2.3 BWR Equation

Thermodynamic properties are evaluated by the Benwdict-Webb-Rubin equation modified by Nishiumi and Saito[1]. No provision is made for transport properties at this moment.

2.3.1 The Names of Subroutine, Library File and Single Shot Program

Library File for UNIX: libjbwr.a
Library File for DOS, Windows95/NT: JBWRMX.LIB
Single Shot Program for UNIX: Not provided
Single Shot Program for DOS, Windows95/NT: BWRMX–SS.EXE

It should be noted that the source programs of JBWRMX.LIB are written in both C-language and FORTRAN. Therefore user’s programming environment must support mixed language programming of C and FORTRAN to use JBWRMX.LIB.

2.3.2 Reference State

By user’s selection of KSTAN, which is the first ARGUMENT of STNKAS, the reference state is determined as shown below.

<table>
<thead>
<tr>
<th>KSTAN</th>
<th>Reference State Specified by KSTAN</th>
<th>value of enthalpy and entropy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>273.15K : saturated liquid of pure component</td>
<td>200kJ/kg, 1.0kJ/(kg·K)</td>
</tr>
<tr>
<td>others</td>
<td>same with KSTAN = 1</td>
<td></td>
</tr>
</tbody>
</table>

2.3.3 Missing SUBPROGRAM

Of the SUBPROGRAMs listed in 1.6, the next is missing in F–PROPATH by BWR equation.

MKTABLE, START1, SUBCRT, SUBMXH, SUBM, SUBPAR, T68, T90

Also, subroutine SUBMIX with either I = 3 or 4 (see 1.7) are not supported in F–PROPATH by BWR equation.

2.3.4 Initialization by SUBROUTINE START2

By the procedure described below, user can use F–PROPATH by BWR equation for any mixture. However in that case a user has to transfer related constants of each component to F–PROPATH. They are relative molecular mass, critical constants(temperature, pressure, volume), acentric factor, coefficients of isobaric specific heat equation at ideal gas state, and interaction parameter.

A user has to write the lines shown below before he or she makes reference to any F–PROPATH by BWR equation SUBPROGRAM.

```
DIMENSION PR1(5),PR2(5),CP1(8),CP2(8)
DATA STATEMENT for PR1,PR2,CP1,CP2
AKI=K
CALL KPAMES(KPA,MESS)
CALL STNKAS(KSTAN,KAS)
CALL START2(J,PR1,PR2,CP1,CP2,AKI)
```

PR1 and PR2 are arrays to which a user transfers constants for component 1 and 2, respectively. CP1 and CP2 are arrays to which a user transfers coefficients of isobaric specific heat equation for component 1 and 2, respectively. AKI is the interaction parameter defined in reference [1].

Elements of PR1 and PR2 mean what are shown below.

- `PR1(1)`: relative molecular mass of component 1 [kg/kmol]
- `PR1(2)`: critical temperature of component 1 [K]
- `PR1(3)`: dummy(critical pressure of component 1 [Pa])
PR1(4) : critical volume of component 1 [m$^3$/kmol]
PR1(5) : acentric factor of component 1 [-]

PR2(1) : relative molecular mass of component 2 [kg/kmol]
PR2(2) : critical temperature of component 2 [K]
PR2(3) : dummy(critical pressure of component 2 [Pa])
PR2(4) : critical volume of component 2 [m$^3$/kmol]
PR2(5) : acentric factor of component 2 [-]

A user is allowed to use one of the following three equations of isobaric specific heat at ideal gas state $(T: \text{temperature [K]})$.

1. $CP[J/(\text{kmol·K})] = A + BT + CT^2 + DT^3 + ET^4$, $CP^*(1) = 2.0$
2. $CP[J/(\text{kmol·K})] = AT^2 + BT + C + DT + ET^2 + FT^3$, $CP^*(1) = 3.0$

Elements of CP1 and CP2 mean what are shown below.
When $CP^*(1) = 1.0$ or 2.0

CP1(1) : number of equation 2.0 or 3.0 for component 1.
CP1(2) : value of A for component 1
CP1(3) : value of B for component 1
CP1(4) : value of C for component 1
CP1(5) : value of D for component 1
CP1(6) : value of E for component 1
CP1(7) : lower valid bound of the equation [K]
CP1(8) : upper valid bound of the equation [K]

CP2(1) : number of equation 2.0 or 3.0 for component 2.
CP2(2) : value of A for component 2
CP2(3) : value of B for component 2
CP2(4) : value of C for component 2
CP2(5) : value of D for component 2
CP2(6) : value of E for component 2
CP2(7) : lower valid bound of the equation [K]
CP2(8) : upper valid bound of the equation [K]

When $CP^*(1) = 3.0$

CP1(1) : number of equation 3.0 for component 1.
CP1(2) : lower valid bound of the equation [K]
CP1(3) : upper valid bound of the equation [K]
CP1(4) : value of A for component 1
CP1(5) : value of B for component 1
CP1(6) : value of C for component 1
CP1(7) : value of D for component 1
CP1(8) : value of E for component 1
CP1(9) : value of F for component 1

CP2(1) : number of equation 3.0 for component 2.
CP2(2) : lower valid bound of the equation [K]
CP2(3) : upper valid bound of the equation [K]
CP2(4) : value of A for component 2
CP2(5) : value of B for component 2
CP2(6) : value of C for component 2
CP2(7) : value of D for component 2
CP2(8) : value of E for component 2
CP2(9) : value of F for component 2
J is the error detection code. When PR1(2) > PR2(2), T_{c1} > T_{c2}, exchange between component 1 and 2 will occur and J = −1 will be returned. For other invalid ARGUMENT(s), J = −2 will occur.

### 2.3.5 Example of User's PROGRAM UNIT

#### Sample Program 1

```fortran
C-----------------------------------------------------------------
C NS-BWR Equation
C This program calculates properties of R22-R114 mixture
C at bubble and dew point at P=2.5[bar] and Z=0.5[kg/kg].
C-----------------------------------------------------------------
C---------------------------------------------
C Definition of array PR1, PR2, CP1 and CP2.
C---------------------------------------------
DIMENSION PR1(5), PR2(5), CP1(9), CP2(9)
C----------------------------------------
C T=[C], P=[bar], quantity=[kg]
C standard state=(saturated liquid at 273.15[K])
C-----------------------------------------
call KPAMES(1,1)
call STNKAS(1,1)
C----------------------------------------------------------------------------
C Putting fundamental constants into PR1 and PR2 using DATA STATEMENT.
C DATA(PR1(I),I=1,5)/MW1[KG/KMOL], TC1[K], dummy, VC1[M^3/KMOL], OMEGA1[-]/
C DATA(PR2(I),I=1,5)/MW2[KG/KMOL], TC2[K], dummy, VC2[M^3/KMOL], OMEGA2[-]/
C----------------------------------------------------------------------------
DATA(PR1(I),I=1,5)/ 86.469, 369.3, -1.0, 0.168555, 0.205/
DATA(PR2(I),I=1,5)/170.922, 418.78, -1.0, 0.296739, 0.234/
C----------------------------------------------------------------------------
C Putting isobaric heat capacity at ideal gas state into CP1 and CP2
C using DATA STATEMENT.
C DATA(CP1(I),I=1,8)/EQUATION NUMBER,TMIN[K],TMAX[K], A,B,C,D,E/
C DATA(CP2(I),I=1,8)/EQUATION NUMBER,TMIN[K],TMAX[K], A,B,C,D,E/
C----------------------------------------------------------------------------
DATA(CP1(I),I=1,9)
& /3.0, 250.0, 350.0,
& -917.3, 28.755, -2.030E-02, 2.5351E-03, -2.185E-06, 7.1E-10/
DATA(CP2(I),I=1,9)
& /2.0, 250.0, 400.0,
& -0.12916, 4.7009E-03, -8.612E-06, 6.05E-09, 0.0, 0.0 /
do 10 I=4,9
CP1(I) = CP1(I) * PR1(1) * 1000
CP2(I) = CP2(I) * PR2(1) * 1000
10 continue
C------------------------------------------
C Setting interaction parameters AKIJ.
C------------------------------------------
AKIJ=0.976
C------------------------------------------
C Execution START2.
C------------------------------------------
call START2(ECODE, PR1, PR2, CP1, CP2, AKIJ)
C------------------------------------------
C Calculation of properties at bubble point and
dew point using SUBPB and output results.
C------------------------------------------
P=2.5
Z=0.5
```
CALL SUBTB(J,TB,P,Z,VB,HB,SB)
CALL SUBTD(J,TD,P,Z,VD,HD,SD)
WRITE(*,*) ' P[bar] =',P
WRITE(*,*) ' Z[kg/kg] =',Z
WRITE(*,1) TB, TD
WRITE(*,2) VB, VD
WRITE(*,3) HB/1000, HD/1000
WRITE(*,4) SB/1000, SD/1000
STOP
END

Output

P[bar] = 2.5
Z[kg/kg] = 0.5
TB[°C] = -14.0 TD = 3.5
VB[m³/kg] = 0.72E-03 VB = 0.75E-01
HB[kJ/kg] = 196.7 HD = 372.0
SB[kJ/kg] = 1.025 SD = 1.683

Sample Program 2

C-----------------------------------------------------------------
C NS-BWR Equation
C This program calculates temperature, volume,entropy and quality
C of R22-R114 mixture
C at P=0.6[MPa], Z=0.5[kg/kg] and H=300[kJ/kg].
C-----------------------------------------------------------------
DIMENSION PR1(5),PR2(5),CP1(9),CP2(9)
call KPAMES(0,1)
call STNKAS(1,1)
DATA(PR1(I),I=1,5)/ 86.469, 369.3, -1.0, 0.168555, 0.205/
DATA(PR2(I),I=1,5)/170.922, 418.78, -1.0, 0.296739, 0.234/
DATA(CP1(I),I=1,9)
& /3.0, 250.0, 350.0,
& -917.3,28.755,-2.030E-02,2.5351E-03,-2.185E-06, 7.1E-10/
C [kJ/kg]
DATA(CP2(I),I=1,9)
& /2.0, 250.0, 400.0,
& -0.12916, 4.7009E-03, -8.612E-06, 6.05E-09, 0.0, 0.0 /
C [kJ/kg]
do 10 I=4,9
C [kJ/kg] -> [J/kmol]
CP1(I) = CP1(I) * PR1(I) * 1000
CP2(I) = CP2(I) * PR2(I) * 1000
10 continue
AKIJ=0.976
call START2(ECODE, PR1, PR2, CP1, CP2, AKIJ)
C-----------------------------------------------------------------
C Calculation of temperature, volume, entropy and quality
C from pressure, whole composition and enthalpy.
C-----------------------------------------------------------------
P = 0.6E+6
Z = 0.5
H = 300.0*1000.0
CALL SUBMIX(2, J, T, P, Z, V, H, S)
Q = QMIX(T, P, Z)
WRITE(*,*) ' P[MPa] =', P/1e+6
WRITE(*,*) ' Z[kg/kg] =', Z
WRITE(*,*) ' H[kJ/kg] =', H/1000
WRITE(*,*) ' T[K] =', T
2.3.6 Sample Output of Single Shot Program

Single shot program of BWR equation is not provided in this version of F-PROPATH.

References
