enthalpy of the feed is the sum of the total enthalpies of both phases; its units

are therefore BTU's, and not BTU/lb. mole. The enthalpy printed out is the actual enthalpy divided by 1000. This is done in order to conserve space.

As mentioned before, all of the routines converge slowly. As a result, if a bad guess is given on the data card, convergence may not readily take place. If this occurs, use the result printed out as your new guess and rerun the problem. This will work on bubble-point and dew-point calculations only.

There is, however, one minor flaw inherent with this equation. If the density of both phases approaches each other (within 5%), the equation will not be able to differentiate between the two phases. As a result, all of the K-values will be close to 1.0 and therefore give erroneous results. This does not occur often, but will occasionally happen near the critical point. If this problem is detected, the program recalculates the problem, but this time it computes equilibrium constants via equation 3-1 instead of through the BWR expression. Although the BWR equation could not be used, this approximate solution is fairly reliable and is therefore given to the user. A remark will appear on the print-out, stating that the ideal K-value equation was used and the results were not obtained via the BWR Equation of State.

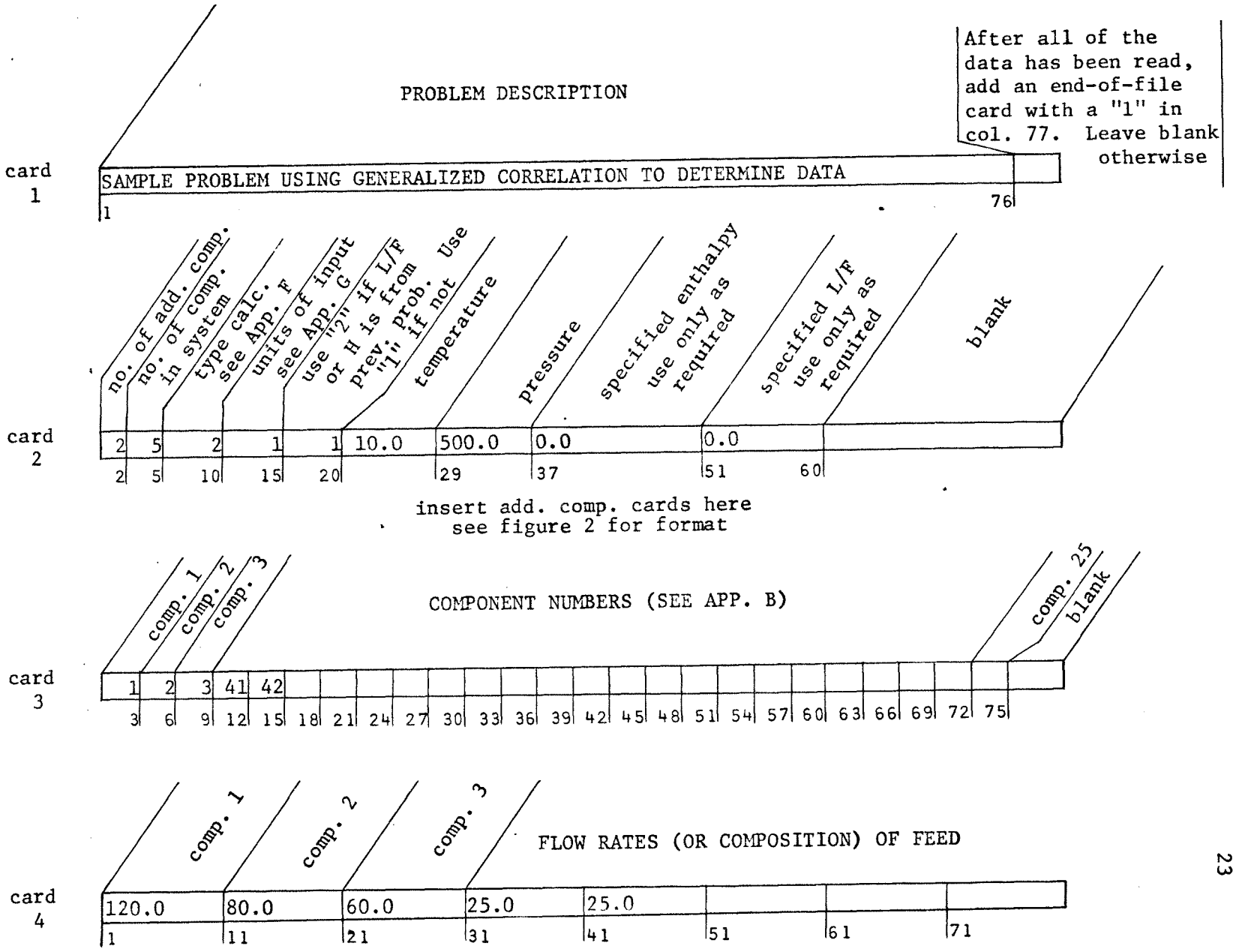

Figure 1

Main Input Cards

component name	"1" is a nonhydrocarbon leave blank otherwise	molecular weight	specific gravity	boiling point	critical temp.	critical press.	critical compressibility factor	blank
ACETYLENE.....		26.04	0.2304	345.2	527.0	906.0	0.274	
AMMONIA.....	1	17.06	0.235	431.5	722.0	1638.0	0.242	
1 20		22	29	36	46	56	66 72	

insert these cards
between cards 2 & 3

	specified comp. (use a "1" if it's the first comp. on card 3, etc)	specified liquid fraction for component	blank
card 5	4	.3697	
	4	14	

Figure 2

Additional Input Cards

```
BUBBLE POINT CALCULATION USING THE FIRST 20 COMPONENTS
   20     1     1     1 -100.0    500.0
  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20
100.0      25.0       10.0       10.0       7.5        7.5        6.0        5.0
2.0        2.0        1.0        1.0        50.0       15.0       8.0        5.0
30.0       1.0        3.0        4.0

SAMPLE PROBLEM USING GENERALIZED CORRELATION TO DETERMINE DATA
 2  5     2     1     1 10.0      500.0
AMMONIA.............117.06  0.235  431.5      722.0      1638.0     0.242
ACETYLENE........... 26.04  0.2304 345.2      527.0      906.0      0.274
  1  2  3 41 42
120.0      80.0       50.0       25.0       25.0

CONSTANT PRESSURE CHECK OF ENTHALPY SPECIFIED ROUTINE
    4     7     1     1 100.0     1000.0     -734800.0
  1  2  3  5
40.0       10.0       20.0       30.0

CONSTANT PRESSURE CHECK OF L/F SUBROUTINE
    4     9     1     1 100.0     1000.0                0.8558
  1  2  3  5
40.0       10.0       20.0       30.0

CONSTANT PRESSURE TEST OF L/F SPEC ROUTINE FOR 1 COMPONENT
    4    11     1     1 100.0     1000.0
  1  2  3  5
40.0       10.0       20.0       30.0
   4 .3697

INSERT THIS CARD LAST TO INDICATE THE END OF FILE                          1
```

Figure 3

Samples of Input

BUBBLE POINT CALCULATION, P SPEC., T VARIABLE.

PROBLEM = SAMPLE PROBLEM USING GENERALIZED CORRELATION TO DETERMINE DATA

THE CALCULATED TEMPERATURE IS -84.01 DEG. F, THE SPECIFIED PRESSURE IS 500.00 PSIA.
-64.28 DEG. C 25.86 M. HG.
375.99 DEG. R 34.02 ATM.
208.88 DEG. K 1017.96 IN. HG.

COMP.	FEED		LIQUID		VAPOR		K
	MOLES	FRAC.	MOLES	FRAC.	MOLES	FRAC.	
METHANE.....	120.0000	.4000	120.0000	.4000	0.0000	.9113	2.2782
ETHANE.....	80.0000	.2667	80.0000	.2667	0.0000	.0505	.1893
PROPANE.....	50.0000	.1667	50.0000	.1667	0.0000	.0045	.0270
AMMONIA.....	25.0000	.0833	25.0000	.0833	0.0000	.0008	.0096
ACETYLENE.....	25.0000	.0833	25.0000	.0833	0.0000	.0330	.3960
TOTAL MOLES	300.0000		300.0000		0.0000		
DENSITY (LB. MOLES/CU. FT.)			1.1579		.1696		
DENSITY (LB/CU. FT.)			29.3827		2.9182		
MOLECULAR WEIGHT			25.376		17.206		
ENTHALPY (KBTU/LB. MOLE)	31561.093		105.204		30.689		

Figure 4

Sample of Output

SECTION V

GENERAL DISCUSSION AND CONCLUSION

For the components included in the program, the BWR equation gives excellent results over a wide range of conditions, as verified by experimental P-V-T data. It can also give fairly reliable results when using the generalized correlation for new components. Tests in the cryogenic region[1] have also proven the equation to be reliable. It has been shown by Chao-Seader[6] to be somewhat better than their own correlation under reasonable conditions, and superior under extreme conditions. There are, however, several areas in the equation where future studies may improve its accuracy.

The main area for study is, of course, the constants themselves. As experimental equipment becomes more refined, many more components will have P-V-T data available. Also, a wider range of P-V-T data can be used to obtain better BWR constants. Once the new constants are obtained, they may be tested to predict phase equilibrium. The best set of BWR constants could then be used to evaluate the phase conditions under study.

Another area for study is the variation of the constants with temperature or pressure. Zudkevitch[12] gives an expression

for C_o as a function of temperature for ten components. Barner and Adler[1] utilize this expression for low temperature enthalpy calculations. Studies are also under way to determine γ as a function of temperature.[1] The program could be modified to include these temperature variations for low temperature applications. However, due to the incomplete work on this subject, it was not included in the present program.

Another topic of study is the mixing rules. The rules used in the program are those suggested by Benedict, Et Al.[5] Studies using this program can be accomplished by simply changing the appropriate cards in subroutine "MIX". The results could then be compared to experimental results to determine the best set of rules. Different sets of rules can also be found in the literature.

In conclusion, it must be said that the BWR equation is probably the most accurate equation of state covering an extremely wide range of conditions. One advantage is the interdependency of the particular components in the mixture. Equations have been made available to establish equilibrium constants, which can be applied to bubble-point, dew-point, and various flash calculations. The program is easy to use, as well as easy to adapt into other programs.

SECTION VI

PROGRAM LISTING

The following program is compatible with the FORTRAN compiler of the Control Data Corporation digital computer, CDC 6600. In addition to the previously mentioned Format designation of implied H or Hollerith conversion, the only other unique statement is the program name designation found on card BWR 1. Variable data set references are used for input and output; these being preset via cards BWR 397 and BWR 398.

The program deck contains the main program as well as the pure component data cards. The user must supply three items in order to use the program. First, proper control cards must preceed the deck. Second, the appropriate control card should follow the last card in the program. This card is the last statement in the program and therefore requires the control card to set it apart from the data. Third, following the data cards for the forty components, input data is supplied as per Section IV. The program is now ready for use.

```
      PROGRAM BWR(INPUT,OUTPUT,TAPE5=INPUT,TAPE6=OUTPUT)                BWR   1
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR   2
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR   3
      NSYS=1                                                            BWR   4
      CALL INPUT                                                        BWR   5
5     IF  (NSYS .NE. 1) CALL DATA                                       BWR   6
      NSYS=NSYS+1                                                       BWR   7
      GO TO 5                                                           BWR   8
10    STOP                                                              BWR   9
      END                                                               BWR  10
```

```
      SUBROUTINE BUBLPT (INDEX,NF)                                      BWR  11
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR  12
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR  13
      COMMON /CODE/ KODE                                                BWR  14
99    FORMAT (* *** E R R O R *** THE RESULTS ARE VIA THE IDEAL K VALUES BWR  15
     1.*)                                                               BWR  16
100   FORMAT(*0NO CONVERGENCE IN BUBBLE POINT ROUTINE.*)                BWR  17
      SUM=0.0                                                           BWR  18
      PSI=1.0                                                           BWR  19
      DO 5 IDO=1,NCP                                                    BWR  20
      I=IDO                                                             BWR  21
5     SUM=SUM+P(I,1)                                                    BWR  22
      KE=1                                                              BWR  23
      GO TO 20                                                          BWR  24
6     KE=2                                                              BWR  25
20    DO 25 IDO=1,NCP                                                   BWR  26
      I=IDO                                                             BWR  27
      X(I)=P(I,1)/SUM                                                   BWR  28
      CALL EQK1(I)                                                      BWR  29
25    Y(I)=X(I)*EQK(I)                                                  BWR  30
      DO 55 LIMIT=1,99                                                  BWR  31
      GO TO (31,32),KE                                                  BWR  32
31    CALL KNUM                                                         BWR  33
      GO TO 30                                                          BWR  34
32    DO 34 I=1,NCP                                                     BWR  35
34    CALL EQK1 (I)                                                     BWR  36
30    SUMY=0.0                                                          BWR  37
      DO 35 IDO=1,NCP                                                   BWR  38
      I=IDO                                                             BWR  39
      Y(I)=X(I)*EQK(I)                                                  BWR  40
35    SUMY=SUMY+Y(I)                                                    BWR  41
      CHECK=ABS(SUMY-1.0)                                               BWR  42
      TERM1=SUMY-1.0                                                    BWR  43
      BLOCK=4.0                                                         BWR  44
      IF (CHECK .GT. 0.050) BLOCK= 50.0*CHECK+0.250/CHECK               BWR  45
      TERM2=TERM1/BLOCK                                                 BWR  46
      SUMY=1.0+TERM2                                                    BWR  47
      IF (CHECK .LT. 0.0001) GO TO 60                                   BWR  48
      GO TO (40,45), INDEX                                              BWR  49
40    P1=P1*SUMY                                                        BWR  50
```

```
      GO TO 55                                                          BWR  51
45    T1=T1/SUMY                                                        BWR  52
55    CONTINUE                                                          BWR  53
      GO TO (56,57), INDEX                                              BWR  54
56    P1=P1/SUMY                                                        BWR  55
      GO TO 60                                                          BWR  56
57    T1=T1*SUMY                                                        BWR  57
60    DO 65 IDO=1,NCP                                                   BWR  58
      I=IDO                                                             BWR  59
      P(I,2)=X(I)*SUM*PSI                                               BWR  60
65    P(I,3)=Y(I)*SUM*(1.0-PSI)                                         BWR  61
      P(29,1)=PSI                                                       BWR  62
      P(30,1)=SUM                                                       BWR  63
      P(30,2)=SUM*PSI                                                   BWR  64
      P(30,3)=SUM*(1.0-PSI)                                             BWR  65
      IF (KE .EQ. 2) GO TO 70                                           BWR  66
      IF (ABS(RHOL-RHOV) .LT. 0.050) GO TO 6                            BWR  67
70    IF (NF .GE. 3) GO TO 75                                           BWR  68
      KODE=INDEX                                                        BWR  69
      CALL TYPE                                                         BWR  70
      IF (NF .NE. 3 .AND. LIMIT .GE. 99) WRITE (NOUT,100)               BWR  71
      CALL PRINT                                                        BWR  72
75    CONTINUE                                                          BWR  73
      CALL HMIX (NF)                                                    BWR  74
      IF (KE .EQ. 2 .AND. NF .NE. 3) WRITE (NOUT,99)                    BWR  75
      RETURN                                                            BWR  76
      END                                                               BWR  77
```

```
      SUBROUTINE DEWPT (INDEX,NF)                                       BWR  78
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR  79
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR  80
      COMMON /CODE/ KODE                                                BWR  81
99    FORMAT (* *** E R R O R *** THE RESULTS ARE VIA THE IDEAL K VALUES BWR  82
     1.*)                                                               BWR  83
100   FORMAT (////,*0NO CONVERGENCE IN THE DEW POINT SUBROUTINE.*)      BWR  84
      PSI=0.0                                                           BWR  85
      SUM=0.0                                                           BWR  86
      DO 5 IDO=1,NCP                                                    BWR  87
      J=IDO                                                             BWR  88
5     SUM=SUM+P(J,1)                                                    BWR  89
      KE=1                                                              BWR  90
      GO TO 30                                                          BWR  91
6     KE=2                                                              BWR  92
30    DO 15 IDO=1,NCP                                                   BWR  93
      I=IDO                                                             BWR  94
      Y(I)=P(I,1)/SUM                                                   BWR  95
      CALL EQK1 (I)                                                     BWR  96
      IF (EQK(I) .LE. 1.0E-15) EQK(I)=1.0E-15                           BWR  97
15    X(I)=Y(I)/EQK(I)                                                  BWR  98
      DO 55 LIMIT=1,99                                                  BWR  99
      GO TO (31,32),KE                                                  BWR 100
31    CALL KNUM                                                         BWR 101
      GO TO 33                                                          BWR 102
32    DO 34 I=1,NCP                                                     BWR 103
34    CALL EQK1 (I)                                                     BWR 104
33    SUMX=0.0                                                          BWR 105
      DO 35 IDO=1,NCP                                                   BWR 106
      I=IDO                                                             BWR 107
      IF (EQK(I) .LE. 1.0E-15) EQK(I)=1.0E-15                           BWR 108
      X(I)=Y(I)/EQK(I)                                                  BWR 109
35    SUMX=SUMX+X(I)                                                    BWR 110
      CHECK=ABS(SUMX-1.0)                                               BWR 111
      TERM1=SUMX-1.0                                                    BWR 112
      BLOCK=4.0                                                         BWR 113
      IF (CHECK .GT. 0.050) BLOCK= 50.0*CHECK+0.250/CHECK               BWR 114
      TERM2=TERM1/BLOCK                                                 BWR 115
      SUMX=1.0+TERM2                                                    BWR 116
      IF (CHECK .LT. 0.0001) GO TO 60                                   BWR 117
```

```
      GO TO (40,45),INDEX                                               BWR 118
40    P1=P1/SUMX                                                        BWR 119
      GO TO 55                                                          BWR 120
45    T1=T1*SUMX                                                        BWR 121
55    CONTINUE                                                          BWR 122
      GO TO (56,57), INDEX                                              BWR 123
56    P1=P1*SUMX                                                        BWR 124
      GO TO 60                                                          BWR 125
57    T1=T1/SUMX                                                        BWR 126
60    DO 65 IDO=1,NCP                                                   BWR 127
      I=IDO                                                             BWR 128
      P(I,2)=X(I)*SUM*PSI                                               BWR 129
65    P(I,3)=Y(I)*SUM*(1.0-PSI)                                         BWR 130
      P(29,1)=PSI                                                       BWR 131
      P(30,1)=SUM                                                       BWR 132
      P(30,2)=SUM*PSI                                                   BWR 133
      P(30,3)=SUM*(1.0-PSI)                                             BWR 134
      IF (KE .EQ. 2) GO TO 70                                           BWR 135
      IF (ABS(RHOL-RHOV) .LT. 0.050) GO TO 6                            BWR 136
70    IF (NF .GE. 3) GO TO 75                                           BWR 137
      KODE=INDEX+2                                                      BWR 138
      CALL TYPE                                                         BWR 139
      IF (NF .NE. 3 .AND. LIMIT .GE. 99) WRITE (NOUT,100)               BWR 140
      CALL PRINT                                                        BWR 141
75    CONTINUE                                                          BWR 142
      CALL HMIX (NF)                                                    BWR 143
      IF (KE .EQ. 2 .AND. NF .NE. 3) WRITE (NOUT,99)                    BWR 144
      RETURN                                                            BWR 145
      END                                                               BWR 146
```

```
      SUBROUTINE FLASH1 (NF)                                            BWR 147
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 148
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 149
      COMMON /CODE/ KODE                                                BWR 150
      DIMENSION F(25)                                                   BWR 151
99    FORMAT(* *** E R R O R *** THE RESULTS ARE VIA THE IDEAL K VALUES. BWR 152
     1 *)                                                               BWR 153
100   FORMAT(* NO CONVERGENCE IN T,P SPEC FLASH CALCULATION.*)          BWR 154
200   FORMAT(*0      L/F = *,F8.4,*        L/V = *,F8.4)               BWR 155
500   FORMAT(////,*0THE GIVEN CONDITIONS ARE OUT OF THE 2-PHASE REGION.* BWR 156
     1,//,* THE BUBBLE POINT AND DEW POINT CALCULATIONS ARE PROVIDED FOR BWR 157
     2 REFERENCE.*)                                                     BWR 158
      LL=0                                                              BWR 159
      PSI=1.00                                                          BWR 160
      SUM=0.0                                                           BWR 161
      DO 5 IDO=1,NCP                                                    BWR 162
      I=IDO                                                             BWR 163
      SUM=SUM+P(I,1)                                                    BWR 164
5     CONTINUE                                                          BWR 165
8     KE=1                                                              BWR 166
      LL=LL+1                                                           BWR 167
      GO TO 7                                                           BWR 168
6     KE=2                                                              BWR 169
7     DO 10 IDO=1,NCP                                                   BWR 170
      I=IDO                                                             BWR 171
      F(I)=P(I,1)/SUM                                                   BWR 172
      CALL EQK1 (I)                                                     BWR 173
      IF (EQK(I) .EQ. 0.0) EQK(I)=0.000001                              BWR 174
      VAL=1.0-1.0/EQK(I)                                                BWR 175
      Y(I)=F(I)/(1.0-PSI*VAL)                                           BWR 176
10    X(I)=Y(I)/EQK(I)                                                  BWR 177
      DO 25 LIMIT=1,75                                                  BWR 178
      GO TO (31,32),KE                                                  BWR 179
31    CALL KNUM                                                         BWR 180
      GO TO 33                                                          BWR 181
32    DO 34 I=1,NCP                                                     BWR 182
34    CALL EQK1 (I)                                                     BWR 183
33    SUMY=0.0                                                          BWR 184
      SUMP=0.0                                                          BWR 185
      DO 20 IDO=1,NCP                                                   BWR 186
```

```
      I=IDO                                                             BWR 187
      IF (EQK(I) .LT. 0.000001) EQK(I)=0.000001                         BWR 188
      VAL=1.0-(1.0/EQK(I))                                              BWR 189
      Y(I)=F(I)/(1.0-PSI*VAL)                                           BWR 190
      X(I)=Y(I)/EQK(I)                                                  BWR 191
      TERM=1.0-PSI*VAL                                                  BWR 192
      IF ((TERM .LT. -1.0E 25) .OR. (TERM .GT. 1.0E 25)) TERM=1.0E 25   BWR 193
      SUMP=SUMP+F(I)*VAL/(TERM**2)                                      BWR 194
20    SUMY=SUMY+Y(I)                                                    BWR 195
      PSIP=PSI-(SUMY-1.0)/SUMP                                          BWR 196
      CHECK=ABS(PSIP-PSI)                                               BWR 197
      IF (CHECK .LT. 0.00010) GO TO 30                                  BWR 198
      PSI=PSIP                                                          BWR 199
25    CONTINUE                                                          BWR 200
30    DO 35 IDO=1,NCP                                                   BWR 201
      I=IDO                                                             BWR 202
      P(I,2)=X(I)*SUM*PSI                                               BWR 203
35    P(I,3)=Y(I)*SUM*(1.0-PSI)                                         BWR 204
      P(30,1)=SUM                                                       BWR 205
      P(30,2)=SUM*PSI                                                   BWR 206
      P(30,3)=SUM*(1.0-PSI)                                             BWR 207
      P(29,1)=PSI                                                       BWR 208
      IF (KE .EQ. 2) GO TO 70                                           BWR 209
      IF (ABS(RHOL-RHOV) .LT. 0.050) GO TO 6                            BWR 210
      TP=T1                                                             BWR 211
      IF((PSI .LT. 0.0) .OR. (PSI .GT. 1.0)) GO TO 50                   BWR 212
      GO TO 70                                                          BWR 213
50    IF (LL .GE. 2) GO TO 70                                           BWR 214
      CALL BUBLPT (2,3)                                                 BWR 215
      TB=T1                                                             BWR 216
      CALL DEWPT  (2,3)                                                 BWR 217
      TD=T1                                                             BWR 218
      IF (TP .LT. TB .OR. TP .GT. TD) GO TO 70                          BWR 219
      PSI=(TP-TD)/(TB-TD)                                               BWR 220
      T1=TP                                                             BWR 221
      IF (LL .EQ. 1) GO TO 8                                            BWR 222
70    IF (NF .GE. 3) GO TO 75                                           BWR 223
      CALL TYPE                                                         BWR 224
      IF (NF .LE. 2 .AND. LIMIT .GE. 75) WRITE (NOUT,100)               BWR 225
      CALL PRINT                                                        BWR 226
```

```
      IF((PSI .LT. 0.0) .OR. (PSI .GT. 1.0)) GO TO 40                   BWR 227
75    CONTINUE                                                          BWR 228
      CALL HMIX (NF)                                                    BWR 229
      ABCD=PSI/(1.-PSI)                                                 BWR 230
      IF (NF .LE. 2) WRITE (NOUT,200) PSI,ABCD                          BWR 231
      IF (KE .EQ. 2 .AND. NF .LE. 2) WRITE (NOUT,99)                    BWR 232
      RETURN                                                            BWR 233
40    IF (NF .LE.2) WRITE (NOUT,500)                                    BWR 234
      CALL BUBLPT (2,1)                                                 BWR 235
      CALL DEWPT (2,1)                                                  BWR 236
      RETURN                                                            BWR 237
      END                                                               BWR 238
```

```
      SUBROUTINE FLASH2 (INDEX,NN)                                      BWR 239
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 240
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 241
      COMMON /CODE/ KODE                                                BWR 242
100   FORMAT(*0NO CONVERGENCE IN ENTHALPY SPEC SUBROUTINE*)             BWR 243
200   FORMAT(*0      L/F = *,F7.4,*          L/V = *,F7.4)             BWR 244
300   FORMAT(*0THE SPECIFIED ENTHALPY IS OUT OF THE TWO PHASE REGION.*, BWR 245
     1/,* THE BUBBLE  POINT AND DEW POINT CALCULATIONS ARE PROVIDED FOR  BWR 246
     2 YOUR REFERENCE.*)                                                BWR 247
      H=P(28,2)                                                         BWR 248
      IF (NN .EQ. 2) H=P(28,1)                                          BWR 249
      SUM=0.0                                                           BWR 250
      DO 1 JK=1,NCP                                                     BWR 251
1     SUM=SUM+P(JK,1)                                                   BWR 252
      CALL BUBLPT (INDEX,3)                                             BWR 253
      HB=P(28,1)                                                        BWR 254
      TB=T1                                                             BWR 255
      PB=P1                                                             BWR 256
      IF (HB .GT. H) GO TO 50                                           BWR 257
      CALL DEWPT (INDEX,3)                                              BWR 258
      TD=T1                                                             BWR 259
      PD=P1                                                             BWR 260
      HD=P(28,1)                                                        BWR 261
      IF (HD .LT. H) GO TO 50                                           BWR 262
      PT=(H-HB)/(HD-HB)                                                 BWR 263
      START=PT*(PB-PD)                                                  BWR 264
      BEGIN=PT*(TD-TB)                                                  BWR 265
      GO TO (5,10),INDEX                                                BWR 266
5     P1=PB-START                                                       BWR 267
      GO TO 15                                                          BWR 268
10    T1=TB+BEGIN                                                       BWR 269
15    DO 30 LIMIT=1,75                                                  BWR 270
      CALL FLASH1 (3)                                                   BWR 271
      TERM1=ABS(P(28,1)-H)                                              BWR 272
      TERM2=ABS(0.000150*H)                                             BWR 273
      IF (TERM1 .LT. TERM2) GO TO 35                                    BWR 274
      TERM5=ABS(HD)+ABS(HB)                                             BWR 275
      TERM6=P(28,1)-H                                                   BWR 276
      TERM7=TERM6/TERM5                                                 BWR 277
18    GO TO (19,24),INDEX                                               BWR 278
```

```
19    TERM7=TERM7/3.0                                          BWR 279
20    P1=P1*(1.0+TERM7)                                        BWR 280
      IF (P1 .GT. PB) P1=PB-1.0                                BWR 281
      IF (P1 .LT. PD) P1=PD+1.0                                BWR 282
      GO TO 30                                                 BWR 283
24    TERM7=TERM7/20.0                                         BWR 284
25    T1=T1*(1.0-TERM7)                                        BWR 285
      IF (T1 .GT. TD) T1=TD-1.0                                BWR 286
      IF (T1 .LT. TB) T1=TB+1.0                                BWR 287
30    CONTINUE                                                 BWR 288
35    CALL TYPE                                                BWR 289
      IF (LIMIT .GE. 75) WRITE (NOUT,100)                      BWR 290
      CALL PRINT                                               BWR 291
      CALL HMIX (2)                                            BWR 292
      ABCD=P(29,1)/(1.0-P(29,1))                               BWR 293
      WRITE (NOUT,200) P(29,1),ABCD                            BWR 294
      RETURN                                                   BWR 295
50    WRITE (NOUT,300)                                         BWR 296
      CALL BUBLPT (INDEX,1)                                    BWR 297
      CALL DEWPT (INDEX,1)                                     BWR 298
      RETURN                                                   BWR 299
      END                                                      BWR 300
```

```
      SUBROUTINE FLASH3 (INDEX,NF)                                      BWR 301
      COMMON /CODE/ KODE                                                BWR 302
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 303
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 304
100   FORMAT(* NO CONVERGENCE IN L/F SPEC SUBROUTINE*)                  BWR 305
      COMMON /SPEC/ LSPEC,FSPEC                                         BWR 306
      FRAC=P(29,2)                                                      BWR 307
200   FORMAT(*0       L/F = *,F8.4,*          L/V = *,F8.4)             BWR 308
      IF (NF .EQ. 2) FRAC=P(29,1)                                       BWR 309
      GO TO (5,10),INDEX                                                BWR 310
5     CALL BUBLPT (1,3)                                                 BWR 311
      GO TO 15                                                          BWR 312
10    CALL BUBLPT(2,3)                                                  BWR 313
15    DO 20 LIMIT=1,50                                                  BWR 314
      IF (ABS(P(29,1)-FRAC) .LT. 0.0001) GO TO 25                       BWR 315
      TERM=P(29,1)-FRAC                                                 BWR 316
      BLOCK=1.50                                                        BWR 317
      IF (ABS(TERM) .GE. 0.04) BLOCK=55.0*ABS(TERM)                     BWR 318
      GO TO (16,17),INDEX                                               BWR 319
16    P1=P1-TERM*P1/BLOCK                                               BWR 320
      GO TO 18                                                          BWR 321
17    T1=T1+TERM*T1/BLOCK                                               BWR 322
18    CALL FLASH1 (3)                                                   BWR 323
      IF (NF .NE. 4) GO TO 20                                           BWR 324
      IF (ABS(X(LSPEC)-FSPEC) .LE. 0.0001) RETURN                       BWR 325
20    CONTINUE                                                          BWR 326
25    SUM=0.0                                                           BWR 327
      FRAC=P(29,1)                                                      BWR 328
      DO 30 IDO=1,NCP                                                   BWR 329
30    SUM=SUM+P(IDO,1)                                                  BWR 330
      DO 35 I=1,NCP                                                     BWR 331
      P(I,2)=X(I)*SUM*FRAC                                              BWR 332
35    P(I,3)=Y(I)*SUM*(1.0-FRAC)                                        BWR 333
      P(30,1)=SUM                                                       BWR 334
      P(30,2)=SUM*FRAC                                                  BWR 335
      P(30,3)=SUM*(1.0-FRAC)                                            BWR 336
70    IF (NF .GE. 3) GO TO 75                                           BWR 337
      CALL TYPE                                                         BWR 338
      IF (NF .NE. 3 .AND. LIMIT .GE. 50) WRITE (NOUT,100)               BWR 339
      CALL PRINT                                                        BWR 340
```

```
      CALL HMIX (NF)                                                    BWR 341
      ABCD=FRAC/(1.0-FRAC)                                              BWR 342
      WRITE (NOUT,200) FRAC,ABCD                                        BWR 343
75    CONTINUE                                                          BWR 344
      RETURN                                                            BWR 345
      END                                                               BWR 346
```

```
      SUBROUTINE FLASH5 (INDEX,NF)                                      BWR 347
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 348
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 349
      COMMON /CODE/ KODE                                                BWR 350
      COMMON /SPEC/ LSPEC,FSPEC                                         BWR 351
200   FORMAT(*0       L/F = *,F8.4,*            L/V = *,F8.4)           BWR 352
1000  FORMAT (I4,F10.4)                                                 BWR 353
1050  FORMAT(* THE LIQUID FRACTION FOR *,5A4,* WAS SPECIFIED AT *,F5.4, BWR 354
     1 /////)                                                           BWR 355
      READ (NIN,1000) LSPEC,FSPEC                                       BWR 356
      PSI=1.0                                                           BWR 357
      P(29,2)=1.0                                                       BWR 358
      K=KOMP(LSPEC)                                                     BWR 359
      DO 50 I=1,3                                                       BWR 360
      PSI=0.10*PSI                                                      BWR 361
5     P(29,2)=P(29,2)-PSI                                               BWR 362
      CALL FLASH3 (INDEX,4)                                             BWR 363
      IF (ABS(X(LSPEC)-FSPEC) .LE. 0.0001) GO TO 55                     BWR 364
      IF (EQK(LSPEC) .GE. 1.0) GO TO 20                                 BWR 365
      IF (X(LSPEC) .LT. FSPEC) GO TO 5                                  BWR 366
      P(29,2)=P(29,2)+PSI                                               BWR 367
      GO TO 50                                                          BWR 368
20    IF (X(LSPEC) .GT. FSPEC) GO TO 5                                  BWR 369
      P(29,2)=P(29,2)+PSI                                               BWR 370
50    CONTINUE                                                          BWR 371
55    CONTINUE                                                          BWR 372
      P(29,2)=P(29,2)-PSI                                               BWR 373
      KODE=INDEX+9                                                      BWR 374
      CALL TYPE                                                         BWR 375
      WRITE (NOUT,1050) (PCP(J,K),J=1,5),FSPEC                          BWR 376
      CALL PRINT                                                        BWR 377
      CALL HMIX (3)                                                     BWR 378
      ABCD=P(29,1)/(1.0-P(29,1))                                        BWR 379
      WRITE (NOUT,200) P(29,1),ABCD                                     BWR 380
      RETURN                                                            BWR 381
      END                                                               BWR 382
```

```
      SUBROUTINE INPUT                                                  BWR 383
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 384
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 385
      COMMON /SYSTEM/ SYS(19)                                           BWR 386
      COMMON /CODE/ KODE                                                BWR 387
8     FORMAT(19A4,I4)                                                   BWR 388
9     FORMAT (25I3)                                                     BWR 389
10    FORMAT(5A4,I3,3F8.2,2F6.4,F10.2,F11.2/I3,2X,F10.5,F10.6,2E15.8,   BWR 390
     1 2F10.5/I3,4E15.8)                                                BWR 391
11    FORMAT(I2,I3,3I5,2F8.2,F14.2,F10.4)                               BWR 392
12    FORMAT(8F10.4)                                                    BWR 393
13    FORMAT (*1THERE IS AN ERROR IN THE PURE COMPONENT DECK.*,/,*0THE P BWR 394
     1ROGRAM HAS BEEN TERMINATED. PLEASE CHECK THE INPUT AND RERUN.*)   BWR 395
      NCPT=40                                                           BWR 396
      NIN=5                                                             BWR 397
      NOUT=6                                                            BWR 398
      KKK=1                                                             BWR 399
      DO 16 I=1,NCPT                                                    BWR 400
      READ (NIN,10)  (PCP(J,I),J=1,5),KX,(PCP(J,I),J=6,12),KY,(PCP      BWR 401
     1(J,I),J=13,18),KZ,(PCP(J,I),J=19,22)                              BWR 402
      IF (KX .NE. KY) KKK=2                                             BWR 403
      IF (KY .NE. KZ) KKK=2                                             BWR 404
      IF (KZ .NE.  I) KKK=2                                             BWR 405
      GO TO (16,17),KKK                                                 BWR 406
17    WRITE (NOUT,13)                                                   BWR 407
      CALL EXIT                                                         BWR 408
16    CONTINUE                                                          BWR 409
      ENTRY DATA                                                        BWR 410
      READ (NIN,8) (SYS(KK),KK=1,19),KODE                               BWR 411
      IF (KODE .GT. 0) CALL EXIT                                        BWR 412
      READ (NIN,11) NC,NCP,KODE,IUNIT,NF,T1,P1,H,FRAC                   BWR 413
      P(29,2)=FRAC                                                      BWR 414
      P(28,2)=H                                                         BWR 415
      IF (NC .GT. 0) CALL NEW (NC)                                      BWR 416
      IF (IUNIT .LE. 4) GO TO 60                                        BWR 417
      IF (IUNIT .LE. 8) GO TO 65                                        BWR 418
      IF (IUNIT .GE. 13) GO TO 70                                       BWR 419
      GO TO 75                                                          BWR 420
60    T1=T1+460.0                                                       BWR 421
      GO TO 75                                                          BWR 422
```

```
65    T1=T1+273.16                                                    BWR 423
70    T1=T1*1.80                                                      BWR 424
75    GO TO (15,77,78,79,15,77,78,79,15,77,78,79,15,77,78,79),IUNIT   BWR 425
77    P1=P1*14.696/760.0                                              BWR 426
      GO TO 15                                                        BWR 427
78    P1=P1*14.696                                                    BWR 428
      GO TO 15                                                        BWR 429
79    P1=P1*14.696/29.92                                              BWR 430
15    CONTINUE                                                        BWR 431
      READ (NIN,9) (KOMP(I),I=1,NCP)                                  BWR 432
      READ (NIN,12) (P(I,1),I=1,NCP)                                  BWR 433
C   A 1 AFTER THE SUBROUTINE TITLE INDICATES CONSTANT TEMP.           BWR 434
18    IF (KODE .EQ. 1) CALL BUBLPT (1,NF)                             BWR 435
      IF (KODE .EQ. 2) CALL BUBLPT (2,NF)                             BWR 436
      IF (KODE .EQ. 3) CALL DEWPT (1,NF)                              BWR 437
      IF (KODE .EQ. 4) CALL DEWPT (2,NF)                              BWR 438
      IF (KODE .EQ. 5) CALL FLASH1 (NF)                               BWR 439
      IF (KODE .EQ. 6) CALL FLASH2 (1,NF)                             BWR 440
      IF (KODE .EQ. 7) CALL FLASH2 (2,NF)                             BWR 441
      IF (KODE .EQ. 8) CALL FLASH3 (1,NF)                             BWR 442
      IF (KODE .EQ. 9) CALL FLASH3 (2,NF)                             BWR 443
      IF (KODE .EQ. 10) CALL FLASH5 (1,NF)                            BWR 444
      IF (KODE .EQ. 11) CALL FLASH5 (2,NF)                            BWR 445
      RETURN                                                          BWR 446
      END                                                             BWR 447
```

```
      SUBROUTINE PRINT                                                  BWR 448
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 449
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 450
      COMMON /SYSTEM/ SYS(19)                                           BWR 451
      COMMON /CODE/ KODE                                                BWR 452
50    FORMAT(*    PROBLEM = *,19A4,/////)                               BWR 453
100   FORMAT(*      THE GIVEN TEMPERATURE IS *,F7.2,* DEG. F ,     THE G BWR 454
     1IVEN PRESSURE IS *,F7.2,* PSIA.*)                                 BWR 455
101   FORMAT(*  THE SPECIFIED TEMPERATURE IS *,F7.2,* DEG. F, THE CALCUL BWR 456
     1ATED PRESSURE IS *,F7.2,* PSIA.*)                                 BWR 457
102   FORMAT(* THE CALCULATED TEMPERATURE IS *,F7.2,* DEG. F,  THE SPECI BWR 458
     1FIED PRESSURE IS *,F7.2,* PSIA.*)                                 BWR 459
105   FORMAT(31X,F7.2,* DEG. C*,28X,F8.2,* M. HG.*)                     BWR 460
110   FORMAT(31X,F7.2,* DEG. R*,28X,F8.2,* ATM.*)                       BWR 461
115   FORMAT(31X,F7.2,* DEG. K*,28X,F8.2,* IN. HG.*,///)                BWR 462
150   FORMAT(*0    COMP.*,23X,*FEED*,15X,*LIQUID*,15X,*VAPOR*,12X,*K*)  BWR 463
175   FORMAT(25X,3(3X,*MOLES*,4X,*FRAC.*,3X))                           BWR 464
200   FORMAT(* *,5A4,2X,8F10.4)                                         BWR 465
300   FORMAT(* TOTAL MOLES*,19X,F10.4,10X,F10.4,10X,F10.4)              BWR 466
350   FORMAT(*0DENSITY (LB/CU. FT.)*,30X,F10.4,10X,F10.4)               BWR 467
400   FORMAT(*0MOLECULAR WEIGHT *,33X,F10.3,10X,F10.3)                  BWR 468
450   FORMAT(*0DENSITY (LB. MOLES/CU. FT.)*,23X,F10.4,10X,F10.4)        BWR 469
      CALL LDENS                                                        BWR 470
      CALL VDENS                                                        BWR 471
      P(26,1)=T1-460.0                                                  BWR 472
      P(27,1)=P1                                                        BWR 473
      WRITE (NOUT,50) (SYS(KK),KK=1,19)                                 BWR 474
      KKK=1                                                             BWR 475
      IF (KODE .EQ. 2 .OR. KODE .EQ. 4) KKK=2                           BWR 476
      IF (KODE .EQ. 7 .OR. KODE .EQ. 9) KKK=2                           BWR 477
      IF (KODE .EQ. 11) KKK=2                                           BWR 478
      IF (KODE .EQ. 05) KKK=3                                           BWR 479
      GO TO (5,10,15),KKK                                               BWR 480
5     WRITE (NOUT,101) P(26,1),P(27,1)                                  BWR 481
      GO TO 20                                                          BWR 482
10    WRITE (NOUT,102) P(26,1),P(27,1)                                  BWR 483
      GO TO 20                                                          BWR 484
15    WRITE (NOUT,100) P(26,1),P(27,1)                                  BWR 485
20    A=(T1/1.80)-273.16                                                BWR 486
      B=P1*0.760/14.696                                                 BWR 487
```

```
      WRITE (NOUT,105) A,B                                              BWR 488
      A=T1                                                              BWR 489
      B=P1/14.696                                                       BWR 490
      WRITE (NOUT,110) A,B                                              BWR 491
      A=T1/1.80                                                         BWR 492
      B=P1*29.92/14.696                                                 BWR 493
      WRITE (NOUT,115) A,B                                              BWR 494
      WRITE (NOUT,150)                                                  BWR 495
      WRITE (NOUT,175)                                                  BWR 496
      WTL=0.0                                                           BWR 497
      WTV=0.0                                                           BWR 498
      DO 250 IDO=1,NCP                                                  BWR 499
      I=KOMP(IDO)                                                       BWR 500
      K=IDO                                                             BWR 501
      WTL=WTL+X(K)*PCP(6,I)                                             BWR 502
      WTV=WTV+Y(K)*PCP(6,I)                                             BWR 503
      F=P(K,1)/P(30,1)                                                  BWR 504
      WRITE (NOUT,200) (PCP(J,I),J=1,5),P(K,1),F,P(K,2),X(K),P(K,3),Y(K) BWR 505
     1,EQK(K)                                                           BWR 506
250   CONTINUE                                                          BWR 507
      WRITE (NOUT,300) P(30,1),P(30,2),P(30,3)                          BWR 508
      DL=RHOL*WTL                                                       BWR 509
      DV=RHOV*WTV                                                       BWR 510
      WRITE (NOUT,450) RHOL,RHOV                                        BWR 511
      WRITE (NOUT,350) DL,DV                                            BWR 512
      WRITE (NOUT,400) WTL,WTV                                          BWR 513
      RETURN                                                            BWR 514
      END                                                               BWR 515
```

```
      SUBROJTINE NEW (NC)                                               BWR 516
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 517
      DIMENSION A(22)                                                   BWR 518
100   FORMAT(5A4,I1,F7.3,F7.4,3F10.3,F7.4)                              BWR 519
      KX=41                                                             BWR 520
      R=0.08205                                                         BWR 521
      DO 10 I=1,NC                                                      BWR 522
      READ (NIN,100) (A(J),J=1,5),NH,A(6),SG,BP,TC,PC,ZC                BWR 523
      A(7)=TC                                                           BWR 524
      A(8)=PC                                                           BWR 525
      TC=TC/1.8                                                         BWR 526
      BP=BP/1.8                                                         BWR 527
      PC=PC/14.696                                                      BWR 528
      R2=R**2                                                           BWR 529
      R3=R**3                                                           BWR 530
      TC2=TC**2                                                         BWR 531
      TC3=TC**3                                                         BWR 532
      TC4=TC**4                                                         BWR 533
      TC5=TC**5                                                         BWR 534
      PC2=PC**2                                                         BWR 535
      PC3=PC**3                                                         BWR 536
      A(9)=3.0*ALOG10(PC)/(TC/BP-1.0)                                   BWR 537
      A(9)=A(9)/7.0-1.0                                                 BWR 538
      A(10)=ZC                                                          BWR 539
      IF (NH .EQ. 1) GO TO 5                                            BWR 540
      A1=0.066190*R3*TC3/PC2                                            BWR 541
      A2=0.264883*R2*TC2/PC                                             BWR 542
      A3=0.046497*R2*TC2/PC2                                            BWR 543
      A4=0.128809*R*TC/PC                                               BWR 544
      A5=0.060965*R3*TC5/PC2                                            BWR 545
      A6=0.181312*R2*TC4/PC                                             BWR 546
      A7=0.001827*R3*TC3/PC3                                            BWR 547
      A8=0.042187*R2*TC2/PC2                                            BWR 548
      GO TO 15                                                          BWR 549
5     A1=0.020830*R3*TC3/PC2                                            BWR 550
      A2=0.284623*R2*TC2/PC                                             BWR 551
      A3=0.027364*R2*TC2/PC2                                            BWR 552
      A4=0.129426*R*TC/PC                                               BWR 553
      A5=0.023222*R3*TC5/PC2                                            BWR 554
      A6=0.157489*R2*TC4/PC                                             BWR 555
```

```
      A7=0.0019427*R3*TC3/PC3                                           BWR 556
      A8=0.052603*R2*TC2/PC2                                            BWR 557
15    A(11)=60407.28743*A1                                              BWR 558
      A(12)=3771.024259*A2                                              BWR 559
      A(13)=256.6019929*A3                                              BWR 560
      A(14)=16.01880282*A4                                              BWR 561
      A(15)=195719.4499*A5                                              BWR 562
      A(16)=12218.12140*A6                                              BWR 563
      A(17)=4110.454410*A7                                              BWR 564
      A(18)=256.6019929*A8                                              BWR 565
      U=(BP*1.80)**0.33333333/SG                                        BWR 566
      API=141.5/SG-131.5                                                BWR 567
      HI=188.25+(3.5442502-(5.2716944E-2-3.5353777E-4*API)*API)*API     BWR 568
     1 -(8.9530784-3.511858E-1*U)*U**2+(43.401618-5.9553889E-3*API)*U   BWR 569
      A(19)=A(6)*HI                                                     BWR 570
      HI=-0.8186204+(-2.8568654E-5+1.7024654E-6*API)*API-1.4886832E-8   BWR 571
     1 *API**3-3.0836492E-4*U**3+(8.8395563E-2+4.2934703E-3*U)*U        BWR 572
      A(20)=A(6)*HI                                                     BWR 573
      A(21)=A(6)*(3.1073165E-4-5.832381E-8*API)                         BWR 574
      A(22)=A(6)*(9.174501019E-11*API-5.6334748E-8)                     BWR 575
      DO 8 J=1,22                                                       BWR 576
8     PCP(J,KX)=A(J)                                                    BWR 577
10    KX=KX+1                                                           BWR 578
      RETURN                                                            BWR 579
      END                                                               BWR 580
```

```
      SUBROUTINE HMIX (NF)                                              BWR 581
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 582
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 583
100   FORMAT(*0ENTHALPY (KBTU/LB. MOLE)*,6X,3(-3PF10.3,10X))           BWR 584
      R=10.7335                                                         BWR 585
      SUML=0.0                                                          BWR 586
      SUMV=0.0                                                          BWR 587
      DO 5 IDO=1,NCP                                                    BWR 588
      I=KOMP(IDO)                                                       BWR 589
      H1=PCP(19,I)+(PCP(20,I)+(PCP(21,I)+(PCP(22,I)*T1)*T1)*T1)         BWR 590
      I=IDO                                                             BWR 591
      SUML=SUML+X(I)*H1                                                 BWR 592
5     SUMV=SUMV+Y(I)*H1                                                 BWR 593
      IF ((RHOL .NE. 0.0) .OR. (RHOV .NE. 0.0)) GO TO 15                BWR 594
      IF (RHOV .EQ. 0.0) GO TO 10                                       BWR 595
      P(28,2)=0.0                                                       BWR 596
      ISET=3                                                            BWR 597
      H0=SUMV                                                           BWR 598
      D=RHOV                                                            BWR 599
      CALL MIX (Y,A,A0,B,B0,C,C0,ALF,GAM)                               BWR 600
      GO TO 20                                                          BWR 601
10    P(28,3)=0.0                                                       BWR 602
      ISET=2                                                            BWR 603
      H0=SUML                                                           BWR 604
      D=RHOL                                                            BWR 605
      CALL MIX (X,A,A0,B,B0,C,C0,ALF,GAM)                               BWR 606
      GO TO 20                                                          BWR 607
15    CONTINUE                                                          BWR 608
      CALL MIX (X,A,A0,B,B0,C,C0,ALF,GAM)                               BWR 609
      H0=SUML                                                           BWR 610
      D=RHOL                                                            BWR 611
      DO 25 ISET=2,3                                                    BWR 612
20    T11=(B0*R*T1-2.0*A0-4.0*C0/(T1**2))*D                             BWR 613
      T22=((2.0*B*R*T1-3.0*A)/2.0)+6.0*ALF*A*(D**5)/5.0                 BWR 614
      GD2=GAM*D**2                                                      BWR 615
      IF (GD2 .EQ. 0.0) GD2=0.0000000001                                BWR 616
      T33=3.0*(1.0-EXP(-GD2))/GD2-(EXP(-GD2)/2.0)+GD2*EXP(-GD2)         BWR 617
      P(28,ISET)=H0+0.1850*(T11+T22+T33)                                BWR 618
      H0=SUMV                                                           BWR 619
      D=RHOV                                                            BWR 620
```

```
      CALL MIX (Y,A,A0,B,B0,C,C0,ALF,GAM)                                BWR 621
25    CONTINUE                                                           BWR 622
      IF (RHOL .EQ. 0.0) P(28,2)=0.0                                     BWR 623
      IF (RHOV .EQ. 0.0) P(28,3)=0.0                                     BWR 624
      P(28,1)=P(30,2)*P(28,2)+P(30,3)*P(28,3)                            BWR 625
      IF (NF .NE. 3) WRITE (NOUT,100) (P(28,I),I=1,3)                    BWR 626
      RETURN                                                             BWR 627
      END                                                                BWR 628
```

```
      SUBROUTINE KNUM                                                   BWR 629
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 630
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 631
      CALL LDENS                                                        BWR 632
      CALL VDENS                                                        BWR 633
15    DO 30 IDO=1,NCP                                                   BWR 634
      K=KOMP(IDO)                                                       BWR 635
      XVALUE=FUG(2,T1,RHOV,K)                                           BWR 636
      YVALUE=FUG(1,T1,RHOL,K)                                           BWR 637
      K=IDO                                                             BWR 638
      IF (XVALUE .EQ. 0.0) XVALUE=0.000001                              BWR 639
      EQK(K)=YVALUE/XVALUE                                              BWR 640
30    CONTINUE                                                          BWR 641
      RETURN                                                            BWR 642
      END                                                               BWR 643
```

```
      SUBROUTINE EQK1 (I)                                               BWR 644
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 645
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 646
      J=KOMP(I)                                                         BWR 647
      TR=T1/PCP(7,J)                                                    BWR 648
      PR=P1/PCP(8,J)                                                    BWR 649
      OMEGA=PCP(9,J)                                                    BWR 650
      CON=ALOG(10.0)                                                    BWR 651
      FP1=0.0                                                           BWR 652
      IF (J .EQ. 1) GO TO 5                                             BWR 653
      IF (J .EQ. 17) GO TO 10                                           BWR 654
      IF (J .EQ. 19) GO TO 11                                           BWR 655
      IF (J .EQ. 25) GO TO 12                                           BWR 656
      FP0=5.75748-3.01761/TR-4.98500*TR+2.02299*(TR**2)+(0.08427+0.26667 BWR 657
     1*TR-0.31138*(TR**2))*PR+(-0.02655+0.02883*TR)*(PR**2)-ALOG10(PR)  BWR 658
      FP1=8.65808*TR-4.23893-1.22050*TR**2-3.15224*TR**3-0.025*(PR-0.60) BWR 659
      GO TO 15                                                          BWR 660
5     FP0=2.43840-2.24550/TR-0.34084*TR+0.00212*(TR**2)-0.00223*(TR**3)+ BWR 661
     1(0.10486-0.03691*TR)*PR-ALOG10(PR)                                BWR 662
      GO TO 15                                                          BWR 663
10    FP0=2.7365534-1.9818310/TR-0.51487289*TR+0.042470988*(TR**2)-     BWR 664
     10.002814385*(TR**3)+(0.021495843*TR-0.029474696)*PR-ALOG10(PR)    BWR 665
      GO TO 15                                                          BWR 666
11    FP0=-30.060874+6.1409853/TR+45.263229*TR-27.303012*TR*TR+5.9152545 BWR 667
     1 *(TR**3)+(0.36838431-0.67916811*TR+0.15546365*(TR**2))*PR+       BWR 668
     2 0.089562849*TR*(PR**2)-ALOG10(PR)                                BWR 669
      GO TO 15                                                          BWR 670
12    FP0=3.0581210-2.6491906/TR+0.37457945*TR-1.14647096*(TR**2)+0.4573 BWR 671
     1 4766*(TR**3)+(1.4272646*TR-0.95721679-0.50242238*TR*TR)*PR+      BWR 672
     2 (0.33859029-0.26678483*TR)*(PR**2)-ALOG10(PR)                    BWR 673
15    FUNCKI=CON*(FP0+OMEGA*FP1)                                        BWR 674
      IF (FUNCKI .GE. 100.0) FUNCKI=100.0                               BWR 675
      EQK(I)=EXP(FUNCKI)                                                BWR 676
      RETURN                                                            BWR 677
      END                                                               BWR 678
```

```
      SUBROUTINE VDENS                                                  BWR 679
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 680
      R=10.7335                                                         BWR 681
      CALL MIX (Y,A,A0,B,B0,C,C0,ALPHA,GAMMA)                           BWR 682
      COR=0.010                                                         BWR 683
      D=0.0                                                             BWR 684
      DIFFE=10.0                                                        BWR 685
      ZZ=0.00000001                                                     BWR 686
101   IF (DIFFE-ZZ) 112,112,102                                         BWR 687
102   DO 106 J=1,200                                                    BWR 688
      D=D+COR                                                           BWR 689
      TERM1=(B0*R*T1-A0-C0/(T1**2))*D**2                                BWR 690
      TERM2=(B*R*T1-A)*(D**3)+A*ALPHA*(D**6)                            BWR 691
      TERM3=(C*(D**3)/(T1**2))*(1.0+GAMMA*(D**2))*EXP(-GAMMA*(D**2))    BWR 692
      F=R*T1*D+TERM1+TERM2+TERM3                                        BWR 693
      DIFE=P1-F                                                         BWR 694
      DIFFE=ABS(DIFE)                                                   BWR 695
103   IF (DIFE) 107,107,106                                             BWR 696
106   CONTINUE                                                          BWR 697
107   IF (COR-ZZ) 112,112,109                                           BWR 698
109   D=D-COR                                                           BWR 699
      COR=0.10*COR                                                      BWR 700
      GO TO 101                                                         BWR 701
112   RHOV=D                                                            BWR 702
      RETURN                                                            BWR 703
      END                                                               BWR 704
```

```
      SUBROUTINE LDENS                                                  BWR 705
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 706
      R=10.7335                                                         BWR 707
      CALL MIX (X,A,A0,B,B0,C,C0,ALPHA,GAMMA)                           BWR 708
      D=2.50                                                            BWR 709
      COR=0.10                                                          BWR 710
      DIFFE=10.0                                                        BWR 711
      ZZ=0.00000001                                                     BWR 712
300   IF (DIFFE-ZZ) 450,450,310                                         BWR 713
310   DO 350 J=1,400                                                    BWR 714
      D=D-COR                                                           BWR 715
      TERM1=(B0*R*T1-A0-C0/(T1**2))*D**2                                BWR 716
      TERM2=(B*R*T1-A)*(D**3)+A*ALPHA*(D**6)                            BWR 717
      TERM3=(C*(D**3)/(T1**2))*(1.0+GAMMA*(D**2))*EXP(-GAMMA*(D**2))    BWR 718
      F=R*T1*D+TERM1+TERM2+TERM3                                        BWR 719
      DIFE=P1-F                                                         BWR 720
      DIFFE=ABS(DIFE)                                                   BWR 721
320   IF (DIFE) 350,355,355                                             BWR 722
350   CONTINUE                                                          BWR 723
355   IF (COR-ZZ) 450,360,360                                           BWR 724
360   D=D+COR                                                           BWR 725
      COR=0.10*COR                                                      BWR 726
      GO TO 300                                                         BWR 727
450   RHOL=D                                                            BWR 728
      RETURN                                                            BWR 729
      END                                                               BWR 730
```

```
      SUBROUTINE MIX (R,A,A0,B,B0,C,C0,ALPHA,GAMMA)                     BWR 731
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 732
      DIMENSION D(8),R(25)                                              BWR 733
      DO 20 J=1,8                                                       BWR 734
20    D(J)=0.0                                                          BWR 735
      DO 11 IDO=1,NCP                                                   BWR 736
      I=KOMP(IDO)                                                       BWR 737
      J=IDO                                                             BWR 738
      IF (PCP(11,I) .LT. 0.0) GO TO 1                                   BWR 739
      D(1)=D(1)+R(J)*(PCP(11,I)**(1.0/3.0))                             BWR 740
      GO TO 2                                                           BWR 741
1     D(1)=D(1)-R(J)*((-PCP(11,I))**(1.0/3.0))                          BWR 742
2     IF (PCP(12,I) .LT. 0.0) GO TO 12                                  BWR 743
      D(2)=D(2)+R(J)*SQRT(PCP(12,I))                                    BWR 744
      GO TO 13                                                          BWR 745
12    D(2)=D(2)-R(J)*SQRT(-PCP(12,I))                                   BWR 746
13    IF (PCP(13,I) .LT. 0.0) GO TO 4                                   BWR 747
      D(3)=D(3)+R(J)*(PCP(13,I)**(1.0/3.0))                             BWR 748
      GO TO 5                                                           BWR 749
4     D(3)=D(3)-R(J)*((-PCP(13,I))**(1.0/3.0))                          BWR 750
5     D(4)=D(4)+R(J)*PCP(14,I)                                          BWR 751
      IF (PCP(15,I) .LT. 0.0)  GO TO 7                                  BWR 752
      D(5)=D(5)+R(J)*(PCP(15,I)**(1.0/3.0))                             BWR 753
      GO TO 8                                                           BWR 754
7     D(5)=D(5)-R(J)*((-PCP(15,I))**(1.0/3.0))                          BWR 755
8     IF (PCP(16,I) .LT. 0.0) GO TO 3                                   BWR 756
      D(6)=D(6)+R(J)*SQRT(PCP(16,I))                                    BWR 757
      GO TO 6                                                           BWR 758
3     D(6)=D(6)-R(J)*SQRT(-PCP(16,I))                                   BWR 759
6     IF (PCP(17,I) .LT. 0.0) GO TO 9                                   BWR 760
      D(7)=D(7)+R(J)*(PCP(17,I)**(1.0/3.0))                             BWR 761
      GO TO 10                                                          BWR 762
9     D(7)=D(7)-R(J)*((-PCP(17,I))**(1.0/3.0))                          BWR 763
10    IF (PCP(18,I) .LT. 0.0) GO TO 14                                  BWR 764
      D(8)=D(8)+R(J)*SQRT(PCP(18,I))                                    BWR 765
      GO TO 11                                                          BWR 766
14    D(8)=D(8)-R(J)*SQRT(-PCP(18,I))                                   BWR 767
11    CONTINUE                                                          BWR 768
      A=D(1)**3                                                         BWR 769
      A0=D(2)**2                                                        BWR 770
```

```
B=D(3)**3                                                    BWR 771
B0=D(4)                                                      BWR 772
C=D(5)**3                                                    BWR 773
C0=D(5)**2                                                   BWR 774
ALPHA=D(7)**3                                                BWR 775
GAMMA=D(8)**2                                                BWR 776
RETURN                                                       BWR 777
END                                                          BWR 778
```

```
      FUNCTION FUG(N,T,D,K)                                             BWR 779
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOJT,KOMP(25)                    BWR 780
      COMMON /EQUIL/ P(30,3),X(25),Y(25),EQK(25),T1,P1,RHOL,RHOV        BWR 781
      REAL U(25)                                                        BWR 782
      DO 3 IDO=1,NCP                                                    BWR 783
      I=IDO                                                             BWR 784
      GO TO (1,2),N                                                     BWR 785
1     U(I)=X(I)                                                         BWR 786
      GO TO 3                                                           BWR 787
2     U(I)=Y(I)                                                         BWR 788
3     CONTINUE                                                          BWR 789
      CALL MIX (U,A,A0,B,B0,C,C0,ALF,GAM)                               BWR 790
      R=10.7335                                                         BWR 791
      T11=R*T*ALOG(D*R*T)                                               BWR 792
      IF ((PCP(12,K) .LT. 0.0) .AND. (PCP(16,K) .LT. 0.0)) GO TO 6      BWR 793
      IF (PCP(12,K) .LT. 0.0) GO TO 8                                   BWR 794
      IF (PCP(16,K) .LT. 0.0) GO TO 10                                  BWR 795
      T22=(B0+PCP(14,K))*R*T-2.0*SQRT(A0*PCP(12,K))-2.0*SQRT(C0*PCP(16,K BWR 796
     1))/(T**2)                                                         BWR 797
      GO TO 15                                                          BWR 798
6     T22=(B0+PCP(14,K))*R*T+2.0*SQRT(-(A0*PCP(12,K)))+2.0*SQRT(-(C0*PCP BWR 799
     1(16,K)))/(T**2)                                                   BWR 800
      GO TO 15                                                          BWR 801
8     T22=(B0+PCP(14,K))*R*T+2.0*SQRT(-(A0*PCP(12,K)))-2.0*SQRT(+(C0*PCP BWR 802
     1(16,K)))/(T**2)                                                   BWR 803
      GO TO 15                                                          BWR 804
10    T22=(B0+PCP(14,K))*R*T-2.0*SQRT(+(A0*PCP(12,K)))+2.0*SQRT(-(C0*PCP BWR 805
     1(16,K)))/(T**2)                                                   BWR 806
15    T22=T22*D                                                         BWR 807
      T32=(A*A*PCP(11,K))**(1.0/3.0)                                    BWR 808
      T31=R*T*(B*B*PCP(13,K))**(1.0/3.0)                                BWR 809
      T33=1.500*(T31-T32)*D*D                                           BWR 810
      T41=A*(ALF*ALF*PCP(17,K))**(1.0/3.0)                              BWR 811
      T42=ALF*(A*A*PCP(11,K))**(1.0/3.0)                                BWR 812
      T44=0.60*(T41+T42)*D**5                                           BWR 813
      T51=3.0*(D**2)*(C*C*PCP(15,K))**(1.0/3.0)                         BWR 814
      GD=GAM*(D**2)                                                     BWR 815
      T52=(1.0-EXP(-GD))/GD                                             BWR 816
      T53=EXP(-GD)/2.0                                                  BWR 817
      T55=T51*(T52-T53)/(T**2)                                          BWR 818
```

```
T61=2.0*(D**2)*C*SQRT(PCP(18,K)/GAM)/(T**2)                    BWR 819
T62=T52-2.0*T53-GD*T53                                         BWR 820
T66=T61*T62                                                    BWR 821
GRAND=T11+T22+T33+T44+T55-T66                                  BWR 822
CON=GRAND/(R*T)                                                BWR 823
IF (CON .GT. 25.0) CON=25.0                                    BWR 824
IF (CON .LT. -25.0) CON=-25.0                                  BWR 825
FUG=EXP(CON)                                                   BWR 826
RETURN                                                         BWR 827
END                                                            BWR 828
```

```
      SUBROUTINE TYPE                                                   BWR 829
      COMMON /MAIN/ PCP(26,75),NCP,NIN,NOUT,KOMP(25)                    BWR 830
      COMMON /CODE/ KODE                                                BWR 831
1     FORMAT(*1BUBBLE POINT CALCULATION, T SPEC., P VARIABLE.*,////)    BWR 832
2     FORMAT(*1BUBBLE POINT CALCULATION, P SPEC., T VARIABLE.*,////)    BWR 833
3     FORMAT(*1DEW POINT CALCULATION, T SPEC., P VARIABLE.*,////)       BWR 834
4     FORMAT(*1DEW POINT CALCULATION, P SPEC., T VARIABLE.*,////)       BWR 835
5     FORMAT(*1FLASH CALCULATION, CONSTANT T AND P, L/F VARIABLE.*,////) BWR 836
6     FORMAT(*1ENTHALPY SPECIFIED, T CONSTANT, P VARIABLE.*,////)       BWR 837
7     FORMAT(*1ENTHALPY SPECIFIED, P CONSTANT, T VARIABLE.*,////)       BWR 838
8     FORMAT(*1LIQUID FRACTION SPECIFIED, T CONSTANT, P VARIABLE.*,////) BWR 839
9     FORMAT(*1LIQUID FRACTION SPECIFIED, P CONSTANT, T VARIABLE.*,////) BWR 840
10    FORMAT(*1L/F SPEC. FOR 1 COMPONENT, T CONSTANT, P VARIABLE.*,////) BWR 841
11    FORMAT(*1L/F SPEC. FOR 1 COMPONENT, P CONSTANT, T VARIABLE.*,////) BWR 842
      GO TO (14,15,16,17,18,19,20,21,22,23,24),KODE                     BWR 843
14    WRITE (NOUT,1)                                                    BWR 844
      RETURN                                                            BWR 845
15    WRITE (NOUT,2)                                                    BWR 846
      RETURN                                                            BWR 847
16    WRITE (NOUT,3)                                                    BWR 848
      RETURN                                                            BWR 849
17    WRITE (NOUT,4)                                                    BWR 850
      RETURN                                                            BWR 851
18    WRITE (NOUT,5)                                                    BWR 852
      RETURN                                                            BWR 853
19    WRITE (NOUT,6)                                                    BWR 854
      RETURN                                                            BWR 855
20    WRITE (NOUT,7)                                                    BWR 856
      RETURN                                                            BWR 857
21    WRITE (NOUT,8)                                                    BWR 858
      RETURN                                                            BWR 859
22    WRITE (NOUT,9)                                                    BWR 860
      RETURN                                                            BWR 861
23    WRITE (NOUT,10)                                                   BWR 862
      RETURN                                                            BWR 863
24    WRITE (NOUT,11)                                                   BWR 864
      RETURN                                                            BWR 865
      END                                                               BWR 866
```

```
METHANE............  1 16.04   343.9   673.1  .0104 .290  2984.12   6995.25
  1  0.86733   0.682401   0.49810600E+09 0.27576300E+09 0.51117  1.53961
  1  0.3683894E+04  0.7880800E+01  0.3505719E-02  0.2446272E-06
ETHANE............  2 30.07   550.0   709.80 .0986 .285  20850.2   15670.7
  2  2.85393   1.00554      0.541314E+10   0.219427E+10 1.00044  3.02790
  2  0.4220126E+04  0.1120242E+02  0.8938123E-02 -0.8065164E-06
PROPANE...........  3 44.10   665.9   617.4  .1524 .277  57248.0   25915.4
  3  5.77355   1.55884      0.252478E+11   0.620993E+10 2.49577  5.64524
  3  0.5068633E+04  0.1510799E+02  0.1540539E-01 -0.2938696E-05
ISO-BUTANE........  4 58.12   734.7   529.1  .1848 .252  117047.0  38587.4
  4  10.8890   2.20329      0.559777E+11   0.103847E+11 4.41496  8.72447
  4  0.6023067E+04  0.1999786E+02  0.2044134E-01 -0.4146112E-05
N-BUTANE..........  5 58.12   765.3   550.7  .2010 .274  113705.0  38029.6
  5  10.2635   1.99211      0.519256E+11   0.121305E+11 4.52693  8.72447
  5  0.6654675E+04  0.2054464E+02  0.1865250E-01 -0.3015783E-05
ISO-PENTANE.......  6 72.15   829.8   483.0  .2223 .268  226902.0  48253.6
  6  17.14409  2.56386      0.136025E+12   0.213367E+11 6.98777  11.8807
  6  0.7475543E+04  0.2465428E+02  0.2446248E-01 -0.4437345E-05
N-PENTANE.........  7 72.15   845.60  489.52 .2539 .269  246147.61 45928.81
  7  17.14409  2.510963   0.16130610E+12 0.25917201E+11  7.43992 12.18858
  7  0.8039759E+04  0.2518989E+02  0.2348587E-01 -0.4174458E-05
NEO-PENTANE.......  8 72.15   780.8   464.0  .1969 .269  210851.64 48885.67
  8  17.14409  2.731686   0.10586282E+12 0.15553609E+11 8.22091  12.83008
  8  0.6949269E+04  0.2517504E+02  0.2602791E-01 -0.5469282E-05
N-HEXANE..........  9 86.18   914.15  439.70 .3007 .264  429901.15 54443.41
  9  28.00323  2.848351   0.29607656E+12 0.40556221E+11 11.55391 17.11146
  9  0.9475028E+04  0.2952267E+02  0.2914070E-01 -0.5911897E-05
N-HEPTANE.........  10 100.21  972.31  396.94 .3498 .260  626106.43 66070.61
 10  38.99170  3.187742   0.48342704E+12 0.57984027E+11 17.9060  23.09415
 10  0.1056589E+05  0.3331526E+02  0.3278746E-01 -0.6696126E-05
N-NONANE..........  11 128.26  1071.29 330.66 .4455 .250  918974.23  105808.85
 11    56.17085  4.477023 9.70906116E+11 8.30756026E+10  76.71274  50.96414
 11  0.1366069E+05  0.4373618E+02  0.4301726E-01 -0.8954736E-05
N-DECANE..........  12 142.29  1114.49 305.68 .4885 .247  7558280.62-1350705.47
 12  504.73569 -99.628417 0.86594713E+09 0.16115702E+10 8.81524  0.0
 12  0.1505435E+05  0.4848591E+02  0.4756158E-01 -0.9858597E-05
ETHYLENE..........  13 28.05   509.5   742.1  .0868 .274  15645.5   12593.6
 13  2.20673   0.891980     0.413360E+10   0.160228E+10 0.73166  2.36844
 13  0.3791992E+04  0.9144806E+01  0.7819394E-02 -0.1522679E-05
PROPYLENE.........  14 42.08   657.2   667.0  .1405 .270  46758.6   23049.2
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 14  4.79997    1.362635    0.20083000E+11    0.536597E+10 1.87312   4.69325
 14  0.4714762E+04  0.1350214E+01  0.1146875E-01  0.1797251E-05
I-BUTYLENE........... 15 56.11    752.2    579.8  .1951 .277   102251.42 33762.92
 15  8.93375    1.858582    0.53307191E+11 0.11329620E+11 3.74417   7.59400
 15  0.5934714E+04  0.1768871E+01  0.1763632E-01 -0.3901157E-05
BENZENE............. 16 78.12    1012.70 714.23 .2125 .275   336468.59 24548.51
 16  19.66341  0.805755    0.23024788E+12 0.41907790E+11 2.87773   7.51843
 16  0.4739947E+04  0.1615755E+02  0.2238763E-01 -0.5355485E-05
NITROGEN............ 17 28.02    227.16   492.3  .0450 .291   1516.36    3937.31
 17  0.597292  0.652648    0.14256400E+09 0.98465700E+08 0.522851 1.35999
 17  0.3192124E+04  0.6956438E+01 -0.3103818E-04  0.2350028E-06
CARBON MONOXIDE..... 18 28.01    239.40   507.0  .093  .294   2213.93    5057.77
 18  0.67527    0.873706    0.20354823E+09 0.10461266E+09 0.55491   1.53961
 18  0.3194209E+04  0.6931740E+01  0.7073785E-04  0.2130755E-06
CARBON DIOXIDE...... 19 44.01    547.56   1071.3 .2310 .275   8248.97    9477.18
 19  1.05699   0.71847     0.29142500E+10 0.17993530E+10 0.34735   1.3824
 19  0.3357740E+04  0.8440110E+01  0.3040541E-02 -0.7897689E-06
SULFUR DIOXIDE...... 20 64.07    775.26   1143.3 .2402 .269   51024.83   7996.23
 20  3.75998    0.419404    0.22184800E 11 0.96992300E 10 0.29577   1.52001
 20  0.3814092E+04  0.9115251E+01  0.2601854E-02  0.5987696E-06
2-METHYL PENTANE.... 21 86.18    896.5    440.0  .2771 .269   448741.58 56301.39
 21  31.17714  2.769651    0.27400720E+12 0.34821646E+11 9.65957   15.90930
 21  0.8577085E+04  0.2888876E+02  0.3209773E-01 -0.7911907E-05
3-METHYL PENTANE.... 22 86.18    896.50   440.1  .2771 .273   360728.16 46017.81
 22  28.80101  1.305613    0.18702168E+12 0.27032594E+10 9.24852   16.13768
 22  0.9476357E+04  0.2956741E+02  0.2890806E-01 -0.5715327E-05
2,2-DIMETHYL BUTANE. 23 86.18    880.9    450.5  .2314 .275   610596.86 44656.47
 23  35.92428  3.077853    0.34217631E+12 0.41046779E+10 8.99778   14.4980
 23  0.8258419E+04  0.2852289E+02  0.3313681E-01 -0.8754726E-05
2,3-DIMETHYL BUTANE. 24 86.20    900.50   455.4  .2466 .297   283648.46 61957.9
 24  20.27156  3.043573    0.22206329E+12 0.31197751E+10 14.77626 19.24513
 24  0.8255574E+04  0.2871950E+02  0.3055211E-01 -0.6444594E-05
HYDROGEN SULFIDE.... 25    34.08   672.48 1306.47 .1056 .2840   14572.52    10558.02
 25      1.41858    .711476 6.06999398E+09 3.26823942E+09     .30788    1.28708
 25 4.99034290E+03-6.42019858E+00 1.06146650E-02-1.95910433E-06
1,3 BUTADIENE....... 26    54.09   765.00   527.52 .2000 .2710   92988.34    28445.96
 26      7.95727  1.685062 5.01240719E+10 1.13950438E+10    4.09023    7.21968
 26 9.56018001E+03 1.95587437E+01 1.65034901E-02-2.56896968E-06
1,2 BUTADIENE....... 27    54.09   802.80   646.62 .2264 .2680 101208.43    30400.98
 27      8.25290  1.716078 6.00795104E+10 1.34114246E+10    4.32027    7.48790
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 27 3.34896790E+03 1.85281791E+01 1.65376577E-02-2.62273205E-06
1-BUTENE............ 28   56.10  755.28  583.43 .1978 .2770 103524.44   29822.98
 28     8.97288  1.789369 5.43943546E+10 1.16450020E+10   4.89778   8.14115
 28 1.12034588E+04 2.12956161E+01 1.70906705E-02-2.62338664E-06
CYCLOPENTANE........ 29   70.13  921.24  654.71 .2031 .2700 149184.22   39538.80
 29    10.60101  1.944945 1.16517422E+11 2.29689728E+10   6.28958   9.61836
 29 9.71295969E+03 1.94732301E+01 2.15526056E-02-3.57479416E-06
CYCLOHEXANE......... 30   84.16  996.66  593.72 .2194 .2740 229709.16   51031.49
 30    15.08789  2.320321 2.10168358E+11 3.46980353E+10  10.67932  13.68933
 30 1.13650756E+04 2.24693202E+01 2.59050465E-02-4.35396423E-06
TOLUENE............. 31   92.13 1069.02  592.25 .2566 .2630 284870.42   58856.20
 31    17.44451  2.494957 2.99856853E+11 4.60401151E+10  13.27666  15.82750
 31 1.29778372E+04 1.87419963E+01 2.84563236E-02-4.92052956E-06
METHYL CYCLOHEXANE.. 32   98.18 1029.96  504.37 .2428 .2510 351290.56   64153.30
 32    22.32766  2.822640 3.43243367E+11 4.65835187E+10  19.22498  20.25802
 32 1.25869247E+04 2.85817530E+01 3.02069764E-02-5.05800364E-06
ETHYL BENZENE....... 33  106.16 1115.46  543.75 .3079 .2600 383935.71   69796.21
 33    22.53210  2.835532 4.40008916E+11 5.94446039E+10  19.48962  20.44351
 33 1.42753089E+04 2.33453177E+01 3.27909565E-02-5.67168702E-06
O-XYLENE............ 34  106.16 1136.70  524.65 .2989 .2600 436416.44   75118.88
 34    25.13347  2.994746 5.19383067E+11 6.64375118E+10  22.96041  22.80374
 34 1.42191924E+04 2.26289737E+01 3.28058846E-02-5.69516937E-06
M-XYLENE............ 35  106.16 1114.20  508.48 .3153 .2700 437559.60   74469.04
 35    25.70817  3.028792 5.00332244E+11 6.32811922E+10  23.75242  23.32518
 35 1.41606068E+04 2.38459175E+01 3.27874477E-02-5.66516767E-06
P-XYLENE............ 36  106.16 1112.40  498.19 .3069 .2500 453610.92   75761.37
 36    26.69437  3.086339 5.17011762E+11 6.41715246E+10  25.13220  24.21996
 36 1.41399513E+04 2.40931645E+01 3.27839145E-02-5.66060986E-06
3-ETHYL HEXANE...... 37  114.22 1020.60  387.97 .3612 .2640 577642.04   81890.36
 37    37.05104  3.636085 5.54197912E+11 5.83870407E+10  41.09619  33.61662
 37 1.37110924E+04 4.01665418E+01 3.50530927E-02-5.74450446E-06
N-PROPYL BENZENE.... 38  120.19 1149.66  459.98 .3432 .2570 587380.53   87643.57
 38    33.44624  3.454677 7.15077890E+11 7.92923852E+10  35.24698  30.34597
 38 1.54305020E+04 2.87512124E+01 3.71179406E-02-6.41081273E-06
CUMENE.............. 39  120.19 1144.80  455.58 .2925 .2600 591242.21   87745.15
 39    33.80905  3.473364 7.13706472E+11 7.87145332E+10  35.82205  30.67515
 39 1.56205094E+04 2.82427863E+01 3.71179406E-02-6.41081273E-06
N-OCTANE............ 40  114.22 1024.92  361.52 .3923 .2500 673751.35   88627.89
 40    43.03352  3.918657 6.51890338E+11 6.37269157E+10  51.44121  39.04456
 40 1.36759318E+04 4.20090869E+01 3.50269109E-02-5.70331988E-06
```

SECTION VII

TABLE OF NOMENCLATURE

a, A_o, b, B_o, c, C_o, α, γ	BWR constants
A	work content (BTU/lb. mole)
E	free energy (BTU/lb. mole)
f	fugacity (psia)
F	feed composition
H	enthalpy (BTU/lb. mole)
K	equilibrium constant
L/F	liquid fraction
N	total number of components
P	pressure (psia)
P_c	critical pressure (psia)
P_r	reduced pressure
R	universal gas constant
S	entropy
T	temperature (°R)
T_c	critical temperature (°R)
T_r	reduced temperature
x	mole fraction - liquid
y	mole fraction - vapor
ρ	density (lb. mole/ft.^{3})

SUBSCRIPTS

i	ith component
n	nth iteration
s	specified

SUPERSCRIPTS

°	ideal state
L	liquid
V	vapor
′	reduced coefficient

PROGRAM VARIABLES

EQK(I)	equilibrium constant for component I
KODE	code for problem type (ie, bubble, dew, etc.)
LIMIT	number of iteration in the subroutines
NC	number of new components added to program
NCP	number of components in system
NIN	reference tape number for input
NOUT	reference tape number for output
P(I,J)	component data in problem I = 1,25 number of moles of component I in (J=1, feed, J=2, liquid phase, J=3, vapor phase)

	I = 26	temperature
	I = 27	pressure
	I = 28	enthalpy
	I = 29	L/F ratio
	I = 30	total moles
P1	pressure in problem	
PCP(I,J)	pure component property of component J	
	I = 1,5	component name
	I = 6	molecular weight
	I = 7	critical temperature
	I = 8	critical pressure
	I = 9	Pitzers' Accentric Factor
	I = 10	critical compressibilty factor
	I = 11,18	BWR constants
	I = 19,22	constants for ideal enthalpy equation
PSI	liquid fraction	
RHOL	liquid density	
RHOV	vapor density	
SYS	problem definition	
T1	temperature in problem	
X(I)	mole fraction of component I in liquid	
Y(I)	mole fraction of component I in vapor	

SECTION VIII

APPENDICES

A. Flow diagrams

B. Acceptable Components

C. BWR Constants

D. Reduced BWR Constants

E. Constants for the Ideal K-value Equations

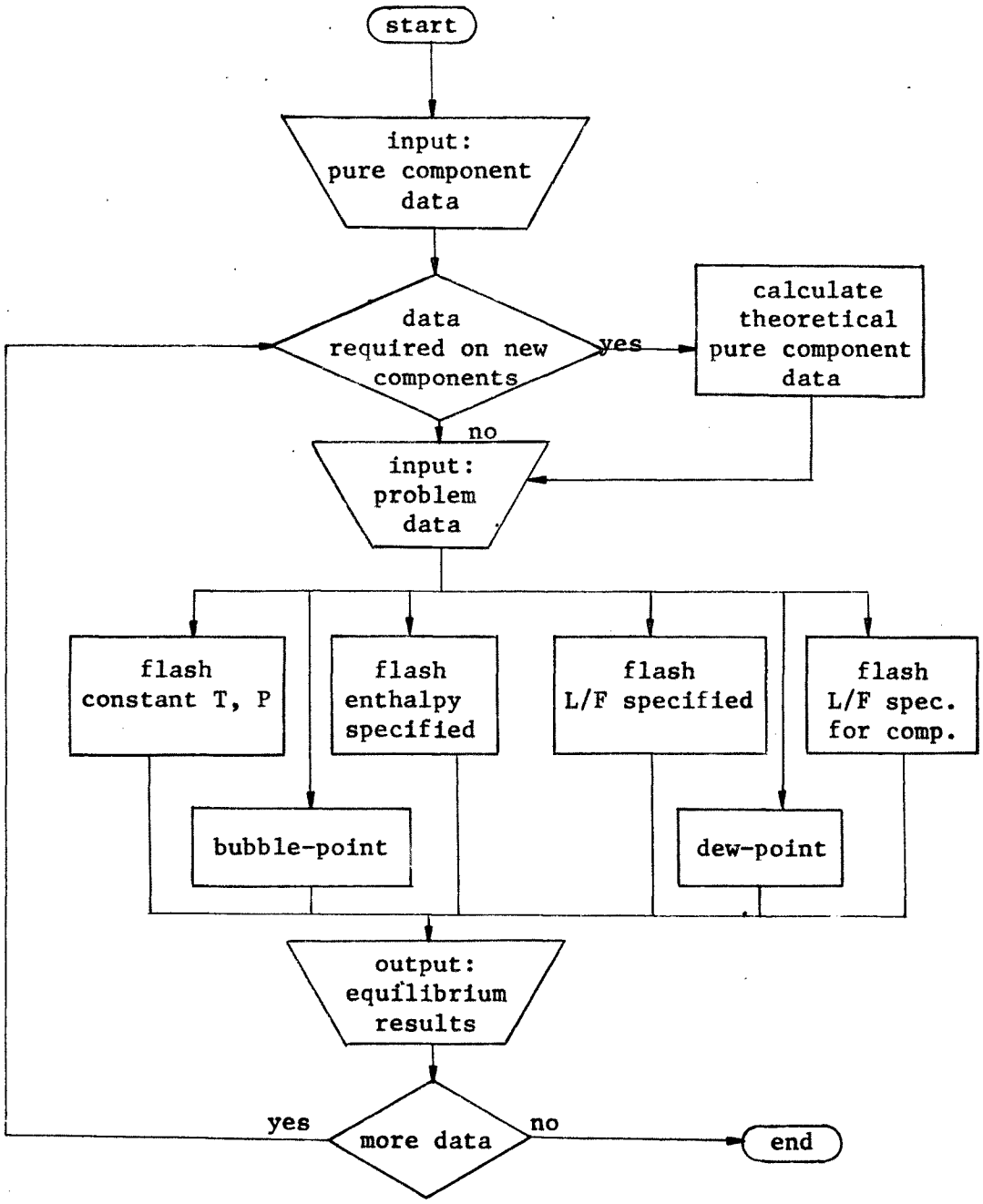
F. Types of Calculations

G. Units for Input

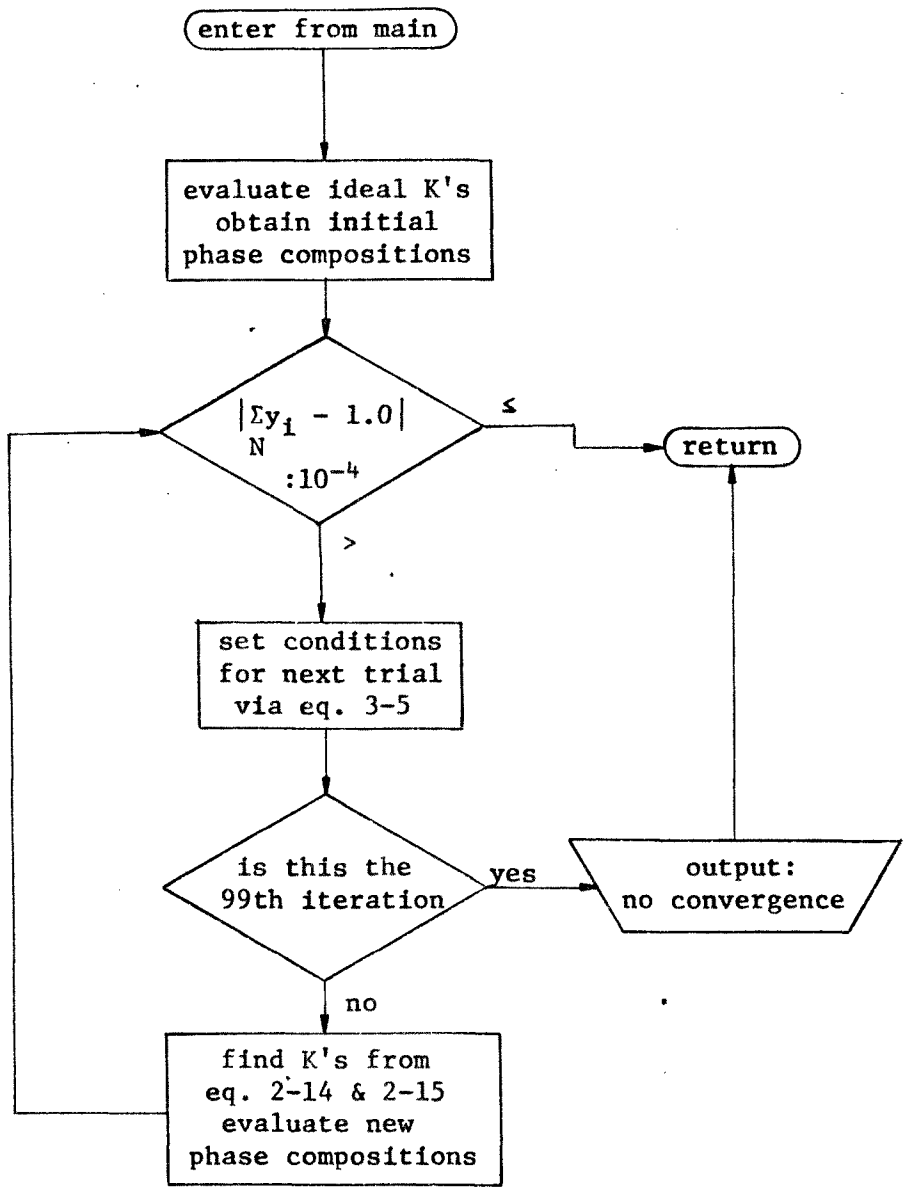
APPENDIX A

FLOW DIAGRAMS

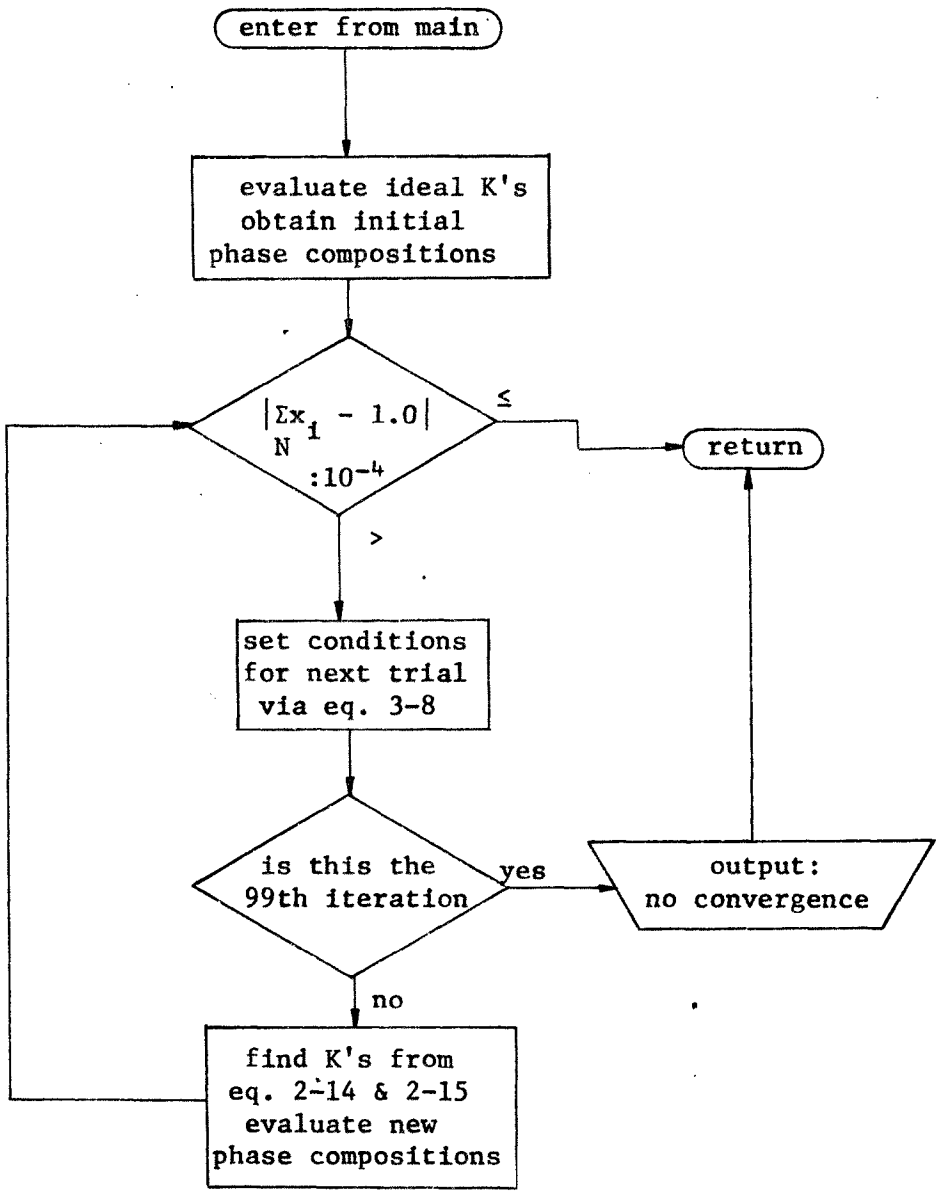
MAIN ROUTINE



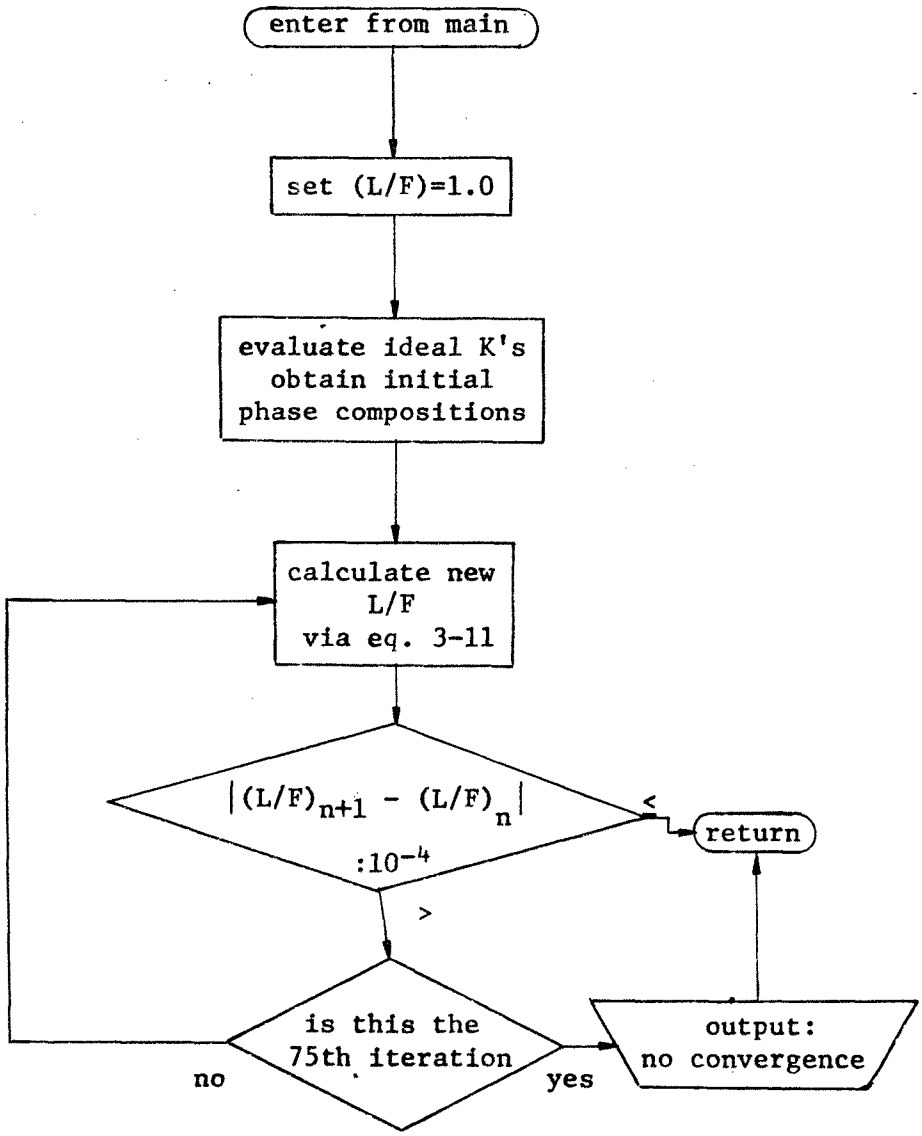
BUBBLE-POINT



DEW-POINT

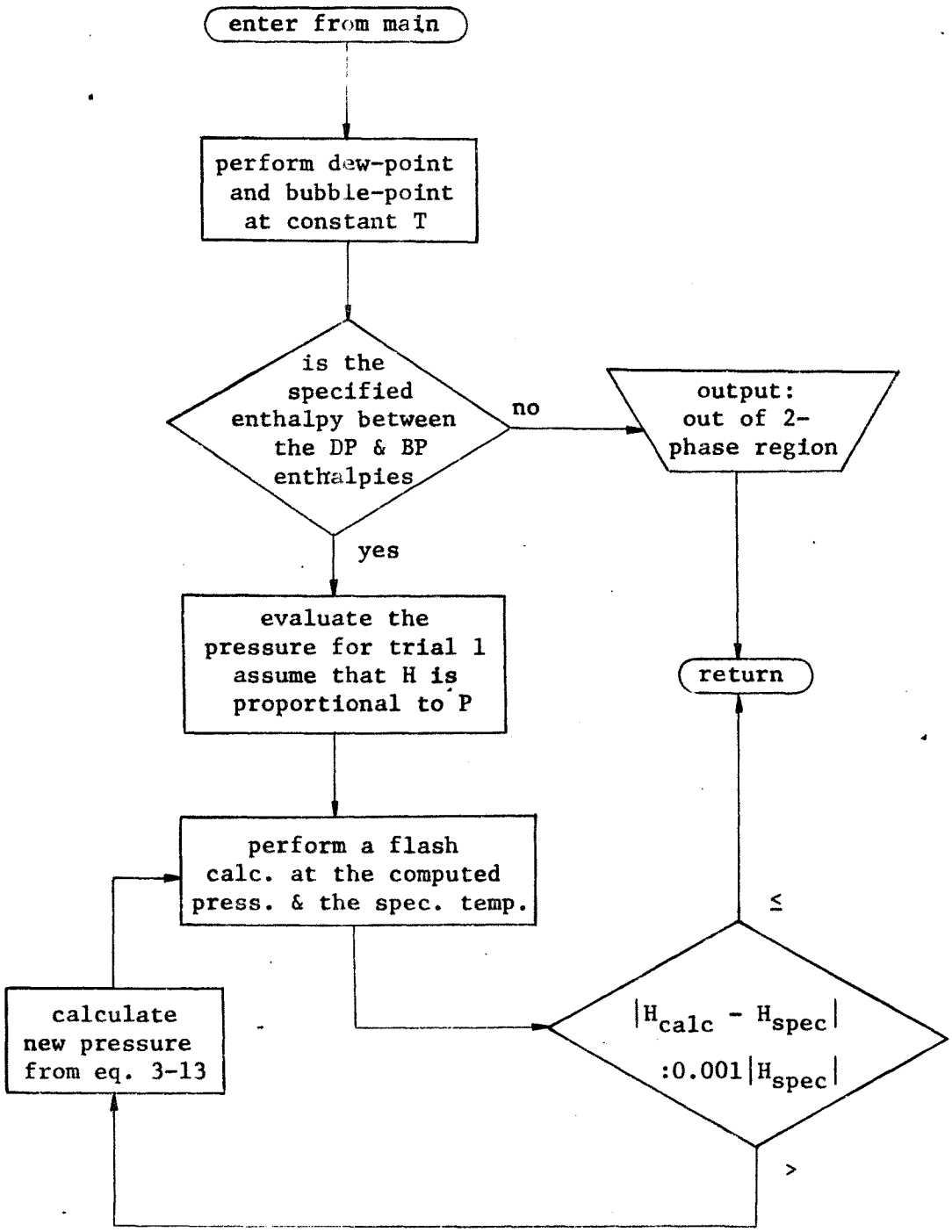

enter from main
evaluate ideal K's
obtain initial
phase compositions
$|\Sigma x_{N_i} - 1.0|$
$:10^{-4}$
≤
return
>
set conditions
for next trial
via eq. 3-8
is this the
99th iteration
yes
output:
no convergence
no
find K's from
eq. 2-14 & 2-15
evaluate new
phase compositions

FLASH - CONSTANT T,P

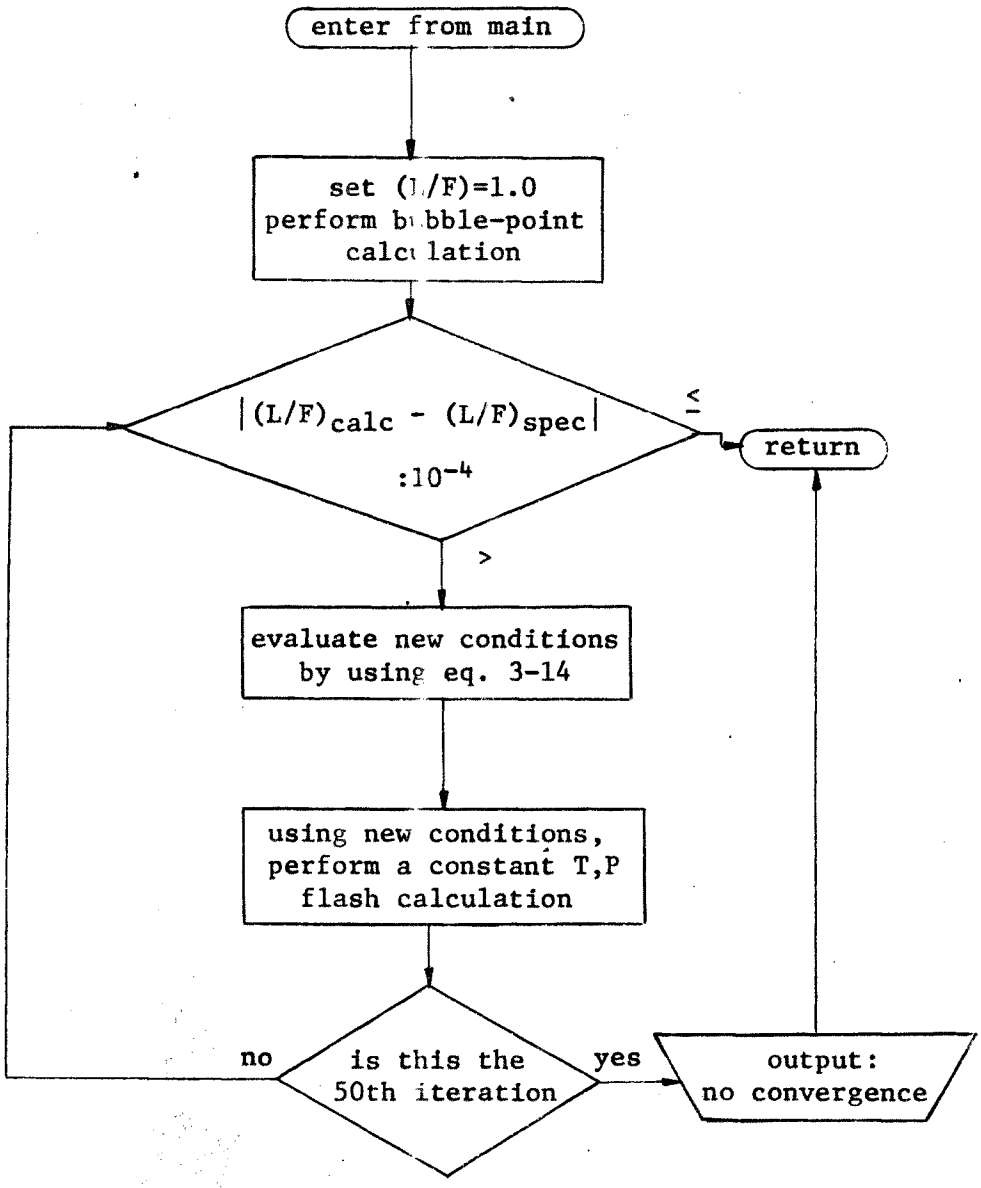


FLASH - ENTHALPY SPECIFIED

(for constant T)

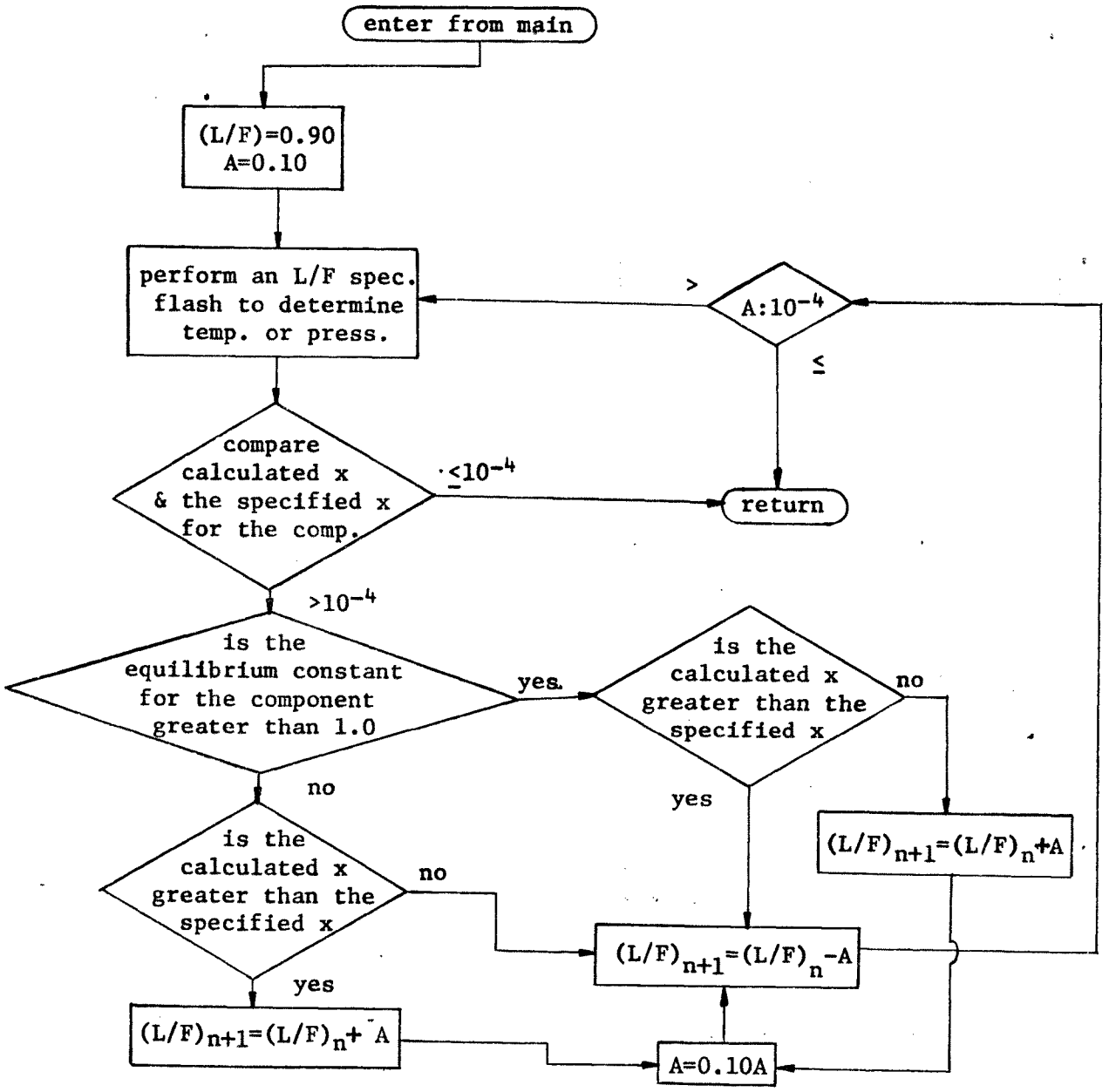


FLASH - L/F SPECIFIED



FLASH - L/F SPECIFIED

FOR ONE COMPONENT



APPENDIX B

ACCEPTABLE COMPONENTS

Benzene.....16
1,2 Butadiene.....27
1,3 Butadiene.....26
Butane (iso).....4
Butane (n).....5
1-Butene.....28
iso-Butylene.....15
Carbon Dioxide.....19
Carbon Monoxide.....18
Cumene.....39
Cyclohexane.....30
Cyclopentane.....29
n-Decane.....12
2,2 Dimethyl Butane...23
2,3 Dimethyl Butane...24
Ethane.....2
Ethyl Benzene.....33
3 Ethyl Hexane.....37
Ethylene.....13
n-Heptane.....10
n-Hexane.....9
Hydrogen Sulfide.....25
Methane.....1
Methyl Cyclohexane....32
2 Methyl Pentane.....21
3 Methyl Pentane.....22
Nitrogen.....17
n-Nonane.....11
n-Octane.....40
Pentane (n).....7
Pentane (neo).....8
Pentane (iso).....6
Propane.....3
n-Propyl Benzene.....38
Propylene.....14
Sulfur Dioxide.....20
Toluene.....31
m-Xylene.....35
o-Xylene.....34
p-Xylene.....36

APPENDIX C

BWR CONSTANTS[5,9]

No.	Component	a	A_o	b	B_o	$c \times 10^{-6}$	$C_o \times 10^{-6}$	α	γ
1	Methane	2984.12	6995.25	0.86733	0.682401	498.1	275.76	0.51117	1.53961
2	Ethane	20850.20	15670.70	2.85393	1.005540	6413.1	2194.27	1.00044	3.02790
3	Propane	57248.00	25915.40	5.77355	1.558840	25247.8	6209.93	2.49577	5.64524
4	iso-Butane	117047.00	38587.40	10.88900	2.203290	55977.7	10384.70	4.41496	8.72447
5	n-Butane	113705.00	38029.60	10.26360	1.992110	61925.6	12130.50	4.52693	8.72447
6	iso-Pentane	226902.00	48253.60	17.14409	2.563860	136025.0	21336.70	6.98777	11.88070
7	n-Pentane	246147.61	45928.81	17.14409	2.510963	161306.1	25917.20	7.43992	12.18858
8	neo-Pentane	210851.64	48885.67	17.14409	2.731686	106862.8	15553.70	8.22091	12.83008
9	n-Hexane	429901.15	54443.41	28.00323	2.848351	296076.6	40556.20	11.55391	17.11146
10	n-Heptane	626106.43	66070.61	38.99170	3.187742	483427.0	57984.00	17.90600	23.09415
11	n-Nonane	918974.23	105808.90	56.17085	4.477023	970906.1	83075.60	76.71274	50.96414
12	n-Decane	7558280.60	-1350705.00	504.73669	-99.828900	866.9	1611.57	8.81524	0.00000
13	Ethylene	15645.50	12593.60	2.20678	0.891980	4133.6	1602.28	0.73166	2.36844
14	Propylene	46758.60	23049.20	4.79997	1.362635	20083.0	5365.97	1.87372	4.69325

Units: see page 79

No.	Component	a	A_o	b	B_o	$c \times 10^{-6}$	$C_o \times 10^{-6}$	α	γ
15	iso-Butylene	102251.40	33762.90	8.93375	1.858582	53807.2	11329.60	3.74417	7.59400
16	Benzene	336468.60	24548.50	19.66341	0.805755	230247.9	41907.80	2.87773	7.51843
17	Nitrogen	1516.36	3937.31	0.59729	0.652648	142.6	98.47	0.52285	1.35999
18	Carbon Monoxide	2213.93	5057.77	0.67527	0.873706	203.5	104.61	0.55491	1.53961
19	Carbon Dioxide	8264.56	10322.80	1.85022	0.799500	2919.7	1693.03	0.34816	1.38411
20	Sulfur Dioxide	51024.80	7996.23	3.75998	0.419404	22184.8	9699.23	0.29577	1.52001
21	2 Methyl Pentane	448741.60	56301.39	31.17714	2.769651	274007.2	34821.65	9.65960	15.90930
22	3 Methyl Pentane	360728.20	46017.81	28.80101	1.305613	187021.7	2703.26	9.24852	16.13768
23	2,2 Dimethyl Butane	610596.00	44656.47	35.92428	3.077853	342176.3	4104.68	8.99778	14.49800
24	2,3 Dimethyl Butane	283648.00	61957.90	20.27156	3.043573	222063.3	3119.78	14.77626	19.24513
25	Hydrogen Sulfide	14572.52	10558.02	1.41858	0.711476	6069.9	3268.24	0.30788	1.28708
26	1,3 Butadiene	92988.34	28445.96	7.95727	1.685062	50124.1	11395.04	4.09023	7.21968
27	1,2 Butadiene	101208.40	30400.98	8.25290	1.716078	60079.5	13411.42	4.32027	7.48790

Units: see page 79

No.	Component	a	A_o	b	B_o	$c \times 10^{-6}$	$C_o \times 10^{-6}$	α	γ
28	1-Butene	103524.4	29822.98	8.97288	1.789369	54394.4	11645.00	4.89778	8.14115
29	Cyclopentane	149184.2	39538.80	10.60101	1.944945	116617.4	22968.97	6.28958	9.61836
30	Cyclohexane	229709.2	51031.49	15.08789	2.320321	210168.4	34698.04	10.67932	13.68933
31	Toluene	184870.4	58856.20	17.44451	2.494957	299856.8	46040.12	13.27666	15.82750
32	Methyl Cyclohexane	351290.0	64153.30	22.32766	2.822640	343243.4	46583.52	19.22498	20.25802
33	Ethyl Benzene	383935.7	69796.21	22.53210	2.835532	440008.9	59444.60	19.48962	20.44351
34	o-Xylene	436416.4	75118.80	25.13347	2.994746	519383.1	66437.51	22.96041	22.80374
35	m-Xylene	437559.6	74469.04	25.70817	3.028792	500332.2	63281.19	23.75242	23.32518
36	p-Xylene	453610.9	75761.37	26.69437	3.086339	517011.8	64171.52	25.13220	24.21996
37	3 Ethyl Hexane	577642.0	81890.36	37.05104	3.636085	554197.9	58387.04	41.09619	33.61662
38	n-Propyl Benzene	587380.5	87643.57	33.44624	3.454677	715077.9	79292.39	35.24698	30.34597
39	Cumene	591242.2	87745.15	33.80905	3.473364	713706.5	78714.53	35.82205	30.67515
40	n-Octane	673751.4	88627.89	43.03352	3.918657	651890.3	63726.92	51.44121	39.04456

Units: see page 79

UNITS FOR

BWR CONSTANTS

$a = (\text{ft.}^3/\text{lb. mole})^3\text{atm.}$

$A_o = (\text{ft.}^3/\text{lb. mole})^2\text{atm.}$

$b = (\text{ft.}^3/\text{lb. mole})^2$

$B_o = (\text{ft.}^3/\text{lb. mole})$

$c = (\text{ft.}^3/\text{lb. mole})^3(°\text{R})^2\text{atm.}$

$C_o = (\text{ft.}^3/\text{lb. mole})^2(°\text{R})^2\text{atm.}$

$\alpha = (\text{ft.}^3/\text{lb. mole})^3$

$\gamma = (\text{ft.}^3/\text{lb. mole})^2$

APPENDIX D

REDUCED BWR CONSTANTS[9]

Hydrocarbon		Nonhydrocarbon
0.066190	a'	0.020830
0.264883	A_o'	0.284623
0.046497	b'	0.027364
0.128809	B_o'	0.129426
0.060966	c'	0.023222
0.181312	C_o'	0.157489
0.001827	α'	0.0019487
0.042187	γ'	0.052603

APPENDIX E

CONSTANTS FOR THE IDEAL K-VALUE EQUATIONS[11]

	CH_4	H_2	N_2	CO_2	H_2S
A_o	2.43840	1.96718	2.7365534	-30.060874	3.0581210
A_1	-2.24550	1.02972	-1.9818310	6.1409853	-2.6491906
A_2	-0.34084	-0.54009	-0.51487289	45.263229	0.37457945
A_3	0.00212	0.0005288	0.042470988	-27.303012	-1.4647096
A_4	-0.00223	0.0	-0.002814385	5.9152545	0.45734766
A_5	0.10486	0.008585	-0.029474696	0.36838431	-0.95721679
A_6	-0.03691	0.0	0.021495843	-0.67916811	1.4272648
A_7	0.0	0.0	0.0	0.15546363	-0.50242238
A_8	0.0	0.0	0.0	0.0	0.33859029
A_9	0.0	0.0	0.0	0.089562849	-0.26678483
A_{10}	0.0	0.0	0.0	0.0	0.0
A_{11}	0.0	0.0	0.0	0.0	0.0
A_{12}	0.0	0.0	0.0	0.0	0.0
A_{13}	0.0	0.0	0.0	0.0	0.0
A_{14}	0.0	0.0	0.0	0.0	0.0

Generalized:

A_o=5.75748	A_3=2.02299	A_7=-0.31138	A_{11}=8.65808
A_1=-3.01761	A_4=0.0	A_8=-0.02655	A_{12}=-1.22060
A_2=-4.98500	A_5=0.08427	A_9=0.02883	A_{13}=-3.15224
	A_6=0.26667	A_{10}=-4.23893	A_{14}=-0.0250

APPENDIX F

TYPES OF CALCULATIONS

CODE	TYPE
1	Bubble-point, constant T
2	Bubble-point, constant P
3	Dew-point, constant T
4	Dew-point, constant P
5	Flash calculation at constant T and P
6	Flash, enthalpy specified, constant T
7	Flash, enthalpy specified, constant P
8	Flash, liquid fraction specified, constant T
9	Flash, liquid fraction specified, constant P
10	Flash, L/F specified for a component, constant T
11	Flash, L/F specified for a component, constant P

APPENDIX G

INPUT CODE FOR UNITS (T,P)

CODE	TEMP.	PRESS.
1	°F	psia
2	°F	mm Hg
3	°F	atm
4	°F	in Hg
5	°C	psia
6	°C	mm Hg
7	°C	atm
8	°C	in Hg
9	°R	psia
10	°R	mm Hg
11	°R	atm
12	°R	in Hg
13	°K	psia
14	°K	mm Hg
15	°K	atm
16	°K	in Hg

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