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C*****
****
C THIS PROGRAM PERFORMS BUBBLE POINT PRESSURE CALCULATION USING PENG-
ROBINSON
C EOS BY MODIFIED RIGOROUS METHOD.
C
*****
***
      IMPLICIT REAL*8 (A-H,O-Z), INTEGER (I-N)
      COMMON/CR/TC,VC,PC,W,AMOLW,AM
      COMMON/TAP/T,P,RT,AOA,BOB,T1,P1
      COMMON/CONS/C1,C2,C3,IL,IV,CPS,R,EPS1,EPS2,KMAX,ISTATE
      COMMON/CID/COMP,DIJ,NUMB
      COMMON/NOS/K,IERR,K1
      COMMON/ENT/VL,VV,ZL,ZV
      DIMENSION ZZ(40),X(40),Y(40),AK(40),ZC(40),ZZ1(40),SRO(600)
      DIMENSION TC(40),VC(40),PC(40),W(40),AMOLW(40),AM(40),TP(600)
      DIMENSION FEED(40),NUMB(40),NUM(40),DIJ(40,40),COMP(40,2)

C      INPUT FILE AND OUTPUT FILE
C*****
      OPEN (UNIT=20,FILE='BINPUT.DAT',ACCESS='SEQUENTIAL',STATUS='OLD')
      OPEN (UNIT=21,FILE='BOUTPUT.DAT',STATUS='NEW')
C*****
      IL=1
      IV=0
          C1=1.0+DSQRT(2.0D0)
      C2=2.0-C1
      C3=C2-C1
      CPS=5.372697
      R=8.20597D-5
      EPS1=1.D-4
      eps2=1.d-5
      KMAX=150

C*****
C      INPUT BLOCK
C*****
C      T1=Temperature at which Bub. point pressure has to be
c      calculated
C      TMAX=Max. Temp. , , , , , ,
C      XINT=Temp. interval.

      TYPE*,'T1=INITIAL TEMP.','TMAX=FINAL TEMP.','XINT=INTERVAL'

      TYPE*,'CALCULATES BUBBLE POINT PRESSURES IN THE TEMP. RANGE'

      TYPE*,'T1 IN K', 'TMAX IN K','XINT'
      ACCEPT*,T1,TMAX,XINT

C*****
C      INPUT FILE
C      NC=NUMBER OF COMPONENTS.NUMB=NUMBERS DESIGNATING THE

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C      COMPONENTS. FEED=MOLE FRACTIONS IN MIXTURE
C*****
      READ(20,*)NC
      READ(20,*) (NUMB(I), I=1,NC)
      READ(20,*) (FEED(I), I=1,NC)
      write(21,2000)
2000  format(2x,'MODIFIED RIGOROUS METHOD',//,1X,'MIXTURE # 2',//)

      CALL EOS(NC)
      DO 3 I=1,NC
3      TOTAL=TOTAL+FEED(I)
      DO 4 I=1,NC
4      ZZ(I)=FEED(I)/TOTAL
      IERR=0.

97     T=T1

C      CALCULATION OF INITIAL PRESSURE

      CALL PINI(NC,ZZ,P1)
      P=P1
      P3=P1/9.869237

      WRITE(21,100)P3
100   FORMAT(2X,'INITIAL GUESS=',F14.4,1X,'MPa')

      CALL APARA(NC)
      RT=R*T
      BOB=P/RT
      AOA=BOB/RT

      DO 90 I=1,NC
90    AK(I)=DEXP(CPS*(1.+W(I))*(1.-TC(I)/T))*PC(I)/P
      CALL BUBP(NC,X,Y,ZZ,AK,VW,BP,ID)
      IF (ID.EQ.1.0)THEN
      TYPE*, 'ITERATIONS REACHED MAXIMUM'
      ENDIF

C*****
C      SUBROUTINE FOR OUTPUT FILE
C*****
      CALL RITE(NC,BP,X,Y,ZZ,AK,VW,ID)

      T1=T1+XINT

      IF(T1.GT.TMAX)GO TO 101
      GO TO 97
101   STOP
      END

      SUBROUTINE PINI(NC,ZZ,P2)
      IMPLICIT REAL*8 (A-H,O-Z), INTEGER(I-N)
      COMMON/CR/TC,VC,PC,W,AMOLW,AM
      COMMON/TAP/T,P,RT,AOA,BOB,T1,P1

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DIMENSION TC(40),VC(40),PC(40),W(40),AMOLW(40),AM(40),ZZ(40)
DIMENSION PS(40),PH(40)
DO 1 I=1,NC
PS(I)=PC(I)*(DEXP(5.373*(1+W(I))*(1.-TC(I)/T)))
IF(T.LE.TC(I))THEN
PH(I)=PS(I)
ELSE
PH(I)=DSQRT(PS(I)*PC(I))
ENDIF
1 CONTINUE
PHT=0.
PHF=0.
DO 2 I=1,NC
PHT=PHT+PH(I)*ZZ(I)
C PHF=PHF+ZZ(I)/PH(I)
2 CONTINUE
P2=PHT
RETURN
END

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SUBROUTINE EOS(NC)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
COMMON/CR/TC,VC,PC,W,AMOLW,AM
COMMON/PAR/B
COMMON/INT/ACIJ
COMMON/CONS/C1,C2,C3,IL,IV,CPS,R,EPS1,EPS2,KMAX,ISTATE
COMMON/CID/COMP,DIJ,NUMB
COMMON/NOS/K,IERR,K1
    DIMENSION COMP(40,2),TC(40),VC(40),PC(40),W(40),AMOLW(40),
1 NUMB(40),AM(40),AIN(350),DIJ(40,40),ACIJ(40,40),AC(40),B(40)
    DIMENSION CN1(40),CN2(40),CP(40),CV(40),CT(40),CW(40),CM(40)
    DATA CN1(1),CN2(1),CP(1),CT(1),CV(1),CW(1),CM(1) / 'METH',
1 'ANE',45.80,190.7,0.0990,0.0130,16.043/
    DATA CN1(2),CN2(2),CP(2),CT(2),CV(2),CW(2),CM(2) / 'ETHA',
1 'NE',48.20,305.43,0.148,0.0986,30.07/
    DATA CN1(3),CN2(3),CP(3),CT(3),CV(3),CW(3),CM(3) / 'PROP',
1 'ANE',42.01,369.9,0.200,0.1524,44.097/
    DATA CN1(4),CN2(4),CP(4),CT(4),CV(4),CW(4),CM(4) / 'I-BU',
1 'TANE',36.00,408.1,0.263,0.1848,58.124/
    DATA CN1(5),CN2(5),CP(5),CT(5),CV(5),CW(5),CM(5) / 'N-BU',
1 'TANE',37.47,425.2,0.255,0.2010,58.124/
    DATA CN1(6),CN2(6),CP(6),CT(6),CV(6),CW(6),CM(6) / 'I-PE',
1 'NTAN',32.90,460.4,0.308,0.2223,72.151/

    DATA CN1(7),CN2(7),CP(7),CT(7),CV(7),CW(7),CM(7) / 'N-PE',
1 'NTAN',33.31,469.8,0.311,0.2539,72.151/
    DATA CN1(8),CN2(8),CP(8),CT(8),CV(8),CW(8),CM(8) / 'N-HE',
1 'XANE',29.92,507.9,0.368,0.3007,86.178/
    DATA CN1(9),CN2(9),CP(9),CT(9),CV(9),CW(9),CM(9) / 'N-HE',
1 'PTAN',27.01,540.16,0.426,0.3498,100.205/
    DATA CN1(10),CN2(10),CP(10),CT(10),CV(10),CW(10),CM(10) /
1 'N-OC', 'TANE',24.64,568.6,0.486,0.4018,114.232/
    DATA CN1(11),CN2(11),CP(11),CT(11),CV(11),CW(11),CM(11) /

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1  'N-NO', 'NANE', 22.50, 594.6, 0.543, 0.4455, 128.259/
DATA CN1 (12), CN2 (12), CP (12), CT (12), CV (12), CW (12), CM (12) /
1  'N-DE', 'CANE', 20.80, 617.6, 0.602, 0.4885, 142.286/
DATA CN1 (13), CN2 (13), CP (13), CT (13), CV (13), CW (13), CM (13) /
1  'N2', ' ', 33.50, 126.2, 0.090, 0.040, 28.013/
DATA CN1 (14), CN2 (14), CP (14), CT (14), CV (14), CW (14), CM (14) /
1  'CO2', ' ', 72.90, 304.2, 0.094, 0.225, 44.01/
DATA CN1 (15), CN2 (15), CP (15), CT (15), CV (15), CW (15), CM (15) /
1  'H2S', ' ', 88.90, 373.6, 0.098, 0.100, 34.076/
DATA CN1 (16), CN2 (16), CP (16), CT (16), CV (16), CW (16), CM (16) /
1  'TOLU', 'ENE ', 41.60, 592.0, 0.316, 0.2596, 92.13/
DATA CN1 (17), CN2 (17), CP (17), CT (17), CV (17), CW (17), CM (17) /
1  'BENZ', 'ENE ', 48.60, 562.1, 0.260, 0.215, 78.11/
DATA CN1 (18), CN2 (18), CP (18), CT (18), CV (18), CW (18), CM (18) /
1  'CYCL', 'O-C6', 40.0, 553.2, 0.308, 0.2133, 84.16/
DATA CN1 (19), CN2 (19), CP (19), CT (19), CV (19), CW (19), CM (19) /
1  'H2O', ' ', 218.3, 647.0, 0.056, 0.348, 18.02/
DATA CN1 (20), CN2 (20), CP (20), CT (20), CV (20), CW (20), CM (20) /
1  'HYDR', 'GANE', 20.20, 43.6, 0.0, 0.0, 2.016/
DATA CN1 (21), CN2 (21), CP (21), CT (21), CV (21), CW (21), CM (21) /
1  'CO', ' ', 34.53, 132.93, 0.0, .0520, 28.01/
DATA CN1 (22), CN2 (22), CP (22), CT (22), CV (22), CW (22), CM (22) /
1  'NH3', ' ', 111.4, 405.11, 0.0, 0.26, 17.03/
DATA CN1 (23), CN2 (23), CP (23), CT (23), CV (23), CW (23), CM (23) /
1  'METH', 'ANOL', 79.9, 512.2, 0.0, 0.559, 32.042/
DATA CN1 (24), CN2 (24), CP (24), CT (24), CV (24), CW (24), CM (24) /
1  'HEL', 'IUM', 6.67, 10.47, 0.0, 0.0, 4.0026/
DATA CN1 (25), CN2 (25), CP (25), CT (25), CV (25), CW (25), CM (25) /
1  'BITU', 'MEN', 6.834, 911.48, 0.0, 1.6591, 544.0/

DATA CN1 (26), CN2 (26), CP (26), CT (26), CV (26), CW (26), CM (26) /
1  'TETR', 'DCAN', 16.02, 694.72, 1.0934, 0.6505, 198.327/
DATA (AIN (I), I=1, 325) / 66*0.0
*      , 0.036, 0.050, 0.080, 0.095, 0.090, 0.095
*      , 7*0.1, 0.130, 0.135, 2*0.13, 3*0.125, 0.1, 0.115, 2*0.11, -0.02, 0.085
*      , 0.084, 0.075, 0.05, 2*0.06, 0.065, 2*0.06, 0.055, 0.05, 0.045, 0.18,
*      0.1, 0.04, 2*0.02, 8*0.0, 0.01, 0.18, 0.09, 0.0, 0.04, 2*0.02, 8*0.0,
*      0.01, 0.16, 0.075, 2*0.0, 0.035, 0.02, 0.02, 8*0.0, 0.01, 2*0.1,
*      3*0.0, 2*0.05, 0.55, 2*0.56, 7*0.48, 0.508, 0.21, 0.164, 3*0.48, -0.15
*      , 11*-0.5, -0.036, -0.3, 0.1, 3*-0.5, 0., 0.02, .026, 0.03, 9*0.04,
*      .012, -0.03, 0.1, 0.105, 0.11, 2*0.1, -0.036, 0.18, .2, 10*0.2, .24,
*      2*0, 3*0.08, -.27, -.183, 0, 0.2, 0.02, .03, 2*.05, 2*.1, 5*.15, .5, -.2,
*      .0, 3*.2, -.08, 15*0., -.4, .4, 5*0., .55, 3*0., .115, .025, 11*0, .095,
*      4*0, .135, 5*0.0, 12*0.0, 2*.1, 0.05, 3*0.0, 0.45, -0.5, 0.04, 2*0.2,
*      -0.5, 0./
IF (NC.EQ.0.0) GO TO 11
DO 1 I=1, NC
J=NUMB (I)
COMP (I, 1)=CN1 (J)
COMP (I, 2)=CN2 (J)
PC (I)=CP (J)
TC (I)=CT (J)
VC (I)=CV (J)
W (I)=CW (J)

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1      AMOLW(I)=CM(J)
      CONTINUE
      NM=NC-1
      IF(NM.EQ.0) GO TO 11
      DO 3 II=1,NM
      I=NUMB(II)
      IP1=II+1.
      DO 3 JJ=IP1,NC
      J=NUMB(JJ)
      IF(J.LT.I) THEN
          KIJ=J+(I-1)*(I-2)/2
          DIJ(JJ,II)=AIN(KIJ)
      ELSE
          KIJ=I+(J-1)*(J-2)/2
          DIJ(JJ,II)=AIN(KIJ)
      ENDIF
3      CONTINUE
11     CONTINUE
      DO 6 I=1,NC
      RTC=R*TC(I)
      RTP=RTC/PC(I)
      AC(I)=0.457235*RTP*RTC
      B(I)=0.077796*RTP
      IF(W(I).GE.0.49)GO TO 7
      AM(I)=0.37464+(1.54226-0.26992*W(I))*W(I)
      GO TO 8
7      AM(I)=0.379642+(1.48503-(0.164423-0.016666*W(I))*W(I))*W(I)
8      CONTINUE
      ACIJ(I,I)=AC(I)
6      DIJ(I,I)=0.0
      IF(NC.EQ.1)RETURN
      DO 10 I=2,NC
      IM1=I-1
      DO 10 J=1,IM1
      ACIJ(I,J)=(1.-DIJ(I,J))*DSQRT(AC(I)*AC(J))
      DIJ(J,I)=DIJ(I,J)
10     ACIJ(J,I)=ACIJ(I,J)
      RETURN
      END

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SUBROUTINE APARA(NC)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
COMMON/TAP/T,P,RT,AOA,BOB,T1,P1
COMMON/CR/TC,VC,PC,W,AMOLW,AM
COMMON/INT/ACIJ
COMMON/AS/AIJ,ALFSQ
COMMON/NOS/K,IERR,K1
DIMENSION TC(40),VC(40),PC(40),W(40),AMOLW(40),AM(40)
DIMENSION ALFSQ(40),ACIJ(40,40),AIJ(40,40)
DO 1 I=1,NC
ALFSQ(I)=1.+AM(I)*(1.-DSQRT(T/TC(I)))
1     AIJ(I,I)=ACIJ(I,I)*ALFSQ(I)*ALFSQ(I)
      IF(NC.EQ.1.)RETURN

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DO 2 I=2,NC
IM1=I-1
DO 2 J=1,IM1
AIJ(I,J)=ACIJ(I,J)*ALFSQ(I)*ALFSQ(J)
2 AIJ(J,I)=AIJ(I,J)
RETURN
END

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SUBROUTINE ABMIX(NC,X,AM,BM,SAM)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
COMMON/AS/AIJ,ALFSQ
COMMON/NOS/K,IERR,K1
COMMON/PAR/B
DIMENSION AIJ(40,40),X(40),SAM(40),ALFSQ(40),B(40)
AM=0.0
BM=0.0
DO 2 I=1,NC
BM=BM+X(I)*B(I)
SAM(I)=0.0
DO 1 J=1,NC
1 SAM(I)=SAM(I)+X(J)*AIJ(I,J)
AM=AM+X(I)*SAM(I)
2 CONTINUE
RETURN
END

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SUBROUTINE VOLUME(AMX,BMX,V,Z,IFASE)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
COMMON/TAP/T,P,RT,AOA,BOB,T1,P1
COMMON/AB/AA,BB
DIMENSION ZR(3),CU(3)
AA=AMX*AOA
BB=BMX*BOB
CU(1)=BB-1
CU(2)=AA-BB*(2.+3.*BB)
CU(3)=BB*(BB*BB+BB-AA)
CALL CUBEQ(IRT,ZR,CU)
IF(IRT)1,1,6
1 IF(IFASE)2,2,3
2 Z=DMAX1(ZR(1),ZR(2),ZR(3))
GO TO 99
3 ZDUM=100.
DO 5 I=1,3
IF(ZR(I))4,4,5
4 ZR(I)=ZDUM
5 CONTINUE
Z=DMIN1(ZR(1),ZR(2),ZR(3))
GO TO 99
6 Z=ZR(1)
99 V=Z/BOB
RETURN
END

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SUBROUTINE CUBEQ(IROOT,Z,B)

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      IMPLICIT REAL*8 (A-H,O-Z) , INTEGER (I-N)
      DIMENSION B (3) , Z (3)
      TRD=1./3.
      B13=B (1) *TRD
      BET=B (3) +B13* (2.*B13*B13-B (2) )
      BO2=0.5*BET
      AO3=TRD* (B (2) -B (1) *B13)
      CUA=AO3*AO3*AO3
      SQB=BO2*BO2
      DEL=SQB+CUA
      IF (DEL) 30, 10, 20
10     IROOT=0
      GAM=DSQRT (-AO3)
      IF (BET) 12, 12, 11
11     Z (1) =-2.*GAM-B13
      Z (2) =GAM-B13
      Z (3) =Z (2)
      RETURN
12     Z (1) =2.*GAM-B13
      Z (2) =-GAM-B13
      Z (3) =Z (2)
      RETURN
20     IROOT=1
      EPS=DSQRT (DEL)
      TAU=-BO2
      RCU=TAU+EPS
      SCU=TAU-EPS
      SIR=1.0
      SIS=1.0
      IF (RCU) 21, 22, 22
21     SIR=-1.0
22     IF (SCU) 23, 24, 24
23     SIS=-1.0
24     R=SIR* (SIR*RCU) **TRD
      S=SIS* (SIS*SCU) **TRD
      Z (1) =R+S-B13
      Z (2) =-0.5* (R+S) -B13
      Z (3) =0.8660254* (R-S)
      RETURN
30     IROOT=-1
      ROOT=DSQRT (-SQB/CUA)
      IF (BET) 32, 31, 31
31     PEI= (1.5707963+DATAN (ROOT/DSQRT (1.-ROOT*ROOT) ) ) *TRD
      GO TO 33
32     PEI=DATAN (DSQRT (1.-ROOT*ROOT) /ROOT) *TRD
33     FACT=2.*DSQRT (-AO3)
      CZ=2.0943951
      DO 34 I=1, 3
34     Z (I) =FACT*DCOS (PEI+CZ* (I-1) ) -B13
      RETURN
      END

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SUBROUTINE FUGA (NC, X, AMX, BMX, Z, SA, FUG, XP)
IMPLICIT REAL*8 (A-H,O-Z) , INTEGER (I-N)

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COMMON/TAP/T,P,RT,AOA,BOB,T1,P1
COMMON/NOS/K,IERR,K1
COMMON/CONS/C1,C2,C3,IL,IV,CPS,R,EPS1,EPS2,KMAX,ISTATE
COMMON/PAR/B
COMMON/AB/AA,BB
COMMON/SST/SAB,TEMP
COMMON/BZ/BLN,ZMBB
DIMENSION SA(40),SAB(40),TEMP(40),FUG(40),B(40),X(40)
ZMBB=Z-BB
ALN=-DLOG(ZMBB)
BLN=AA*DLOG((Z+C2*BB)/(Z+C1*BB))/BB/C3
DO 3 I=1,NC
BIOB=B(I)/BMX
SAB(I)=SA(I)*2/AMX-BIOB
TEMP(I)=(Z-1)*BIOB-BLN*SAB(I)
FOXP=TEMP(I)+ALN
3 FUG(I)=X(I)*XP*DEXP(FOXP)
RETURN
END
SUBROUTINE RITE(NC,TP,X,Y,ZZ,AK,VW,ID)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
COMMON/TAP/T,P,RT,AOA,BOB,T1,P1
COMMON/CR/TC,VC,PC,W,AMOLW,AM
COMMON/CID/COMP,DIJ,NUMB
COMMON/RF/RATIO
COMMON/ENT/VL,VV,ZL,ZV
COMMON/NOS/K,IERR,K1
DIMENSION ZZ(40),X(40),Y(40),AK(40),COMP(40,2),RATIO(40)
DIMENSION TC(40),VC(40),PC(40),W(40),AMOLW(40),AM(40)
PSI=TP/9.869237

WRITE(21,61)PSI,T1
      WRITE(21,116)K

      IF(IERR.LE.1) THEN
WRITE(21,1000)
1000 FORMAT(3X,'COMP',9X,'Z',9X,'X',7X,'Y',11X,'K',8X,'Ri',/)
      WRITE(21,114)((COMP(I,J),J=1,2),ZZ(I),X(I),Y(I),AK(I),
1 RATIO(I),I=1,NC)

      ELSEIF(IERR.EQ.2.) THEN
WRITE(21,72)
      ELSEIF(IERR.EQ.3) THEN
WRITE(21,73)
      ELSEIF(IERR.EQ.4) THEN
WRITE(21,74)
      ELSEIF(IERR.EQ.5) THEN
WRITE(21,75)
      ENDIF
61 FORMAT(1X,/,,'BUBB. PRESS=',f14.3,'MPA',2X,'temperature='
1 ,f8.2,'k')
72 FORMAT(1X,'UNREALISTIC VOLUME')
73 FORMAT(1X,'CALCULATION INTERRUPTED')
74 FORMAT(1X,'PRESSURE IS NEGATIVE')

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75   FORMAT(1X, 'PRESSURE ITER DIVERGENT')
114  FORMAT(1X, 2A4, 5F10.5)
115  FORMAT(1X, 4F16.7)
116  FORMAT(1X, 'NO. OF ITERATIONS=', I4, '/')
      RETURN
      END

      SUBROUTINE BUBP(NC, X, Y, ZZ, AK, VW, BP, ID)
      IMPLICIT REAL*8 (A-H, O-Z), INTEGER (I-N)
      COMMON/CONS/C1, C2, C3, IL, IV, CPS, R, EPS1, EPS2, KMAX, ISTATE
      COMMON/TAP/T, P, RT, AOA, BOB, T1, P1
      COMMON/RF/RATIO
      COMMON/CR/TC, VC, PC, W, AMOLW, AM
      COMMON/ENT/VL, VV, ZL, ZV
      COMMON/NOS/K, IERR, K1
      COMMON/EQ/AKO
      COMMON/PTXY/ROXY
      COMMON/SWIT/AKL, RX, EPSU
      COMMON/NT/NCP, NCM
      COMMON/AB/AA, BB
      DIMENSION X(40), Y(40), ZZ(40), AK(40), TC(40), PC(40), VC(40)
      DIMENSION RATIO(40), FL(40), FV(40), SAL(40), SAV(40), W(40)
      1   , AMOLW(40), AM(40), RVPT(40), ROXY(40, 41), DEL(40), SRO(0:600)
      1   , AKL(40, 0:100), ASRO(0:100), TP(0:200)
      K=0.0
      p3=p/9.869237
      rx=0.7
C*****
      type*, 'ks=NO OF SS ITERATIONS REQUIRED BEFORE RIGOROUS
      1   METHOD, PUT KS=1, IF DIVERGES PUT KS=3'
      ACCEPT*, KS

      BP=P
      DO 1 I=1, NC
      X(I)=ZZ(I)
1     CONTINUE

      CALL ABMIX(NC, X, AML, BML, SAL)
      SUMY=0.0
      DO 2 I=1, NC
      Y(I)=AK(I)*X(I)
2     SUMY=SUMY+Y(I)
      DO 3 I=1, NC
3     Y(I)=Y(I)/SUMY
      GO TO 13
12    IF(BP.LE.0.0) GO TO 24
      BOB=BP/RT
      AOA=BOB/RT
13   CONTINUE
      CALL VOLUME(AML, BML, VL, ZL, IL)
      IF(VL.LE.BML) GO TO 25
      CALL FUGA(NC, X, AML, BML, ZL, SAL, FL, BP)
      CALL ABMIX(NC, Y, AMV, BMV, SAV)
      CALL VOLUME(AMV, BMV, VV, ZV, IV)

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IF(VV.LE.BMV) GO TO 25
CALL FUGA(NC,Y,AMV,BMV,ZV,SAV,FV,BP)

DO 41 I=1,NC
IF(FV(I).EQ.0.0) THEN
RATIO(I)=0.0
ELSE
RATIO(I)=FL(I)/FV(I)
ENDIF
41 CONTINUE
K=K+1
if(k.gt.kmax)go to 21
SUMY=0.0
DO 42 I=1,NC
42 Y(I)=RATIO(I)*Y(I)
SUMY=SUMY+Y(I)
DO 5 I=1,NC
5 Y(I)=Y(I)/SUMY
CONTINUE
BP=BP*(2.-1./SUMY)
IF(K.LT.kS)GO TO 12

k=0
NCP=NC+1
NCM=NC-1
71 CONTINUE
k1=k+1
sp=bp/9.869237
IF(BP.LE.0.0)GO TO 24
BOB=BP/RT
AOA=BOB/RT
CALL VOLUME(AML,BML,VL,ZL,IL)
IF(VL.LE.BML)GO TO 25
CALL FUGA(NC,X,AML,BML,ZL,SAL,FL,BP)
CALL DRVS(NC,X,AML,BML,ZL,SAL,IL,BP)
DO 8 I=1,NC
8 RVPT(I)=ROXY(I,1)
CALL ABMIX(NC,Y,AMV,BMV,SAV)
CALL VOLUME(AMV,BMV,VV,ZV,IV)
IF(VV.LE.BMV)GO TO 25
CALL FUGA(NC,Y,AMV,BMV,ZV,SAV,FV,BP)
CALL DRVS(NC,Y,AMV,BMV,ZV,SAV,IV,BP)
SRO(K)=0.
DO 9 I=1,NC
IF(FV(I).EQ.0.0)GO TO 9
RATIO(I)=FL(I)/FV(I)
ROXY(I,NCP)=1.-RATIO(I)
9 SRO(K)=SRO(K)+(DABS(ROXY(I,NCP)))**2
sro(k)=sro(k)/nc
TP(K)=BP*14.696
ASRO(K)=DLOG10(SRO(K))
DO 10 I=1,NC
IF(ROXY(I,NCP).EQ.1.0)GO TO 10
IF((DABS(ROXY(I,NCP))).GE.EPS2) GO TO 11

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```

10    CONTINUE
      GO TO 99
11    IF(K.GT.KMAX) GO TO 21
      DO 100 I=1,NC
      ROXY(I,1)=RATIO(I)*(RVPT(I)-ROXY(I,1))
      DO 100 J=2,NC
100   ROXY(I,J)=-RATIO(I)*ROXY(I,J)
      RYN=RATIO(NC)/Y(NC)
      DO 200 JK=2,NC
      JM=JK-1
      ROXY(JM,JK)=ROXY(JM,JK)-RATIO(JM)/Y(JM)
200   ROXY(NC,JK)=ROXY(NC,JK)+RYN
      CALL LINSYS(NC,ROXY,DEL)
      DO 890 I=1,NC
      IF((DABS(DEL(I))).GT.0.0) GO TO 900
890   CONTINUE
      GO TO 23
900   BP=BP+DEL(1)
      DO 300 I=2,NC
      Y(I-1)=Y(I-1)+DEL(I)
300   Y(NC)=Y(NC)-DEL(I)
      DO 201 I=1,NC
      AKL(I,K)=Y(I)
201   CONTINUE
C*****
C FOR CALCULATION USING NEWTON METHOD DELETE THE FOLLOWING 11 LINES
C*****
      IF(K.Gt.1) THEN
      T=K/3.
      M=K/3.
      ENDIF
      IF((T-M).EQ.0.0) THEN
      rat1=sro(k)/sro(k-1)
      rat2=sro(k-1)/sro(k-2)
      if((rat1.lt.1).and.(rat2.lt.1.)) then
      CALL SWITCH(NC,X,Y,AK,BP,REL,SRO)
      ENDIF
      endif
C*****
      K=K+1
      GO TO 71

23    TYPE*, 'IERR=3'
      GO TO 99

21    ID=1
      RETURN
99    DO 20 I=1,NC
      IF(X(I).EQ.0.0) THEN
      AK(I)=0.0
      ELSE
      AK(I)=Y(I)/X(I)
      ENDIF

```

```

20  CONTINUE
    RETURN
25  TYPE*, ' IERR=2 '
    RETURN
24  TYPE*, ' IERR=4 '
    RETURN

    END
    SUBROUTINE SWITCH (NC, X, Y, AK, BP, REL, SRO)
    IMPLICIT REAL*8 (A-H, O-Z), INTEGER (I-N)
    COMMON/NOS/K, IERR, K1
    COMMON/SWIT/AKL, RX, EPSU
    DIMENSION AKL(40, 0:100), RLK(40), X(40)
1   , Y(40), AK(40), SRO(0:100), RLKJ(100)
    IF (SRO(K) .LT. 1.D-06) GO TO 9
    SUMY=0.

    DO 30 I=1, NC
    F=0.
    DO 2 J=1, 3
    RLKJ(J)=DABS((AKL(I, K)-AKL(I, K-J))/J)
    IF (RLKJ(J) .GT. F) THEN
    F=RLKJ(J)
    F1=J
    ENDIF
2   CONTINUE
    RLK(I)=(AKL(I, K)-AKL(I, K-F1))/F1
c   RLK(I)=DMIN1(RLKJ(1), RLKJ(2), RLKJ(3))
    Y(I)=Y(I)+RX*RLK(I)
    SUMY=Y(I)+SUMY
30  CONTINUE
    DO 40 I=1, NC
    Y(I)=Y(I)/SUMY
40  CONTINUE
9   RETURN
    END

    SUBROUTINE DRVS (NC, X, AMX, BMX, Z, SA, IFASE, BP)
    IMPLICIT REAL*8 (A-H, O-Z), INTEGER (I-N)
    COMMON/CR/TC, VC, PC, W, AMOLW, AM
    COMMON/AS/AIJ, ALFSQ
    COMMON/TAP/T, P, RT, AOA, BOB, T1, P1
    COMMON/CONS/C1, C2, C3, IL, IV, CPS, R, EPS1, EPS2, KMAX, ISTATE
    COMMON/NOS/K, IERR, K1
    COMMON/AB/AA, BB
    COMMON/SST/SAB, TEMP
    COMMON/PAR/B
    COMMON/PTXY/ROXY
    COMMON/BZ/BLN, ZMBB
    COMMON/NT/NCP, NCM
    DIMENSION AM(40), TC(40), VC(40), PC(40), W(40), AMOLW(40)
    DIMENSION ALFSQ(40), ACIJ(40, 40), AIJ(40, 40), B(40), ROXY(40, 41)
    DIMENSION X(40), SA(40), SAB(40), TEMP(40)
    U0=AA-(3*BB+2.)*BB

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```

U3=AA/BB/(Z+C1*BB)/(Z+C2*BB)
U5=6.*BB+2.
Z50=Z*(Z-U5)-U0
DENO=Z*(3.*Z-2.*(1.-BB))+U0
R3=2.*BLN/AMX
AOP=AA/BP
BOP=BB/BP
ZOP=AOP*ZMBB+BOP*Z50
ZOP=-ZOP/DENO
U1=ZOP/BMX
U2=(ZOP-BOP)/ZMBB
U4=(Z*BOP-BB*ZOP)*U3
DO 10 I=1,NC
10 ROXY(I,1)=B(I)*U1-U2-U4*SAB(I)
IF(IFASE.EQ.1.)GO TO 5
DO 70 J=1,NCM
AXY=2.*(SA(J)-SA(NC))*AOA
BXY=(B(J)-B(NC))*BOB
ZXY=AXY*ZMBB+BXY*Z50
ZXY=-ZXY/DENO
R1=BXY/BB
R2=(ZXY-BXY)/ZMBB
R4=U3*(Z*BXY-BB*ZXY)
R5=((SAB(J)-SAB(NC))*BLN+ZXY)/BMX
L=J+1
DO 70 I=1,NC
ROXY(I,L)=R1*TEMP(I)+R2+R3*(AIJ(J,I)-AIJ(NC,I))
1 +R4*SAB(I)-R5*B(I)
70 ROXY(I,L)=-ROXY(I,L)
5 RETURN
END
SUBROUTINE LINSYS(N,AM,X)
IMPLICIT REAL*8(A-H,O-Z),INTEGER(I-N)
DIMENSION AM(40,41),IP(40),JP(40),X(40)
NB=N+1
DO 1 I=1,N
1 IP(I)=0.
DO 6 M=1,N
PIVOT=0.0
DO 4 I=1,N
DO 2 MM=1,M
IF(I.EQ.IP(MM))GO TO 4
2 CONTINUE
DO 3 J=1,N
IF(DABS(PIVOT).GT.DABS(AM(I,J)))GO TO 3
PIVOT=AM(I,J)
IP(M)=I
JP(M)=J
3 CONTINUE
4 CONTINUE
K=IP(M)
L=JP(M)
IF(PIVOT.EQ.0.0)GO TO 113
DO 41 J=1,NB

```

```
41   AM(K, J) = AM(K, J) / PIVOT
    DO 43 I=1, N
      IF(I.EQ.K) GO TO 43
      AN = AM(I, L)
      DO 42 J=1, NB
62    AM(I, J) = AM(I, J) - AM(K, J) * AN
      AM(I, L) = 0.
43   CONTINUE
6    CONTINUE
      DO 8 I=1, N
        DO 7 J=1, N
          IF(AM(I, J).NE.0.0) GO TO 8
7    CONTINUE
      GO TO 113
8    CONTINUE
      DO 9 M=1, N
        I = IP(M)
        J = JP(M)
9    X(J) = AM(I, NB)
      RETURN
113  DO 12 I=1, N
12   X(I) = 0.0
      RETURN
     END
```