

References

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## Appendix

- A. Appendix Pascal Program Criteria for initial estimate.
- B. Appendix Pascal Program Three-Phase Flash Computation by Soave-Redlich-Kwong Equation of State.
- C. Appendix Pascal Program Three-Phase Flash Computation by Harmens & Knapp Equation of state.
- D. Appendix Pascal Program Three-Phase Flash Computation by Peng and Robinson Equation of State.
- E. Appendix Pascal Program Three-Phase Flash Computation by Graboski and Daubert Equation of state.

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PROGRAM CRITERIAFORINITIALESTIMATEI
CONST
  G=0.3333;RR=0.082;P=48.95;TT=298.15;
TYPE
  CLASS =RECORD
    NAME:STRING(10);
    END;
VAR
  COMP:ARRAY[1..3]OF CLASS;
  XL1:ARRAY[1..3]OF REAL;  XL2:ARRAY[1..3]OF REAL;
  TC:ARRAY[1..3]OF REAL;  Y:ARRAY[1..3]OF REAL;
  PC:ARRAY[1..3]OF REAL;  W:ARRAY[1..3]OF REAL;
  KL1:ARRAY[1..4]OF REAL;  KL2:ARRAY[1..4]OF REAL;
  Z:ARRAY[1..4]OF REAL;  XT1:ARRAY[1..3]OF REAL;
  YT1:ARRAY[1..3]OF REAL;  XT1:ARRAY[1..3]OF REAL;
  Y1:ARRAY[1..3]OF REAL;  YT2:ARRAY[1..3]OF REAL;
  XT2:ARRAY[1..3]OF REAL;  T,Q1,Q2,Q3,Q4,Q5,Q6:REAL;
  I,J,NU:INTEGER;  ETHANE:STRING(10);
  KFI:TEXT;
  FUNCTION PWR(E:REAL;H:REAL):REAL;
  BEGIN
    PWR:=EXP(E*LN(H));
  END;
  FUNCTION TAN(X:REAL):REAL;
  BEGIN
    TAN:=SIN(X)/COS(X);
  END;
BEGIN
  NU:=3;

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  WRITELN('19,'INITIAL ESTIMATE COMPOSITIONS');
  WRITELN('15,'-----',
    '-----');
  WRITELN('15,'COMP','18,'TC':5,'PC':10,'W':10,'Y':8,'XL1':
  10,'XL2':8,'Z':17);
  WRITELN('15,'-----',
    '-----');
  ASSIGN(KFI,'WUN.TXT');
  RESET(KFI);
  FOR I:=1 TO NU DO
  BEGIN
    READLN(KFI,COMP[I].NAME,TC[I],PC[I],W[I],Y[I],XL1[I],XL2[I]);
  END;
  CLOSE(KFI);
  YT[1]:=0.0888;
  YT[3]:=0.0001;
  YT[2]:=1-YT[1]-YT[3];
  XT1[1]:=0.0345;
  XT1[2]:=0.8920;
  XT1[3]:=1-XT1[1]-XT1[2];
  XT2[1]:=0.0497;
  XT2[2]:=0.9432;
  XT2[3]:=1-XT2[1]-XT2[2];
  FOR I:=1 TO NU DO
  BEGIN
    Z[I]=(YT[I]+XT1[I]+XT2[I])/3;
    WRITELN('15,COMP[I].NAME:8,TC[I]:10:4,PC[I]:10:4,
    W[I]:10:4,Y[I]:8:4,XL1[I]:8:4,XL2[I]:8:4,Z[I]:8:4);
  END;

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```

WRITELN('15, '-----',
        '-----');
WRITELN;
FOR I1=1 TO NU DO
BEGIN
KL1(I1)=Y(I1)/XL1(I1);
KL2(I1)=Y(I1)/XL2(I1);
END;
Q1=0;      Q2=0;
Q3=0;      Q4=0;
Q5=0;      Q6=0;
  FOR I1=1 TO NU DO
  BEGIN
Q11=Q1+Z(I1)*KL1(I1);
Q21=Q2+Z(I1)/KL1(I1);
Q31=Q3+Z(I1)*KL2(I1);
Q41=Q4+Z(I1)/KL2(I1);
Q51=Q5+Z(I1)*KL1(I1)/KL2(I1);
Q61=Q6+Z(I1)*KL2(I1)/KL1(I1);
END;
WRITELN('10, 'SUM(Z(I1)*KL1(I1)) =', Q11(8:4));
WRITELN('10, 'SUM(Z(I1)/KL1(I1)) =', Q21(8:4));
WRITELN('10, 'SUM(Z(I1)*KL2(I1)) =', Q31(8:4));
WRITELN('10, 'SUM(Z(I1)/KL2(I1)) =', Q41(8:4));
WRITELN('10, 'SUM(Z(I1)*KL1(I1)/KL2(I1)) =', Q51(8:4));
WRITELN('10, 'SUM(Z(I1)*KL2(I1)/KL1(I1)) =', Q61(8:4));
WRITELN;
END.

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PROGRAM SRK;
CONST
  G=0.3333; RR=0.082; P=48.95; TT=298.15;
TYPE
  CLASS = RECORD
    NAME: STRING(10);
    END;
VAR
  COMP: ARRAY(1..3) OF CLASS;
  DD: ARRAY(1..3) OF REAL;
  PRI: ARRAY(1..3) OF REAL;
  KL: ARRAY(1..3) OF REAL;
  MP: ARRAY(1..3) OF REAL;
  WT: ARRAY(1..3) OF REAL;
  TC: ARRAY(1..3) OF REAL;
  PC: ARRAY(1..3) OF REAL;
  WI: ARRAY(1..3) OF REAL;
  XI: ARRAY(1..3) OF REAL;
  YI: ARRAY(1..3) OF REAL;
  ZI: ARRAY(1..3) OF REAL;
  YI: ARRAY(1..3) OF REAL;
  Y2I: ARRAY(1..3) OF REAL;
  BIJ: ARRAY(1..3, 1..3) OF REAL;
  AI: ARRAY(1..4, 1..4) OF REAL;
  BI: ARRAY(1..4, 1..4) OF REAL;
  ZI: ARRAY(1..3) OF REAL;
  ZHI: ARRAY(1..3) OF REAL;
  ZTI: ARRAY(1..3) OF REAL;
  BTI: ARRAY(1..3) OF REAL;
  ALI: ARRAY(1..2) OF REAL;
  TRI: ARRAY(1..2) OF REAL;
  BLI: ARRAY(1..3) OF REAL;
  XLI: ARRAY(1..3) OF REAL;
  XL2I: ARRAY(1..3) OF REAL;
  QVI: ARRAY(1..3) OF REAL;
  QLI: ARRAY(1..3) OF REAL;
  QL2I: ARRAY(1..3) OF REAL;
  KLI: ARRAY(1..3) OF REAL;
  KL2I: ARRAY(1..3) OF REAL;
  MMI: ARRAY(1..3) OF REAL;
  AII: ARRAY(1..3) OF REAL;
  AIJ: ARRAY(1..3, 1..3) OF REAL;
  UUI: ARRAY(1..3) OF REAL;
  QMI: ARRAY(1..3) OF REAL;
  AEI: ARRAY(1..3) OF REAL;
  DEI: ARRAY(1..3) OF REAL;
  CI: ARRAY(1..4, 1..4) OF REAL;
  ATI: ARRAY(1..3) OF REAL;
  ZLI: ARRAY(1..3) OF REAL;

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XX1:ARRAY(1..4)OF REAL;      KK1:ARRAY(1..3)OF REAL;
X1:ARRAY(1..3)OF REAL;      X2:ARRAY(1..3)OF REAL;
KK2:ARRAY(1..3)OF REAL;      XT1:ARRAY(1..3)OF REAL;
X12:ARRAY(1..3)OF REAL;      YT1:ARRAY(1..3)OF REAL;
HU1:ARRAY(1..15)OF REAL;     EU1:ARRAY(1..15)OF REAL;
HU2:ARRAY(1..15)OF REAL;     EU2:ARRAY(1..15)OF REAL;
T, ZL, ZV, AT, DT, U, DPT, APT1, BPT1, CPT1, ERROR3, ERROR4: REAL;
BPT, APT, CPT, V, V1, V2, V3, DT, ZJ, F, F1, F2, F3, F4: REAL;
QM, RQ, ZK, ZA, AMAX, DQ11, DQ12, DQ21, DQ22: REAL;
O1, O2, U1, U2, DP, AP, ERROR1, ERROR2: REAL;
I, J, N, K, NG, NU, TH, DP, L, MT, OU: INTEGER;
CO2: STRING(15);
TRIDECANE: STRING(15);
KF1: TEXT;
FUNCTION PWR(E: REAL; H: REAL): REAL;
  BEGIN
    PWR := EXP(E*LN(H));
  END;
FUNCTION TAN(X: REAL): REAL;
  BEGIN
    TAN := SIN(X)/COS(X);
  END;
BEGIN
  NU := 3;
  WRITELN('FILE = DUO3.PAS');
  WRITELN;
  WRITELN('T=', TT:8:2, 'I4', 'K', 'I4', 'P=', P:8:2);
  WRITELN('I19, INITIAL ESTIMATE COMPOSITIONS');
  WRITELN('I5, -----',

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-----');
WRITELN('I5, 'COMP', 'I8, 'TC'15, 'PC'110, 'W'110, 'Y'18,
'XL1'110, 'XL2'10, 'Z'17);
WRITELN('I5, -----',
-----');
  ASSIGN(KF1, 'WUN.TXT');
  RESRT(KF1);
  FOR I:=1 TO NU DO
    BEGIN
      READLN(KF1, COMP(I), NAME, TCC(I), PCC(I), W(I), Y(I), XL1(I), XL2(I));
    END;
  CLOSE(KF1);
  FOR I:=1 TO NU DO
    BEGIN
      PRC(I) = P/PCC(I);          TRC(I) = TT/TCC(I);
      MMC(I) = 0.480 + 1.574*W(I) - 0.176*W(I)*W(I);
      KLC(I) = (1 + MMC(I) - MMC(I)*SQRT(TRC(I)));
      DDC(I) = KLC(I)*KLC(I);
    END;
  FOR I:=1 TO NU DO
    BEGIN
      AIJC(I, I) = 0.42747*DDC(I)*RR*RR*TCC(I)*TCC(I)/PCC(I);
      BIJC(I, I) = 0.08664*RR*TCC(I)/PCC(I);
    END;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:= 1 TO NU DO
        BEGIN
          AIJC(I, J) = SQRT(AIJC(I, I))*SQRT(AIJC(J, J));

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      BIJ(I,J):=(BIJ(I,I)+BIJ(J,J))/2;
    END;
  END;
  AT:=0;      BT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          AT:=AT+Y(I)*Y(J)*AIJ(I,J);
          BT:=BT+Y(I)*Y(J)*BIJ(I,J);
        END;
      END;
    END;
  ALI(I):=0;      BLI(I):=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          ALI(I)=ALI(I)+XL(I)*XL(J)*AIJ(I,J);
          BLI(I)=BLI(I)+XL(I)*XL(J)*BIJ(I,J);
        END;
      END;
    END;
  ALI(2):=0;      BLI(2):=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          ALI(2)=ALI(2)+XL2(I)*XL2(J)*AIJ(I,J);
          BLI(2)=BLI(2)+XL2(I)*XL2(J)*BIJ(I,J);
        END;
      END;
    END;

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  END;
  FOR I:=1 TO NU DO
    BEGIN
      AEC(I):=AIJ(I,I)*P/(RR*RR*TT*TT);
      BEC(I):=BIJ(I,I)*P/(RR*TT);
    END;
  AT:=AT*P/(RR*RR*TT*TT);      BT:=BT*P/(RR*TT);
  QM:=AT-BT-BT*BT;      RQ:=AT*BT;
  ZK:=1;
  FOR I:=1 TO 10 DO
    BEGIN
      F1=ZK*ZK*ZK-ZK*ZK+(AT-BT-BT*BT)*ZK-AT*BT;
      F1:=3*ZK*ZK-2*ZK+QM;
      F4:=-F/F1;
      ZA:=ZK+F4;
      ZK:=ZA;
    END;
  ZL:=ZK;
  FOR I:=1 TO 2 DO
    BEGIN
      AT(I):=ALI(I)*P/(RR*RR*TT*TT);
      BT(I):=BLI(I)*P/(RR*TT);
      QM(I):=AT(I)-BT(I)-BT(I)*BT(I);
    END;
  ZL(I):=0; ZL(2):=0;
  FOR I:=1 TO 10 DO
    BEGIN
      F1=ZL(I)*ZL(I)*ZL(I)-ZL(I)*ZL(I)+
        (AT(I)-BT(I)-BT(I)*BT(I))*ZL(I)-AT(I)*BT(I);

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F1:=3*ZL1(1)*ZL1(1)-2*ZL1(1)+QM1(1);
F4:=- (F/F1);
ZA:=ZL1(1)+F4;
ZL1(1):=ZA;
END;
FOR I:=1 TO 10 DO
BEGIN
F1:=ZL1(2)*ZL1(2)*ZL1(2)-ZL1(2)*ZL1(2)+
(AT1(2)-BT1(2)-BT1(2)*BT1(2))*ZL1(2)-AT1(2)*BT1(2);
F1:=3*ZL1(2)*ZL1(2)-2*ZL1(2)+QM1(2);
F4:=- (F/F1);
ZA:=ZL1(2)+F4;
ZL1(2):=ZA;
END;
V1:=ZL*RR*TT/P1;          V2:=ZL1(1)*RR*TT/P1;
V3:=ZL1(2)*RR*TT/P1;      YTC(2):=0.9111;
YTC(3):=0.0001;           YTC(1):=1-YTC(2)-YTC(3);
XT1(1):=0.0345;           XT1(2):=0.8920;
XT1(3):=1-XT1(1)-XT1(2); XT2(1):=0.0497;
XT2(2):=0.9432;           XT2(3):=1-XT2(1)-XT2(2);
AP1:=V2/(V1+V2+V3);       BP1:=V3/(V1+V2+V3);
FOR I:=1 TO NU DO
BEGIN
Z(I):=(YTC(I)+XT1(I)+XT2(I))/3;
WRITELN('15,COMP(I).NAME:5,TCC(I):10:4,PCC(I):10:4,WC(I):10:4,
YC(I):8:4,XL1(I):8:4,XL2(I):8:4,Z(I):8:4);
END;
WRITELN;                WRITELN;
WRITELN('120,'COMPRESSIBILITY OF MIXTURE');

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WRITELN('15,'-----');
'-----');
WRITELN('120,'V','110,'L1','110,'L2');
WRITELN('15,'-----');
'-----');
WRITELN('115,ZL1:8:4,'14,ZL1(1):8:4,'14,ZL1(2):8:4);
WRITELN('15,'-----');
'-----');
WRITELN;
WRITELN('120,'MOLAR VOLUME OF MIXTURE(L/G-MOL)');
WRITELN('15,'-----');
'-----');
WRITELN('120,'V','110,'L1','110,'L2');
WRITELN('15,'-----');
'-----');
WRITELN('115,V1:8:4,'14,V2:8:4,'14,V3:8:4);
WRITELN('15,'-----');
'-----');
WRITELN;
WRITELN(BT1(1):8:4,BT1(2):8:4,BT1:8:4);
WRITELN;
WRITELN('120,'MIXTURE FUGACITY COEFFICIENTS');
WRITELN('15,'-----');
'-----');
WRITELN('17,'COMP','15,'QV:17,'QL1':10,'QL2':10,'17,
'KL1','17,'KL2');
WRITELN('15,'-----');
'-----');
FOR I:=1 TO NU DO

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BEGIN
  QV1(I) = EXP((ZL-I)*BEC(I)/BT-LN(ZL-BT)-
    (2*SQRT(AEC(I))/SQRT(AT)-BEC(I)/BT)*
    LN((ZL+BT)/ZL)*AT/BT);
  QL1(I) = EXP((ZL1(I)-1)*BEC(I)/BT1(I)-LN(ZL1(I)-BT1(I))-
    (2*SQRT(AEC(I))/SQRT(AT1(I))-BEC(I)/BT1(I))*
    LN((ZL1(I)+BT1(I))/ZL1(I))*AT1(I)/BT1(I));
  QL2(I) = EXP((ZL1(2)-1)*BEC(I)/BT1(2)-LN(ZL1(2)-BT1(2))-
    (2*SQRT(AEC(I))/SQRT(AT1(2))-BEC(I)/BT1(2))*
    LN((ZL1(2)+BT1(2))/ZL1(2))*AT1(2)/BT1(2));
  KL1(I) = QL1(I)/QV1(I);      KL2(I) = QL2(I)/QV1(I);
  WRITELN('15,COMP(I).NAME:0,QV1(I):10:4,QL1(I):10:4,
  QL2(I):10:4,KL1(I):10:4,KL2(I):10:4);
END;
WRITELN('15, '-----',
  '-----');
WRITELN(AP:8:4,BP:8:4);
U1=0.4548;      U2=0.33;      GU1=1;
WHILE GU<8 DO
  BEGIN
    Q1=0;
    Q2=0;
    FOR I=1 TO NU DO
      BEGIN
        Q1=Q1+(Z(I)*KL2(I)*(1-KL1(I)))/(KL1(I)*KL2(I)+U1
          *KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I)));
        Q2=Q2+(Z(I)*KL1(I)*(1-KL2(I)))/(KL1(I)*KL2(I)+U1
          *KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I)));
      END;
  END;

```

```

A(1,3)=-Q1; A(2,3)=-Q2; DQ11=0; DQ12=0; DQ22=0;
FOR I=1 TO NU DO
  BEGIN
    DQ11=DQ11+(-Z(I)*KL2(I)*KL2(I)*(1-KL1(I))*(1-KL1(I))
    /((KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I)))*
    (KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I))));
    DQ12=DQ12+(-Z(I)*KL1(I)*KL2(I)*(1-KL1(I))*(1-KL2(I))
    /((KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I)))*
    (KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I))));
    DQ22=DQ22+(-Z(I)*KL1(I)*KL1(I)*(1-KL2(I))*(1-KL2(I))
    /((KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I)))*
    (KL1(I)*KL2(I)+U1*KL2(I)*(1-KL1(I))+U2*KL1(I)*(1-KL2(I))));
  END;
DQ21=DQ12; A(1,1)=DQ11; A(1,2)=DQ12; A(2,1)=DQ21;
A(2,2)=DQ22;      KI=1;TN=2;DP=1;LI=1;
WHILE DP<2 DO
  BEGIN
    IF A(K,K)=0 THEN
      BEGIN
        AMAX=A(K,K);
        FOR I=1 TO 2 DO
          BEGIN
            IF AMAX<A(I,L) THEN
              BEGIN
                AMAX=A(I,L);
              END;
          END;
        END;
        WRITELN(AMAX:8:4);
        FOR I=1 TO 2 DO

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BEGIN
  IF AMAX=AC(1,L) THEN
    MT:=1;
  END;
  WRITELN('MT=',MT:4);
  FOR J:=1 TO 2 DO
    BEGIN
      CCK,J:=AC(MT,J);
      CCMT,J:=ACK,J;
    END;
  FOR J:=1 TO 2 DO
    BEGIN
      ACMT,J:=CCMT,J;
      ACK,J:=CCK,J;
    END;
  END;
  FOR N:=TN TO 2 DO
    BEGIN
      FOR J:=DP TO 3 DO
        BEGIN
          BC(N,J)=AC(N,J)-AC(N,K)*ACK,J/ACK,K;
        END;
      AC(N,1)=BC(N,1);  AC(N,2)=BC(N,2);
      AC(N,3)=BC(N,3);  AC(N,4)=BC(N,4);
    END;
    K:=K+1; TN:=TN+1; DP:=DP+1; L:=L+1;
  END;
  XX(2):=AC(2,3)/AC(2,2);
  XX(1):=(AC(1,3)-AC(1,2)*XX(2))/AC(1,1);

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```

U1:=U1+XX(1); U2:=U2+XX(2); HU1(GU):=Q1; HU2(GU):=Q2;
EU1(GU):=U1; EU2(GU):=U2; GU:=GU+1;
END;
WRITELN('','5','Q1','','5','Q2','','5','U1','','5','U2');
FOR I:=1 TO 7 DO
  BEGIN
    WRITELN(HU1(I):8:4,HU2(I):8:4,EU1(I):8:4,EU2(I):8:4);
  END;
  WRITELN;
  AP:=1-U1-U2;  BP:=U1/(U1+U2);
  FOR I:=1 TO NU DO
    BEGIN
      X1(I):=Z(I)/(AP*KL1(I)+(1-AP)*(BP+(1-BP)*KL1(I)/KL2(I)));
      X2(I):=Z(I)/(AP*KL2(I)+(1-AP)*(BP*KL2(I)/KL1(I)+1-BP));
      Y1(I)=KL1(I)*X1(I);  Y2(I)=KL2(I)*X2(I);
      KK1(I)=Y1(I)/X1(I);  KK2(I)=Y2(I)/X2(I);
    END;
    APT:=0; BPT:=0; CPT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT:=APT+ABS(XL1(I)-X1(I));
      BPT:=BPT+ABS(XL2(I)-X2(I));
      CPT:=CPT+ABS(Y(I)-Y1(I));
    END;
    APT:=0;  BPT:=0;  CPT:=0;  DPT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT:=APT+X1(I);  BPT:=BPT+X2(I);
      CPT:=CPT+Y1(I);  DPT:=DPT+Y2(I);

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END;
ERROR1:=APT1;   ERROR2:=BPT1;   ERROR3:=CPT1;
WRITELN(' '10,'ERROR1=',ERROR1:8:4,' '15,'ERROR2=',ERROR2:8:4,
        ' '15,'ERROR3=',ERROR3:8:4);
WRITELN;
WRITELN(' '13,'COMPOSITIONS AFTER RUN BY S-R-K EQUATION OF STATE');
WRITELN(' '15,'-----');
        '-----');
WRITELN(' '10,'COMP', ' '10,'Y1', ' '16,'Y2', ' '17,'X1', ' '16,
        'X2', ' '15,'KL1', ' '15,'KL2');
WRITELN(' '15,'-----');
        '-----');
FOR I:=1 TO NU DO
BEGIN
WRITELN(' '10,COMP(I).NAME,Y1(I):8:4,Y2(I):8:4,
        X1(I):8:4,X2(I):8:4,KL1(I):8:4,KL2(I):8:4);
END;
WRITELN(' '15,'-----');
        '-----');
WRITELN(' '10,'TOTAL', ' '15,CPT:8:4,DPT:8:4,APT:8:4,BPT:8:4);
WRITELN(' '15,'-----');
        '-----');
END.

```

```

PROGRAM HARMENS&KNAPP;
USES PRINTER;
CONST
G=0.3333;RR=0.082;P=47.35;TT=303.15;
TYPE
CLASS =RECORD
NAME:STRING(10);
END;
VAR
COMP:ARRAY[1..3]OF CLASS;
DD:ARRAY[1..3]OF REAL;   AL:ARRAY[1..2]OF REAL;
PR:ARRAY[1..3]OF REAL;   TR:ARRAY[1..2]OF REAL;
KL:ARRAY[1..3]OF REAL;   BL:ARRAY[1..3]OF REAL;
MP:ARRAY[1..3]OF REAL;   XL:ARRAY[1..3]OF REAL;
XL2:ARRAY[1..3]OF REAL;   TC:ARRAY[1..3]OF REAL;
PC:ARRAY[1..3]OF REAL;   QL:ARRAY[1..3]OF REAL;
W:ARRAY[1..3]OF REAL;    QL2:ARRAY[1..3]OF REAL;
X:ARRAY[1..3]OF REAL;    KL1:ARRAY[1..3]OF REAL;
Y:ARRAY[1..3]OF REAL;    KL2:ARRAY[1..3]OF REAL;
Z:ARRAY[1..3]OF REAL;    MM:ARRAY[1..3]OF REAL;
Y1:ARRAY[1..3]OF REAL;   A1:ARRAY[1..3]OF REAL;
Y2:ARRAY[1..3]OF REAL;   A1J:ARRAY[1..3,1..3]OF REAL;
B1J:ARRAY[1..3,1..3]OF REAL;  UU:ARRAY[1..3]OF REAL;
A:ARRAY[1..4,1..4]OF REAL;   QM:ARRAY[1..3]OF REAL;
B:ARRAY[1..4,1..4]OF REAL;   AE:ARRAY[1..3]OF REAL;
ZT:ARRAY[1..3]OF REAL;      BE:ARRAY[1..3]OF REAL;
ZH:ARRAY[1..3]OF REAL;      C:ARRAY[1..4,1..4]OF REAL;
ZTP:ARRAY[1..3]OF REAL;     AT:ARRAY[1..3]OF REAL;
BT:ARRAY[1..3]OF REAL;     ZL:ARRAY[1..3]OF REAL;
XX:ARRAY[1..4]OF REAL;      KK:ARRAY[1..3]OF REAL;
X1:ARRAY[1..3]OF REAL;     X2:ARRAY[1..3]OF REAL;

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```

KE2:ARRAY(1..3)OF REAL;      XT1:ARRAY(1..3)OF REAL;
XT2:ARRAY(1..3)OF REAL;      YT:ARRAY(1..3)OF REAL;
HU1:ARRAY(1..15)OF REAL;     EU1:ARRAY(1..15)OF REAL;
HU2:ARRAY(1..15)OF REAL;     EU2:ARRAY(1..15)OF REAL;
BI:ARRAY(1..3)OF REAL;       RA:ARRAY(1..3)OF REAL;
RAA:ARRAY(1..3)OF REAL;      ZC:ARRAY(1..3)OF REAL;
HC:ARRAY(1..3)OF REAL;       KO:ARRAY(1..3)OF REAL;
KTR:ARRAY(1..3)OF REAL;      APP:ARRAY(1..3)OF REAL;
RI:ARRAY(1..3)OF REAL;       CL:ARRAY(1..3)OF REAL;
UC:ARRAY(1..3,1..3)OF REAL;  WW:ARRAY(1..3)OF REAL;
BY:ARRAY(1..3)OF REAL;       AA:ARRAY(1..3)OF REAL;
BB:ARRAY(1..3)OF REAL;       QV:ARRAY(1..3)OF REAL;

T,ZL,ZV,AT,BT,U,DPT,APT1,BPT1,CPT1,ERROR3,ERROR4:REAL;
BPT,APT,CPT,V,V1,V2,V3,DT,ZJ,F,F1,F2,F3,F4:REAL;
QM,RQ,ZK,ZA,AMAX,DQ11,DQ12,DQ21,DQ22:REAL;
Q1,Q2,U1,U2,BP,AP,ERROR1,ERROR2,FW,DFW,BD:REAL;
LV,L1,L2,CT,WT,AK:REAL;
I,J,N,K,NG,HU,TN,DP,L,MT,GU:INTEGER;
CO2:STRING(15);
TRIDECANE:STRING(15);
KFI:TEXT;
FUNCTION PWR(E:REAL;H:REAL):REAL;
  BEGIN
    PWR:=EXP(E*LN(H));
  END;
FUNCTION TAN(X:REAL):REAL;
  BEGIN
    TAN:=SIN(X)/COS(X);
  END;

```

```

BEGIN
  NU:=3;
  WRITELN(LST,'FILE = HARMENS & KNAPP.PAS');
  WRITELN;
  WRITELN(LST,'T=',TT:8:2,'I4','K','I4','P=',PI:8:2);
  WRITELN(LST,'I19,'INITIAL ESTIMATE COMPOSITIONS');
  WRITELN(LST,'I5,'-----',
  '-----');
  WRITELN(LST,'I5,'COMP','I8','TC'I5,'PC'I10,'W'I10,'Y'I8,'XL'I
  I10,'XL2'I8,'Z'I7);
  WRITELN(LST,'I5,'-----',
  '-----');
  ASSIGN(KFI,'DEMO6.TXT');
  RESET(KFI);
  FOR I:=1 TO NU DO
    BEGIN
      READLN(KFI,COMP(I).NAME,TC(I),PC(I),WC(I),YC(I),XL(I),XL2(I));
    END;
  CLOSE(KFI);
  FOR I:=1 TO NU DO
    BEGIN
      PR(I)=P/PC(I);
      TR(I)=TT/TC(I);
      ZC(I)=0.3211-0.080*WC(I)+0.0384*WC(I)*WC(I);
      BC(I)=0.10770+0.76405*ZC(I)-1.24282*ZC(I)*ZC(I)+
      0.9621*ZC(I)*ZC(I)*ZC(I);
    END;
  FOR I:=1 TO NU DO
    BEGIN

```

```

IF WC(I) <= 0.2 THEN
AA(I) = 0.50 + 0.27767 * WC(I) + 2.17225 * WC(I) * WC(I)
IF WC(I) > 0.2 THEN
AA(I) = 0.41311 + 1.14657 * WC(I)
END
FOR I = 1 TO NU DO
BEGIN
IF WC(I) <= 0.2 THEN
BB(I) = -0.022 + 0.338 * WC(I) - 0.045 * WC(I) * WC(I)
IF WC(I) > 0.2 THEN
BB(I) = 0.0118
END
FOR J = 1 TO NU DO
BEGIN
IF TR(I) <= J THEN
DD(I) = (1 + AA(I) - AA(I) * SQRT(TR(I)) - BB(I) + BB(I) / TR(I)) *
(1 + AA(I) - AA(I) * SQRT(TR(I)) - BB(I) + BB(I) / TR(I))
DD(I) = 1 - (0.6258 + 1.5227 * WC(I)) * LN(TR(I)) + (0.1533 + 0.41 * WC(I))
* LN(TR(I)) * LN(TR(I))
END
FOR I = 1 TO NU DO
BEGIN
RA(I) = 1 - 3 * ZC(I) + 3 * ZC(I) * ZC(I) + BC(I) * ZC(I) * (3 - 6 * ZC(I)
+ BC(I) * ZC(I))
RB(I) = BC(I) * ZC(I)
END
FOR I = 1 TO NU DO
BEGIN
AIJ(I, J) = RA(I) * DD(I) * RR * RR * TC(I) * TC(I) / PC(I)

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BIJ(I, J) = RB(I) * RR * TC(I) / PC(I)
UC(I, J) = 1 + (1 - 3 * ZC(I)) / (BC(I) * ZC(I))
END
FOR I = 1 TO NU DO
BEGIN
FOR J = 1 TO NU DO
BEGIN
AIJ(I, J) = SQRT(AIJ(I, I)) * SQRT(AIJ(J, J))
BIJ(I, J) = (BIJ(I, I) + BIJ(J, J)) / 2
UC(I, J) = (UC(I, I) + UC(J, J)) / 2
END
END
AT = 0
BT = 0
CT = 0
FOR I = 1 TO NU DO
BEGIN
FOR J = 1 TO NU DO
BEGIN
AT = AT + YC(I) * YC(J) * AIJ(I, J)
BT = BT + YC(I) * YC(J) * BIJ(I, J)
CT = CT + YC(I) * YC(J) * UC(I, J)
END
END
AL(I) = 0
BL(I) = 0
CL(I) = 0
FOR I = 1 TO NU DO
BEGIN
FOR J = J TO NU DO
BEGIN
AL(I) = AL(I) + XL(I) * XL(J) * AIJ(I, J)
BL(I) = BL(I) + XL(I) * XL(J) * BIJ(I, J)

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```

          CL1(I)=CL1(I)+XL1(I)*XL1(J)*UC1(I,J)
        ENDI
      ENDI
      AL1(2)=0;          BL1(2)=0;          CL1(2)=0;
      FOR I=1 TO NU DO
        BEGIN
          FOR J=1 TO NU DO
            BEGIN
              AL1(2)=AL1(2)+XL2(I)*XL2(J)*A1J(I,J);
              BL1(2)=BL1(2)+XL2(I)*XL2(J)*B1J(I,J);
              CL1(2)=CL1(2)+XL2(I)*XL2(J)*UC1(I,J);
            ENDI
          ENDI
        ENDI
      FOR I=1 TO NU DO
        BEGIN
          AEC(I)=A1J(I,I)*P/(RR*RR*TT*TT);
          BEC(I)=B1J(I,I)*P/(RR*TT);
        ENDI
      WT=1-CT;          WW1(I)=1-CL1(I);          WW1(2)=1-CL1(2);
      AT=AT*P/(RR*RR*TT*TT);
      BT=BT*P/(RR*TT);
      ZK=1;
      FOR I=1 TO 10 DO
        BEGIN
          F1=ZK*ZK*ZK-(1+BT-CT*BT)*ZK*ZK+(AT+WT*BT*BT-CT*BT
            -CT*BT*BT)*ZK-AT*BT-WT*BT*BT-WT*BT*BT*BT;
          F11=3*ZK*ZK-2*(1+BT-CT*BT)*ZK+(AT+WT*BT*BT-CT*BT
            -CT*BT*BT);
          F41=-F/F1;

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```

          ZA1=ZK+F41;
          ZK1=ZA1;
        ENDI
      ENDI
      ZL1=ZK1;
      FOR I=1 TO 2 DO
        BEGIN
          AT1(I)=AL1(I)*P/(RR*RR*TT*TT);
          BT1(I)=BL1(I)*P/(RR*TT);
        ENDI
      ZL1(I)=0; ZL1(2)=0;
      FOR I=1 TO 2 DO
        BEGIN
          FOR J=1 TO 10 DO
            BEGIN
              F1=ZL1(I)*ZL1(I)*ZL1(I)-(1+BT1(I)-CL1(I)*BT1(I))*ZL1(I)*ZL1(I)
                +(AT1(I)+WW1(I)*BT1(I)*BT1(I)-CL1(I)*BT1(I)-CL1(I)*BT1(I)*BT1(I))
                *ZL1(I)-AT1(I)*BT1(I)-WW1(I)*BT1(I)*BT1(I)-WW1(I)
                *BT1(I)*BT1(I)*BT1(I);
              F11=3*ZL1(I)*ZL1(I)-2*(1+BT1(I)-CL1(I)*BT1(I))*ZL1(I)+(AT1(I)+WW1(I)
                *BT1(I)*BT1(I)-CL1(I)*BT1(I)-CL1(I)*BT1(I)*BT1(I));
              F41=-F/F11;
              ZA1=ZL1(I)+F41;
              ZL1(I)=ZA1;
            ENDI
          ENDI
          V1=ZL1*RR*TT/P;          V2=ZL1(I)*RR*TT/P;
          V3=ZL1(2)*RR*TT/P;      YTC(2)=0.9871;
          YTC(3)=0.0001;          YTC(1)=1-YTC(2)-YTC(3);
          XT1(I)=0.0053;          XT1(2)=0.9252;

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```

XT1(3)=1-XT1(1)-XT1(2) XT2(1)=0.0092
XT2(2)=0.9837 XT2(3)=1-XT2(1)-XT2(2)
AP1=V2/(V1+V2+V3) BP1=V3/(V1+V2+V3)
FOR I=1 TO NU DO
  BEGIN
    Z(I)=(Y(I)*XT1(I)+XT2(I))/3
    WRITELN(LST,'15,COMP(I).NAMR15,TCC(I):10:4,PCC(I):10:4,
    WC(I):10:4,YC(I):8:4,XL1(I):8:4,XL2(I):8:4,Z(I):8:4)
    END
    WRITELN(LST)
  WRITELN(LST,'120,COMPRESSIBILITY OF MIXTURE')
  WRITELN(LST,'15,-----',
  '-----')
  WRITELN(LST,'120,V','110,L1','110,L2')
  WRITELN(LST,'15,-----',
  '-----')
  WRITELN(LST,'115,ZL:8:4,'14,ZL1(I):8:4,'14,ZL1(2):8:4)
  WRITELN(LST,'15,-----',
  '-----')
  WRITELN(LST)
  WRITELN(LST,'120,MOLAR VOLUME OF MIXTURE(L/G-MOL)')
  WRITELN(LST,'15,-----',
  '-----')
  WRITELN(LST,'120,V','110,L1','110,L2')
  WRITELN(LST,'15,-----',
  '-----')
  WRITELN(LST,'115,V1:8:4,'14,V2:8:4,'14,V3:8:4)
  WRITELN(LST,'15,-----',
  '-----')

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```

WRITELN(LST)
WRITELN(BT1(1):8:4,BT1(2):8:4,BT1(3):8:4)
WRITELN
WRITELN(LST,'120,MIXTURE FUGACITY COEFFICIENTS')
WRITELN(LST,'15,-----',
  '-----')
WRITELN(LST,'17,COMP','15,QV:17,QL1:110,
  'QL2:110','17,KL1','17,KL2')
WRITELN(LST,'15,-----',
  '-----')
BY(1)=0 BY(2)=0 BY(3)=0
FOR I=1 TO NU DO
  BEGIN
    BY(1)=BY(1)+Y(I)*TCC(I)/PCC(I) BY(2)=BY(2)+XL1(I)*TCC(I)/PCC(I)
    BY(3)=BY(3)+XL2(I)*TCC(I)/PCC(I) B(I)=TCC(I)/PCC(I)
    END
    LV1=LN((2*ZL+BT*(CT+SQRT(CT*CT-4*WT)))/
    (2*ZL+BT*(CT-SQRT(CT*CT-4*WT))))
    L1=LN((2*ZL1(I)+BT1(I)*(CL1(I)+SQRT(CL1(I)*CL1(I)-4*WW1(I)))/
    (2*ZL1(I)+BT1(I)*(CL1(I)-SQRT(CL1(I)*CL1(I)-4*WW1(I))))
    L2=LN((2*ZL1(2)+BT1(2)*(CL1(2)+SQRT(CL1(2)*CL1(2)-4*WW1(2)))/
    (2*ZL1(2)+BT1(2)*(CL1(2)-SQRT(CL1(2)*CL1(2)-4*WW1(2))))
    AK1=AT*RR*RR*TT*TT/P1
    FOR I=1 TO NU DO
      BEGIN
        QV(I)=EXP((ZL-1)*B(I)/BY(I)-LN(ZL-BT)+AT*(B(I)/BY(I)
        -2*SQRT(A1J(I,I)/AK)))/(BT*SQRT(CT*CT-4*WT))*LV)
        QL1(I)=EXP((ZL1(I)-1)*B(I)/BY(2)-LN(ZL1(I)-BT1(I))+AT1(I)
        *(B(I)/BY(2)-2*SQRT(A1J(I,I)/AL1(I)))/(BT1(I)*SQRT

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```

      (CL1[1]*CL1[1]-4*WW1[1])*L1);
QL2[1]=EXP((ZL1[2]-1)*B1[1]/BY[3]-LN(ZL1[2]-BT1[2])+AT1[2])
*(B1[1]/BY[3]-2*SQR(AT1[1,1]/AL1[2]))/(BT1[2]*
  SQR(CL1[2]*CL1[2]-4*WW1[2])*L2);
KL1[1]=QL1[1]/QV[1];      KL2[1]=QL2[1]/QV[1];
WRITELN(LST,'15,COMP[1].NAME:8,QV[1]:10:4,QL1[1]:10:4,
  QL2[1]:10:4,KL1[1]:10:4,KL2[1]:10:4);
END;
WRITELN(LST,'15,-----',
  '-----');
WRITELN(AP:8:4,BP:8:4);
U1:=0.3909;      U2:=0.45;      GU:=1;
WHILE GU<8 DO
  BEGIN
    Q1:=0;      Q2:=0;
    FOR I:=1 TO NU DO
      BEGIN
        Q1:=Q1+(Z[1]*KL2[1]*(1-KL1[1]))/(KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])
          +U2*KL1[1]*(1-KL2[1]));
        Q2:=Q2+(Z[1]*KL1[1]*(1-KL2[1]))/(KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])
          +U2*KL1[1]*(1-KL2[1]));
      END;
      AC[1,3]:=-Q1;  AC[2,3]:=-Q2;  DQ11:=0;  DQ12:=0;  DQ22:=0;
      FOR I:=1 TO NU DO
        BEGIN
          DQ11:=DQ11+(-Z[1]*KL2[1]*KL2[1]*(1-KL1[1])*(1-KL1[1]))
            /((KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1]))*
              (KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1])));
          DQ12:=DQ12+(-Z[1]*KL1[1]*KL2[1]*(1-KL1[1])*(1-KL2[1]))

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```

            /((KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1]))*
              (KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1])));
          DQ22:=DQ22+(-Z[1]*KL1[1]*KL1[1]*(1-KL2[1])*(1-KL2[1]))
            /((KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1]))*
              (KL1[1]*KL2[1]+U1*KL2[1]*(1-KL1[1])+U2*KL1[1]*(1-KL2[1])));
        END;
      DQ21:=DQ12;  AC[1,1]:=DQ11;  AC[1,2]:=DQ12;  AC[2,1]:=DQ21;
      AC[2,2]:=DQ22;      KI:=1;  TNI:=2;  DPI:=1;  LI:=1;
      WHILE DP<2 DO
        BEGIN
          IF ACK,KJ=0 THEN
            BEGIN
              .AMAX:=ACK,KJ;
              FOR I:=1 TO 2 DO
                BEGIN
                  IF AMAX<AC[I,L] THEN
                    BEGIN
                      AMAX:=AC[I,L];
                    END;
                END;
              WRITELN(AMAX:8:4);
              FOR I:=1 TO 2 DO
                BEGIN
                  IF AMAX=AC[I,L] THEN
                    MT:=I;
                END;
              WRITELN('MT=',MT:4);
              FOR J:=1 TO 2 DO
                BEGIN

```

```

      C(K,J)=A(MT,J)
      C(MT,J)=A(K,J)
    END
  FOR J=1 TO 2 DO
    BEGIN
      A(MT,J)=C(MT,J)
      A(K,J)=C(K,J)
    END
  END
  FOR N=TN TO 2 DO
    BEGIN
      FOR J=DP TO 3 DO
        BEGIN
          B(N,J)=A(N,J)-A(N,K)*A(K,J)/A(K,K)
        END
        A(N,1)=B(N,1)
        A(N,2)=B(N,2)
        A(N,3)=B(N,3)
        A(N,4)=B(N,4)
      END
      K=K+1
      DP=DP+1
      TN=TN+1
      L=L+1
    END
    XX(2)=A(2,3)/A(2,2)
    XX(1)=(A(1,3)-A(1,2)*XX(2))/A(1,1)
    U1=U1+XX(1)
    U2=U2+XX(2)
    HU1(GU)=U1
    HU2(GU)=U2
    EU1(GU)=U1
    EU2(GU)=U2
    GU=GU+1
  
```

```

    END
    WRITELN(LST,' '15,'Q1',' '15,'Q2',' '15,'U1',' '15,'U2')
  FOR I=1 TO 7 DO
    BEGIN
      WRITELN(LST,HU1(I):8:4,HU2(I):8:4,EU1(I):8:4,EU2(I):8:4)
    END
    WRITELN(LST)
    AP=1-U1-U2
    BP=U1/(U1+U2)
    FOR I=1 TO NU DO
      BEGIN
        X1(I)=Z(I)/(AP*KL1(I)+(1-AP)*(BP+(1-BP)*KL1(I)/KL2(I)))
        X2(I)=Z(I)/(AP*KL2(I)+(1-AP)*(BP*KL2(I)/KL1(I)+1-BP))
        Y1(I)=KL1(I)*X1(I)
        Y2(I)=KL2(I)*X2(I)
        KK1(I)=Y1(I)/X1(I)
        KK2(I)=Y2(I)/X2(I)
      END
      APT=0
      BPT=0
      CPT=0
    FOR I=1 TO NU DO
      BEGIN
        APT=APT+ABS(XL1(I)-X1(I))
        BPT=BPT+ABS(XL2(I)-X2(I))
        CPT=CPT+ABS(YC(I)-Y1(I))
      END
      APT=0
      BPT=0
      CPT=0
      DPT=0
    FOR I=1 TO NU DO
      BEGIN
        APT=APT+X1(I)
        BPT=BPT+X2(I)
        CPT=CPT+Y1(I)
        DPT=DPT+Y2(I)
      END
      ERROR1=APT
      ERROR2=BPT
      ERROR3=CPT
    
```

```

WRITELN(LST, ' :10, 'ERROR1=' , ERROR1:8:4, ' :5, 'ERROR2=' ,
ERROR2:8:4, ' :5, 'ERROR3=' , ERROR3:8:4);
WRITELN(LST);
WRITELN(LST, ' :13, 'COMPOSITIONS AFTER RUN BY S-R-K EQUATION OF STATE');
WRITELN(LST, ' :15, '-----',
'-----');
WRITELN(LST, ' :10, 'COMP', ' :10, 'Y1', ' :16, 'Y2', ' :17, 'X1', ' :
6, 'X2', ' :5, 'KL1', ' :5, 'KL2');
WRITELN(LST, ' :15, '-----',
'-----');
FOR I:=1 TO NU DO
BEGIN
WRITELN(LST, ' :10, COMP[I].NAME, Y1[I]:8:4, Y2[I]:8:4, X1[I]:8:4,
X2[I]:8:4, KL1[I]:8:4, KL2[I]:8:4);
END;
WRITELN(LST, ' :5, '-----',
'-----');
WRITELN(LST, ' :10, 'TOTAL', ' :15, CPT:8:4, DPT:8:4, APT:8:4, BPT:8:4);
WRITELN(LST, ' :15, '-----',
'-----');
END.

```

```

PROGRAM PengRobinson;
USES PRINTER;
CONST
G=0.3333;RR=0.082;P=79.29;TT=301.15;
TYPE
CLASS =RECORD
NAME:STRING[10];
END;
VAR
COMP:ARRAY[1..3]OF CLASS;
DD:ARRAY[1..3]OF REAL; A1:ARRAY[1..2]OF REAL;
PR:ARRAY[1..3]OF REAL; TR:ARRAY[1..2]OF REAL;
KL:ARRAY[1..3]OF REAL; BL:ARRAY[1..3]OF REAL;
MP:ARRAY[1..3]OF REAL; XL:ARRAY[1..3]OF REAL;
WT:ARRAY[1..3]OF REAL; XL2:ARRAY[1..3]OF REAL;
TC:ARRAY[1..3]OF REAL; QV:ARRAY[1..3]OF REAL;
PC:ARRAY[1..3]OF REAL; QL:ARRAY[1..3]OF REAL;
W:ARRAY[1..3]OF REAL; QL2:ARRAY[1..3]OF REAL;
X:ARRAY[1..3]OF REAL; KL1:ARRAY[1..3]OF REAL;
Y:ARRAY[1..3]OF REAL; KL2:ARRAY[1..3]OF REAL;
Z:ARRAY[1..3]OF REAL; MM:ARRAY[1..3]OF REAL;
Y1:ARRAY[1..3]OF REAL; A11:ARRAY[1..3]OF REAL;
Y2:ARRAY[1..3]OF REAL; A1J:ARRAY[1..3,1..3]OF REAL;
BIJ:ARRAY[1..3,1..3]OF REAL; UU:ARRAY[1..3]OF REAL;
A:ARRAY[1..4,1..4]OF REAL; QM:ARRAY[1..3]OF REAL;
B:ARRAY[1..4,1..4]OF REAL; AE:ARRAY[1..3]OF REAL;
ZT:ARRAY[1..3]OF REAL; BE:ARRAY[1..3]OF REAL;
ZH:ARRAY[1..3]OF REAL; C:ARRAY[1..4,1..4]OF REAL;
ZTP:ARRAY[1..3]OF REAL; AT:ARRAY[1..3]OF REAL;

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BT1:ARRAY[1..3]OF REAL;      ZL1:ARRAY[1..3]OF REAL;
XX:ARRAY[1..4]OF REAL;      KK:ARRAY[1..3]OF REAL;
X1:ARRAY[1..3]OF REAL;      X2:ARRAY[1..3]OF REAL;
KK2:ARRAY[1..3]OF REAL;     XT1:ARRAY[1..3]OF REAL;
XT2:ARRAY[1..3]OF REAL;     YT:ARRAY[1..3]OF REAL;
KO:ARRAY[1..3]OF REAL;      K1:ARRAY[1..3]OF REAL;
KK1:ARRAY[1..3]OF REAL;     SU1:ARRAY[1..3]OF REAL;
SU2:ARRAY[1..3]OF REAL;     SU3:ARRAY[1..3]OF REAL;
UT1:ARRAY[1..15]OF REAL;    UT2:ARRAY[1..15]OF REAL;
QU1:ARRAY[1..15]OF REAL;    QU2:ARRAY[1..15]OF REAL;
T,ZL,ZV,AT,BT,U,DPT,APT1,BPT1,CPT1,ERROR3,ERROR4:REAL;
BPT,APT,CPT,V,V1,V2,V3,DT,ZJ,F,F1,F2,F3,F4,A1,B1:REAL;
QM,RQ,ZK,ZA,AMAX,DQ11,DQ12,DQ21,DQ22:REAL;
Q1,Q2,U1,U2,BP,AP,ERROR1,ERROR2:REAL;
I,J,N,K,NG,NU,TH,DP,L,MT,GU:INTEGER;
CO2:STRING[15];
TRIDECANE:STRING[15];
KFI:TEXT;
FUNCTION PWR(E:REAL;H:REAL):REAL;
  BEGIN
    PWR:=EXP(E*LN(H))
  END;
FUNCTION TAN(X:REAL):REAL;
  BEGIN
    TAN:=SIN(X)/COS(X)
  END;
BEGIN
  NU:=3;
  WRITELN(LST,'FILE = PRW.PAS');  WRITELN(LST);

```

```

  WRITELN(LST,'T=',TT:8:2,' '14,'K',' '14,'P=',P:8:2);
  WRITELN(LST,' '19,'INITIAL ESTIMATE COMPOSITIONS');
  WRITELN(LST,' '15,'-----',
    '-----');
  WRITELN(LST,' '15,'COMP',' '18,'TC'15,'PC'110,'W'110,'Y'18,'
    XL1'110,'XL2'18,'Z'17);
  WRITELN(LST,' '15,'-----',
    '-----');
  ASSIGN(KFI,'DEMO7.TXT');
  RESET(KFI);
  FOR I:=1 TO NU DO
  BEGIN
    READLN(KFI,COMP[I].NAME,TCC[I],PCC[I],WCI,YCI,XL1[I],XL2[I]);
  END;
  CLOSE(KFI);
  FOR I:=1 TO NU DO
  BEGIN
    PRC[I]=P/PCC[I];          TRC[I]=TT/TCC[I];
    MMC[I]=0.37464+1.54226*WCI-0.26992*WCI*WCI;
    KLC[I]=(1+MMC[I]-MMC[I]*SORT(TRC[I])); DDE[I]=KLC[I]*KLC[I];
  END;
  FOR I:=1 TO NU DO
  BEGIN
    AIJ[I,I]=0.45724*DDI[1]*RR*RR*TCC[I]*TCC[I]/PCC[I];
    BIJ[I,I]=0.07780*RR*TCC[I]/PCC[I];
  END;
  FOR I:=1 TO NU DO
  BEGIN
    FOR J:= 1 TO NU DO

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      BEGIN
    AIJ[1,J]:=SQRT(AIJ[1,I])*SQRT(AIJ[J,J]);
      END;
    END;
  AT:=0;      AL1[1]:=0;      AL1[2]:=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          AT:=AT+Y[I]*Y[J]*AIJ[1,J];
          AL1[1]:=AL1[1]+XL1[I]*XL1[J]*AIJ[1,J];
          AL1[2]:=AL1[2]+XL2[I]*XL2[J]*AIJ[1,J];
        END;
      END;
    BT:=0;      BL1[1]:=0;      BL1[2]:=0;
    FOR I:=1 TO NU DO
      BEGIN
        BT:=BT+Y[I]*BIJ[1,I];      BL1[1]:=BL1[1]+XL1[I]*BIJ[1,I];
        BL1[2]:=BL1[2]+XL2[I]*BIJ[1,I];
      END;
    AT:=AT*P/(RR*RR*TT*TT);  BT:=BT*P/(RR*TT);  QM:=AT-3*BT*BT-2*BT;
    RQ:=AT*BT;      ZK:=1;
    FOR I:=1 TO 10 DO
      BEGIN
        F:=ZK*ZK*ZK-(1-BT)*ZK*ZK+(AT-3*BT*BT-2*BT)*ZK-(AT*BT-BT*BT-
          BT*BT*BT);
        F1:=3*ZK*ZK-2*(1-BT)*ZK+QM;
        F4:=- (F/F1);
        ZA:=ZK+F4;

```

```

      ZK:=ZA;
    END;
    ZL1:=ZK;
  FOR I:=1 TO 2 DO
    BEGIN
      AT1[I]:=AL1[I]*P/(RR*RR*TT*TT);
      BT1[I]:=BL1[I]*P/(RR*TT);
      QM1[I]:=AT1[I]-3*BT1[I]*BT1[I]-2*BT1[I];
    END;
    ZL1[1]:=0; ZL1[2]:=0;
  FOR I:=1 TO 2 DO
    BEGIN
      FOR J:=1 TO 10 DO
        BEGIN
          F:=ZL1[I]*ZL1[I]*ZL1[I]-(1-BT1[I])*ZL1[I]*ZL1[I]+QM1[I];
          *ZL1[I]-(AT1[I]*BT1[I]-BT1[I]*BT1[I]-BT1[I]*BT1[I]*BT1[I]);
          F1:=3*ZL1[I]*ZL1[I]-2*(1-BT1[I])*ZL1[I]+QM1[I];
          F4:=- (F/F1);
          ZA:=ZL1[I]+F4;
          ZL1[I]:=ZA;
        END;
      END;
    V1:=ZL*RR*TT/P;  V2:=ZL1[1]*RR*TT/F;  V3:=ZL1[2]*RR*TT/P;
    YT[1]:=0.9521;  YT[2]:=0.0470;  YT[3]:=1-YT[1]-YT[2];
    XT1[1]:=0.7016;  XT1[2]:=0.0093;  XT1[3]:=1-XT1[1]-XT1[2];
    XT2[1]:=0.9684;  XT2[2]:=0.0302;  XT2[3]:=1-XT2[1]-XT2[2];
    AP:=V2/(V1+V2+V3);  BP:=V3/(V1+V2+V3);
  FOR I:=1 TO NU DO
    BEGIN

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      Z[I]= (YTC[I]+XT1[I]+XT2[I])/3;
WRITELN(LST, ' :5, COMPE [I].NAME:5, TCE [I]:10:4, PCE [I]:10:4, WE [I]
:10:4, YC [I]:8:4, XL1C [I]:8:4, XL2C [I]:8:4, Z [I]:8:4);
      END;
      WRITELN(LST);
      WRITELN(LST, ' :20, 'COMPRESSIBILITY OF MIXTURE');
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST, ' :20, 'V', ' :10, 'L1', ' :10, 'L2');
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST, ' :15, ZL:8:4, ' :4, ZL1C [I]:8:4, ' :4, ZL1C [2]:8:4);
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST);
      WRITELN(LST, ' :20, 'MOLAR VOLUME OF MIXTURE(L/G-MOL)');
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST, ' :20, 'V', ' :10, 'L1', ' :10, 'L2');
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST, ' :15, V1:8:4, ' :4, V2:8:4, ' :4, V3:8:4);
      WRITELN(LST, ' :5, '-----',
      '-----');
      WRITELN(LST);
      WRITELN(LST, ' :15, BT1C [I]:8:4, BT1C [2]:8:4, BT:8:4);
      WRITELN(LST);
      WRITELN(LST, ' :20, 'MIXTURE FUGACITY COEFFICIENTS');
      WRITELN(LST, ' :5, '-----',

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      '-----');
WRITELN(LST, ' :17, 'COMP', ' :15, 'QV':17, 'QL1':10, 'QL2'
:10, ' :17, 'KL1', ' :17, 'KL2');
WRITELN(LST, ' :5, '-----',
      '-----');
      a1:=AT*RR*RR*TT*TT/P;          b1:=BT*RR*TT/P;
      FOR I:=1 TO NU DO
      BEGIN
        SU1[I]=0;          SU2[I]=0;          SU3[I]=0;
        FOR K:=1 TO NU DO
        BEGIN
          SU1[I]=SU1[I]+Y[K]*A1J[I, K];
          SU2[I]=SU2[I]+XL1C [K]*A1J[I, K];
          SU3[I]=SU3[I]+XL2C [K]*A1J[I, K];
        END;
      END;
      FOR I:=1 TO NU DO
      BEGIN
        QV[I]=EXP(BIJ[I, I]*(ZL-1)/b1-LN(ZL-BT)-(LN((ZL+2.414*BT)
/(ZL-0.414*BT)))*(2*SU1[I]/a1-BIJ[I, I]/b1)*AT/(2.828*BT));
        QL1[I]=EXP(BIJ[I, I]*(ZL1C [I]-1)/BL1C [I]-LN(ZL1C [I]-BT1C [I])
-(LN((ZL1C [I]+2.414*BT1C [I])/(ZL1C [I]-0.414*BT1C [I])))
*(2*SU2[I]/AL1C [I]-BIJ[I, I]/BL1C [I])*AT1C [I]/(2.828*BT1C [I]));
        QL2[I]=EXP(BIJ[I, I]*(ZL1C [2]-1)/BL1C [2]-LN(ZL1C [2]-BT1C [2])
-(LN((ZL1C [2]+2.414*BT1C [2])/(ZL1C [2]-0.414*BT1C [2])))
*(2*SU3[I]/AL1C [2]-BIJ[I, I]/BL1C [2])*AT1C [2]/(2.828*BT1C [2]));
        KL1[I]=QL1[I]/QV[I];          KL2[I]=QL2[I]/QV[I];
      WRITELN(LST, ' :5, COMPE [I].NAME:8, QV [I]:10:4, QL1 [I]
:10:4, QL2 [I]:10:4, KL1 [I]:10:4, KL2 [I]:10:4);

```

```

END;
WRITELN(LST, ' :5, '-----',
        '-----');
WRITELN(AP:8:4, BP:8:4);
U1:=0.8009;    U2:=0.2055;    GU:=1;
WHILE GU<7 DO
  BEGIN
    Q1:=0;    Q2:=0;
    FOR I:=1 TO NU DO
      BEGIN
        Q1:=Q1+(Z[I]*KL2[I]*(1-KL1[I]))/(KL1[I]*KL2[I]+U1*KL2[I]
          *(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
        Q2:=Q2+(Z[I]*KL1[I]*(1-KL2[I]))/(KL1[I]*KL2[I]+U1*KL2[I]
          *(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
      END;
    A[1,3]:=-Q1; A[2,3]:=-Q2; DQ11:=0; DQ12:=0; DQ22:=0;
    FOR I:=1 TO NU DO
      BEGIN
        DQ11:=DQ11+(-Z[I]*KL2[I]*KL2[I]*(1-KL1[I])*(1-KL1[I]))
          /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
            (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
        DQ12:=DQ12+(-Z[I]*KL1[I]*KL2[I]*(1-KL1[I])*(1-KL2[I]))
          /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
            (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
        DQ22:=DQ22+(-Z[I]*KL1[I]*KL1[I]*(1-KL2[I])*(1-KL2[I]))
          /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
            (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
      END;
    DQ21:=DQ12;    A[1,1]:=DQ11;    A[1,2]:=DQ12;

```

```

A[2,1]:=DQ21;    A[2,2]:=DQ22;    K:=1; TN:=2; DP:=1; L:=1;
  WHILE DP<2 DO
    BEGIN
      IF A[K,K]=0 THEN
        BEGIN
          AMAX:=A[K,K];
          FOR I:=1 TO 2 DO
            BEGIN
              IF AMAX<A[I,L] THEN
                BEGIN
                  AMAX:=A[I,L];
                END;
            END;
          WRITELN(AMAX:8:4);
          FOR I:=1 TO 2 DO
            BEGIN
              IF AMAX=A[I,L] THEN
                MT:=I;
            END;
          WRITELN('MT=', MT:4);
          FOR J:=1 TO 2 DO
            BEGIN
              C[K,J]:=A[MT,J];
              C[MT,J]:=A[K,J];
            END;
          FOR J:=1 TO 2 DO
            BEGIN
              A[MT,J]:=C[MT,J];
              A[K,J]:=C[K,J];

```

```

      END;
    END;
  FOR NI=TN TO 2 DO
    BEGIN
      FOR JI=DP TO 3 DO
        BEGIN
          BCN,JJ:=ACN,JJ-ACN,KJ*AKK,JJ/ACK,KJ;
        END;
      ACN,1J:=BCN,1J; ACN,2J:=BCN,2J;
      ACN,3J:=BCN,3J; ACN,4J:=BCN,4J;
    END;
    K:=K+1; TN:=TN+1; DP:=DP+1; LI=L+1;
  END;
  XX[2J]:=AC[2,3J]/AC[2,2J];
  XX[1J]:=(AC[1,3J]-AC[1,2J]*XX[2J])/AC[1,1J];
  U1:=U1+XX[1J]; U2:=U2+XX[2J]; UT1[GUJ]=U1;
  UT2[GUJ]=U2; QU1[GUJ]=Q1; QU2[GUJ]=Q2; GU:=GU+1;
  END;
  WRITELN(LST,' :5,'U1',' :10,'U2',' :12,'Q1',' :10,'Q2');
  FOR I:=1 TO 6 DO
    BEGIN
      WRITELN(LST,UT1[I]:8:4,' :5,UT2[I]:8:4,' :5,QU1[I]:8:4,
        ' :5,QU2[I]:8:4);
    END;
  WRITELN;
  AP:=1-U1-U2; BP:=U1/(U1+U2);
  FOR I:=1 TO NU DO
    BEGIN
      X1[I]:= Z[I]/(AP*KL1[I]+(1-AP)*(BP+(1-BP)*KL1[I]/KL2[I]));

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```

      X2[I]:= Z[I]/(AP*KL2[I]+(1-AP)*(BP*KL2[I]/KL1[I]+1-BP));
      Y1[I]:=KL1[I]*X1[I]; Y2[I]:=KL2[I]*X2[I];
      KK1[I]:=Y1[I]/X1[I]; KK2[I]:=Y1[I]/X2[I];
    END;
    APT1:=0; BPT1:=0; CPT1:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT1:=APT1+ABS(XL1[I]-X1[I]);
      BPT1:=BPT1+ABS(XL2[I]-X2[I]);
      CPT1:=CPT1+ABS(Y[I]-Y1[I]);
    END;
    APT:=0; BPT:=0; CPT:=0; DPT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT:=APT+X1[I]; BPT:=BPT+X2[I];
      CPT:=CPT+Y1[I]; DPT:=DPT+Y2[I];
    END;
    ERROR1:=APT; ERROR2:=BPT; ERROR3:=CPT;
    WRITELN(LST,' :10,'ERROR1=' ,ERROR1:8:4,' :5,'ERROR2=' ,
      ERROR2:8:4,' :5,'ERROR3=' ,ERROR3:8:4);
    WRITELN(LST);
    WRITELN(LST,' :13,'COMPOSITIONS AFTER RUN BY S-R-K EQUATION OF STATE');
    WRITELN(LST,' :5,'-----',
      '-----');
    WRITELN(LST,' :10,'COMP',' :10,'Y1',' :6,'Y2',' :7,'X1',
      ' :6,'X2',' :5,'KL1',' :5,'KL2');
    WRITELN(LST,' :5,'-----',
      '-----');
  FOR I:=1 TO NU DO

```



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161 BEGIN
WRITELN(LST, ':10,COMP[1].NAME,Y[1]:8:4,Y2[1]:8:4,
        X1[1]:8:4,X2[1]:8:4,KL1[1]:8:4,KL2[1]:8:4);
END;
WRITELN(LST, ':5, '-----',
        '-----');
WRITELN(LST, ':10, 'TOTAL', ':5,CPT:8:4,DPT:8:4,APT:8:4,BPT:8:4);
WRITELN(LST, ':5, '-----',
        '-----');
END.

```

```

PROGRAM GraboskiDaubert;
CONST
G=0.3333;RR=0.082;P=48.95;TT=298.15;
TYPE
CLASS =RECORD
NAME:STRING[10];
END;
VAR
COMP:ARRAY[1..3]OF CLASS;
DD:ARRAY[1..3]OF REAL;
PR:ARRAY[1..3]OF REAL;
KL:ARRAY[1..3]OF REAL;
MP:ARRAY[1..3]OF REAL;
WT:ARRAY[1..3]OF REAL;
TC:ARRAY[1..3]OF REAL;
PC:ARRAY[1..3]OF REAL;
W:ARRAY[1..3]OF REAL;
X:ARRAY[1..3]OF REAL;
Y:ARRAY[1..3]OF REAL;
Z:ARRAY[1..3]OF REAL;
Y1:ARRAY[1..3]OF REAL;
Y2:ARRAY[1..3]OF REAL;
BIJ:ARRAY[1..3,1..3]OF REAL;
A:ARRAY[1..4,1..4]OF REAL;
B:ARRAY[1..4,1..4]OF REAL;
ZT:ARRAY[1..3]OF REAL;
ZH:ARRAY[1..3]OF REAL;
ZTP:ARRAY[1..3]OF REAL;
BT1:ARRAY[1..3]OF REAL;
AL1:ARRAY[1..2]OF REAL;
TR:ARRAY[1..2]OF REAL;
BL1:ARRAY[1..3]OF REAL;
XL1:ARRAY[1..3]OF REAL;
XL2:ARRAY[1..3]OF REAL;
QV:ARRAY[1..3]OF REAL;
QL1:ARRAY[1..3]OF REAL;
QL2:ARRAY[1..3]OF REAL;
KL1:ARRAY[1..3]OF REAL;
KL2:ARRAY[1..3]OF REAL;
MM:ARRAY[1..3]OF REAL;
AI1:ARRAY[1..3]OF REAL;
AIJ:ARRAY[1..3,1..3]OF REAL;
UU:ARRAY[1..3]OF REAL;
QM1:ARRAY[1..3]OF REAL;
AE:ARRAY[1..3]OF REAL;
BE:ARRAY[1..3]OF REAL;
C:ARRAY[1..4,1..4]OF REAL;
AT1:ARRAY[1..3]OF REAL;
ZL1:ARRAY[1..3]OF REAL;

```

```

XX:ARRAY[1..4]OF REAL;      KK1:ARRAY[1..3]OF REAL;
X1:ARRAY[1..3]OF REAL;      X2:ARRAY[1..3]OF REAL;
KK2:ARRAY[1..3]OF REAL;      XT1:ARRAY[1..3]OF REAL;
XT2:ARRAY[1..3]OF REAL;      YT:ARRAY[1..3]OF REAL;
HU1:ARRAY[1..15]OF REAL;     EU1:ARRAY[1..15]OF REAL;
HU2:ARRAY[1..15]OF REAL;     EU2:ARRAY[1..15]OF REAL;
T,ZL,ZV,AT,BT,U,DPT,APT1,BPT1,CPT1,ERROR3,ERROR4:REAL;
BPT,APT,CPT,V,V1,V2,V3,DT,ZJ,F,F1,F2,F3,F4:REAL;
QM,RQ,ZK,ZA,AMAX,DQ11,DQ12,DQ21,DQ22:REAL;
Q1,Q2,U1,U2,BP,AP,ERROR1,ERROR2:REAL;
I,J,N,K,NG,NU,TN,DP,L,MT,GU:INTEGER;
CO2:STRING[15];
TRIDECANE:STRING[15];
KF1:TEXT;
FUNCTION PWR(E:REAL;H:REAL):REAL;
  BEGIN
    PWR:=EXP(E*LN(H))
  END;
FUNCTION TAN(X:REAL):REAL;
  BEGIN
    TAN:=SIN(X)/COS(X)
  END;
BEGIN
  NU:=3;
  WRITELN('FILE = DUO3.PAS');
  WRITELN;
  WRITELN('T=',TT:8:2,'':4,'K',':':4,'P=',P:8:2);
  WRITELN('':19,'INITIAL ESTIMATE COMPOSITIONS');
  WRITELN('':15,'-----');

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-----');
WRITELN('':5,'COMP',':':8,'TC':5,'PC':10,'W':10,'Y':8,
'XL1':10,'XL2':8,'Z':7);
WRITELN('':5,'-----');
-----');
  ASSIGN(KF1,'WUN.TXT');
  RESET(KF1);
  FOR I:=1 TO NU DO
    BEGIN
      READLN(KF1,COMP[I],NAME,TC[I],PC[I],WC[I],Y[I],XL1[I],XL2[I]);
      END;
      CLOSE(KF1);
      FOR I:=1 TO NU DO
        BEGIN
          PR[I]:=P/PC[I];      TR[I]:=TT/TC[I];
          MM[I]:=0.48508+1.55171*WC[I]-0.15613*WC[I]*W[I];
          KL[I]:=(1+MM[I]-MM[I]*SQRT(TR[I]));
          DD[I]:=KL[I]*KL[I];
        END;
        FOR I:=1 TO NU DO
          BEGIN
            AIJ[I,I]:=0.42747*DD[I]*RR*RR*TC[I]*TC[I]/PC[I];
            BIJ[I,I]:=0.08664*RR*TC[I]/PC[I];
          END;
          FOR I:=1 TO NU DO
            BEGIN
              FOR J:= 1 TO NU DO
                BEGIN
                  AIJ[I,J]:=SQRT(AIJ[I,I])*SQRT(AIJ[J,J]);

```

```

      BIJCI,JJ)=(BIJCI,IJ+BIJCJ,JJ)/2;
      END;
    END;
  END;
  AT:=0;      BT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          AT:=AT+YCIJ)*Y[CJ]*AIJCI,JJ;
          BT:=BT+YCIJ)*Y[CJ]*BIJCI,JJ;
        END;
      END;
    END;
  AL1CI)=0;      BL1CI)=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          AL1CI)=AL1CI)+XL1CI)*XL1CJ)*AIJCI,JJ;
          BL1CI)=BL1CI)+XL1CI)*XL1CJ)*BIJCI,JJ;
        END;
      END;
    END;
  AL1C2)=0;      BL1C2)=0;
  FOR I:=1 TO NU DO
    BEGIN
      FOR J:=1 TO NU DO
        BEGIN
          AL1C2)=AL1C2)+XL2CI)*XL2CJ)*AIJCI,JJ;
          BL1C2)=BL1C2)+XL2CI)*XL2CJ)*BIJCI,JJ;
        END;
      END;
    END;

```

```

  END;
  FOR I:=1 TO NU DO
    BEGIN
      AEI)=AIJCI,IJ)*P/(RR*RR*TT*TT);
      BEI)=BIJCI,IJ)*P/(RR*TT);
    END;
  AT:=AT*P/(RR*RR*TT*TT);      BT:=BT*P/(RR*TT);
  QM:=AT-BT-BT*BT;      RQ:=AT*BT;
  ZK:=1;
  FOR I:=1 TO 10 DO
    BEGIN
      F1=ZK*ZK*ZK-ZK*ZK+(AT-BT-BT*BT)*ZK-AT*BT;
      F1:=3*ZK*ZK-2*ZK+QM;
      F4:=- (F/F1);
      ZA:=ZK+F4;
      ZK:=ZA;
    END;
  ZL:=ZK;
  FOR I:=1 TO 2 DO
    BEGIN
      AT1CI)=AL1CI)*P/(RR*RR*TT*TT);
      BT1CI)=BL1CI)*P/(RR*TT);
      QM1CI)=AT1CI)-BT1CI)-BT1CI)*BT1CI);
    END;
  ZL1CI)=0; ZL1C2)=0;
  FOR I:=1 TO 10 DO
    BEGIN
      F:=ZL1CI)*ZL1CI)*ZL1CI)-ZL1CI)*ZL1CI)+
      (AT1CI)-BT1CI)-BT1CI)*BT1CI)*ZL1CI)-AT1CI)*BT1CI);

```

```

F1:=3*ZL1[1]*ZL1[1]-2*ZL1[1]+QM1[1];
F4:=- (F/F1);
ZA:=ZL1[1]+F4;
ZL1[1]:=ZA;
END;
FOR I:=1 TO 10 DO
BEGIN
F:=ZL1[2]*ZL1[2]*ZL1[2]-ZL1[2]*ZL1[2]+
(AT1[2]-BT1[2]-BT1[2]*BT1[2])*ZL1[2]-AT1[2]*BT1[2];
F1:=3*ZL1[2]*ZL1[2]-2*ZL1[2]+QM1[2];
F4:=- (F/F1);
ZA:=ZL1[2]+F4;
ZL1[2]:=ZA;
END;
V1:=ZL*RR*TT/P;          V2:=ZL1[1]*RR*TT/P;
V3:=ZL1[2]*RR*TT/P;      Y2[2]:=0.91111;
YT[3]:=0.0001;           Y2[1]:=1-Y2[2]-Y2[3];
XT1[1]:=0.0345;          XT1[2]:=0.8920;
XT1[3]:=1-XT1[1]-XT1[2]; XT2[1]:=0.0497;
XT2[2]:=0.9432;          XT2[3]:=1-XT2[1]-XT2[2];
AP:=V2/(V1+V2+V3);      BP:=V3/(V1+V2+V3);
FOR I:=1 TO NU DO
BEGIN
Z[I]:=(YT[I]+XT1[I]+XT2[I])/3;
WRITELN(' :5,COMP',I,NAME;5,TC[I];10;4,PC[I];10;4,WC[I];10;4,
Y[I];8;4,XL1[I];8;4,XL2[I];8;4,Z[I];8;4);
END;
WRITELN;                WRITELN;
WRITELN(' :20,COMPRESSIBILITY OF MIXTURE');

```

```

WRITELN(' :15,-----');
'-----');
WRITELN(' :20, 'V', ' :10, 'L1', ' :10, 'L2');
WRITELN(' :15,-----');
'-----');
WRITELN(' :15,ZL;8;4, ' :4,ZL1[1];8;4, ' :4,ZL1[2];8;4);
WRITELN(' :15,-----');
'-----');
WRITELN;
WRITELN(' :20, 'MOLAR VOLUME OF MIXTURE(L/G-MOL)');
WRITELN(' :15,-----');
'-----');
WRITELN(' :20, 'V', ' :10, 'L1', ' :10, 'L2');
WRITELN(' :15,-----');
'-----');
WRITELN(' :15,V1;8;4, ' :4,V2;8;4, ' :4,V3;8;4);
WRITELN(' :15,-----');
'-----');
WRITELN;
WRITELN(BT1[1];8;4,BT1[2];8;4,BT;8;4);
WRITELN;
WRITELN(' :20, 'MIXTURE FUGACITY COEFFICIENTS');
WRITELN(' :15,-----');
'-----');
WRITELN(' :7, 'COMP', ' :5, 'QV';7, 'QL1';10, 'QL2';10, ' :7,
'KL1', ' :7, 'KL2');
WRITELN(' :15,-----');
'-----');
FOR I:=1 TO NU DO

```

```

BEGIN
  QV[1] := EXP((ZL-1)*BEC[1]/BT-LN(ZL-BT)-
    (2*SQRT(AEC[1])/SQRT(AT)-BEC[1]/BT)*
    LN((ZL+BT)/ZL)*AT/BT);
  QL1[1] := EXP((ZL1[1]-1)*BEC[1]/BT1[1]-LN(ZL1[1]-BT1[1])-
    (2*SQRT(AEC[1])/SQRT(AT1[1])-BEC[1]/BT1[1])*
    LN((ZL1[1]+BT1[1])/ZL1[1])*AT1[1]/BT1[1]);
  QL2[1] := EXP((ZL1[2]-1)*BEC[1]/BT1[2]-LN(ZL1[2]-BT1[2])-
    (2*SQRT(AEC[1])/SQRT(AT1[2])-BEC[1]/BT1[2])*
    LN((ZL1[2]+BT1[2])/ZL1[2])*AT1[2]/BT1[2]);
  KL1[1] := QL1[1]/QV[1];      KL2[1] := QL2[1]/QV[1];
  WRITELN(' :5,COMP[1].NAME:8,QV[1]:10:4,QL1[1]:10:4,
  QL2[1]:10:4,KL1[1]:10:4,KL2[1]:10:4);
END;
WRITELN(' :5, '-----',
  '-----');
WRITELN(AP:8:4,BP:8:4);
U1:=0.4548;      U2:=0.33;      GU:=1;
WHILE GU<8 DO
  BEGIN
    Q1:=0;
    Q2:=0;
    FOR I:=1 TO NU DO
      BEGIN
        Q1:=Q1+(Z[I]*KL2[I]*(1-KL1[I]))/(KL1[I]*KL2[I]+U1
          *KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
        Q2:=Q2+(Z[I]*KL1[I]*(1-KL2[I]))/(KL1[I]*KL2[I]+U1
          *KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]));
      END;
    END;
  END;

```

```

AC1,3]:=-Q1; AC2,3]:=-Q2; DQ11:=0; DQ12:=0; DQ22:=0;
FOR I:=1 TO NU DO
  BEGIN
    DQ11:=DQ11+(-Z[I]*KL2[I]*KL2[I]*(1-KL1[I])*(1-KL1[I]))
      /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
      (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I])));
    DQ12:=DQ12+(-Z[I]*KL1[I]*KL2[I]*(1-KL1[I])*(1-KL2[I]))
      /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
      (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I])));
    DQ22:=DQ22+(-Z[I]*KL1[I]*KL1[I]*(1-KL2[I])*(1-KL2[I]))
      /((KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I]))*
      (KL1[I]*KL2[I]+U1*KL2[I]*(1-KL1[I])+U2*KL1[I]*(1-KL2[I])));
  END;
DQ21:=DQ12; AC1,1]:=DQ11; AC1,2]:=DQ12; AC2,1]:=DQ21;
AC2,2]:=DQ22;      K:=1;TN:=2;DP:=1;L:=1;
  WHILE DP<2 DO
    BEGIN
      IF A[K,K]=0 THEN
        BEGIN
          AMAX:=A[K,K];
          FOR I:= 1 TO 2 DO
            BEGIN
              IF AMAX<A[I,L] THEN
                BEGIN
                  AMAX:=A[I,L];
                END;
            END;
          END;
          WRITELN(AMAX:8:4);
          FOR I:=1 TO 2 DO

```

```

BEGIN
  IF AMAX=AC1,L THEN
    MT:=1;
  END;
  WRITELN('MT=',MT,4);
  FOR J:=1 TO 2 DO
    BEGIN
      C[K,J]:=A[MT,J];
      C[MT,J]:=A[K,J];
    END;
  FOR J:=1 TO 2 DO
    BEGIN
      A[MT,J]:=C[MT,J];
      A[K,J]:=C[K,J];
    END;
  END;
  FOR N:=TN TO 2 DO
    BEGIN
      FOR J:=DP TO 3 DO
        BEGIN
          B[N,J]:=A[N,J]-A[N,K]*A[K,J]/A[K,K];
        END;
      A[N,1]:=B[N,1];  A[N,2]:=B[N,2];
      A[N,3]:=B[N,3];  A[N,4]:=B[N,4];
    END;
    K:=K+1; TN:=TN+1; DP:=DP+1; L:=L+1;
  END;
  XX[2]:=A[2,3]/A[2,2];
  XX[1]:=(A[1,3]-A[1,2]*XX[2])/A[1,1];

```

```

U1:=U1+XX[1]; U2:=U2+XX[2]; HU1[GU]:=Q1; HU2[GU]:=Q2;
EU1[GU]:=U1; EU2[GU]:=U2; GU:=GU+1;
END;
WRITELN('15,'Q1','15,'Q2','15,'U1','15,'U2');
FOR I:=1 TO 7 DO
  BEGIN
    WRITELN(HU1[I]:8:4,HU2[I]:8:4,EU1[I]:8:4,EU2[I]:8:4);
  END;
  WRITELN;
  AP:=1-U1-U2;  BP:=U1/(U1+U2);
  FOR I:=1 TO NU DO
    BEGIN
      X1[I]:=Z[I]/(AP*KL1[I]+(1-AP)*(BP+(1-BP)*KL1[I]/KL2[I]));
      X2[I]:=Z[I]/(AP*KL2[I]+(1-AP)*(BP*KL2[I]/KL1[I]+1-BP));
      Y1[I]:=KL1[I]*X1[I];  Y2[I]:=KL2[I]*X2[I];
      KK1[I]:=Y1[I]/X1[I];  KK2[I]:=Y2[I]/X2[I];
    END;
    APT1:=0; BPT1:=0; CPT1:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT1:=APT1+ABS(XL1[I]-X1[I]);
      BPT1:=BPT1+ABS(XL2[I]-X2[I]);
      CPT1:=CPT1+ABS(Y[I]-Y1[I]);
    END;
    APT:=0;  BPT:=0;  CPT:=0;  DPT:=0;
  FOR I:=1 TO NU DO
    BEGIN
      APT:=APT+X1[I];  BPT:=BPT+X2[I];
      CPT:=CPT+Y1[I];  DPT:=DPT+Y2[I];

```

```

END;
ERROR1:=APT1;   ERROR2:=BPT1;   ERROR3:=CPT1;
WRITELN('':10,'ERROR1=',ERROR1:8:4,'':5,'ERROR2=',ERROR2:8:4,
        '':5,'ERROR3=',ERROR3:8:4);
WRITELN;
WRITELN('':13,'COMPOSITIONS AFTER RUN BY S-R-K EQUATION OF STATE');
WRITELN('':5,'-----',
        '-----');
WRITELN('':10,'COMP',':':10,'Y1',':':6,'Y2',':':7,'X1',':':6,
        'X2',':':5,'KL1',':':5,'KL2');
WRITELN('':5,'-----',
        '-----');
FOR I:=1 TO NU DO
  BEGIN
    WRITELN('':10,COMP[I].NAME,Y1[I]:8:4,Y2[I]:8:4,
            X1[I]:8:4,X2[I]:8:4,KL1[I]:8:4,KL2[I]:8:4);
    END;
    WRITELN('':5,'-----',
            '-----');
    WRITELN('':10,'TOTAL',':':5,CPT:8:4,DPT:8:4,APT:8:4,BPT:8:4);
    WRITELN('':5,'-----',
            '-----');
  END.

```

### Biography

Mr. Chet Rattanamalakorn was born at Rardburee, Thailand on November 27, 1959. He graduated B.S. (Chemistry) from faculty of science Ramkhamhaeng university in 1983. He worked in chemist position at Pure Chem Co, Ltd. and Sai 5 gases product Co, Ltd.. He has been a graduate student in chemical department in Chulalongkorn university.