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APPENDIX

APPENDIX I

PHYSICAL PROPERTY CONSTANTS OF NATURAL GAS

The following physical property constants are listed :

M = Molecular Weight

TB = Normal Boiling Point Temperature

TC = Critical Temperature

PC = Critical Pressure

ZC = Critical Compressibility Factor

ω = Acentric Factor

Components	M	TB		TC		PC		ZC	ω
		^oR	K	^oR	K	Psia	MPa		
CO_2	44.010	350.4	185.29	548.00	304.44	1073.00	7.395	0.275	0.225
N_2	28.016	193.3	77.35	227.20	126.22	492.00	3.391	0.292	0.040
C_1	16.042	201.0	111.67	343.30	190.72	673.10	4.639	0.290	0.014
C_2	30.068	332.2	184.54	549.77	305.43	708.30	4.881	0.288	0.099
C_3	44.094	416.0	231.10	665.95	370.00	617.40	4.255	0.278	0.152
i-C_4	58.120	470.6	261.26	734.65	408.14	529.10	3.646	0.283	0.185
n-C_4	58.120	490.8	231.65	765.31	425.17	550.70	3.795	0.274	0.201
i-C_5	72.146	541.8	300.82	829.80	461.00	483.00	3.329	0.269	0.222
n-C_5	72.146	556.6	309.22	845.60	469.78	489.50	3.374	0.268	0.254
C_6	86.172	615.4	341.89	914.20	507.89	439.70	3.030	0.264	0.301
C_7	100.198	668.9	371.59	972.31	540.17	396.90	2.735	0.260	0.350
C_8	114.224	717.9	398.82	1024.31	569.06	362.10	2.496	0.256	0.402
C_9	128.250	763.1	423.95	1073.00	596.11	345.00	2.378	0.250	0.446
C_{10}	142.276	805.1	447.27	1114.70	619.28	306.00	2.109	0.246	0.489
C_{11}	156.302	844.3	469.04	1153.70	640.94	282.00	1.943	0.243	0.501
C_{12}	170.378	881.0	489.44	1187.70	659.83	263.00	1.813	0.237	0.539

APPENDIX II

GENERALIZED VAPOR PRESSURE EQUATION FOR NONPOLAR SUBSTANCES

The reduced vapor pressure relationship takes the form (40)

$$\ln P_R = \beta \left[\frac{1}{T_R^m} - 1 \right] + \gamma [T_R^n - 1] \quad (1)$$

For n-paraffin,

$$n = 7.0 \quad (2)$$

$$s = (T_B \ln P_C)/(T_C - T_B) \quad (3)$$

$$m = 0.78425\, e^{0.089315s} - 8.5217/e^{0.74826s} \quad (4)$$

$$\beta = -4.26700 - \frac{221.79}{s^{2.5}\, e^{0.03848s^{2.5}}} + \frac{3.8126}{e^{2272.44/s^3}} + \Delta^* \quad (5)$$

The term is significant only with quantum gases i.e. helium, n-hydrogen, and neon. For all other substances, the term $\Delta^* = 0$.

$$\gamma = as + b\beta \quad (6)$$

$$a = (1/T_{RB} - 1)/(1 - T_{RB}^7) \quad (6a)$$

$$b = (1/T_{RB}^m - 1)/(1 - T_{RB}^7) \quad (6b)$$

For a substance lacking any experimental information, the predicted will be associated with an average percentage deviation of 0.97, provided reliable values of the normal boiling point and its corresponding critical values are available.

Equation (1) offers a capability to calculate vapor pressure of both polar and nonpolar substances because the heuristical development of this relationship is completely general. The application of these relationship must be restricted to nonpolar substances. For polar substances, correct vapor pressure parameters β, γ, and m for nonpolar substances are needed in order to establish a completely general method applicable to all type of substances.

APPENDIX III

DESCRIPTIONS AND LISTINGS OF SUBROUTINES FOR VAPOR-LIQUID EQUILIBRIUM CALCULATIONS

The computer subroutines for vapor-phase and liquid-phase fugacity coefficient by the Soave-Redlich-Kwong equation of state, flash calculations, dew point and bubble point calculations, are described and listed in this Appendix. These subroutines are are written in FORTRAN IV, they should be compatible with most computer systems with FORTRAN IV compilers.

These subroutines are capable of treating multicomponent system with up to 20 components. For compatibility with diverse, user-written main programs, they employ vector of length N, where N ($\leqslant$20) is the number of components involved, in their argument lists.

```
C#####################################################################
C#####                        MAIN PROGRAM                     #######
C##  SCALING DOWN OF FLASH CALCULATION OF NATURAL GAS WITH THE      ###
C##                    AID OF PSEUDOCOMPONENTS                       ##
C#####################################################################
C  OBJECTIVES: -TO SCALE DOWN THE CALCULATION OF PROPERTIES OF
C                NATURAL GAS
C              -TO DEVELOP SIMPLE AND EASY MODEL FOR PREDICTION
C  LIST OF SYMBOL IN THIS PROGRAM
C     N-- THE NUMBER OF COMPONENT
C     M-- THE LIGHTEST COMPONENT WHICH IS GROUPED
C     X-- COMPOSITION IN LIQUID PHASE
C     Y-- COMPOSITION IN VAPOR PHASE
C     K-- EQUILIBRIUM RATIO (Y(I)/X(I))
C     ZF-- FEED COMPOSITION
C     P-- TOTAL PRESSURE
C     T-- SYSTEM TEMPERATURE
C     TC AND PC ARE CRITICAL TEMPERATURE AND PRESSURE,RESPECTIVELY
C     W -- ACENTRIC FACTOR
C     FEED-- FEED RATE (MOLE/HR)
C     VAP-- VAPOR TO FEED RATIO(V/F)
C     R-- THE UNIVERSAL GAS CONSTANT
C     AAD-- AVERAGE ABSOLUTE DEVIATION
C
      REAL L,K
      INTEGER ID,NAME,N,NN,M
      COMMON/VALUE/N,T,P,R,FEED,VAP,V,L,NIT
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20)
      COMMON/PROP/ID(20),NAME(20),TC(20),PC(20),W(20),K(20),COEF(20,20)
      COMMON/PSEUDO/TCLX(20),TOLY(20),PSTC(20),PSPC(20),PSW(20),ZF1(20)
      COMMON/ERROR/ERRX(20),ERRY(20),XX(20),YY(20)
      READ (5,7) N
      READ (5,8) (ID(I),I=1,N)
      READ (5,9) (NAME(I),I=1,N)
      READ (5,11) ((COEF(I,J),J=1,N),I=1,N)
      READ (5,13) (TC(I),PC(I),W(I),I=1,N)
      READ (5,15) (ZF(I),I=1,N)
      READ (5,17) (XX(I),I = 1,N)
      READ (5,18) (YY(I),I = 1,N)
      READ (5,19) FEED,VAP
      READ (5,21) T,P,R
      WRITE (6,25)N
      WRITE (6,27)T,P,R
      WRITE (6,29)FEED,VAP
    7 FORMAT (2I3)
    8 FORMAT (16I2)
    9 FORMAT (16A4)
   11 FORMAT (16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/
     * 16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3)
   13 FORMAT (3(2F7.2,F5.4)/3(2F7.2,F5.4)/3(2F7.2,F5.4)/3(2F7.2,F5.4)/
     * 3(2F7.2,F5.4)/(2F7.2,F5.4))
   15 FORMAT (6F9.6/6F9.6/4F9.6)
```

```
   17 FORMAT (8F6.3/8F6.3)
   18 FORMAT (6F9.6/6F9.6/4F9.6)
   19 FORMAT (2F9.6)
   21 FORMAT (3F6.2)
   25 FORMAT (/5X,'THE AMOUNT OF COMPONENT,N  = ',I3)
   27 FORMAT (/5X,'T = ',F7.2,3X,'F',7X,'P = ',F7.2,3X,'PSIA',7X,'R = ',
     * F7.3,3X,'PSIA-CUBIC FT/LB-MOLE R')
   29 FORMAT(/5X,'FEED RATE = ',F9.6,3X,'MOLE/HR',5X,'V/F = ',F9.6//)
C
      IT = 1
      T = T + 460.0
      DO 90 I = 1,N
      XX(I) = XX(I)/100.0
   90 YY(I) = YY(I)/100.0
      WRITE (6,95)
      WRITE (6,96)
      WRITE (6,97)
      WRITE (6,98)
   95 FORMAT (7X,'INITIAL VALUE OF LIQUID AND VAPOR PHASE COMPOSITION')
   96 FORMAT (7X,50('_'))
   97 FORMAT (/9X,'ID',5X,'COMPONENT',7X,'X',14X,'Y')
   98 FORMAT (7X,50('_'))
      SUMX = 0.0
      SUMY = 0.0
      DO 100 I = 1,N
      ZF(I) = ZF(I)/100.0
      Y(I) = ZF(I)
      SUMY = SUMY+Y(I)
      X(I) = 1.0/N
      SUMX = SUMX+X(I)
      WRITE (6,103)ID(I),NAME(I),X(I),Y(I)
  103 FORMAT (8X,I2,7X,A4,5X,F10.6,5X,F10.6)
  100 CONTINUE
  104 FORMAT (7X,50('_'))
  105 FORMAT (20X,'SUM =',F11.6,4X,F11.6)
  106 FORMAT (7X,50('_'))
      WRITE (6,104)
      WRITE (6,105)SUMX,SUMY
      WRITE (6,106)
  115 DO 120 I = 1,N
      X1(I) = X(I)
  120 Y1(I) = Y(I)
      IT = IT+1
      CALL SRK
      CALL FLASH
      DO 130 I = 1,N
      X2(I) = X(I)
      Y2(I) = Y(I)
  130 CONTINUE
      STOLX = 0.0
      STOLY = 0.0
      DO 140 I = 1,N
      TOLX(I) = X2(I)-X1(I)
      TOLY(I) = Y2(I)-Y1(I)
      STOLX = STOLX+ABS(TOLX(I))
      STOLY = STOLY+ABS(TOLY(I))
  140 CONTINUE
```

```
      AADXX = STOLX/N
      AADYY = STOLY/N
      IF (AADXX .LE. 0.005 .AND. AADYY .LE. 0.0005) GO TO 155
      DO 150 I = 1,N
      X(I) = X2(I)
      Y(I) = Y2(I)
  150 CONTINUE
      GO TO 115
C  NORMALIZED LIQUID AND VAPOR PHASE COMPOSITION
  155 SUMX2 = 0.0
      SUMY2 = 0.0
      DO 157 I = 1,N
      X2(I) = X2(I)
      SUMX2 = SUMX2+X2(I)
      Y2(I) = Y2(I)
  157 SUMY2 = SUMY2+Y2(I)
      SUMX = 0.0
      SUMY = 0.0
      DO 160 I = 1,N
      X(I) = X2(I)/SUMX2
      SUMX = SUMX + X(I)
      Y(I) = Y2(I)/SUMY2
      SUMY = SUMY + Y(I)
  160 CONTINUE
      SERRX = 0.0
      SERRY = 0.0
      DO 170 I = 1,N
      ERRX(I) = X(I) - XX(I)
      SERRX = SERRX + ABS(ERRX(I))
      ERRY(I) = Y(I) - YY(I)
      SERRY = SERRY + ABS(ERRY(I))
  170 CONTINUE
      AADX = SERRX*100.0/N
      AADY = SERRY*100.0/N
      WRITE (6,180)VAP,V,L
      WRITE (6,182)IT
      WRITE (6,184)
      WRITE (6,186)
      WRITE (6,188)
      WRITE (6,190)(ID(I),NAME(I),XX(I),YY(I),X(I),Y(I),
     * K(I),ERRX(I),ERRY(I),I = 1,N)
      WRITE (6,192)
      WRITE (6,194)SUMX,SUMY,AADX,AADY
      WRITE (6,196)
  180 FORMAT (/T12,'V/F = ',F11.9/T12,'V = ',F11.5,
     * 3X,'MOLE/HR'/T12,'L = ',F11.9,3X,'MOLE/HR')
  182 FORMAT (/7X,'NO. OF ITERATION = ',I3/)
  184 FORMAT (2X,127('_'))
  186 FORMAT (5X,'ID',5X,'COMPONENT',8X,'X(EXP)',7X,'Y(EXP)',10X,
     * 'X(MODEL)',6X,'Y(MODEL)',8X,'K(MODEL)',9X,'ERRX',11X,'ERRY')
  188 FORMAT (2X,127('_'))
  190 FORMAT (4X,I3,7X,A4,7X,F10.5,5X,F10.5,5X,F10.5,5X,F10.6,
     * 6X,F10.5,5X,F10.5,5X,F10.6)
  192 FORMAT (2X,127('_'))
  194 FORMAT (48X,'SUM = ',F11.5,4X,F11.6,14X,'%AAD = ',F10.5,5X,F10.6)
  196 FORMAT (2X,127('_'))
      STOP
      END
```

```
C#############################################################################
C#####                         MAIN PROGRAM                            #######
C##  SCALING DOWN OF FLASH CALCULATION OF NATURAL GAS WITH THE            ###
C##                      AID OF PSEUDOCOMPONENTS                          ##
C#############################################################################
C  OBJECTIVES: -TO SCALE DOWN THE CALCULATION OF PROPERTIES OF
C                NATURAL GAS
C              -TO DEVELOP SIMPLE AND EASY MODLE FOR PREDICTION
C
C  NOMENCLATURES IN THIS PROGRAM
C     N-- THE TOTAL NUMBER OF COMPONENT
C     M-- THE LIGHTEST COMPONENT WHICH IS GROUPED
C     X-- COMPOSITION IN LIQUID PHASE
C     Y-- COMPOSITION IN VAPOR PHASE
C     K-- EQUILIBRIUM RATIO (Y(I)/X(I))
C     ZF-- FEED COMPOSITION
C     P-- TOTAL PRESSURE
C     T-- SYSTEM TEMPERATURE
C     TC AND PC ARE CRITICAL TEMPERATURE AND PRESSURE,RESPECTIVELY
C     W -- ACENTRIC FACTOR
C     FEED-- FEED RATE (MOLE/HR)
C     VAP-- VAPOR TO FEED RATIO(V/F)
C     R-- THE UNIVERSAL GAS CONSTANT
      REAL L,K,KK,K1
      INTEGER ID,NAME,N,NN,M,ERR
      COMMON/VALUE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PSEUDO/COEF(20,20),PSTC(20),PSPC(20),PSW(20),KK(20),K1(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YO(20),TC(20),PC(20),W(20)
      COMMON/PROP1/LTC(20),LPC(20),LW(20),HTC(20),HPC(20),HW(20)
      READ (5,7) N,M
      READ (5,8) (ID(I),I=1,N)
      READ (5,9) (NAME(I),I=1,N)
      READ (5,11) ((COEF(I,J),J=1,N),I=1,N)
      READ (5,13) (TC(I),PC(I),W(I),I=1,N)
      READ (5,15) (ZF(I),I=1,N)
      READ (5,17) (XO(I),I = 1,N)
      READ (5,18) (YO(I),I = 1,N)
      READ (5,19) FEED,VAP
      READ (5,21) T,P,R
      WRITE (6,25)N
      WRITE (6,27)T,P,R
      WRITE (6,29)FEED,VAP
    7 FORMAT (2I3)
    8 FORMAT (16I2)
    9 FORMAT (16A4)
   11 FORMAT (16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/
     * 16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3/16F4.3)
   13 FORMAT (3(2F7.2,F5.4)/3(2F7.2,F5.4)/3(2F7.2,F5.4)/3(2F7.2,F5.4)/
     * 3(2F7.2,F5.4)/(2F7.2,F5.4))
   15 FORMAT (6F9.6/6F9.6/4F9.6)
```

```
   17 FORMAT (3F6.3/3F6.3)
   18 FORMAT (6F9.6/6F9.6/6F9.6)
   19 FORMAT (2F9.6)
   21 FORMAT (3F6.2)
   25 FORMAT (/5X,'THE AMOUNT OF COMPONENT,N  = ',I3)
   27 FORMAT (/5X,'T = ',F7.2,3X,'F',7X,'P = ',F7.2,3X,'PSIA',7X,'R = ',
     * F7.3,3X,'PSIA-CUBIC FT/LB-MOLE R')
   29 FORMAT(/5X,'FEED RATE = ',F9.6,3X,'MOLE/HR',5X,'V/F = ',F9.6//)
C
      IT = 1
      T = T+460.0
      DO 90 I = 1,N
      XO(I) = XO(I)/100.0
   90 YO(I) = YO(I)/100.0
      WRITE (6,95)
      WRITE (6,96)
      WRITE (6,97)
      WRITE (6,98)
   95 FORMAT (7X,'INITIAL VALUE OF LIQUID AND VAPOR PHASE COMPOSITION')
   96 FORMAT (7X,50('_'))
   97 FORMAT (/9X,'ID',5X,'COMPONENT',7X,'X',14X,'Y')
   98 FORMAT (7X,50('_'))
      SUMX = 0.0
      SUMY = 0.0
      DO 100 I = 1,N
      ZF(I) = ZF(I)/100.0
      Y(I) = ZF(I)
      SUMY = SUMY+Y(I)
      X(I) = 1.0/N
      SUMX = SUMX+X(I)
      WRITE (6,103)ID(I),NAME(I),X(I),Y(I)
  103 FORMAT (8X,I2,7X,A4,5X,F10.6,5X,F10.6)
  100 CONTINUE
      WRITE (6,104)
      WRITE (6,105)SUMX,SUMY
      WRITE (6,106)
  104 FORMAT (7X,50('_'))
  105 FORMAT (20X,'SUM =',F11.6,4X,F11.6)
  106 FORMAT (7X,50('_'))
      DO 110 I = 1,N
      TC1(I) = TC(I)
      PC1(I) = PC(I)
      W1(I) = W(I)
      X1(I) = X(I)
      Y1(I) = Y(I)
      ZF2(I) = ZF(I)
  110 CONTINUE
C  GROUPED HEAVY-PSEUDOCOMPONENTS(CM+)
      SUMX = 0.0
      SUMY = 0.0
      SUMZF = 0.0
      DO 130 I = M,N
      SUMX = SUMX+X(I)
      SUMY = SUMY+Y(I)
  130 SUMZF = SUMZF+ZF(I)
      NN = M
      X(M) = SUMX
```

```
      Y(M) = SUMY
      ZF(M) = SUMZF
      TC(M) = TC(M+2)
      PC(M) = PC(M+2)
      W(M) = W(M+2)
      DO 135 I = 1,NN
  135 ZF3(I) = ZF(I)
      CALL SRK
      CALL FLASH
      NN = NN-1
      DO 140 I = 1,NN
      KK(I) = K(I)
      XX(I) = X(I)
  140 YY(I) = Y(I)
      DO 145 I = M,N
      XX(I) = X1(I)
  145 YY(I) = Y1(I)
      DO 150 I = 1,N
      X2(I) = XX(I)
  150 Y2(I) = YY(I)
C  GROUPED LIGHT-PSEUDOCOMPONENT (CM-)
      MM = M-1
      NN = N-M+4
      SUMZ = 0.0
      DO 160 I = 3,MM
  160 SUMZ = SUMZ+ZF2(I)
      ZF2(3) = SUMZ
      DO 163 I = 4,NN
  163 ZF2(I) = ZF2(I+M-4)
  170 DO 165 I = 1,NN
  165 ZF(I) = ZF2(I)
      DO 175 I = 1,N
      X(I) = X2(I)
  175 Y(I) = Y2(I)
      CALL LIGHT
      CALL SRK
      CALL FLASH
      DO 180 I = M,N
      KK(I) = K(I-2)
      XX(I) = X(I-2)
      YY(I) = Y(I-2)
  180 CONTINUE
      DO 190 I = 1,N
      KK(I) = KK(I)
      X2(I) = XX(I)
  190 Y2(I) = YY(I)
      IT = IT+1
      DO 200 I = 1,N
      X(I) = X2(I)
  200 Y(I) = Y2(I)
C  GROUPED HEAVY-PSEUDOCOMPONENT (CM+)
      CALL HEAVY
      CALL SRK
      DO 210 I = 1,M
  210 ZF(I) = ZF3(I)
      CALL FLASH
      NN = NN-1
```

```
      DO 220 I = 1,NN
      KK(I) = K(I)
      XX(I) = X(I)
  220 YY(I) = Y(I)
      SUMX2 = 0.0
      SUMY2 = 0.0
      DO 240 I = 1,N
      KK(I) = KK(I)
      X2(I) = XX(I)
      SUMX2 = SUMX2+X2(I)
      Y2(I) = YY(I)
      SUMY2 = SUMY2+Y2(I)
  240 CONTINUE
      SUMX = 0.0
      SUMY = 0.0
      DO 250 I = 1,N
      X(I) = X2(I)/SUMX2
      SUMX = SUMX + X(I)
      Y(I) = Y2(I)/SUMY2
      SUMY = SUMY + Y(I)
  250 CONTINUE
      SERRX = 0.0
      SERRY = 0.0
      DO 255 I = 1,N
      ERRX(I) = X2(I)-XO(I)
      SERRX = SERRX+ABS(ERRX(I))
      ERRY(I) = Y2(I)-YO(I)
      SERRY = SERRY+ABS(ERRY(I))
  255 CONTINUE
      AADX = SERRX*100.0/N
      AADY = SERRY*100.0/N
      WRITE (6,300)VAP,V,L
      WRITE (6,305)IT
      WRITE (6,310)
      WRITE (6,315)
      WRITE (6,320)
      WRITE (6,325)(ID(I),NAME(I),XO(I),YO(I),X(I),Y(I),
     * KK(I),ERRX(I),ERRY(I),I = 1,N)
      WRITE (6,330)
      WRITE (6,335)SUMX,SUMY,AADX,AADY
      WRITE (6,340)
  300 FORMAT (/T12,'V/F = ',F11.9/T12,'V = ',F11.9,
     * 3X,'MOLE/HR'/T12,'L = ',F11.9,3X,'MOLE/HR')
  305 FORMAT (/7X,'NO. OF ITERATION = ',I3/)
  310 FORMAT (2X,127('_'))
  315 FORMAT (5X,'ID',5X,'COMPONENT',8X,'X(EXP)',8X,'Y(EXP)',9X,
     * 'X(MODEL)',6X,'Y(MODEL)',9X,'K(MODEL)',7X,'ERR ',11X,'ERRY')
  320 FORMAT (2X,127('_'))
  325 FORMAT (4X,I3,7X,A4,7X,F10.5,5X,F10.5,5X,F10.5,5X,F10.6,
     * 6X,F10.5,5X,F10.5,5X,F10.6)
  330 FORMAT (2X,127('_'))
  335 FORMAT (48X,'SUM = ',F11.5,4X,F11.6,14X,'%AAD = ',F10.5,5X,F10.6)
  340 FORMAT (2X,127('_'))
      STOP
      END
```

```
C
C.....................................................................
C               SUBROUTINE LIGHT-PSEUDOCOMPONENT                      C
C.....................................................................
C
      SUBROUTINE LIGHT
      COMMON/VALUE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PSEUDO/COEF(20,20),PSTC(20),PSPC(20),PSW(20),KK(20),K1(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YO(20),TC(20),PC(20),W(20)
      COMMON/PROP1/LTC(20),LPC(20),LW(20),HTC(20),HPC(20),HW(20)
      REAL L,LTC,LPC,LW
C GROUPED LIGHT-PSEUDOCOMPONENT (C1+)
      SUMX = 0.0
      SUMY = 0.0
C NORMALIZED PSEUDOCOMPONENT(C1+)
      MM = M-1
      DO 299 I = 1,N
      LTC(I) = TC1(I)
      LPC(I) = PC1(I)
299   LW(I) = W1(I)
      DO 300 I = 3,MM
      SUMX = SUMX+X(I)
300   SUMY = SUMY+Y(I)
      SUMTC = 0.0
      SUMPC = 0.0
      SUMW = 0.0
      DO 310 I = 3,MM
      PSTC(I) = LTC(I)*X(I)
      SUMTC = SUMTC+PSTC(I)
      PSPC(I) = LPC(I)*X(I)
      SUMPC = SUMPC+PSPC(I)
      PSW(I) = LW(I)*X(I)
      SUMW = SUMW+PSW(I)
310   CONTINUE
      X(3) = SUMX
      Y(3) = SUMY
      LTC(3) = SUMTC/SUMX
      LPC(3) = SUMPC/SUMX
      LW(3) = SUMW/SUMX
C     NN = N-M+4
      DO 320 I = 4,NN
      X(I) = X(I+M-4)
      Y(I) = Y(I+M-4)
      LTC(I) = LTC(I+M-4)
      LPC(I) = LPC(I+M-4)
320   LW (I) = LW(I+M-4)
      DO 330 I = 1,NN
      X(I) = X(I)
      Y(I) = Y(I)
      TC(I) = LTC(I)
      PC(I) = LPC(I)
330   W(I) = LW(I)
      RETURN
      END
```

```
C
C.......................................................................
C                        SUBROUTINE HEAVY-PSEUDOCOMPONENT              C
C.......................................................................
C
      SUBROUTINE HEAVY
      COMMON/VALLE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPD/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XY(20)
      COMMON/COMPD1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PSEUDO/COEF(20,20),PSTC(20),PSPC(20),PSW(20),KK(20),K1(20)
      COMMON/PROP/NAME(20),ID(20),XD(20),YD(20),TC(20),PC(20),W(20)
      COMMON/PROP1/LTC(20),LPC(20),LW(20),HTC(20),HPC(20),HW(20)
      REAL L
C REGROUPED HEAVY-PSEUDOCOMPONENT(CM+)
      DO 400 I = 1,N
      HTC(I) = TC1(I)
      HPC(I) = PC1(I)
 400  HW(I) = W1(I)
      SUMX = 0.0
      SUMY = 0.0
      DO 405 I = M,N
      SUMX = SUMX+X(I)
 405  SUMY = SUMY+Y(I)
      SUMTC = 0.0
      SUMPC = 0.0
      SUMW = 0.0
      DO 410 I = M,N
      PSTC(I) = HTC(I)*X(I)
      SUMTC = SUMTC+PSTC(I)
      PSPC(I) = HPC(I)*X(I)
      SUMPC = SUMPC+PSPC(I)
      PSW(I) = HW(I)*X(I)
      SUMW = SUMW+PSW(I)
 410  CONTINUE
      X(M) = SUMX
      Y(M) = SUMY
      HTC(M) = SUMTC/SUMX
      HPC(M) = SUMPC/SUMX
      HW(M) = SUMW/SUMX
      NN = M
      DO 420 I = 1,NN
      X(I) = X(I)
      Y(I) = Y(I)
      TC(I) = HTC(I)
      PC(I) = HPC(I)
      W(I) = HW(I)
 420  CONTINUE
      RETURN
      END
```

```
C
C...........................................................................C
C                              FLASH CALCULATION                            C
C...........................................................................C
C
      SUBROUTINE FLASH
C
C**** USED NEWTON'S METHOD FOR SOLVING V/F
C**** V/F IS CALLED "FRACTION VAPORIZATION"
C**** VAP IS NOTATION OF V/F
C
      REAL L,K
      COMMON/VALUE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YC(20),TC(20),PC(20),W(20)
      COMMON/VARFD/F(20),D(20),F2(20)
   25 SUMF = 0.0
      SUMD = 0.0
      DO 30 I = 1,NN
      F(I) = ZF(I)*(K(I)-1)/(((K(I)-1)*VAP)+1)
      SUMF = SUMF+F(I)
      D(I) = ZF(I)*(K(I)-1)**2/(((K(I)-1)*VAP)+1)**2
      SUMD = SUMD+D(I)
   30 CONTINUE
      VAP1 = VAP+(SUMF/SUMD)
      IF (VAP1 .LT. 0.0) VAP1 = VAP/2.0
      IF (VAP1 .GT. 1.0) VAP1 = (1.0+VAP)/2.0
      IF (ABS((VAP1-VAP)/VAP) .LE. 0.0001) GOTO 50
      VAP = VAP1
      GO TO 25
   50 V = VAP1*FEED
      L = FEED-V
      SUMX = 0.0
      SUMY = 0.0
      DO 60 I = 1,NN
      X(I) = ZF(I)/(((K(I)-1)*VAP)+1)
      SUMX = SUMX+X(I)
      Y(I) = K(I)*X(I)
      SUMY = SUMY+Y(I)
   60 CONTINUE
      RETURN
      END
```

```
C
C........................................................................
C                        SUBROUTINE CHECK                               C
C........................................................................
C
      SUBROJTINE CHECK
      COMMON/VALLE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERR)(2C),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y (2C),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W)(2C),K(20),YY(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YO(2C),TC(20),PC(2C),W(20)
      COMMON/VARFD/F(2C),D(20),F2(20)
C
      REAL K
      VAP1 = 0.0
  900 SUMF2 = 0.0
      DO 1000 I = 1,N
      F2(I) = ZF(I)*(K(I)-1)/(((K(I)-1)*VAP1)+1)
      SJMF2 = SUMF2+F2(I)
 1000 CONTINUE
      IF (SJMF2 .LT. 0.0) GO TO 1110
      VAP1 = VAP1+1.0
      GO TJ 900
 1110 WRITE (6,1120)
 1120 FORMAT (/5X,'THE TWO-PHASE IS EXIST'//)
      RETURN
      END
```

```
C
C......................................................................
C                       SOAVE-REDLICH KWONG EQUATION OF STATE           C
C......................................................................
C
      SUBROUTINE SRK
C     TC AND PC ARE CRITICAL TEMPERATURE AND PRESSURE,RESPECTIVELY
C     W IS ACENTRIC FACTOR
C     TR IS REDUCED TEMPERATURE
C     COEF(N) IS A SYMBOL OF K(I,J)
C     Z IS COMPRESSIBILITY FACTOR
C
      REAL L,K
      COMMON/VALUE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PSEUDO/COEF(20,20),PSTC(20),PSPC(20),PSW(20),KK(20),K1(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YO(20),TC(20),PC(20),W(20)
      COMMON/VAR1/ZZ(20),B(20),BB(20),SLOPE(20),AC(20),STORE(20)
      COMMON/VAR2/TR(20),ALFA(20),PHIL(20),PHIV(20),SUMA(20)
      COMMON/VAR3/ACALFA(20,20),AALFA(20,20),DUMMY1(20),DUMMY3(20)
C
C     IPH =1 -- VAPOR PHASE
      IPH = 1
      DO 16 I=1,NN
   16 ZZ(I) = Y(I)
   17 SUMB = 0.0
      DO 25 I = 1,NN
      B(I) = 0.08664*R*TC(I)/PC(I)
      BB(I) = ZZ(I)*B(I)
      SUMB = SUMB+BB(I)
   25 CONTINUE
      B1 = P*SUMB/(T*R)
      DO 30 J = 1,NN
      TR(J) = T/TC(J)
      SLOPE(J) = 0.480+1.574*W(J)+0.176*W(J)*W(J)
      ALFA(J) = 1+SLOPE(J)*(1-TR(J)**0.5)
      AC(J) = 0.42747**0.5*R*TC(J)/PC(J)**0.5
   30 CONTINUE
      SUMAA = 0.0
      DO 35 I = 1,NN
      SUMA(I) = 0.0
      DO 40 J = 1,NN
      ACALFA(I,J) = ZZ(J)*AC(I)*AC(J)*ALFA(I)*ALFA(J)*(1-COEF(I,J))
      SUMA(I) = SUMA(I)+ACALFA(I,J)
      AALFA(I,J) = ZZ(I)*ZZ(J)*AC(I)*AC(J)*ALFA(I)*ALFA(J)*(1-COEF(I,J))
      SUMAA = SUMAA+AALFA(I,J)
   40 CONTINUE
   35 CONTINUE
      A = SUMAA*P/(R*R*T*T)
      Q = A-B1-B1*B1
      RR = A*B1
      CALL ROOTZ(Z,Q,RR,IPH,B1)
      IF (IPH) 90,55,45
C  CALCULATE VAPOR PHASE FUGACITY COEFFICIENT
   45 DO 50 I = 1,NN
      DUMMY1(I) = B(I)/SUMB*(Z-1)
```

```
      DUMMY2 = ALOG(Z-B1)
      DUMMY3(I) = (2*SUMA(I)/SUMAA)-(B(I)/SUMB)
      DUMMY4 = B1/Z
      DUMMY5 = ALOG(1+DUMMY4)
      STORE(I) = DUMMY1(I)-DUMMY2-A/B1*DUMMY3(I)*DUMMY5
      PHIV(I) = EXP(STORE(I))
C     PHIV(I) = EXP(B(I)/SUMB*(Z-1)-ALOG(Z-B1)-
C    1(A/B1*(2*SUMA(I)/SUMAA-B(I)/SUMB)*ALOG(1+B1/Z)))
   50 CONTINUE
C
C     IPH = 0 --LIQUID PHASE
      IPH = 0
      DO 51 I =1,NN
   51 ZZ(I) = X(I)
      GOTO 17
C  CALCULATE LIQUID PHASE FUGACITY COEFFICIENT
   55 DO 60 I = 1,NN
      DUMMY1(I) = B(I)/SUMB*(Z-1)
      DUMMY2 = ALOG(Z-B1)
      DUMMY3(I) = (2*SUMA(I)/SUMAA)-(B(I)/SUMB)
      DUMMY4 = B1/Z
      DUMMY5 = ALOG(1+DUMMY4)
      STORE(I) = DUMMY1(I)-DUMMY2-A/B1*DUMMY3(I)*DUMMY5
      PHIL(I) = EXP(STORE(I))
C     PHIL(I) = EXP(B(I)/SUMB*(Z-1)-ALOG(Z-B1)-
C    1(A/B1*(2*SUMA(I)/SUMAA-B(I)/SUMB)*ALOG(1+B1/Z)))
   60 CONTINUE
      DO 70 I = 1,NN
      K(I) = PHIL(I)/PHIV(I)
   70 CONTINUE
   90 RETURN
      END
C
C**** SUBROUTINE FOR DETERMNINING COMPRESSIBILITY FACTOR,Z
      SUBROUTINE ROOTZ(Z,Q,RR,IPH,B1)
      IF (Q .GT. .33333) GOTO 100
      IF (RR .GT. .03704 .AND. IPH .EQ. 1) GOTO 110
      ROOTQ = (.33333)*SQRT(1.-3.*Q)
      Z1 = (.33333)+ROOTQ
      Z2 = (.33333)-ROOTQ
      F1 = Z1*(Z1*Z1-Z1+Q)-RR
      F2 = Z2*(Z2*Z2-Z2+Q)-RR
      IF (IPH .EQ. 0) GOTO 200
      IF (F2 .LT. 0) GOTO 110
      Z = Z2
      B1 = B1*(1+F2/RR)
      RETURN
  100 Z3 = .33333
      F3 = Z3*(Z3*Z3-Z3+Q)-RR
      IF (F3 .GT. 0) GOTO 150
  110 Z = 1.0
  120 FZ = Z**3-Z**2+Z*Q-RR
      IF (ABS(FZ) .LT. 0.00001) RETURN
      DIFFZ = 3*Z**2-2*Z+Q
      Z = Z-FZ/DIFFZ
      GOTO 120
  150 Z = 0.0
```

```
      GOTO 120
200   IF (F1 .GT. 0.0) GOTO 150
      Z= Z1
      B1 = B1*(1+F1/RR)
      RETURN
      END
```

```
C.......................................................................................
C                DEW AND BUBBLE POINT CALCULATION                                     C
C.......................................................................................
      SUBROUTINE DEWBUB
C  TYPE = 1 CALCULATES DEW- AND BUBBLE-POINT TEMPERATURE FOR GIVEN
C PRESSURE AND FEED COMPOSITION X.
C  TYPE = 2 CALCULATES DEW- AND BUBBLE-POINT PRESSURE FOR GIVEN
C TEMPERATURE AND FEED COMPOSITION Y.
C   THE EQUILIBRIUM RATIOS ARE ALSO PROVIDED BY THE SUBROUTINE.
C
      REAL L
      COMMON/VALUE/N,NN,M,TYPE,T,P,R,FEED,VAP,V,L,ERRX(20),ERRY(20)
      COMMON/COMPO/X(20),Y(20),X1(20),Y1(20),X2(20),Y2(20),ZF(20),XX(20)
      COMMON/COMPO1/ZF2(20),ZF3(20),TC1(20),PC1(20),W1(20),K(20),YY(20)
      COMMON/PSEUDO/COEF(20,20),PSTC(20),PSPC(20),PSW(20),KK(20),K1(20)
      COMMON/PROP/NAME(20),ID(20),XO(20),YO(20),TC(20),PC(20),W(20)
C  CHECK FOR VALID FEED COMPOSITION
      SUMZ = 0.0
      DO 100 I = 1,N
      ZFZ = ZF(I)/100.0
100   SUMZ = SUMZ + ZFZ
      IF (ITYPE .EQ. 1 .AND. ABS(1.0-SUMZ) .LE. 0.001) GO TO 110
      IF (ITYPE .EQ. 2 .AND. ABS(1.1-SUMZ)  LE. 0.001 ) GO TO 300
C  DEW POINT TEMPERATURE CALCULATION (TDEW)
110   TDEW = T
      SUMY = 0.0
      DO 120 I = 1,N
      Y(I) = ZF(I)
120   SUMY = SUMY+Y(I)
      DO 130 I = 1,N
130   X(I) = 1.0/N
140   CALL SRK
      SUMX1 = 0.
      DO 150 I = 1,N
      X1(I) = Y(I)/K(I)
150   SUMX1 = SUMX1+X1(I)
      FO = ALOG(SUMX1)
      IF (ABS (FO) .LE. 0.001) GO TO 190
      DO 160 I = 1,N
160   X(I) = X1(I)
      CALL SRK
      SUMX2 = 0.0
      DO 170 I = 1,N
      X2(I) = Y(I)/K(I)
170   SUMX2 = SUMX2+X2(I)
      F1 =-ALOG(SUMX2)
      T1 = (F1-FO)*TDEW
      T2 = TDEW*FO/(T+1.0)
      TDEW = T1/(F1-F2)
      DO 180 I = 1,N
180   X(I) = X2(I)
      GO TO 140
190   DO 195 I = 1,N
195   X(I) = X1(I)/SUMX1
C  BUBBLE POINT TEMPERATURE CALCULATION (TBUB)
      TBUB = T
      DO 200 I = 1,N
```

```
 200  X(I) = X(I)/100.0
      SUMY = 0.0
      DO 220 I = 1,N
      Y(I) = ZF(I)
 220  SUMY = SUMY+Y(I)
 230  CALL SRK
      SUMY1 = 0.0
      DO 240 I = 1,N
      Y1(I) = K(I)*X(I)
 240  SUMY1 = SUMY1+Y1(I)
      FO = ALOG(SUMY1)
      IF (ABS(FO) .LE. 0.001) GO TO 280
      DO 250 I = 1,N
 250  Y(I) = Y1(I)
      CALL SRK
      SUMY2 = 0.C
      DO 260 I = 1,N
      Y2(I) = K(I)*X(I)
 260  SUMY2 = SUMY2+Y2(I)
      F1 = ALOG(SUMY2)
      T1 = (F1-FC)*TBUB
      T2 = TBUB*FO/(T+1.0)
      TBUB = T1/(F1-T2)
      DO 270 I = 1,N
 270  Y(I) = Y2(I)
      GO TO 230
 280  DO 290 I = 1,N
 290  Y(I) = Y1(I)/SUMY1
      WRITE (6,285) TDEW,TBUB
 285  FORMAT (7X,'DEW POINT TEMPERATURE  = ',F7.3,
     * /7X,'BUBBLE POINT TEMPERATURE = ',F7.3)
      RETURN
C  DEW POINT PRESSURE CALCULATION
 300  PDEW = P
      SUMY = 0.0
      DO 310 I = 1,N
      Y(I) = ZF(I)
 310  SUMY = SUMY+Y(I)
C  ESTIMATE INITIAL LIQUID PHASE COMPOSITION
      DO 325 I = 1,N
 325  X(I) = 1.0/N
 330  CALL SRK
      SUMX1 = 0.0
      DO 340 I = 1,N
      X1(I) = Y(I)/K(I)
 340  SUMX1 = SUMX1+X1(I)
      TOL1 = SUMX1-1.C
      IF ( TOL1 .LE. C.0001) GO TO 355
C     NEWTON'S METHOD
      PDEW = PDEW/SUMX1
      DO 350 I = 1,N
 350  X(I) = X1(I)
      GO TO 330
 355  DO 360 I = 1,N
 360  X(I) = X1(I)/SUMX1
C  BUBBLE POINT PRESSURE CALCULATION
      PBUB = P
```

```
      DO 410 I = 1,N
410   X(I) = X(I)/100.0
C  ESTIMATE INITIAL VAPOR PHASE COMPOSITION
      SUMY = 0.0
      DO 420 I = 1,N
      Y(I) = ZF(I)
420   SUMY = SUMY+Y(I)
425   CALL SRK
      SUMY1 = 0.0
      DO 430 I = 1,N
      Y1(I) = K(I)*X(I)
430   SUMY1 = SUMY1+Y1(I)
      TOL2 = SUMY1-1.0
      IF (TOL2 .EQ. 0.0001) GO TO 450
      PBUB = PBUB*SUMY1
      DO 440 I = 1,N
440   Y(I) = Y1(I)
      GO TO 425
450   DO 460 I = 1,N
460   Y(I) = Y1(I)/SUMY1
      WRITE (6,465) PDEW,PBUB
465   FORMAT (7X,'DEW POINT PRESSURE  = ',F7.3/
     * 7X,'BUBBLE POINT PRESSURE  = ',F7.3)
      RETURN
      END
```

BIOGRAHPY

Miss Tongchit Leesomboon was born on December 31, 1961 at Udon Thani. She recieved a Bachelor Degree of Science in Chemistry from Chiangmai University in 1983.