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APPENDIX

MAIN PROGRAM AND SUBROUTINE

Program COEF is the main program that reads the control parameters for the optimization,inputs the pure component properties, binary equilibrium data.

Subroutine BULBP this subroutine does bubble point pressure calculation for each data point by calling subroutine PHIMIX . The squares of bubble pressure deviation ratio are provides for subroutine FOBR and FOBN

Subroutine BRACK this subroutine is used to locate two values of a single variable (binary interaction parameter) between which the objective function has a minimum.

Subroutine FIBO this subroutine is used to locate the optimum of a single variable (here it is binary interaction parameter) objective function. The subroutine returns a final interval of uncertainty, and if desired, an estimate of the optimal value of the variable obtained by quadratic interpolation.

Function FOBR this function calculates the objective function assigned. It sum up the squares of deviation provided by subroutine FOBN

Function FOBN this is a nagative funtion of FOBR

Subroutine PHIMIX this subroutine calculates vapor and liquid phases fugacity coefficients of both components in the binary mixture by the Graboski and Daubert version of SRK, or the original SRK, or the Peng and Robinson equation of state. Compressibility factors and molar volumes in both vapor and liquid phases calculate by calling NUM

Subroutine NUM this subroutine solves a cubic equation using a Newton convergence technique.

```
C     ***************************************************************
C     *
C     ***************     MAIN  PROGRAM  IDENTIFICATION     ***************
C     *
C     *       THIS MAIN PROGRAM DRIVES SUBROUTINE BRACK AND FIBO TO
C     *       SEARCH OPTIMUM BINARY INTERACTION CONSTANT.THE OPTION
C     *       OF GRA,SRK OR PR EQUATIONS OF STATE ARE USED FOR BOTH
C     *       VAPOR AND LIQUID PHASES OF BUBBLE POINT PRESSURE
C     *       CALCULATION.
C     *
C     ***************************************************************
C     *
C     ***************     VARIABLE IDENTIFICATION     ***************
C     *
C     *******                 CONTROL PARAMETER                 *******
C     *
C     *       IEQ             = TYPE OF EQUATION OF STATE.
C     *                 0     = PENG AND ROBINSON (PR)
C     *                 1     = SOAVE
C     *                 2     = GRABOSKI AND DAUBERT (GRA)
C     *                 3     = LEIVA
C     *                 4     = ISHIKAWA (ISHI)
C     *       ICAL              = CALCULATION OPTION IDENTIFICATION
C     *                 0     = OPTIMIZATION
C     *                 1     = CALCULATION ONLY
C     *
C     *******              CONSTANT IDENTIFICATION              *******
C     *
C     *       HV              = THE DESIRED FINAL INTERVAL IF UNCERTAINTY
C     *                         TRY 0.0001
C     *       AXO             = STARTING VALUE OF SEARCHING PARAMETER.
C     *                         TRY 0    OR -0.3
C     *       AXF             = LIMITING VALUE OF SEARCHING PARAMETER.
C     *                         TRY 0.25 OR 0.
C     *       DAX             = INITIAL STEP SIZE ,TRY 0.01
C     *
C     *******                SIMPLE VARIABLE                *******
C     *
C     *       COMP            = NAME OF COMPONENT
C     *       NDATA           = NUMBER OF DATA POINTS
C     *       NCOMP           = NUMBER OF COMPONENTS
C     *       NSUP            = NUMBER OF SUPERCRITICAL COMPONENTS
C     *       NSUB            = NUMBER OF SUBCRITICAL COMPONENTS
C     *       T               = TEMPERATURE                 ; DEG K
C     *       P               = PRESSURE                    ; ATM
C     *       V               = MOLAR VOLUME                ; CC/G MOLE
C     *
C     *******                ARRAY IDENTIFICATION                ********
C     *
C     *       TC              = CRITICAL TEMPERATURE        ; DEG K
C     *       PC              = CRITICAL PRESSURE           ; ATM
C     *       VC              = CRITICAL VOLUME             ; CC/G MOLE
C     *       W               = PITZER ACENTIC FACTOR
C     *       KIJ             = BINARY INTERACTION PARAMETER
C     *       X               = LIQUID MOLE FRACTION
C     *       Y               = VAPOR  MOLE FRACTION
C     *       K               = VAPOR LIQUID EQUILIBRIUM RATIO
C     *
C     ********             SUBROUTINE  AND FUNCTION NAME             ******
C     *
C     *         BRACK         = BRACKET INTERVAL OF KIJ
C     *         FIBO          = COMPUTES OPTIMUM KIJ
C     *         BULBP         = COMPUTES BUBBLE POINT PRESSURE
C     *
C     ***************************************************************
C     *
C     *       WRITTEN BY A. SAWANGPHANYANGKUL:  FEB,1986
C     *
C     ***************************************************************
```

```
      CHARACTER *80 TITLE1,TITLE2
      CHARACTER * 15 COMP
      REAL K1CAL,K2CAL,K1EXP,K2EXP
      COMMON/AA/XEXP(2),YCAL(2),PHIV(2),PHIL(2),P
      COMMON/A /VC(2)
      COMMON/BB/COMP(2)
      COMMON/CC/TC(2),PC(2),W(2)
      COMMON/DD/PEXP(200),Y1EXP(200),X1EXP(200)
      COMMON/EE/NDATA
      COMMON/II/ COA(2,3),COB(2,3),CONA(2),CONB(2)
      COMMON/IC/IZ
      COMMON/WW/NSUB,TR(2),WA(2),WB(2)
      COMMON/P_IKE/BI(2),AIJ(2,2)
      COMMON/STATE/R,T
      COMMON/PRIA/VVCAL,VLCAL
      COMMON/EPSC/IEQ,MDC
      EXTERNAL FOBR
      EXTERNAL FOBN
      ICAL = 1
C---- READ THE TITLE CARD
      READ(5,150) TITLE1
  150 FORMAT(A80)
C---- READ CONTROL PARAMETERS
      READ(5,170) IEQ,IZ
  170 FORMAT(2I3)
      READ(5,180) AXO,AXF,DAX,HN
  180 FORMAT(4F10.0)
         AMNHX= 1.0
      WRITE(6,190) AXO,AXF,DAX,HN
  190 FORMAT(1H1,///,28X,'SEARCH OPTIMUM BINARY INTERACTION (KIJ),WITH'/
     1/,35X,'AXO         =         ',F8.4/,35X,'AXF         =         ',F8.4/
     2 ,35X,'DAX         =         ',F8.4/,35X,'HN          =         ',F8.4)
      WRITE(6,200)
  200 FORMAT(///,20X,'          PURE COMPONENT PHYSICAL PROPERTIES'//10X,
     1'      NO.       COMPONENT      PC(ATM)       TC(DEG K)       VC(CC/MO
     2LE)          W')
C---- READ AND WRITE PURE COMPONENT PHYSICAL PROPERTIES
      DO 5 I=1,2
      READ(5,210) PC(I),TC(I),VC(I),W(I),COMP(I)
  210 FORMAT(4F10.4,A15)
      WRITE(6,220) I,COMP(I),PC(I),TC(I),VC(I),W(I)
  220 FORMAT(15X,I2,7X,A10,3(F10.1,5X),F10.3)
    5 CONTINUE
C
           R      = 82.057
```

```
      6     READ(5,230) NDATA,TITLE2
    230     FORMAT(I3,A60)
            IF(NDATA .EQ. 0) STOP
            READ(5,300) TEMP
    300     FORMAT(F10.2)
                 T      =  TEMP+273.16
            NSUP = 0
            DO 10 I=1,2
                 TR(I)  =  T/TC(I)
            IF(TR(I) .GT. 1.0) NSUP=NSUP+1
     10     CONTINUE
      C
      C------CALCULATE WA,WB FOR SUPERCRITICAL COMPONENTS
            IF(NSUP .EQ. 0) GOTO 40
      C
            IF(IEQ .GT. 0) GOTO 20
            DO 15 I=1,NSUP
                 WA(I)  =  0.42747
                 WB(I)  =  0.08664
     15     CONTINUE
            GOTO 40
     20     IF(IEQ .EQ. 4) GOTO 30
            DO 25 I=1,NSUP
                 WA(I)  =  0.45724
                 WB(I)  =  0.07780
     25     CONTINUE
            GOTO 40
     30     DO 35 I=1,NSUP
                 WA(I)  =  0.467123
                 WB(I)  =  0.108762
     35     CONTINUE
      C      CALCULATE WA,WB FOR SUBCRITICAL COMPONENTS
     40     IF(NSUP .EQ. 2) GOTO 50
            NSUP =  NSUP+1
            IF(IEQ .EQ. 1) GOTO 41
            IF(IEQ .EQ. 2) GOTO 42
            IF(IEQ .EQ. 3) GOTO 43
            IF(IEQ .EQ. 4) GOTO 44
            CALL PR
            GOTO 45
     41     CALL SOAVE
            GOTO 45
     42     CALL GRA
            GOTO 45
     43     CALL LEIVA
            GOTO 45
     44     CALL ISHI
     45     WRITE(6,111)
    111     FORMAT(1H1,/////,40X,'WA',8X,'WB',/)
            DO 50 I=1,2
            WRITE(6,222) COMP(I),WA(I),WB(I)
     50     CONTINUE
    222     FORMAT(25X,A10,2F10.5)
      C      CALCULATE A AND B FOR PURE COMPONENTS
            DO 55 I=1,2
                 BI(I)  =    WB(I)*R*TC(I)/PC(I)
                AIJ(I,I)  =    WA(I)*R*R*TC(I)*TC(I)/PC(I)
```

```
 55   CONTINUE
C------READ AND WRITE INPUT DATA
 65    DO 70 I=1,NDATA
       READ(5,320) PEXP(I)
       READ(5,320) Y1EXP(I)
       READ(5,320) X1EXP(I)
 320   FORMAT(F10.0)
 70    CONTINUE
C
C----   SKIP OPTIMIZATION PART IF ICAL=1
       IF (ICAL .EQ. 1) GOTO 75
C------ OPTIMIZE INTERACTION CANSTANT
       CALL BRACK(FOBN,AXO,AXF,DAX,AX1,FB1,AX2,FB2,AX3,FB3,IERR)
       CALL FIBO(FOBR,AMNMX,AX1,AX3,HN,BX1,BX4,BXM,BYM)
C
C
 75    WRITE(6,350) TITLE1
 350   FORMAT(1HL,///,5X,'EXPERIMENTAL AND CALCULATED RESULTS FOR BINARY
      *SYSTEM, ',A40/100('-')/27X,'EXPERIMENTAL',15X,
      *' CALCULATED',15X,'DEVIATIONS'/21X,25(' '),5X,15(' '),5X,25(' ')
      */5X,'T(K)',12X,'P,ATM',6X,'Y1',8X,'X1',8X,'P,ATM',6X,'Y1',8X,'P',
      *6X,'DP/P',7X,'Y1'/100('-'))
       WRITE(6,355) T
 355   FORMAT(2X,F7.2)
C
C
C ---- CALCULATE PREDICTED VALUES AND STATISTIC NUMBERS --
          SMDP2   =  0.0
          SMDPR2  =  0.0
          SMDY2   =  0.0
          SMDP    =  0.0
          SMDPR   =  0.0
          SMDY    =  0.0
C
       DO 80 I=1,NDATA
          BXM     =  0.1021
       CALL BUBBP(BXM,FB,I)
          DP      =  PEXP(I) - P
          DP2     =  DP*DP
          DPR     = (DP/PEXP(I))*100.0
          DPR2    =  DPR*DPR
          DY      =  Y1EXP(I)- YCAL(I)
          DY2     =  DY*DY
C
          SMDP2   =  SMDP2  + DP2
          SMDPR2  =  SMDPR2 + DPR2
          SMDY2   =  SMDY2  + DY2
          SMDP    =  SMDP   + ABS(DP)
          SMDPR   =  SMDPR  + ABS(DPR)
          SMDY    =  SMDY   + ABS(DY)
C
       WRITE(6,360) I,PEXP(I),Y1EXP(I),X1EXP(I),P,YCAL(I),DP,DPR,DY
 360   FORMAT(14X,I2,F10.2,2F10.4,F10.2,F10.4,2F10.2,F10.4)
 80    CONTINUE
C
       WRITE(6,333)
 333   FORMAT(100('-'))
```

```
C
C         RMSD      =  SQRT(BYM/NDATA)
          RMDP      =  SQRT(SMDP2/NDATA)
          RMDPR     =  SQRT(SMDPR2/NDATA)
          RMDY      =  SQRT(SMDY2/NDATA)
C
          EP        =  SMDP/NDATA
          EPR       =  SMDPR/NDATA
          EY        =  SMDY/NDATA
C
          WRITE(6,370) EP,EPR,EY
  370     FORMAT(5X,'AVG. ERROR',51X,2F10.2,F10.4)
          WRITE(6,380) RMDP,RMDPR,RMDY
  380     FORMAT(5X,'ROOT MEAN SQUARE DEVIATION',35X,2F10.2,F10.4/100('_'))
C------   WRITE NOTES
          WRITE(6,400)
  400     FORMAT(////,25X,'** NOTE **')
          IF(ICAL .EQ. 0) WRITE(6,420) BXM
  420     FORMAT(20X,'BINARY INTERACTION CONSTANT EVALUATION',/,
         *20X,'OPTIMAL BINARY INTERACTION CONSTANT =',E12.5)
          IF(ICAL.EQ.1) WRITE(6,450) BXM
  450     FORMAT(20X,'CALCULATED AT BINARY INTERACTION CONSTANT =',F8.4)
          IF(IEQ .EQ. 0) WRITE(6,600)
          IF(IEQ .EQ. 1) WRITE(6,610)
          IF(IEQ .EQ. 2) WRITE(6,620)
          IF(IEQ .EQ. 3) WRITE(6,630)
          IF(IEQ .EQ. 4) WRITE(6,640)
          WRITE(6,670) TITLE2
          GOTO 6
  600     FORMAT(20X,'PR EQUATION OF STATE')
  610     FORMAT(20X,'ORIGINAL SRK EQUATION OF STATE')
  620     FORMAT(20X,'GRA EQUATION OF STATE')
  630     FORMAT(20X,'LEIVA EQUATION OF STATE')
  640     FORMAT(20X,'ISHI EQUATION OF STATE')
  670     FORMAT(11X,A80)
          END
C
```

```
      SUBROUTINE BULBP(AX,FB,II)
C     ******************************************************************
C     *                                                                *
C     *  THIS SUBROUTINE DOES BUBBLE POINT PRESSURE CALCULATION FOR    *
C     *  EACH DATA POINT. IT CALCULATES BUBLLE PRESSURE DEVIATION,     *
C     *  BUBBLE PRESSURE AND VAPOR PHASE COMPOSITION.                  *
C     *                                                                *
C     *  SUBROUTINE USED : PHIMIX                                      *
C     *                                                                *
C     ******************************************************************
      COMMON/AA/XEXP(2),YCAL(2),PHIV(2),PHIL(2),P
      COMMON/CC/TC(2),PC(2),W(2)
      COMMON/DD/PEXP(200),Y1EXP(200),X1EXP(200)
      COMMON/PRIA/VVCAL,VLCAL
      COMMON/EPSC/IEQ,MDC
C     DIMENSION CRC(2)
C
          XEXP(1)   =  X1EXP(II)
          XEXP(2)   =  1.0 - XEXP(1)
C------ INITIAL ESTIMATE OF P, ATM
                P   =  PEXP(II)
C------ INITIALIZE PHIV TO ONE
      DO 70 K=1,2
        PHIV(K)   =  1.0
   70 CONTINUE
      NLAP = 0
   80 CONTINUE
C------ CALCULATE VAPOR PHASE MOLE FRACTIONS AND TOTAL PRESSURE
          YSUM      =  0.0
      CALL PHIMIX(P,XEXP,IEQ,AX,0,PHIL,VL,ZL)
      DO 90 K=1,2
          YCAL(K)   =  PHIL(K)*XEXP(K)/PHIV(K)
          YSUM      =  YSUM + YCAL(K)
   90 CONTINUE
C
C------ CHECK CONVERGENCE OF Y
      IF( ABS(YSUM-1.0) .LE. 0.0001) GOTO 110
            P       =  P*YSUM
C------ NORMALIZE Y
      DO 95 K=1,2
        YCAL(K)   =  YCAL(K)/YSUM
   95 CONTINUE
      CALL PHIMIX(P,YCAL,IEQ,AX,1,PHIV,VV,ZV)
       NLAP = NLAP+1
      IF(NLAP.GT.35) GOTO 100
      GOTO 80
  100 WRITE(6,101)
  101 FORMAT(20X,'OVER 35 NLAP IN BULBP')
  110 CONTINUE
                VVCAL     =  VV
                VLCAL     =  VL
                 DPR      =  1.0 - P/PEXP(II)
                 DY       =  Y1EXP(II) - YCAL(1)
                 FB       =  DPR*DPR + DY*DY
   31 RETURN
      END
```

```
      SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
C*************************************************************
C  PURPOSE :   CALCULATE THE FUGACITY COEFFICIENTS OF EITHER
C              A GAS OR LIQUID PHASE.
C
C          P,Y,T,IEQ,CRC,FK,NOP,MUST KNOW AS CALLING
C
C          P       = PRESSURE. ATM
C          Y       = VAPOR OR LIQUID PHASE MOLE FRACTIONS
C          T       = TEMPERATURE . DEG KELVIN
C          IEQ     = IDENTIFICATION NUMBER OF EQUATION OF STATE
C     *        0   = PR
C     *        1   = SRK
C     *        2   = GRA
C     *        3   = LEIVA
C     *        4   = ISHI
C
C*************************************************************
      REAL LZB,LZAB,LVBV,LB2V
      COMMON/STATE/R,T
      COMMON/PURE/BI(2),AIJ(2,2)
      COMMON/CC/TC(2),PC(2),W(2)
      COMMON/IC/IZ
      DIMENSION Y(2),PHILN(2),PHI(2),AI(2),COF(4)
C
C------CALCULATE A AND B FOR BINARY MIXTURE
 10         AM          =  0.0
            BM          =  0.0
      DO 25 I=1,2
            AI(I)       =  0.0
            BM          =  BM+Y(I)*BI(I)
      DO 25 J=1,2
      IF(J .EQ. I) GOTO 15
            AIJ(I,J) =  SQRT(AIJ(I,I)*AIJ(J,J))*(1.0-FK)
      GOTO 20
 15         AIJ(I,J) =  AIJ(I,I)
 20         AI(I)       =  AI(I) + Y(J)*AIJ(I,J)
            AM          =  AM + Y(I)*Y(J)*AIJ(I,J)
 25   CONTINUE
      IF(IEQ .EQ. 0) GOTO 50
            PBRT     =  P*BM/(R*T)
            PBRT2    =  PBRT*PBRT
            ABRT     =  P*AM/(R*T*R*T)
              PP     =  1.0
              QQ     =  ABRT-PBRT-PBRT2
              RR     =  ABRT*PBRT
         CALL NUM(QQ,RR,IPH,PBRT,Z)
C------CALCULATE MOLAR VOLUME
            V        =  Z*R*T/P
C------ CALCULATE FUGACITY COEFFICIENTS OF COMPONENTS
C             LIQUID PHASE  IPH=0
C             VAPOR PHASE   IPH=1
C------
            ZB       =  (Z-1.0)/BM
            ZPB      =  Z-PBRT
            ZPZ      =  1.0+PBRT/Z
      IF(ZPB .LE. 0.0 .OR. ZPZ .LE. 0.0) GOTO 80
```

```
      LZB    =    ALOG(ZPB)
      LZAB   =    ALOG(ZPZ)*ABRT/PBRT
      DO 30 I=1,2
      PHILN(I) =  BI(I)*ZB-LZB-(2.0*AI(I)/AM-BI(I)/BM)*LZAB
      IF(PHILN(I) .LT. -174.0) PHILN(I)=-174.0
      IF(PHILN(I) .LT. 174.0) GOTO 29
      WRITE(6,100)
      PHILN(I)   =    0.0
   29 PHI(I)     =    EXP(PHILN(I))
   30 CONTINUE
  100 FORMAT(10X,'LOG OF PHI .GT. 174 IN PHIMIX,PHI SET TO 1')
      RETURN
C
C-------- FOR PENG AND ROBINSON EQUATION OF STATE(1976)
   50 PBRT     =    P*BM/(R*T)
      PBRT2    =    PBRT*PBRT
      PBRT3    =    PBRT2*PBRT
      ABRT     =    P*AM/(R*T*R*T)
      PP       =    (1.0-PBRT)
      QQ       =    ABRT-(3.0*PBRT2)-(2.0*PBRT)
      RR       =    ABRT*PBRT-PBRT2-PBRT3
      CALL NUMP(PP,QQ,RR,IPH,PBRT,Z)
C
      V        =    Z*R*T/P
C     PRINT,' V    =',V
      ZB       =   (Z-1.0)/BM
      ZPB      =    Z-PBRT
      ZPZ      =   (Z+2.414*PBRT)/(Z-0.414*PBRT)
      IF(ZPB .LE. 0.0 .OR. ZPZ .LE. 0.0) GOTO 80
      LZB      =    ALOG(ZPB)
      LZAB     =    ALOG(ZPZ)*(ABRT/(2.828427*PBRT))
      DO 60 I=1,2
      PHILN(I) =    BI(I)*ZB-LZB-(2.0*AI(I)/AM-BI(I)/BM)*LZAB
      IF(PHILN(I) .LT. -174.0) PHILN(I)=-170.0
      IF(PHILN(I) .LT. 174.0) GOTO 59
      WRITE(6,100)
      PHILN(I)   =    0.0
   59 PHI(I)     =    EXP(PHILN(I))
   60 CONTINUE
      RETURN
C
C-------ERROR ADJUSTMENT
   80 DO 90 I=1,2
      IF(IPH .EQ. 1) PHI(I)=1.0
      IF(IPH .EQ. 0) PHI(I)=0.2
   90 WRITE(6,200) I,PHI(I)
  200 FORMAT(10X,'NAGATIVE LOG CALCD IN PHIMIX, PHI(',I1,')=',F4.1,
     *'ASSUMPTION WAS FORCED TO MAKE.')
      RETURN
      END
C
```

```
      SUBROUTINE NUM(QQ,RR,IPH,PBRT,Z)
C
C     PURPOSE :    SOLVES CUBIC EQUATION OF STATES (SOAVE EOS)
C                  FOR COMPRESSIBILITY FACTORS.
C                  THE ALGORITHM IS BASED ON T. GUNDERSEN(1982).
C
        FZ3 = (1./3.)**3 - (1./3.)**2 + QQ*(1./3.) - RR
      IF(QQ .GT. 1./3. .AND. FZ3 .GT. 0.) GOTO 40
      IF(QQ .GT. 1./3. .AND. FZ3 .LT. 0.) GOTO 50
      IF(RR .GT. 1./27. .AND. IPH .EQ. 1) GOTO 50
         Z1 = 1./3. - 1./3.*SQRT(1.0-3.0*QQ)
         Z2 = 1./3. + 1./3.*SQRT(1.0-3.0*QQ)
        FZ1 = Z1*Z1*Z1 - Z1*Z1 + Z1*QQ - RR
        FZ2 = Z2*Z2*Z2 - Z2*Z2 + Z2*QQ - RR
      IF(IPH .NE. 0) GOTO 20
      IF(FZ1 .GT. 0.0) GOTO 40
         Z = Z1
       PBRT = PBRT*(1.0 + FZ1/RR)
      PRINT,'LIQUID ROOT WAS FOUND BUT WAS NOT REAL '
      GOTO 60
20    IF (FZ2 .LT. 0.0) GOTO 50
         Z = Z2
       PBRT = PBRT*(1.0 + FZ2/RR)
      PRINT,'VAPOR ROOT WAS FOUND BUT WAS NOT REAL '
      GOTO 60
C        SOLVE CUBIC EQUATION BY NEWTON-RAPHSON METHOD
C        INITIAL VALUE:    Z = 0.0  , FOR IPH = 0
C                          Z = 1.0  , FOR IPH = 1
C
40       Z = 0.0
      NLOOP = 0
      GOTO 52
50       Z = 1.0
      NLOOP = 0
52    NLOOP = NLOOP+1
      IF (NLOOP .GT. 25) GOTO 55
         FZ = Z*Z*Z - Z*Z + Z*QQ - RR
         SLOPE = (3.0*Z*Z - 2.0*Z + QQ)
         ZN = Z-(FZ/SLOPE)
         ERR = ABS((ZN-Z)/ZN)
          Z = ZN
      IF(ERR .LE. 0.000001) GOTO 60
      GOTO 52
55    WRITE(6,100)
100   FORMAT(10X,'OVER 25 LOOPS OF NEWRAP CALCULATIONS')
60    WRITE(6,150) IPH,QQ,RR
      WRITE(6,200) Z
150   FORMAT('0     ROOTS OF CUBIC EQUATION ,WITH'/
     1       '0     IPH      = ',I3/6X,'0     QQ       = ',F12.8/
     2       '      RR       = ',F12.8)
200   FORMAT('0     Z        = ',F12.8)
      RETURN
      END
```

```
      SUBROUTINE ANAL(PP,QQ,RR,IPH,Z)
C-----------------------------------------------------------------------
C     PURPOSE :     SOLVES CUBIC EQUATION OF STATES (SOAVE EOS)
C                   FOR COMPRESSIBILITY FACTORS.
C                   BY ANALYTICAL METHOD.
C-----------------------------------------------------------------------
      DIMENSION A(4),B(3),ZZ(3)
        A(1) = 1.0
        A(2) = PP
        A(3) = QQ
        A(4) = RR
C     WRITE(6,105)
C 105 FORMAT('0 ---- CASE 0'/
C    1       'THERE ARE 3 REAL ROOTS'/
C    2       'THIS CASE DOES NOT OCCUR IN RK EQ.'/
C    3       '0       CASE 1'/
C    4       'THERE IS ONLY ONE REAL ROOT'/
C    5       'WHICH GIVES THE Z IN THE MONO PHASE'///)
      B(1) = A(2)/A(1)
      B1OV3 = B(1)/3.0
      B(2)  = A(3)/A(1)
      B(3)  = A(4)/A(1)
        ALF   = B(2)-B(1)*B1OV3
        BET   = 2.0*B1OV3**3-B(2)*B1OV3+B(3)
        BETOV2 = BET/2.0
        ALFOV3 = ALF/3.0
        CU3OV3 = ALFOV3**3
        SQBOV2 = BETOV2**2
        DEL    = SQBOV2+CU3OV3
      IF(DEL)40,20,30
   20 MTYPE=0
      GAM=SQRT(-ALFOV3)
      IF (BET) 22,22,21
   21   ZZ(1)  = -2.0*GAM B1OV3
        ZZ(2)  = GAM-B1OV3
        ZZ(3)  = ZZ(2)
      GOTO 50
   22   ZZ(1)  = 2.0*GAM-B1OV3
        ZZ(2)  =-GAM-B1OV3
        ZZ(3)  = ZZ(2)
      GOTO 50
   30 MTYPE=1
      EPS  =  SQRT(DEL)
      TAU  =  BETOV2
      RCU  =  TAU+EPS
      SCU  =  TAU EPS
      SIR=1.0
      SIS=1.0
      IF(RCU) 31,32,32
   31 SIR= 1.0
   32 IF (SCU) 33,34,34
   33 SIS= 1.0
   34 RS  = SIR*(SIR*RCU)**0.33333333
      S   = SIS*(SIS*SCU)**0.33333333
        ZZ(1)  = RS+S-B1OV3
        ZZ(2)  = -(RS+S)/2.0 B1OV3
        ZZ(3)  = 0.86602540*(RS-S)
```

```
      GOTO 50
   40 MTYPE= 1
      QUOT   = SOBOV2/CUAOV3
      ROOT   = SQRT(-QUOT)
      IF(DET) 42,41,41
   41 PEI    = (1.5707963 + ATAN(ROOT/SQRT(1.0 - ROOT**2)))/3.0
      GOTO 43
   42 PEI    =  ATAN(SQRT(1.0 ROOT**2)/ROOT)/3.0
   43 FACT   =  2.0*SQRT(-ALFOV3)
        ZZ(1)  = FACT*COS(PEI)-B1OV3
        ZZ(2)  = FACT*COS(PEI+2.094395) B1OV3
        ZZ(3)  = FACT*COS(PEI+4.188790)-B1OV3
C     WRITE(6,110) IPH,A(3),A(4)
C     WRITE(6,120) ZZ(1),ZZ(2),ZZ(3)
   50 IF(IPH) 80,80,55
   55 IF(MTYPE) 60,70,70
   60 Z=AMAX1(ZZ(1),ZZ(2),ZZ(3))
C     WRITE(6,130) Z
      GOTO 200
   70   Z  = ZZ(1)
C     WRITE(6,140) Z,MTYPE
      GOTO 200
   80 IF(MTYPE) 90,95,95
   90   Z  = AMIN1(ZZ(1),ZZ(2),ZZ(3))
C     WRITE(6,150) Z
      GOTO 200
   95   Z  = ZZ(1)
C     WRITE(6,160) Z,MTYPE
  200 RETURN
C 110 FORMAT('0     ROOTS OF CUBIC EQUATION,WITH'/
C    1       '0     IPH      =',I1/6X,'Q        =',F12.8/
C    2       '      R        =',F12.8)
C 120 FORMAT('0     Z(1)     =',F12.8/6X,'Z(2)     =',F12.8/
C    1       '      Z(3)     =',F12.8)
C 130 FORMAT('0     ZV       =',F12.8,' (MAX. VALUE)')
C 140 FORMAT('0     ZV       =',F12.8,' (CASE',I2,')')
C 150 FORMAT('0     ZL       =',F12.8,' (MIN. VALUE)')
C 160 FORMAT('0     ZL       =',F12.8,' (CASE',I2,')')
      END
```

```
      SUBROUTINE FIBO(Y,AMNMX,A,B,HN,X1,X4,XM,YM)
      DIMENSION F(26)
      DATA F/1.,1.,2.,3.,5.,8.,13.,21.,34.,55.,89.,144.,233.,377.,610.,
     *987.,1597.,2584.,4181.,6765.,10946.,17711.,28657.,46368.,75025.,
     *121393./
    1 FORMAT(1H0,'NEED MORE FIBONACCI NUMBERS FOR SPECIFIED ACCURACY.')
    2 FORMAT(1H0//1X,'FIBONACCI SEARCH OVER RANGE(',E11.4,1H,,E11.4,1H)/
     *)
    3 FORMAT(1H ,'RANGE = (',E12.5,1H,,E12.5,1H),5X,'X2,Y2 = (',E12.5,1H
     *,,E12.5,1H),5X,'X3,Y3 = (',E12.5,1H,,E12.5,1H))
    4 FORMAT(1H0,10X,'NOTE THAT THE ESTIMATED OPTIMUM IS A BOUNDARY POIN
     *T.'/)
    5 FORMAT(1H0,//,10X,'QUADRATIC INTERPOLATION FOR FINAL ESTIMATE')
    6 FORMAT(1H0,10X,'FINAL INTERVAL OF UNCERTAINTY = (',E12.5,1H,,E12.5
     *,1H),5X,'LENGTH =',E12.5//10X,'ESTIMATE Y(OPT) =',E12.5,' AT X =',
     *E12.5,//10X,I2,' TRIALS REQUIRED'/)
      ICD  = 1
      IPRNT= 1
      X1=A
      X4=B
      K=2
      Y1=1.0E10
      Y4=1.0E10
      H1=B-A
      GOTO (15,20),ICD
   15 HR=0.5*HN/H1
      GOTO 25
   20 HR=HN/H1
   25 DO 30 J=3,26
      IF(F(J)/F(J-1)-HR) 35,35,30
   30 CONTINUE
      WRITE(6,1)
      STOP
   35  N=J
      GOTO (40,41),IPRNT
   40 WRITE(6,2) A,B
      NT=0
   41 NM3=N-3
      DO 200 M=1,NM3
      MM=N-M+1
      S=F(MM)*H1/F(N)
      GOTO (50,50,70),K
   50 X2=X1+S
      Y2=Y(X2)*AMNMX
      GOTO(55,60),IPRNT
   55 GOTO (57,70),K
   56 NT=NT+1
      YY=Y2*AMNMX
      YZ=Y3*AMNMX
      WRITE(6,3) X1,X4,X2,YY,X3,YZ
   60 GOTO(80,70,70),K
   70 X3=X4-S
      Y3=Y(X3)*AMNMX
      GOTO (75,80),IPRNT
   75 NT=NT+1
      YY=Y3*AMNMX
      YZ=Y2*AMNMX
```

```
      WRITE(6,3) X1,X4,X2,YZ,X3,YY
   80 IF(Y2-Y3) 90,90,100
   90   K=3
        X1=X2
        Y1=Y2
        X2=X3
        Y2=Y3
        GOTO 200
  100   K=1
        X4=X3
        Y4=Y3
        X3=X2
        Y3=Y2
  200 CONTINUE
        GOTO (210,300,250),K
  210 X2=X3
        Y2=Y3
        IF(Y1-1.0E10) 300,220,300
  220 Y1=Y(X1)*AMNMX
        IF(Y1-Y2) 290,290,225
  225 XM=X1
        YM=Y1
        X4=X3
        WRITE(6,4)
        GOTO 400
  250 IF(Y4-1.0E10) 300,260,300
  260 Y4=Y(X4)*AMNMX
        IF(Y4-Y2) 290,290,270
  270 XM=X4
        YM=Y4
        X1=X2
        WRITE(6,4)
        GOTO 400
  290 XM=X2
        YM=Y2
        GOTO 400
  300 GOTO (310,350),ICD
  310 B1=(Y2-Y1)/(X2 X1)
        B2=((Y4-Y1)/(X4-X1)-B1)/(X4 X2)
        XM=0.5*(X1+X2)-B1/(B2+B2)
        YM=Y(XM)
        GOTO (320,450),IPRNT
  320 NT=NT+1
        WRITE(6,5)
        GOTO 400
  350 DEL=0.01*(X4 X1)
        IF(DEL 1.0E-6) 365,370,370
  365 XM=X2
        GOTO 400
  370 X3=X2+DEL
        Y3=Y(X3)
        GOTO (375,380),IPRNT
  375 NT=NT+1
        YY=Y3*AMNMX
        YZ=Y2*AMNMX
        WRITE(6,3) X1,X4,X2,YZ,X3,YY
  380 IF(Y2-Y3) 385,385,390
```

```
115    385  X1=X2
116         XM=X3
117         YM=Y3
118         GOTO 400
119    390  X4=X3
120         XM=X2
121         YM=Y2
122    400  GOTO (410,450),IPRNT
123    410  H1=X4-X1
124         WRITE(6,6) X1,X4,H1,YM,XM,NT
125    450  RETURN
126         END
```

```
      FUNCTION FOBR(AX)
C     ******************************************************************
C     * THIS FUNCTION CALCULATES OBJECTIVE FUNCTION OF BUBBLE
C     * PRESSURE VARIANCE FOR SUBROUTINE FIBO.
C     * SUBROUTINE USED : FUNB
C     ******************************************************************
      COMMON/EE/NDATA
      FOBR=0.0
      DO 10 J=1,NDATA
      CALL BULP(AX,FB,J)
   10 FOBR=FOBR+FB
      RETURN
      END
C
      FUNCTION FOBN(AX)
C     ******************************************************************
C     * THIS FUNCTION IS THE NAGATIVE FUNCTION OF FOBR. IT CALCULATES
C     * OBJECTIVE FUNCTION OF BUBBLE PRESSURE VCARIANCE FOR SUBROUTINE
C     *-BRACK.
C     ******************************************************************
      FOBN=-FOBR(AX)
      RETURN
      END
```

```
      SUBROUTINE BRACK(F,XO,XF,DX,X1,F1,X2,F2,X3,F3,IERR)
C
C     BRACKETS AN INTERVAL ON X LINE WHICH CONTAINS AN MAXIMUM OF F(X)
C
  997 FORMAT(1H1,////,25X,'     BRACK CALLED ;       XO     =    '
     1,1PE12.5,'     XF     =     ',E12.5/)
  999 FORMAT(30X,'X  = ',1PE12.5,'  F  = ',E12.5)
  996 FORMAT(23X,'        OPTIMUM IS BETWEEN    X     =    ',1PE12.5,'
     1   AND           ',E12.5//30(30X,'           X     =    ',1PE12.5,'
     2     F     =     ',E12.5/))
  995 FORMAT(19X,'OPTIMUM IS AT THE STARTING POINT X  =    ',1PE12.5,' AT
     1WHICH F     =     ',E12.5/40X,'A BETTER VALUE CAN PROBABLY BE FOUND
     2BY CHANGING THE SIGN OF THE INITIAL STEP DX'/)
  994 FORMAT(19X,'EITHER OPTIMUM IS BEYOND THE PRESET LIMIT XF =',E12.5,
     1 'OR F IS MONOTONIC'//30X,'                 X     =    ',E12.5,'
     2     F     =     ',E12.5/)
      IPR=1
      WRITE(6,997) XO,XF
      DX = 0.01
      D=SIGN(1.0,DX)
      XFM=XF*D
      X1=XO
      F1=F(X1)
      X2=X1+DX
      F2=F(X2)
      IF(IPR.EQ.1) WRITE(6,999) X1,F1,X2,F2
      IF(F1-F2) 50,50,200
   50 DX=DX+DX
      X3=X2+DX
      X3M=X3*D
      IF(X3M .GT. XFM) X3=XF
      F3=F(X3)
      IF(IPR .EQ. 1) WRITE(6,999) X3,F3
      IF(F2-F3) 70,175,150
   70 IF(X3 .EQ. XF) GOTO 250
      X1=X2
      F1=F2
      X2=X3
      F2=F3
      GOTO 50
  150 IERR=0
      IF(D) 160,160,170
  160 X4=X3
      X3=X1
      X1=X4
      F4=F3
      F3=F1
      F1=F4
  170 IF(IPR .EQ. 3) RETURN
      WRITE(6,996) X1,X3,X1,F1,X2,F2,X3,F3
      RETURN
  175 X1=X2
      F1=F2
      X2=0.5*(X1+X3)
      F2=F(X2)
      GOTO 150
  200 XT=XO+1.0E-4*D*ABS(XO)
```

```
      IF(XT .EQ. 0.0) XT=1.0E-4*0
      FT=F(XT)
      IF(F1-FT) 210,210,205
205   IERR=1
      X3=X2
      F3=F2
      X2=XT
      F2=FT
      IF(IPR  .EQ. 3) RETURN
      WRITE(6,995) X1,F1
      RETURN
210   X3=X2
      F3=F2
      X2=XT
      F2=FT
      GOTO 150
250   XT=XF-1.0E-4*0*ABS(XF)
      IF(XT .EQ. 0.0) XT=  -1.0E-4*0
      FT=F(XT)
      IF(F3 FT) 260,260,255
255   IERR=2
      X1=X2
      F1=F2
      X2=XT
      F2=FT
      WRITE(6,994) XF,X3,F3
      RETURN
260   X1=X2
      F1=F2
      X2=XT
      F2=FT
      GOTO 150
      END
```

```
      SUBROUTINE LEIVA
      COMMON/CC/ TC(2),PC(2),W(2)
      COMMON/WW/ NSUB,TR(2),WA(2),WB(2)
      DO 10 I = 1,2
        AW1 = 0.60424+0.95362*W(I)-0.33760*W(I)*W(I)
        AW2 = 0.65870 1.09907*W(I)+0.46498*W(I)*W(I)
      WA(I) = 0.42747*EXP(AW1+AW2*TR(I))
        BW1 = 0.15389-0.73725*W(I)+0.15117*W(I)*W(I)
        BW2 = 0.23715+0.56228*W(I) 0.10689*W(I)*W(I)
      WB(I) = 0.08664*EXP(BW1+BW2*TR(I))
   10 CONTINUE
      RETURN
      END
      SUBROUTINE PR
      COMMON/CC/ TC(2),PC(2),W(2)
      COMMON/WW/ NSUB,TR(2),WA(2),WB(2)
      DO 10 I=NSUB,2
       WB(I) = 0.0788)
            S = 0.37464+1.54226*W(I)-0.26992*W(I)*W(I)
        ALF = 1.+S*(1-SQRT(TR(I)))
       ALF2 = ALF*ALF
      WA(I) = 0.45724*ALF2
   10 CONTINUE
      RETURN
      END
      SUBROUTINE ISHI
      COMMON/CC/ TC(2),PC(2),W(2)
      COMMON/WW/ NSUB,TR(2),WA(2),WB(2)
      COMMON/II/ COA(2,3),COB(2,3),CONA(2),CONB(2)
      DIMENSION SWA(2),SWB(2)
      DO 15 I = NSUB,2
       SWA(I)  = 0.0
       SWB(I)  = 0.0
      DO 10 J = 1,3
       SWA(I)  = SWA(I) + COA(I,J)*TR(I)**J
       SWB(I)  = SWB(I) + COB(I,J)*TR(I)**J
   10 CONTINUE
       WA(I)  = CONA(I) + SWA(I)
       WB(I)  = CONB(I) + SWB(I)
   15 CONTINUE
      RETURN
      END
      SUBROUTINE SOAVE
      COMMON/CC/ TC(2),PC(2),W(2)
      COMMON/WW/ NSUB,TR(2),WA(2),WB(2)
      DO 10 I = 1,2
        WB(I) = 0.08664
            S = 0.480 + 1.574*W(I)   0.176*W(I)*W(I)
        ALF = 1.0 + S*(1-SQRT(TR(I)))
       ALF2 = ALF*ALF
      WA(I) = 0.42747*ALF2
   10 CONTINUE
      RETURN
      END
      SUBROUTINE GRA
      COMMON/CC/ TC(2),PC(2),W(2)
      COMMON/STATE/ R,T
```

```
      COMMON/WW/ NSUB,TR(2),WA(2),WB(2)
      DO 10 I = NSUB,2
       WB(I) = 0.03664
          S  = 0.48508 + 1.55171*W(I)   0.15613*W(I)*W(I)
        ALF  = 1.0 + S*(1- SQRT(TR(I)))
       ALF2  = ALF*ALF
       WA(I) = 0.42747*ALF2
   10 CONTINUE
      RETURN
      END
```

VITA

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