

References

1. Soave, G., "Equilibrium Constants from a Modified Redlich-Kwong Equation of State", Chem. Eng. Sci., 27(6), 1197-1203, 1972.
2. Peng, D.Y., and D.B. Robinson, "A New Two-Constant Equation of State", Ind. Eng. Chem. Fundam., 15(1), 59-64, 1976.
3. Schmidt, G., and H. Wenzel, "A Modified Van der Waals Type Equation of State", Chem. Eng. Sci., 35, 1503-1512, 1980.
4. Harmens, A., and H. Knapp, "Three-Parameter Cubic Equation of State for Normal Substances", Ind. Eng. Chem. Fundam., 19, 291-294, 1980.
5. Petel, N.C., and A.S. Teja, "A New Cubic Equation of State for Fluids and Fluid Mixtures", Chem. Eng. Sci., 37(3), 463-473, 1982.
6. Redlich, O., and J.N.S. Kwong, "An Equation of State. Fugacities of Gaseous Solutions", Chem. Rev., 44, 233-244, 1949.
7. Fuller, G.G., "A Modified SRK EOS Capable of Representing the Liquid State", Ind. Eng. Chem. Fundam., 15, 257, 1976.
8. Kumar, K.H., and K.E. Starling, Ind. Eng. Chem. Fundam., 21, 255, 1982.

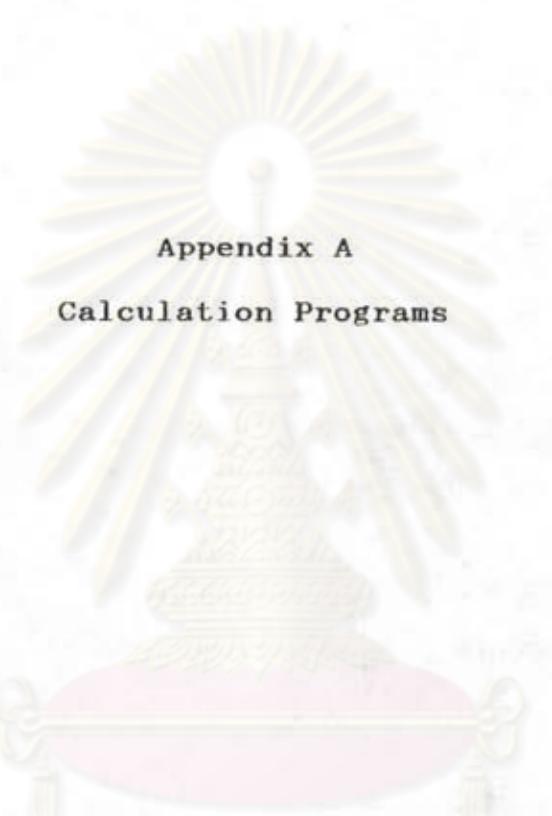
9. Adachi, Y., H. Sugie, and B.C.Y. Lu, J. Chem. Eng.
(Japan), 18, 20, 1985.
10. Graboski, M.S., "A Modified Soave Equation of State for
Phase Equilibrium Calculations", Ind. Eng. Chem.
Process Des. Dev., 17, 443, 1978.
11. Tsonopoulos, C., and J.L. Heidman, "From Redlich-Kwong
to the Present", Fluid Phase Equilibria, 24,
1-23, 1985.
12. T.H. Ahmed, "Comparative study of Eight Equations of
State for Predicting Hydrocarbon Volumetric
Phase Behavior", SPE Reservoir Engineering,
337-348, 1988.
13. Zudkevitch, D., and J. Joffe, "Correlation and
Prediction of VLE with the RK EOS ", A.I.Ch.E
Journal, 16, 112-119, 1970.
14. Ho-mu-Lin, "Modified SOAVE EOS for Phase Equilibrium
Calculations", Ind. Eng. Chem. Process Des.
Dev., 19, 501-505, 1980.
15. Radisz, Ho-mu-Lin, Kwang-Chu Chao, "High Pressure VLE in
Asymmetric Mixtures Using New Mixing Rules",
Ind. Eng. Chem. Process Des. Dev., 21, 653,
1982.
16. Graboski, M.S., "A Modified Soave Equation of State for
Phase Equilibrium Calculations: Systems
Containing CO₂, H₂S, N₂ and CO₂", Ind. Eng.
Chem. Process Des. Dev., 17, 448, 1978.

17. Kato, M., W.K. Chung, and B.C-Y. Lu, "Binary Interaction Coefficients of the RK EOS", Chem. Eng. Sci., 31, 733-736, 1976.
18. Al-Sahhaf, "VLE in the N₂+CO₂+CH₂ System", Ind. Eng. Chem. Fundam., 22, 372, 1983.
19. Moyson, Huron, and Vidal, "Prediction of the Solubility of H₂ in HC Solvents through Cubic EOS", Chem. Eng. Sci., 38, 1085-1092, 1983.
20. Plockner, U., H. Knapp, and J. Prausnitz, "Calculation of High Pressure VLE from a Corresponding States Correlation with Emphasis on Asymmetric Mixtures", Ind. Eng. Chem. Process Des. Dev., 17, 324-332, 1979.
21. Evelein, and Moore, "Prediction of Phase Equilibria in Sour Natural Gas Systems Using the SRK EOS", ibid., 18, 618, 1979.
22. Pauvonic, R., S. Jovanovic, and A. Mihajlov, "Rapid Computation of Binary Interaction Coefficients of an Equation of State for Vapor-Liquid Equilibrium Calculations. Applications of the RKS Equation", Fluid Phase Equilibria, 6, 141-148, 1981.
23. Kuester, J.L., and J.H. Mize, "Optimization Techniques with Fortran", McGraw-Hill, New York, pp.286, 1973.

24. Davalos, J., W.R. Andersen, R.E. Phelps, and A.J. Kidnay, "VLE at 250.00 K for Systems Containing Methane, Ethane, and Carbon Dioxide", J. Chem. Eng. Data, 21(1), 81-84, 1976.
25. Haman, S.E.M., and C.Y. Lu, "Isothermal VLE in Binary System Propane-Carbon Dioxide", J. Chem. Eng. Data, 21(2), 200-204, 1976.
26. Besserer, G.J., and D.B. Robinson, "Equilibrium-Phase Properties of i-Butane-Carbon Dioxide System", J. Chem. Eng. Data, 18(3), 298-304, 1973.
27. -----, "Equilibrium-Phase Properties of n-Pentane-Carbon Dioxide System", J. Chem. Eng. Data, 18(4), 417-419, 1973.
28. Kalra, H., H. Kubato, and D.B. Robinson, "Equilibrium Phase Properties of Carbon Dioxide-n-Heptane System", J. Chem. Eng. Data, 23(4), 317-321, 1978.
29. Sebastian, H.M., J.J. Simnick, H.M. Lin, and K.C. Chao, "VLE in Binary Mixture of Carbon Dioxide-n-Decane and Carbon Dioxide-n-Hexadecane", J. Chem. Eng. Data, 25(2), 138-140, 1980.
30. Wichterle, I., and R. Kobayashi, "VLE of Methane-Ethane System at Low Temperatures and High Pressures", J. Chem. Eng. Data, 17(1), 9-12, 1972.

31. Gupta, M.K., G.C. Gardner, M.J. Hegarty, and A.J. Kidney, "Liquid-Vapor Equilibria for the $N_2 + CH_4 + C_2H_6$ System from 260 to 280 K", J. Chem. Eng. Data, 25, 313-318, 1980.
32. Wichterle, I., and R. Kobayashi, "VLE of Methane-Propane System at Low Temperatures and High Pressures", J. Chem. Eng. Data, 17(1), 4-8, 1972.
33. Akers, W.W., J.F. Burns, and W.R. Fairchild, "Low-Temperature Phase Equilibria Methane-Propane System", Ind. Eng. Chem., 46(12), 2531-2534, 1954.
34. Kalra, L.C., "Low Temperature K Data for Methane-n-Butane", J. Chem. Eng. Data, 19(1), 67, 1974.
35. Prodany, N.W., and B. Williams, "VLE in Methane-Hydrocarbon Systems", J. Chem. Eng. Data, 16(1), 1-6, 1971.
36. Shim, J., and J.P. Kohn, "Multi Phase and Volumetric Equilibria of Methane-n-Hexane Binary System at Temperature between 110 and 150 C", J. Chem. Eng. Data, 7(1), 3-8, 1962.
37. Chappelear, P.S., and R. Kobayashi, "VLE of the Methane-n-Hexane System", J. Chem. Eng. Data, 22(4), 402, 1977.
38. Matschke, D.E., and G. Thodos, "Vapor-Liquid Equilibria for the Ethane-Propane System", J. Chem. Eng. Data, 7(2), 232-234, 1962.

39. Besserer G.J., and D.B. Robinson, "Equilibrium-Phase Properties of i-Butane-Ethane System", J. Chem. Eng. Data, 18(3), 301-304, 1973.
40. Reamer H.H., B.H. Sage, and W.N. Lacey, "Phase Equilibria in Hydrocarbon System. Volumetric and Phase Behavior of Ethane-n-Pentane System", J. Chem. Eng. Data, 5(1), 44-50, 1960.
41. Chueh, P.L., and J.M. Prausnitz, "Calculation of High-Pressure Vapor-Liquid Equilibria", Applied Thermodynamics Symposium, 6(3), 34-52, 1968.
42. Gundersen, T., "Numerical Aspects of the Implementation of Cubic EOS in Flash Calculation Routines", Comp & Chem. Eng., 6(3), 245, 1982.
43. Ellott, J.R., and T.E. Daubert, "Revised Procedures for Phase Equilibrium Calculations with the Soave Equation of State", Ind. Eng. Chem. Process Des. Dev., 24, 743-748, 1985.
44. Kato, K., K. Nakahama, and M. Hirata, "Generalized Interaction Parameters for the Peng-Robinson Equation of State : Carbondioxide-n-Paraffin Binary Systems", Fluid Phase Equilibria, 7, 219-231, 1981.



Appendix A

Calculation Programs

ศูนย์วิทยบรังษย์ฯ
จุฬาลงกรณ์มหาวิทยาลัย

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10 REM *****
12 REM **
13 REM ** PROGRAM FOR CREATING A DATA FILE
14 REM **
15 REM *****
16 DIM NS(10),MW(10),TC(10),PC(10),W(10)
17 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
18 CLS
19 LOCATE 3,5:PRINT "Name of data file to be created : "
20 COLOR 0,15:LOCATE 3,42:INPUT D$
21 COLOR 0,2
22 OPEN "D",#1,D$
23 LOCATE 5,5:INPUT "Number of components : ",N
24 LOCATE ,5:INPUT "Temp. of mixture(deg.C) : ",T
25 LOCATE ,5:INPUT "Number of data points : ",NDATA
26 WRITE #1,N,T,NDATA
27 PRINT
28 FOR II=1 TO N
29 PRINT
30 LOCATE .7:PRINT "Component (";II;") :"
31 INPUT "Component name : ",NS(II)
32 INPUT "Molecular weight : ",MW(II)
33 INPUT "Critical temperature(K) : ",TC(II)
34 INPUT "Critical pressure(atm) : ",PC(II)
35 INPUT "Acentric factor(omega) : ",W(II)
36 WRITE #1,NS(II),MW(II),TC(II),PC(II),W(II)
37 NEXT II
38 CLS
39 FOR I=1 TO NDATA
40 PRINT "DATA POINT NO. ";I
41 PRINT : PRINT
42 LOCATE ,5:INPUT "Press. of mixture(atm) : ",PEXP(I)
43 NEXT I
44 CLS
45 FOR I=1 TO NDATA
46 PRINT : PRINT
47 PRINT TAB(5) "Component ";NS(I)
48 PRINT
49 INPUT "Vapor mole fraction y : ",YEXP(1,I)
50 NEXT I
51 CLS
52 FOR I=1 TO NDATA
53 PRINT : PRINT
54 PRINT TAB(5) "Component ";NS(I)
55 PRINT
56 INPUT "Liquid mole fraction x : ",XEXP(1,I)
57 NEXT I
58 FOR I=1 TO NDATA
59 YEXP(2,I) = 1-YEXP(1,I) : XEXP(2,I) = 1-XEXP(1,I)
60 WRITE #1,PEXP(I)
61 WRITE #1,YEXP(1,I),XEXP(1,I)
62 WRITE #1,YEXP(2,I),XEXP(2,I)
63 NEXT I
64 CLOSE #1
65 STOP : END

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10 REM *****
11 REM **
12 REM ** PROGRAM FOR SEARCHING THE OPTIMUM Kij
13 REM ** FOR THE PATEL-TEJA EQUATION OF STATE
14 REM ** USING THE BUBBLE POINT PRESSURE CRITERION
15 REM **
16 REM *****
17 REM *****
18 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
19 CLS : COLOR 0,2
20 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
21 OPEN "I",#1,D$
22 INPUT #1,N,T,NDATA
23 T = T+ 273.16
24 FOR II=1 TO N
25 INPUT #1,M$(II),MW(II),TC(II),PC(II),W(II)
26 NEXT II
27 FOR I=1 TO NDATA
28 INPUT #1,PEXP(I)
29 FOR II=1 TO N
30 INPUT #1,YEXP(II,I),XEXP(II,I)
31 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 240
32 NEXT II
33 NEXT I
34 CLS
35 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
36 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILN(20),Z(20)
37 DIM NC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20),DP(100)
38 DIM FIB(50)
39 ALPHA=.01
40 LOCATE 10,26 : PRINT "SPECIFY RANGE OF Kij FOR INITIAL SEARCH"
41 LOCATE 12,26 : INPUT "FROM AF = ",AF
42 LOCATE ,26 : INPUT "TO BF = ",BF
43 DEL = BF-AF
44 CLS :PRINT TAB(5) "FIBONACCI SINGLE VARIABLE PROCEDURE"
45 REM ***** DEFINE THE FIRST THREE FIBONACCI NUMBERS
46 FIB0 = 1!
47 FIB(1) = 1!
48 FIB(2) = 2!
49 REM ***** CALCULATE THE REMAINING FIBONACCI NUMBERS
50 BBF = 1/ALPHA
51 IF (BBF-2) <= 0 THEN GOTO 480
52 JJF = 2
53 JJF = JJF+1
54 FIB(JJF) = FIB(JJF-1)+FIB(JJF-2)
55 CCF = FIB(JJF)
56 IF (CCF-BBF) >= 0 THEN GOTO 550
57 GOTO 430
58 PRINT "ACCURACY SPECIFIED IN FUNC NOT SUFFICIENT"
59 PRINT "PROGRAM RESET ALPHA, ALPHA = 0.01"
60 ALPHA = .01
61 GOTO 400
62 REM *****
63 REM ***** FIRST STEP IN THE TABLEAU *****
64 REM *****
65 IFF = 0

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560 KKF = JJF-2
570 IKF = JJF-2
580 BL = BF-AF
590 ALL = FIB(IKF)*BL/FIB(JJF)
600 WF = AF+ALL
610 VF = BF-ALL
620 XF = WF :GOSUB 1250 :TF = DPR
630 XF = VF :GOSUB 1250 :UF = DPR
640 JKF = 1
650 PRINT "K"TAB(10)"LK"TAB(20)"AK"TAB(30)"BK"TAB(40)"LLK"TAB(50)"X"TAB(60)"Y"
660 PRINT JKF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
670 REM *****
680 REM ***** SUCCEEDING STEPS IN THE TABLEAU *****
690 REM *****
700 IKF = IKF-1
710 JJF = JJF-1
720 FOR IFF=1 TO KKF
730 IF (UF-TF) > 0 THEN GOTO 900
740 AF = AF+ALL
750 BL = BF-AF
760 WF = VF
770 XF = WF :GOSUB 1250 :TF = DPR
780 ALL = FIB(IKF)*BL/FIB(JJF)
790 VF = BF-ALL
800 XF = VF :GOSUB 1250 :UF = DPR
810 IIF = IFF+1
820 IKF = IKF-1
830 JJF = JJF-1
840 IF (IKF-1) >= 0 THEN GOTO 860
850 IKF = 1
860 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
870 PRINT TAB(50)VF TAB(60)UF
880 GOTO 1040
890 REM *****
900 BF = BF-ALL
910 BL = BF-AF
920 VF = WF
930 XF = VF :GOSUB 1250 :UF = DPR
940 ALL = FIB(IKF)*BL/FIB(JJF)
950 WF = AF+ALL
960 XF = WF :GOSUB 1250 :TF = DPR
970 IIF = IFF+1
980 IKF = IKF-1
990 JJF = JJF-1
1000 IF (IKF-1) >= 0 THEN GOTO 1020
1010 IKF = 1
1020 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)VF TAB(60)UF
1030 PRINT TAB(50)WF TAB(60)TF
1040 NEXT IFF
1050 REM *****
1060 REM CALCULATION OF THE FINAL RANGE OF THE DEPENDENT VARIABLE
1070 REM *****
1080 EPS = .001*WF
1090 DL = WF+EPS
1100 XF = DL :GOSUB 1250 :YL = DPR

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1110 IF (YL-TF) > 0 THEN GOTO 1160
1120 XF = BF :GOSUB 1250 :BFF = DPR
1130 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";BF
1140 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";BFF
1150 GOTO 1190
1160 XF = AF :GOSUB 1250 :AFF = DPR
1170 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";AF
1180 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";AFF
1190 ACC = (WF-AF)/DEL
1200 LPRINT :LPRINT "THE ACCURACY IS ";ACC
1210 LPRINT "THE REQUIRED ACCURACY WAS ";ALPHA
1220 LPRINT TAB(10) "FOR ";N$(1);"(1) - ";N$(2);"(2)"
1230 LPRINT TAB(10) "AT TEMP. = ";T;"K"
1240 STOP :END
1250 REM *****
1260 REM ***** SUBROUTINE BUBL FUNC(X,Y) *****
1270 REM *****
1280 DPR = 0
1290 FK = XF
1300 R = 82.057
1310 FOR I = 1 TO N
1320 TR(I) = T/TC(I)
1330 NEXT I
1340 REM ***** PATEL - TEJA EOS *****
1350 FOR I = 1 TO N
1360 CC = .329032-.076799*W(I)+.0211947*W(I)*W(I)
1370 FF = .452413+1.30982*W(I)+.295937*W(I)*W(I)
1380 WC(I) = 1-3*CC
1390 WB(I) = .32429*CC-.022005
1400 ALF = 1! + FF*(1 - SQR(TR(I)))
1410 ALF2 = ALF*ALF
1420 WAA = 3*CC^2+3*(1-2*CC)*WB(I)+WB(I)^2+(1-3*CC)
1430 WA(I) = WAA*ALF2
1440 NEXT I
1450 REM ***** CALCULATE A AND B FOR PURE COMPONENTS *****
1460 FOR I = 1 TO N
1470 CI(I) = WC(I)*R*TC(I)/PC(I)
1480 BI(I) = WB(I)*R*TC(I)/PC(I)
1490 AIJ(I,I) = WA(I)*R*R*TC(I)*TC(I)/PC(I)
1500 NEXT I
1510 REM ***** BUBL CALCULATION *****
1520 FOR III=1 TO NDATA
1530 P = PEXP(III)
1540 REM ***** INITIALIZE PHIV TO ONE *****
1550 FOR K = 1 TO N
1560 PHIV(K) = 1!
1570 NEXT K
1580 NLAP = 0
1590 REM ***** CALCULATE VAPOR PHASE MOLE FRACTIONS AND TOTAL PRESSURE
1600 YSUM = 0!
1610 GOSUB 1960
1620 REM ***** PHIMIX XEXP(I,III) *****
1630 FOR K = 1 TO N
1640 YCAL(K) = PHIL(K)*XEXP(K,III)/PHIV(K)
1650 YSUM = YSUM + YCAL(K)

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1660 NEXT K
1670 REM ***** CHECK CONVERGENCE OF Y *****
1680 IF ABS(YSUM-1!) < .0001 THEN GOTO 1810
1690 P = P*YSUM
1700 REM ***** NORMALIZE Y *****
1710 FOR K = 1 TO N
1720 YCAL(K) = YCAL(K)/YSUM
1730 NEXT K
1740 GOSUB 2210
1750 REM PHIMIX Y(I)
1760 NLAP = NLAP + 1
1770 IF NLAP > 35 THEN GOTO 1800
1780 GOTO 1600
1790 CLS : LOCATE 12,25
1800 PRINT "OVER 35 NLAP IN BULBP"
1810 CLS
1820 LOCATE 10,26 :PRINT "PCAL = ";P
1830 FOR I=1 TO N
1840 LOCATE ,26 :PRINT "YCAL(";I;") =";YCAL(I)
1850 NEXT I
1860 LOCATE ,26 :PRINT "VVCAL = ";VV
1870 LOCATE ,26 :PRINT "VLCAL = ";VL
1880 DP(III) = 1! - P/PEXP(III)
1890 DP(III) = ABS(DP(III))
1900 DY = YEXP(1,III) - YCAL(1)
1910 DPR = DPR+DP(III)
1920 NEXT III
1930 DPR = DPR/NDATA
1940 LPRINT:LPRINT TAB(7) "AT K = ";FK;" AAD = ";DPR
1950 RETURN
1960 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V,Z)
1970 REMCALCULATE A AND B FOR BINARY MIXTURE
1980 IPH = 0
1990 AM = 0!
2000 BM = 0!
2010 CM = 0!
2020 FOR I = 1 TO N
2030 AI(I) = 0!
2040 BM = BM + XEXP(I,III)*BI(I)
2050 CM = CM + XEXP(I,III)*CI(I)
2060 FOR J = 1 TO N
2070 IF J = I THEN GOTO 2100
2080 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J)*(1! - FK))
2090 GOTO 2110
2100 AIJ(I,J) = AIJ(I,I)
2110 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
2120 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
2130 NEXT J
2140 NEXT I
2150 GOSUB 2460
2160 FOR I = 1 TO N
2170 PHI(I) = PHI(I)
2180 NEXT I
2190 VL=V : ZL=Z
2200 RETURN

```

2210 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
2220 REM ....CALCULATE A AND B FOR BINARY MIXTURE
2230 IPH = 1
2240 AM = 0!
2250 BM = 0!
2260 CM = 0!
2270 FOR I = 1 TO N
2280 AI(I) = 0!
2290 BM = BM + YCAL(I)*BI(I)
2300 CM = CM + YCAL(I)*CI(I)
2310 FOR J = 1 TO N
2320 IF J = I THEN GOTO 2350
2330 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J)*(1! - FK))
2340 GOTO 2360
2350 AIJ(I,J) = AIJ(I,I)
2360 AI(I) = AI(I) + YCAL(J)*AIJ(I,J)
2370 AM = AM + YCAL(1)*YCAL(J)*AIJ(I,J)
2380 NEXT J
2390 NEXT I
2400 GOSUB 2460
2410 FOR I = 1 TO N
2420 PHIV(I) = PHI(I)
2430 NEXT I
2440 VV=V :ZV=Z
2450 RETURN
2460 REM ***** FOR PATEL AND TAJA EQUATION OF STATE *****
2470 PBRT = P*BM/R/T
2480 PBRT2 = PBRT*PBRT
2490 PCRT = P*CM/R/T
2500 ABRT = P*AM/R/T/R/T
2510 PP = -(PCRT - 1)
2520 QQ = ABRT - 2*PBRT*PCRT - PBRT - PCRT - PBRT2
2530 RR = -(PBRT*PCRT + PBRT2*PCRT - ABRT*PBRT)
2540 GOSUB 2890
2550 REM CALL ANAL(PP,QQ,RR,IPH,Z)
2560 V = Z*R*T/P
2570 PRINT " MOLAR VOLUME .V = "; V
2580 ZB = R*T/(V-BM)
2590 QUE = V+(BM+CM)/2
2600 DSM = SQR(BM*CM+((BM+CM)^2)/4)
2610 SQQ = QUE^2 - DSM^2
2620 QD = (QUE+DSM)/(QUE-DSM)
2630 ZPB = Z - PBRT
2640 IF ZPB <= 0! OR QD <= 0! THEN GOTO 2810
2650 LZB = LOG(ZPB)*R*T
2660 LQD = LOG(QD)
2670 FOR I = 1 TO N
2680 C3B = CI(I)*(3*BM+CM)+BI(I)*(3*CM+BM)
2690 PHILN(I) = BI(I)*ZB - LZB - AI(I)/DSM*LQD
2700 PHILN(I) = PHILN(I) + AM*(BI(I)+CI(I))/(2*SQQ)
2710 PHILN(I) = PHILN(I) + AM/(8*DSM^3)*C3B*(LQD-2*QUE*DSM/SQQ)
2720 PHILN(I) = PHILN(I)/R/T
2730 IF PHILN(I) < -174! THEN PHILN(I) = -170!
2740 IF PHILN(I) < 174! THEN GOTO 2770
2750 PRINT "LOG OF PHI .GT. 174 IN PHIMIX.PHI SET TO 1"

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2760 PHILN(I) = 0!
2770 PHI(I) = EXP(PHILN(I))
2780 PRINT " FUGACITY COEFF. PHI(.I.) :" ; PHI(I)
2790 NEXT I
2800 RETURN
2810 REM *****...ERROR ADJUSTMENT...
2820 FOR I = 1 TO N
2830 IF IPH = 1 THEN PHI(I) = 1!
2840 IF IPH = 0 THEN PHI(I) = .2
2850 PRINT "NEGATIVE VALUE FOR MOLAR VOLUMN CALC. IN PHIMIX"
2860 PRINT "SO LET ASSUME PHI(" ; I ; ") :" ; PHI(I)
2870 NEXT I
2880 RETURN
2890 REM *****
2900 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
2910 REM INITIAL VALUE ; Z = 0.0 , FOR IPH = 0
2920 REM Z = 1.0 , FOR IPH = 1
2930 IF IPH = 1 GOTO 2970
2940 Z = 0!
2950 NLOOP = 0
2960 GOTO 2990
2970 Z = 1!
2980 NLOOP = 0
2990 NLOOP = NLOOP + 1
3000 IF NLOOP > 25 THEN GOTO 3080
3010 FZ = Z*Z*Z - Z*Z*PP + Z*QQ - RR
3020 SLOPE = (3!*Z*Z - 2!*Z*PP + QQ)
3030 ZN = Z - (FZ/SLOPE)
3040 EROR = ABS((ZN-Z)/ZN)
3050 Z = ZN
3060 IF EROR < .0001 THEN GOTO 3100
3070 GOTO 2990
3080 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
3090 CLS
3100 LOCATE 10,26 :PRINT " ROOTS OF CUBIC EQUATION WITH"
3110 LOCATE ,26 :PRINT " IPH = " ; IPH
3120 LOCATE ,26 :PRINT " P = " ; PP
3130 LOCATE ,26 :PRINT " Q = " ; QQ
3140 LOCATE ,26 :PRINT " R = " ; RR
3150 LOCATE ,26 :PRINT " Z = " ; Z
3160 RETURN

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บริการรัฐบาล
ศูนย์การณ์มหาวิทยาลัย

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10 REM *****
20 REM **
30 REM ** PROGRAM FOR SEARCHING THE OPTIMUM Kij
40 REM ** FOR THE PATEL-TEJA EQUATION OF STATE
50 REM ** USING THE FUGACITY CRITERION
60 REM **
70 REM *****
80 DIM N$(20),MW(20),TC(20),PC(20),W(20)
90 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
100 CLS : COLOR 0,2
110 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
120 OPEN "I",#1,D$
130 INPUT #1,N,T,NDATA
140 T = T+ 273.16
150 FOR II=1 TO N
160 INPUT #1,N$(II),MW(II),TC(II),PC(II),W(II)
170 NEXT II
180 FOR I=1 TO NDATA
190 INPUT #1,PEXP(I)
200 FOR II=1 TO N
210 INPUT #1,YEXP(II,I),XEXP(II,I)
220 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 250
230 NEXT II
240 NEXT I
250 CLS
260 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
270 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILH(20),Z(20)
280 DIM WC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20),DEV(100),DFU(100)
290 DIM FIB(50)
300 ALPHA=.01
310 LOCATE 10,26 : PRINT "SPECIFY RANGE OF Kij FOR INITIAL SEARCH"
320 LOCATE 12,26 : INPUT "FROM AF = ",AF
330 LOCATE 14,26 : INPUT "TO BF = ",BF
340 DEL = BF-AF
350 CLS :PRINT TAB(5) "FIBONACCI SINGLE VARIABLE PROCEDURE"
360 REM ***** DEFINE THE FIRST THREE FIBONACCI NUMBERS
370 FIB0 = 1!
380 FIB(1) = 1!
390 FIB(2) = 2!
400 REM ***** CALCULATE THE REMAINING FIBONACCI NUMBERS
410 BBF = 1/ALPHA
420 IF (BBF-2) <= 0 THEN GOTO 490
430 JJF = 2
440 JJF = JJF+
450 FIB(JJF) = FIB(JJF-1)+FIB(JJF-2)
460 CCF = FIB(JJF)
470 IF (CCF-BBF) >= 0 THEN GOTO 560
480 GOTO 440
490 PRINT "ACCURACY SPECIFIED IN FUNC NOT SUFFICIENT"
500 PRINT "PROGRAM RESET ALPHA. ALPHA = 0.01"
510 ALPHA = .01
520 GOTO 410
530 REM *****
540 REM ***** FIRST STEP IN THE TABLEAU *****
550 REM *****

```

560 IFF = 0
570 KKF = JJF-2
580 IKF = JJF-2
590 BL = BF-AF
600 ALL = FIB(IKF)*BL/FIB(JJF)
610 WF = AF+ALL
620 VF = BF-ALL
630 XF = WF :GOSUB 1260 :TF = DPR
640 XF = VF :GOSUB 1260 :UF = DPR
650 JKF = 1
660 PRINT "K"TAB(10)"LK"TAB(20)"AK"TAB(30)"BK"TAB(40)"LLK"TAB(50)"X"TAB(60)"Y"
670 PRINT JKF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
680 REM *****
690 REM ***** SUCCEEDING STEPS IN THE TABLEAU *****
700 REM *****
710 IKF = IKF-1
720 JJF = JJF-1
730 FOR IFF=1 TO KKF
740 IF (UF-TF) > 0 THEN GOTO 910
750 AF = AF+ALL
760 BL = BF-AF
770 WF = VF
780 XF = WF :GOSUB 1260 :TF = DPR
790 ALL = FIB(IKF)*BL/FIB(JJF)
800 VF = BF-ALL
810 XF = VF :GOSUB 1260 :UF = DPR
820 IIF = IFF+1
830 IKF = IKF-1
840 JJF = JJF-1
850 IF (IKF-1) >= 0 THEN GOTO 870
860 IKF = 1
870 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
880 PRINT TAB(50)VF TAB(60)UF
890 GOTO 1050
900 REM *****
910 BF = BF-ALL
920 BL = BF-AF
930 VF = WF
940 XF = VF :GOSUB 1260 :UF = DPR
950 ALL = FIB(IKF)*BL/FIB(JJF)
960 WF = AF+ALL
970 XF = WF :GOSUB 1260 :TF = DPR
980 IIF = IFF+1
990 IKF = IKF-1
1000 JJF = JJF-1
1010 IF (IKF-1) >= 0 THEN GOTO 1030
1020 IKF = 1
1030 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)VF TAB(60)UF
1040 PRINT TAB(50)WF TAB(60)TF
1050 NEXT IFF
1060 REM *****
1070 REM CALCULATION OF THE FINAL RANGE OF THE DEPENDENT VARIABLE
1080 REM *****
1090 EPS = .001*WF
1100 DL = WF+EPS

```

1110 XF = DL :GOSUB 1260 :YL = DPR
1120 IF (YL-TF) > 0 THEN GOTO 1170
1130 XF = BF :GOSUB 1260 :BFF = DPR
1140 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";BF
1150 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";BFF
1160 GOTO 1200
1170 XF = AF :GOSUB 1260 :AFF = DPR
1180 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";AF
1190 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";AFF
1200 ACC = (WF-AF)/DEL
1210 LPRINT :LPRINT "THE ACCURACY IS ";ACC
1220 LPRINT "THE REQUIRED ACCURACY WAS ";ALPHA
1230 LPRINT :LPRINT TAB(10) "FOR ";N$(1);"(1) - ";N$(2);"(2)"
1240 LPRINT :LPRINT TAB(10) "AT TEMP. = ";T;"K"
1250 STOP :END
1260 REM *****
1270 REM ***** SUBROUTINE BUBL FUNC(X,Y) *****
1280 REM *****
1290 DPR = 0
1300 FK = XF
1310 R = 82.057
1320 FOR I = 1 TO N
1330 TR(I) = T/TC(I)
1340 NEXT I
1350 REM ***** PATEL - TEJA EOS *****
1360 FOR I = 1 TO N
1370 CC = .329032-.076799*W(I)+.0211947*W(I)*W(I)
1380 FF = .452413+1.30982*W(I)+.295937*W(I)*W(I)
1390 WC(I) = 1-3*CC
1400 WB(I) = .32429*CC-.022005
1410 ALF = 1! + FF*(1 - SQR(TR(I)))
1420 ALF2 = ALF*ALF
1430 WAA = 3*CC^2+3*(1-2*CC)*WB(I)+WB(I)^2+(1-3*CC)
1440 WA(I) = WAA*ALF2
1450 NEXT I
1460 REM ***** CALCULATE A AND B FOR PURE COMPONENTS *****
1470 FOR I =1 TO N
1480 CI(I) = WC(I)*R*TC(I)/PC(I)
1490 BI(I) = WB(I)*R*TC(I)/PC(I)
1500 AIJ(I,I) = WA(I)*R*R*TC(I)*TC(I)/PC(I)
1510 NEXT I
1520 REM ***** FUGACITY COEFF. CALCULATION *****
1530 FOR III=1 TO NDATA
1540 FOR III=1 TO NDATA
1550 P = PEXP(III)
1560 GOSUB 1750
1570 REM ***** PHIMIX XEXP(I,III) *****
1580 GOSUB 2000
1590 REM ***** PHIMIX YEXP(I,III) *****
1600 CLS
1610 LOCATE 10,26 :PRINT "PCAL = ";P
1620 LOCATE ,26 :PRINT "VVCAL = ";VV
1630 LOCATE ,26 :PRINT "VLCAL = ";VL
1640 DFU(III) = 0
1650 FOR I=1 TO N

```

1660 FUGAL(I) = PHIL(I)*XEXP(I,III)*P
1670 FUGAV(I) = PHI(V,I)*YEXP(I,III)*P
1680 DEV(I) = (ABS(FUGAL(I)-FUGAV(I)))/FUGAV(I)
1690 DFU(III) = DFU(III) + DEV(I)
1700 NEXT I
1710 DPR = DPR + DFU(III)
1720 NEXT III
1730 LPRINT: LPRINT TAB(7)"AT K = ";FK;" DEV. F = ";DPR
1740 RETURN
1750 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V,Z)
1760 REMCALCULATE A AND B FOR BINARY MIXTURE
1770 IPH = 0
1780 AM = 0!
1790 BM = 0!
1800 CM = 0!
1810 FOR I = 1 TO N
1820 AI(I) = 0!
1830 BM = BM + XEXP(I,III)*BI(I)
1840 CM = CM + XEXP(I,III)*CI(I)
1850 FOR J = 1 TO N
1860 IF J = I THEN GOTO 1890
1870 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1880 GOTO 1900
1890 AIJ(I,J) = AIJ(I,I)
1900 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
1910 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
1920 NEXT J
1930 NEXT I
1940 GOSUB 2250
1950 FOR I = 1 TO N
1960 PHIL(I) = PHI(I)
1970 NEXT I
1980 VL=V : ZL=Z
1990 RETURN
2000 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
2010 REMCALCULATE A AND B FOR BINARY MIXTURE
2020 IPH = 1
2030 AM = 0!
2040 BM = 0!
2050 CM = 0!
2060 FOR I = 1 TO N
2070 AI(I) = 0!
2080 BM = BM + YEXP(I,III)*BI(I)
2090 CM = CM + YEXP(I,III)*CI(I)
2100 FOR J = 1 TO N
2110 IF J = I THEN GOTO 2140
2120 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
2130 GOTO 2150
2140 AIJ(I,J) = AIJ(I,I)
2150 AI(I) = AI(I) + YEXP(J,III)*AIJ(I,J)
2160 AM = AM + YEXP(I,III)*YEXP(J,III)*AIJ(I,J)
2170 NEXT J
2180 NEXT I
2190 GOSUB 2250
2200 FOR I = 1 TO N

```

2210 PHIV(I) = PHI(I)
2220 NEXT I
2230 VV=V :ZV=2
2240 RETURN
2250 REM ***** FOR PATEL AND TAJA EQUATION OF STATE *****
2260 PBRT = P*BM/R/T
2270 PBRT2 = PBRT*PBRT
2280 PCRT = P*CM/R/T
2290 ABRT = P*AM/R/T/R/T
2300 PP = -(PCRT - 1)
2310 QQ = ABRT - 2*PBRT*PCRT - PBRT - PCRT - PBRT2
2320 RR = -(PBRT*PCRT + PBRT2*PCRT - ABRT*PBRT)
2330 GOSUB 2680
2340 REM CALL ANAL(PP,QQ,RR,IPH,Z)
2350 V = Z*R*T/P
2360 PRINT " MOLAR VOLUMN V = "; V
2370 ZB = R*T/(V-BM)
2380 QUE = V+(BM+CM)/2
2390 DSM = SQR(BM*CM+((BM+CM)^2)/4)
2400 SQQ = QUE^2 - DSM^2
2410 QD = (QUE+DSM)/(QUE-DSM)
2420 ZPB = Z - PBRT
2430 IF ZPB <= 0! OR QD <= 0! THEN GOTO 2600
2440 LZB = LOG(ZPB)*R*T
2450 LQD = LOG(QD)
2460 FOR I = 1 TO N
2470 C38 = CI(I)*(3*BM+CM)+BI(I)*(3*CM+BM)
2480 PHILN(I) = BI(I)*ZB - LZB - AI(I)/DSM*LQD
2490 PHILN(I) = PHILN(I) + AM*(BI(I)+CI(I))/(2*SQQ)
2500 PHILN(I) = PHILN(I) + AM/(8*DSM^3)*C38*(LQD-2*QUE*DSM/SQQ)
2510 PHILN(I) = PHILN(I)/R/T
2520 IF PHILN(I) < -174! THEN PHILN(I) = -170!
2530 IF PHILN(I) > 174! THEN GOTO 2560
2540 PRINT "LOG OF PHI .GT. 174 IN PHIMIX.PHI SET TO 1"
2550 PHILN(I) = 0!
2560 PHI(I) = EXP(PHILN(I))
2570 PRINT " FUGACITY COEFF. PHI("I,") =";PHI(I)
2580 NEXT I
2590 RETURN
2600 REM *****...ERROR ADJUSTMENT...
2610 FOR I = 1 TO N
2620 IF IPH = 1 THEN PHI(I) = 1!
2630 IF IPH = 0 THEN PHI(I) = .2
2640 PRINT "NEGATIVE VALUE FOR MOLAR VOLUMN CALC. IN PHIMIX"
2650 PRINT "SO LET ASSUME PHI("I,") =";PHI(I)
2660 NEXT I
2670 RETURN
2680 REM *****
2690 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
2700 REM INITIAL VALUE ; Z = 0.0 , FOR IPH = 0
2710 REM Z = 1.0 , FOR IPH = 1
2720 IF IPH = 1 GOTO 2760
2730 Z = 0!
2740 NLOOP = 0
2750 GOTO 2780

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```
2760 Z      =  1!
2770 NLOOP = 0
2780 NLOOP = NLOOP + 1
2790 IF NLOOP > 25 THEN GOTO 2870
2800 FZ    =  Z*Z*Z - Z*Z*PP + Z*QQ - RR
2810 SLOPE =  (3!*Z*Z - 2!*Z*PP + QQ)
2820 ZN   =  Z-(FZ/SLOPE)
2830 EROR = ABS((ZN-Z)/ZN)
2840 Z      =  ZN
2850 IF EROR < .0001 THEN GOTO 2890
2860 GOTO 2780
2870 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
2880 CLS
2890 LOCATE 10,26 :PRINT "    ROOTS OF CUBIC EQUATION ,WITH"
2900 LOCATE ,26 :PRINT "    IPH      = ";IPH
2910 LOCATE ,26 :PRINT "    P        = ";PP
2920 LOCATE ,26 :PRINT "    Q        = ";QQ
2930 LOCATE ,26 :PRINT "    R        = ";RR
2940 LOCATE ,26 :PRINT "    Z        = ";Z
2950 RETURN
```

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10 REM *****
20 REM **
30 REM **          BUBBLE POINT PRESSURE CALCULATION PROGRAM      **
40 REM **          FOR THE PATEL-TEJA EQUATION OF STATE          **
50 REM **
60 REM *****
70 DIM N$(20),MW(20),TC(20),PC(20),W(20)
80 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
90 CLS : COLOR 0,2
100 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
110 OPEN "I",#1,D$
120 INPUT #1,M,T,NDATA
130 T = T+ 273.16
140 FOR II=1 TO N
150 INPUT #1,N$(II),MW(II),TC(II),PC(II),W(II)
160 NEXT II
170 FOR I=1 TO NDATA
180 INPUT #1,PEXP(I)
190 FOR II=1 TO N
200 INPUT #1,YEXP(II,I),XEXP(II,I)
210 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 240
220 NEXT II
230 NEXT I
240 CLS
250 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
260 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILN(20),ZZ(20)
270 DIM WC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20)
280 DIM DP(100),DPP(100),DY(100)
290 REM *****
300 REM ***** SUBROUTINE BUBL FUNC(X,Y) *****
310 REM *****
320 LOCATE 10,26 : INPUT "THE OPTIMUM VALUE OF Kij = ".FK
330 LPRINT TAB(10) "PATEL-TEJA EQUATION OF STATE"
340 LPRINT TAB(10) "MIXTURE : ";N$(1);"(1) - ";N$(2);"(2)"
350 LPRINT TAB(10) "TEMP. =";T;"K"
360 LPRINT TAB(10) "Kij = ";FK
370 LPRINT : LPRINT TAB(10) "REF. SHIM & KOHN (1962)"
380 LPRINT TAB(6) -----
-----
390 LPRINT TAB(16)"EXPERIMENTAL" TAB(43)"CALCULATED" TAB(63)"DEVIATIONS"
400 LPRINT TAB(8)----- TAB(39)----- TAB(59)-----"
410 LPRINT TAB(10)"P(atm)" TAB(21)"X(1)" TAB(31)"Y(1)" TAB(40)"P(atm)" TAB(51)"Y
(1)" TAB(61)"!DP!" TAB(69)"!DY(1)!"
420 LPRINT TAB(6) -----
-----
430 R = 82.057
440 FOR I = 1 TO N
450 TR(I) = T/TC(I)
460 NEXT I
470 REM ***** PATEL - TEJA EOS *****
480 FOR I = 1 TO N
490 CC = .329032-.076799*W(I)+.0211947*W(I)*W(I)
500 FF = .452413+.30982*W(I)+.295937*W(I)*W(I)
510 WC(I) = 1-3*CC
520 WB(I) = .32429*CC-.022005
530 ALF = 1! + FF*(1 - SQR(TR(I)))
540 ALF2 = ALF*ALF
550 WAA = 3*CC^2+3*(1-2*CC)*WB(I)+WB(I)^2+(1-3*CC)

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```

560 WA(I) = WAA*ALF2
570 NEXT I
580 REM ***** CALCULATE A AND B FOR PURE COMPONENTS *****
590 FOR I =1 TO N
600 CI(I) = WC(I)*R*TC(I)/PC(I)
610 BI(I) = WB(I)*R*TC(I)/PC(I)
620 AIJ(I,I) = WA(I)*R*R*TC(I)*TC(I)/PC(I)
630 NEXT I
640 REM ***** BUBL CALCULATION *****
650 FOR III=1 TO NDATA
660 P = PEXP(III)
670 REM ***** INITIALIZE PHIV TO ONE *****
680 FOR K = 1 TO N
690 PHIV(K) = 1!
700 NEXT K
710 NLAP = 0
720 REM ***** CALCULATE VAPOR PHASE MOLE FRACTIONS AND TOTAL PRESSURE
730 YSUM = 0!
740 GOSUB 1110
750 REM ***** PHIMIX XEXP(I,III) *****
760 FOR K = 1 TO N
770 YCAL(K) = PHIL(K)*XEXP(K,III)/PHIV(K)
780 YSUM = YSUM + YCAL(K)
790 NEXT K
800 REM ***** CHECK CONVERGENCE OF Y *****
810 IF ABS(YSUM-1) < .0001 THEN GOTO 940
820 P = P*YSUM
830 REM ***** NORMALIZE Y *****
840 FOR K = 1 TO N
850 YCAL(K) = YCAL(K)/YSUM
860 NEXT K
870 GOSUB 1360
880 REM PHIMIX Y(I)
890 NLAP = NLAP + 1
900 IF NLAP > 35 THEN GOTO 930
910 GOTO 730
920 CLS : LOCATE 12,25
930 PRINT "OVER 35 NLAP IN BULBP"
940 CLS
950 LOCATE 10,26 :PRINT "PCAL = ";P
960 FOR I=1 TO N
970 LOCATE ,26 :PRINT "YCAL(";I;") =";YCAL(I)
980 NEXT I
990 LOCATE ,26 :PRINT "VVCAL = ";VV
1000 LOCATE ,26 :PRINT "VLCAL = ";VL
1010 DPP(III) = ABS(PEXP(III)-P)
1020 DP(III) = DPP(III)/PEXP(III)
1030 DY(III) = ABS(YEXP(1,III) - YCAL(1))
1040 DPR = DPR+DP(III)
1050 LPRINT TAB(8) USING "###.###";PEXP(III),XEXP(1,III),YEXP(1,III),P,YCAL(1),
),DPP(III),DY(III)
1060 NEXT III
1070 DPR = DPR/NDATA*100
1080 LPRINT TAB(6) -----
1090 LPRINT TAB(10) "WITH MIN. ADD. =";DPR
1100 END

```

```

1110 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V,Z)
1120 REM ....CALCULATE A AND B FOR BINARY MIXTURE
1130 IPH = 0
1140 AM = 0!
1150 BM = 0!
1160 CM = 0!
1170 FOR I = 1 TO N
1180 AI(I) = 0!
1190 BM = BM + XEXP(I,III)*BI(I)
1200 CM = CM + XEXP(I,III)*CI(I)
1210 FOR J = 1 TO N
1220 IF J = I THEN GOTO 1250
1230 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1240 GOTO 1260
1250 AIJ(I,J) = AIJ(I,I)
1260 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
1270 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
1280 NEXT J
1290 NEXT I
1300 GOSUB 1610
1310 FOR I = 1 TO N
1320 PHIL(I) = PHI(I)
1330 NEXT I
1340 VL=V : ZL=Z
1350 RETURN
1360 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
1370 REM ....CALCULATE A AND B FOR BINARY MIXTURE
1380 IPH = 1
1390 AM = 0!
1400 BM = 0!
1410 CM = 0!
1420 FOR I = 1 TO N
1430 AI(I) = 0!
1440 BM = BM + YCAL(I)*BI(I)
1450 CM = CM + YCAL(I)*CI(I)
1460 FOR J = 1 TO N
1470 IF J = I THEN GOTO 1500
1480 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1490 GOTO 1510
1500 AIJ(I,J) = AIJ(I,I)
1510 AI(I) = AI(I) + YCAL(J)*AIJ(I,J)
1520 AM = AM + YCAL(I)*YCAL(J)*AIJ(I,J)
1530 NEXT J
1540 NEXT I
1550 GOSUB 1610
1560 FOR I = 1 TO N
1570 PHIV(I) = PHI(I)
1580 NEXT I
1590 VV=V : ZV=Z
1600 RETURN
1610 REM ***** FOR PATEL AND TAJA EQUATION OF STATE *****
1620 PBRT = P*BM/R/T
1630 PBRT2 = PBRT*PBRT
1640 PCRT = P*CM/R/T
1650 ABRT = P*AM/R/T/R/T

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1660 PP = -(PCRT - 1)
1670 QQ = ABRT - 2*PBRT*PCRT - PBRT - PCRT - PERT2
1680 RR = -(PBRT*PCRT + PBRT2*PCRT - ABRT*PBRT)
1690 GOSUB 2040
1700 REM CALL ANAL(PP,QQ,RR,1PH,2)
1710 V = Z*R*T/P
1720 PRINT " MOLAR VOLUME V = "; V
1730 ZB = R*T/(V-BM)
1740 QUE = V+(BM+CM)/2
1750 DSM = SQR(BM*CM+((BM+CM)^2)/4)
1760 SQQ = QUE^2 - DSM^2
1770 QD = (QUE+DSM)/(QUE-DSM)
1780 ZPB = Z - PBRT
1790 IF ZPB <= 0! OR QD <= 0! THEN GOTO 1960
1800 LZB = LOG(ZPB)*R*T
1810 LQD = LOG(QD)
1820 FOR I = 1 TO N
1830 C3B = CI(I)*(3*BM+CM)+BI(I)*(3*CM+BM)
1840 PHILN(I) = BI(I)*ZB - LZB - AI(I)/DSM*LQD
1850 PHILN(I) = PHILN(I) + AM*(BI(I)+CI(I))/(2*SQQ)
1860 PHILN(I) = PHILN(I) + AM/(B*DSM^3)*C3B*(LQD-2*QUE*DSM/SQQ)
1870 PHILN(I) = PHILN(I)/R/T
1880 IF PHILN(I) < -174! THEN PHILN(I) = -170!
1890 IF PHILN(I) < 174! THEN GOTO 1920
1900 PRINT "LOG OF PHI .GT. 174 IN PHIMIX, PHI SET TO 1"
1910 PHILN(I) = 0!
1920 PHI(I) = EXP(PHILN(I))
1930 PRINT " FUGACITY COEFF. PHI(",I,") = ";PHI(I)
1940 NEXT I
1950 RETURN
1960 REM *****...ERROR ADJUSTMENT...
1970 FOR I = 1 TO N
1980 IF IPH = 1 THEN PHI(I) = 1!
1990 IF IPH = 0 THEN PHI(I) = .2
2000 PRINT "NEGATIVE VALUE FOR MOLAR VOLUME CALC. IN PHIMIX"
2010 PRINT "SO LET ASSUME PHI(";I,") = ";PHI(I)
2020 NEXT I
2030 RETURN
2040 REM *****
2050 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
2060 REM INITIAL VALUE ; Z = 0.0 , FOR IPH = 0
2070 REM Z = 1.0 , FOR IPH = 1
2080 IF IPH = 1 GOTO 2120
2090 Z = 0!
2100 NLOOP = 0
2110 GOTO 2140
2120 Z = 1!
2130 NLOOP = 0
2140 NLOOP = NLOOP + 1
2150 IF NLOOP > 25 THEN GOTO 2230
2160 FZ = Z*Z*Z - Z*Z*PP + Z*QQ - RR
2170 SLOPE = (3!*Z*Z - 2!*Z*PP + QQ)
2180 ZN = Z-(FZ/SLOPE)
2190 EROR = ABS((ZN-Z)/ZN)
2200 Z = ZN

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```
2210 IF EROR < .0001 THEN GOTO 2250
2220 GOTO 2140
2230 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
2240 CLS
2250 LOCATE 10,26 :PRINT " ROOTS OF CUBIC EQUATION ,WITH"
2260 LOCATE ,26 :PRINT " IPH = ";IPH
2270 LOCATE ,26 :PRINT " P = ";PP
2280 LOCATE ,26 :PRINT " Q = ";QQ
2290 LOCATE ,26 :PRINT " R = ";RR
2300 LOCATE ,26 :PRINT " Z = ";Z
2310 RETURN
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จุฬาลงกรณ์มหาวิทยาลัย

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10 REM *****
20 REM **
30 REM ** PROGRAM FOR SEARCHING THE OPTIMUM Kij
40 REM ** FOR THE SCHMIDT-WENZEL EQUATION OF STATE
50 REM ** USING THE BUBBLE POINT PRESSURE CRITERION
60 REM **
70 REM *****
80 DIM N$(20),MW(20),TC(20),PC(20),W(20)
90 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
100 CLS : COLOR 0,2
110 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
120 OPEN "I",#1,D$
130 INPUT #1,N,T,NDATA
140 T = T+ 273.16
150 FOR II=1 TO N
160 INPUT #1,N$(II),MW(II),TC(II),PC(II),W(II)
170 NEXT II
180 FOR I=1 TO NDATA
190 INPUT #1,PEXP(I)
200 FOR II=1 TO N
210 INPUT #1,YEXP(II,I),XEXP(II,I)
220 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 250
230 NEXT II
240 NEXT I
250 CLS
260 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
270 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILN(20),ZZ(20)
280 DIM WC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20),DP(100)
290 DIM FIB(50)
300 ALPHA=.01
310 LOCATE 10,26 : PRINT "SPECIFY RANGE OF Kij FOR INITIAL SEARCH"
320 LOCATE 12,26 : INPUT "FROM AF = ",AF
330 LOCATE ,26 : INPUT "TO BF = ",BF
340 DEL = BF-AF
350 CLS :PRINT TAB(5) "FIBONACCI SINGLE VARIABLE PROCEDURE"
360 REM ***** DEFINE THE FIRST THREE FIBONACCI NUMBERS
370 FIB0 = 1!
380 FIB(1) = 1!
390 FIB(2) = 2!
400 REM ***** CALCULATE THE REMAINING FIBONACCI NUMBERS
410 BBF = 1/ALPHA
420 IF (BBF-2) <= 0 THEN GOTO 490
430 JJF = 2
440 JJF = JJF+1
450 FIB(JJF) = FIB(JJF-1)+FIB(JJF-2)
460 CCF = FIB(JJF)
470 IF (CCF-BBF) >= 0 THEN GOTO 560
480 GOTO 440
490 PRINT "ACCURACY SPECIFIED IN FUNC NOT SUFFICIENT"
500 PRINT "PROGRAM RESET ALPHA, ALPHA = 0.01"
510 ALPHA = .01
520 GOTO 410
530 REM *****
540 REM ***** FIRST STEP IN THE TABLEAU *****
550 REM *****

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560 IFF = 0
570 KKF = JJF-2
580 IKF = JJF-2
590 BL = BF-AF
600 ALL = FIB(IKF)*BL/FIB(JJF)
610 WF = AF+ALL
620 VF = BF-ALL
630 XF = WF :GOSUB 1260 :TF = DPR
640 XF = VF :GOSUB 1260 :UF = DPR
650 JKF = 1
660 PRINT "K"TAB(10)"LK"TAB(20)"AK"TAB(30)"BK"TAB(40)"LLK"TAB(50)"X"TAB(60)"Y"
670 PRINT JKF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
680 REM *****
690 REM ***** SUCCEEDING STEPS IN THE TABLEAU *****
700 REM *****
710 IKF = IKF-1
720 JJF = JJF-1
730 FOR IFF=1 TO KKF
740 IF (UF-TF) > 0 THEN GOTO 910
750 AF = AF+ALL
760 BL = BF-AF
770 WF = VF
780 XF = WF :GOSUB 1260 :TF = DPR
790 ALL = FIB(IKF)*BL/FIB(JJF)
800 VF = BF-ALL
810 XF = VF :GOSUB 1260 :UF = DPR
820 IIF = IFF+1
830 IKF = IKF-1
840 JJF = JJF-1
850 IF (IKF-1) >= 0 THEN GOTO 870
860 IKF = 1
870 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
880 PRINT TAB(50)VF TAB(60)UF
890 GOTO 1050
900 REM *****
910 BF = BF-ALL
920 BL = BF-AF
930 VF = WF
940 XF = VF :GOSUB 1260 :UF = DPR
950 ALL = FIB(IKF)*BL/FIB(JJF)
960 WF = AF+ALL
970 XF = WF :GOSUB 1260 :TF = DPR
980 IIF = IFF+1
990 IKF = IKF-1
1000 JJF = JJF-1
1010 IF (IKF-1) >= 0 THEN GOTO 1030
1020 IKF = 1
1030 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)VF TAB(60)UF
1040 PRINT TAB(50)WF TAB(60)TF
1050 NEXT IFF
1060 REM *****
1070 REM CALCULATION OF THE FINAL RANGE OF THE DEPENDENT VARIABLE
1080 REM *****
1090 EPS = .001*WF
1100 DL = WF+EPS

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1110 XF = DL :GOSUB 1260 :YL = DPR
1120 IF (YL-TF) > 0 THEN GOTO 1170
1130 XF = BF :GOSUB 1260 :BFF = DPR
1140 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";BF
1150 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";BFF
1160 GOTO 1200
1170 XF = AF :GOSUB 1260 :AFF = DPR
1180 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";AF
1190 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";AFF
1200 ACC = (WF-AF)/DEL
1210 LPRINT :LPRINT "THE ACCURACY IS ";ACC
1220 LPRINT "THE REQUIRED ACCURACY WAS ";ALPHA
1230 LPRINT :LPRINT TAB(10) "FOR ";N$(1);"(1) - ";N$(2);"(2)"
1240 LPRINT :LPRINT TAB(10) "AT TEMP. = ";T;"K"
1250 STOP :END
1260 REM *****
1270 REM ***** SUBROUTINE BUBL FUNC(X,Y) *****
1280 REM *****
1290 DPR = 0
1300 FK = XF
1310 R = 82.057
1320 FOR I = 1 TO N
1330 TR(I) = T/TC(I)
1340 NEXT I
1350 REM ***** Schmidt - Wenzel EOS *****
1360 FOR I = 1 TO N
1370 BETA = .25989 - .0217*W(I) + .00375*W(I)*W(I)
1380 CC = 1/(3*(1+BETA*W(I)))
1390 WB(I) = BETA*CC
1400 WAA = (1-CC*(1-BETA))^3
1410 IF W(I) > .3671 THEN GOTO 1440
1420 MO = .465 + 1.347*W(I) - .528*W(I)*W(I)
1430 GOTO 1450
1440 MO = .5361 + .9593*W(I)
1450 MONE = MO + ((5*TR(I)-3*MO-1)^2)/70
1460 MTWO = MO + .71*((TR(I)-.779)^2)
1470 IF W(I) <= .4 THEN MM = MONE
1480 GOTO 1520
1490 IF W(I) >= .55 THEN MM = MTWO
1500 GOTO 1520
1510 MM = MTWO*(W(I)-.4)/.15 + MONE*(.55-W(I))/.15
1520 IF TR(I) > 1 THEN GOTO 1550
1530 ALF = 1 + MM*(1-SQR(TR(I)))
1540 GOTO 1560
1550 ALF = 1-(.4774+1.328*W(I))*LOG(TR(I))
1560 ALF2 = ALF*ALF
1570 WA(I) = WAA*ALF2
1580 NEXT I
1590 REM ***** CALCULATE A AND B FOR PURE COMPONENTS *****
1600 FOR I =1 TO N
1610 BI(I) = WB(I)*R*TC(I)/PC(I)
1620 AIJ(I,I) = WA(I)*R*R*TC(I)*TC(I)/PC(I)
1630 NEXT I
1640 REM ***** BUBL CALCULATION *****
1650 FOR III=1 TO NDATA

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1660 P = PEXP(III)
1670 REM ***** INITIALIZE PHIV TO ONE *****
1680 FOR K = 1 TO N
1690 PHIV(K) = 1!
1700 NEXT K
1710 NLAP = 0
1720 REM ***** CALCULATE VAPOR PHASE MOLE FRACTIONS AND TOTAL PRESSURE
1730 YSUM = 0!
1740 GOSUB 2090
1750 REM ***** PHIMIX XEXP(I,III) *****
1760 FOR K = 1 TO N
1770 YCAL(K) = PHIL(K)*XEXP(K,III)/PHIV(K)
1780 YSUM = YSUM + YCAL(K)
1790 NEXT K
1800 REM ***** CHECK CONVERGENCE OF Y *****
1810 IF ABS(YSUM-1!) < .0001 THEN GOTO 1940
1820 P = P*YSUM
1830 REM ***** NORMALIZE Y *****
1840 FOR K = 1 TO N
1850 YCAL(K) = YCAL(K)/YSUM
1860 NEXT K
1870 GOSUB 2370
1880 REM PHIMIX Y(I)
1890 NLAP = NLAP + 1
1900 IF NLAP > 35 THEN GOTO 1930
1910 GOTO 1730
1920 CLS : LOCATE 12,25
1930 PRINT "OVER 35 NLAP IN BULBP"
1940 CLS
1950 LOCATE 10,26 :PRINT "PCAL = ";P
1960 FOR I=1 TO N
1970 LOCATE ,26 :PRINT "YCAL(";I;") =";YCAL(I)
1980 NEXT I
1990 LOCATE ,26 :PRINT "VVCAL = ";VV
2000 LOCATE ,26 :PRINT "VLCAL = ";VL
2010 DP(III) = 1! - P/PEXP(III)
2020 DPR = ABS(DP(III))
2030 DY = YEXP(1,III) - YCAL(1)
2040 DPR = DPR+DP(III)
2050 NEXT III
2060 DPR = DPR/NDATA
2070 LPRINT:LPRT TAB(7) "AT K = ";FK;" AAD = ";DPR
2080 RETURN
2090 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V.Z)
2100 REM ....CALCULATE A AND B FOR BINARY MIXTURE
2110 IPH = 0
2120 AM = 0 : BM = 0
2130 WM = 0 : WNUM = 0 : WDEN = 0
2140 FOR I = 1 TO N
2150 AI(I) = 0!
2160 BM = BM + XEXP(I,III)*BI(I)
2170 WNUM = WNUM + W(I)*XEXP(I,III)*BI(I)^.7
2180 WDEN = WDEN + XEXP(I,III)*BI(I)^.7
2190 FOR J = 1 TO N
2200 IF J = I THEN GOTO 2230

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2210 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
2220 GOTO 2240
2230 AIJ(I,J) = AIJ(I,I)
2240 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
2250 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
2260 NEXT J
2270 NEXT I
2280 WM = WNUM/WDEN
2290 UBAR = WM*3+1
2300 WBAR = -3*WM
2310 GOSUB 2650
2320 FOR I = 1 TO N
2330 PHIL(I) = PHI(I)
2340 NEXT I
2350 VL=V : ZL=Z
2360 RETURN
2370 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
2380 REM ....CALCULATE A AND B FOR BINARY MIXTURE
2390 IPH = 1
2400 AM = 0 : BM = 0
2410 WM = 0 : WNUM = 0 : WDEN = 0
2420 FOR I = 1 TO N
2430 AI(I) = 0!
2440 BM = BM + YCAL(I)*BI(I)
2450 WNUM = WNUM + W(I)*YCAL(I)*BI(I)^.7
2460 WDEN = WDEN + YCAL(I)*BI(I)^.7
2470 FOR J =1 TO N
2480 IF J = I THEN GOTO 2510
2490 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
2500 GOTO 2520
2510 AIJ(I,J) = AIJ(I,I)
2520 AI(I) = AI(I) + YCAL(J)*AIJ(I,J)
2530 AM = AM + YCAL(I)*YCAL(J)*AIJ(I,J)
2540 NEXT J
2550 NEXT I
2560 WM = WNUM/WDEN
2570 UBAR = WM*3+1
2580 WBAR = -3*WM
2590 GOSUB 2650
2600 FOR I = 1 TO N
2610 PHIV(I) = PHI(I)
2620 NEXT I
2630 VV=V : ZV=Z
2640 RETURN
2650 REM ***** FOR SCHMIDT AND WENZEL EQUATION OF STATE *****
2660 PBRT = P*BM/R/T
2670 PBRT2 = PBRT*PBRT
2680 PBRT3 = PBRT2*PBRT
2690 ABRT = P*AM/R/T/R/T
2700 PP = -(UBAR*PBRT-PBRT-1)
2710 QQ = WBAR*PBRT2-UBAR*PBRT2-UBAR*PBRT+ABRT
2720 RR = WBAR*PBRT3+WBAR*PBRT2+ABRT*PBRT
2730 GOSUB 3020
2740 REM CALL ANAL(PP,QQ,RR,IPH,Z)
2750 V = Z*R*T/P

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2760 PRINT "      MOLAR VOLUMN   V   = "; V
2770 KBAR   = (UBAR^2+4*UBAR-4)^.5
2780 ZB    = (Z - 1!)/BM
2790 ZPB   = Z - PBRT
2800 ZPZ   = (Z + (UBAR+KBAR)/2*PBRT)/(Z + (UBAR-KBAR)/2*PBRT)
2810 IF ZPB <= 0! OR ZPZ <= 0! THEN GOTO 2940
2820 LZB   = LOG(ZPB)
2830 LZAB  = LOG(ZPZ)*(ABRT/(KBAR*PBRT))
2840 FOR I = 1 TO N
2850 PHILN(I) = BI(I)*ZB - LZB - (2!*AI(I)/AM - BI(I)/BM)*LZAB
2860 IF PHILN(I) < -174! THEN PHILN(I) = -174!
2870 IF PHILN(I) < 174! THEN GOTO 2900
2880 PRINT "LOG OF PHI .GT. 174 IN PHIMIX, PHI SET TO 1"
2890 PHILN(I) = 0!
2900 PHI(I) = EXP(PHILN(I))
2910 PRINT "      FUGACITY COEFF.  PHI(";I,")      =" ; PHI(I)
2920 NEXT I
2930 RETURN
2940 REM *****...ERROR ADJUSTMENT...*****
2950 FOR I = 1 TO N
2960 IF IPH = 1 THEN PHI(I) = 1!
2970 IF IPH = 0 THEN PHI(I) = .2
2980 PRINT "NAGATIVE VALUE FOR MOLAR VOLUMN CALC. IN PHIMIX"
2990 PRINT "SO LET ASSUME PHI(";I,") = "; PHI(I)
3000 NEXT I
3010 RETURN
3020 REM *****
3030 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
3040 REM      INITIAL VALUE ;  Z = 0.0 , FOR IPH = 0
3050 REM                      Z = 1.0 , FOR IPH = 1
3060 IF IPH = 1 GOTO 3100
3070 Z = 0!
3080 NLOOP = 0
3090 GOTO 3120
3100 Z = 1!
3110 NLOOP = 0
3120 NLOOP = NLOOP + 1
3130 IF NLOOP > 25 THEN GOTO 3210
3140 FZ = Z*Z*Z - Z*Z*PP + Z*QQ - RR
3150 SLOPE = (3!*Z*Z - 2!*Z*PP + QQ)
3160 ZN = Z-(FZ/SLOPE)
3170 EROR = ABS((ZN-Z)/ZN)
3180 Z = ZN
3190 IF EROR < .0001 THEN GOTO 3230
3200 GOTO 3120
3210 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
3220 CLS
3230 LOCATE 10,26 :PRINT "      ROOTS OF CUBIC EQUATION ,WITH"
3240 LOCATE ,26 :PRINT "      IPH      = ";IPH
3250 LOCATE ,26 :PRINT "      P      = ";PP
3260 LOCATE ,26 :PRINT "      Q      = ";QQ
3270 LOCATE ,26 :PRINT "      R      = ";RR
3280 LOCATE ,26 :PRINT "      Z      = ";Z
3290 RETURN

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10 REM *****
20 REM **
30 REM ** PROGRAM FOR SEARCHING THE OPTIMUM Kij
40 REM ** FOR THE SCHMIDT-WENZEL EQUATION OF STATE
41 REM ** USING THE FUGACITY CRITERION
42 REM **
43 REM *****
50 DIM N$(20),MW(20),TC(20),PC(20),W(20)
60 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
70 CLS : COLOR 0,2
80 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
90 OPEN "I",#1,D$
100 INPUT #1,N,T,NDATA
110 T = T+ 273.16
120 FOR II=1 TO N
130 INPUT #1,N$(II),MW(II),TC(II),PC(II),W(II)
140 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
150 FOR I=1 TO NDATA
160 INPUT #1,PEXP(I)
170 FOR II=1 TO N
180 INPUT #1,YEXP(II,I),XEXP(II,I)
190 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 220
200 NEXT II
210 NEXT I
220 CLS
230 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
240 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILN(20),ZZ(20)
250 DIM WC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20),DEV(100),DFU(100)
260 DIM FIB(50)
270 ALPHA=.01
280 LOCATE 10,26 : PRINT "SPECIFY RANGE OF Kij FOR INITIAL SEARCH"
290 LOCATE 12,26 : INPUT "FROM AF = ",AF
300 LOCATE ,26 : INPUT "TO BF = ",BF
310 DEL = BF-AF
320 CLS :PRINT TAB(5) "FIBONACCI SINGLE VARIABLE PROCEDURE"
330 REM ***** DEFINE THE FIRST THREE FIBONACCI NUMBERS
340 FIB0 = 1!
350 FIB(1) = 1!
360 FIB(2) = 2!
370 REM ***** CALCULATE THE REMAINING FIBONACCI NUMBERS
380 BBF = 1/ALPHA
390 IF (BBF-2) <= 0 THEN GOTO 460
400 JJF = 2
410 JJF = JJF+1
420 FIB(JJF) = FIB(JJF-1)+FIB(JJF-2)
430 CCF = FIB(JJF)
440 IF (CCF-BBF) >= 0 THEN GOTO 530
450 GOTO 410
460 PRINT "ACCURACY SPECIFIED IN FUNC NOT SUFFICIENT"
470 PRINT "PROGRAM RESET ALPHA, ALPHA = 0.01"
480 ALPHA = .01
490 GOTO 380
500 REM *****
510 REM ***** FIRST STEP IN THE TABLEAU *****
520 REM *****
530 IFF = 0
540 KXF = JJF-2
550 IKF = JJF-2

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560 BL = BF-AF
570 ALL = FIB(IKF)*BL/FIB(JJF)
580 WF = AF+ALL
590 VF = BF-ALL
600 XF = WF :GOSUB 1230 :TF = DPR
610 XF = VF :GOSUB 1230 :UF = DPR
620 JKF = 1
630 PRINT "K"TAB(10)"LK"TAB(20)"AK"TAB(30)"BK"TAB(40)"LLK"TAB(50)"X"TAB(60)"Y"
640 PRINT JKF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
650 REM *****
660 REM ***** SUCCEEDING STEPS IN THE TABLEAU *****
670 REM *****
680 IKF = IKF-1
690 JJF = JJF-1
700 FOR IFF=1 TO KKF
710 IF (UF-TF) > 0 THEN GOTO 880
720 AF = AF+ALL
730 BL = BF-AF
740 WF = VF
750 XF = WF :GOSUB 1230 :TF = DPR
760 ALL = FIB(IKF)*BL/FIB(JJF)
770 VF = BF-ALL
780 XF = VF :GOSUB 1230 :UF = DPR
790 IIF = IFF+1
800 IKF = IKF-1
810 JJF = JJF-1
820 IF (IKF-1) >= 0 THEN GOTO 840
830 IKF = 1
840 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)WF TAB(60)TF
850 PRINT TAB(50)VF TAB(60)UF
860 GOTO 1020
870 REM *****
880 BF = BF-ALL
890 BL = BF-AF
900 VF = WF
910 XF = VF :GOSUB 1230 :UF = DPR
920 ALL = FIB(IKF)*BL/FIB(JJF)
930 WF = AF+ALL
940 XF = WF :GOSUB 1230 :TF = DPR
950 IIF = IFF+1
960 IKF = IKF-1
970 JJF = JJF-1
980 IF (IKF-1) >= 0 THEN GOTO 1000
990 IKF = 1
1000 PRINT IIF TAB(10)BL TAB(20)AF TAB(30)BF TAB(40)ALL TAB(50)VF TAB(60)UF
1010 PRINT TAB(50)WF TAB(60)TF
1020 NEXT IFF
1030 REM *****
1040 REM CALCULATION OF THE FINAL RANGE OF THE DEPENDENT VARIABLE
1050 REM *****
1060 EPS = .001*WF
1070 DL = WF+EPS
1080 XF = DL :GOSUB 1230 :YL = DPR
1090 IF (YL-TF) > 0 THEN GOTO 1140
1100 XF = BF :GOSUB 1230 :BFF = DPR

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1110 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";BF
1120 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";BFF
1130 GOTO 1170
1140 XF = AF :GOSUB 1230 :AFF = DPR
1150 LPRINT :LPRINT "THE FINAL FEASIBLE REGION X =";WF;"TO";AF
1160 LPRINT "WITH FUNCTION VALUES Y =";TF;"TO";AFF
1170 ACC = (WF-AF)/DEL
1180 LPRINT :LPRINT "THE ACCURACY IS ";ACC
1190 LPRINT "THE REQUIRED ACCURACY WAS ";ALPHA
1200 LPRINT :LPRINT TAB(10) "FOR ";N$(1);"(1) - ";N$(2);"(2)"
1210 LPRINT :LPRINT TAB(10) "AT TEMP. = ";T;"K"
1220 STOP :END
1230 REM ****
1240 REM ***** SUBROUTINE BUBL FUNC(X,Y) ****
1250 REM ****
1260 DPR = 0
1270 FK = XF
1280 R = 82.057
1290 FOR I = 1 TO N
1300 TR(I) = T/TC(I)
1310 NEXT I
1320 REM ***** Schmidt - Wenzel EOS ****
1330 FOR I = 1 TO N
1340 BETA = .25989 - .0217*W(I) + .00375*W(I)*W(I)
1350 CC = 1/(3*(1+BETA*W(I)))
1360 WB(I) = BETA*CC
1370 WAA = (1-CC*(1-BETA))^3
1380 IF W(I) > .3671 THEN GOTO 1410
1390 MO = .465 + 1.347*W(I) - .528*W(I)*W(I)
1400 GOTO 1420
1410 MO = .5361 + .9593*W(I)
1420 MONE = MO + ((5*TR(I)-3*MO-1)^2)/70
1430 MTWO = MO + .71*((TR(I)-.779)^2)
1440 IF W(I) <= .4 THEN MM = MONE
1450 GOTO 1490
1460 IF W(I) >= .55 THEN MM = MTWO
1470 GOTO 1490
1480 MM = MTWO*(W(I)-.4)/.15 + MONE*(.55-W(I))/.15
1490 IF TR(I) > 1 THEN GOTO 1520
1500 ALF = 1 + MM*(1-SQR(TR(I)))
1510 GOTO 1530
1520 ALF = 1-(.4774+1.328*W(I))*LOG(TR(I))
1530 ALF2 = ALF*ALF
1540 WA(I) = WAA*ALF2
1550 NEXT I
1560 REM ***** CALCULATE A AND B FOR PURE COMPONENTS ****
1570 FOR I = 1 TO N
1580 BI(I) = WB(I)*R*TC(I)/PC(I)
1590 AIJ(I,I) = WA(I)*R*TC(I)*TC(I)/PC(I)
1600 NEXT I
1610 REM ***** FUGACITY COEFF. CALCULATION ****
1620 FOR III=1 TO NDATA
1630 FOR III=1 TO NDATA
1640 P = PEXP(III)
1650 GOSUB 1840

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1660 REM ***** PHIMIX XEXP(I,III) *****
1670 GOSUB 2120
1680 REM ***** PHIMIX YEXP(I,III) *****
1690 CLS
1700 LOCATE 10,26 :PRINT "PCAL = ";P
1710 LOCATE ,26 :PRINT "VVCAL = ";VV
1720 LOCATE ,26 :PRINT "VLCAL = ";VL
1730 DFU(III) = 0
1740 FOR I=1 TO N
1750 FUGAL(I) = PHIL(I)*XEXP(I,III)*P
1760 FUGAV(I) = PHIV(I)*YEXP(I,III)*P
1770 DEV(I) = (ABS(FUGAL(I)-FUGAV(I)))/FUGAV(I)
1780 DFU(III) = DFU(III) + DEV(I)
1790 NEXT I
1800 DPR = DPR + DFU(III)
1810 NEXT III
1820 LPRINT:LPRINT TAB(7)"AT K = ";FK; DEV. F = ";DPR
1830 RETURN
1840 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V,Z)
1850 REM ....CALCULATE A AND B FOR BINARY MIXTURE
1860 IPH = 0
1870 AM = 0 : BM = 0
1880 WM = 0 : WNUM = 0 : WDEN = 0
1890 FOR I = 1 TO N
1900 AI(I) = 0!
1910 BM = BM + XEXP(I,III)*BI(I)
1920 WNUM = WNUM + W(I)*XEXP(I,III)*BI(I)^.7
1930 WDEN = WDEN + XEXP(I,III)*BI(I)^.7
1940 FOR J = 1 TO N
1950 IF J = I THEN GOTO 1980
1960 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1970 GOTO 1990
1980 AIJ(I,J) = AIJ(I,I)
1990 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
2000 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
2010 NEXT J
2020 NEXT I
2030 WM = WNUM/WDEN
2040 UBAR = WM*3+1
2050 WBAR = -3*WM
2060 GOSUB 2400
2070 FOR I = 1 TO N
2080 PHIL(I) = PHI(I)
2090 NEXT I
2100 VL=V : ZL=Z
2110 RETURN
2120 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
2130 REM ....CALCULATE A AND B FOR BINARY MIXTURE
2140 IPH = 1
2150 AM = 0 : BM = 0
2160 WM = 0 : WNUM = 0 : WDEN = 0
2170 FOR I = 1 TO N
2180 AI(I) = 0!
2190 BM = BM + YEXP(I,III)*BI(I)
2200 WNUM = WNUM + W(I)*YEXP(I,III)*BI(I)^.7

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2210 WDEN      = WDEN + YEXP(I,III)*BI(I)^.7
2220 FOR J = 1 TO N
2230 IF J = I THEN GOTO 2260
2240 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(I! - FK)
2250 GOTO 2270
2260 AIJ(I,J) = AIJ(I,I)
2270 AI(I)     = AI(I) + YEXP(J,III)*AIJ(I,J)
2280 AM        = AM + YEXP(I,III)*YEXP(J,III)*AIJ(I,J)
2290 NEXT J
2300 NEXT I
2310 WM        = WNUM/WDEN
2320 UBAR      = WM*3+1
2330 WBAR      = -3*WM
2340 GOSUB 2400
2350 FOR I = 1 TO N
2360 PHIV(I) = PHI(I)
2370 NEXT I
2380 VV=V :ZV=Z
2390 RETURN
2400 REM ***** FOR SCHMIDT AND WENZEL EQUATION OF STATE *****
2410 PBRT = P*BM/R/T
2420 PBRT2 = PBRT*PBRT
2430 PBRT3 = PBRT2*PBRT
2440 ABRT = P*AM/R/T/R/T
2450 PP = -(UBAR*PBRT-PBRT-1)
2460 QQ = WBAR*PBRT2-UBAR*PBRT2-UBAR*PBRT+ABRT
2470 RR = WBAR*PBRT3+WBAR*PBRT2+ABRT*PBRT
2480 GOSUB 2770
2490 REM CALL ANAL(PP,QQ,RR,IPH,Z)
2500 V = Z*R*T/P
2510 PRINT "          MOLAR VOLUMN      V      = "; V
2520 KBAR = (UBAR^2+4*UBAR-4)^.5
2530 ZB = (Z - 1!)/BM
2540 ZPB = Z - PBRT
2550 ZPZ = (Z + (UBAR+KBAR)/2*PBRT)/(Z + (UBAR-KBAR)/2*PBRT)
2560 IF ZPB <= 0! OR ZPZ <= 0! THEN GOTO 2690
2570 LZB = LOG(ZPB)
2580 LZAB = LOG(ZPZ)*(ABRT/(KBAR*PBRT))
2590 FOR I = 1 TO N
2600 PHILN(I) = BI(I)*ZB - LZB - (2!*AI(I)/AM - BI(I)/BM)*LZAB
2610 IF PHILN(I) < -174! THEN PHILN(I) = -170!
2620 IF PHILN(I) < 174! THEN GOTO 2650
2630 PRINT "LOG OF PHI .GT. 174 IN PHIMIX, PHI SET TO 1"
2640 PHILN(I) = 0!
2650 PHI(I) = EXP(PHILN(I))
2660 PRINT "          FUGACITY COEFF.    PHI(",I,")      =";PHI(I)
2670 NEXT I
2680 RETURN
2690 REM *****...ERROR ADJUSTMENT...
2700 FOR I = 1 TO N
2710 IF IPH = 1 THEN PHI(I) = 1!
2720 IF IPH = 0 THEN PHI(I) = .2
2730 PRINT "NAGATIVE VALUE FOR MOLAR VOLUMN CALC. IN PHIMIX"
2740 PRINT "SO LET ASSUME PHI(";I,") =";PHI(I)
2750 NEXT I

```

```

2760 RETURN
2770 REM *****
2780 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
2790 REM      INITIAL VALUE : Z = 0.0 , FOR IPH = 0
2800 REM                  Z = 1.0 , FOR IPH = 1
2810 IF IPH = 1 GOTO 2850
2820 Z      = 0!
2830 NLOOP = 0
2840 GOTO 2870
2850 Z      = 1!
2860 NLOOP = 0
2870 NLOOP = NLOOP + 1
2880 IF NLOOP > 25 THEN GOTO 2960
2890 FZ     = Z*Z*Z - Z*Z*PP + Z*QQ - RR
2900 SLOPE  = (3*Z*Z - 2*Z*PP + QQ)
2910 ZN    = Z-(FZ/SLOPE)
2920 EROR  = ABS((ZN-Z)/ZN)
2930 Z      = ZN
2940 IF EROR < .0001 THEN GOTO 2980
2950 GOTO 2870
2960 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
2970 CLS
2980 LOCATE 10,26 :PRINT " ROOTS OF CUBIC EQUATION ,WITH"
2990 LOCATE ,26 :PRINT " IPH    = ";IPH
3000 LOCATE ,26 :PRINT " P      = ";PP
3010 LOCATE ,26 :PRINT " Q      = ";QQ
3020 LOCATE ,26 :PRINT " R      = ";RR
3030 LOCATE ,26 :PRINT " Z      = ";Z
3040 RETURN

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```

10 REM *****
20 REM **
30 REM ** BUBBLE POINT PRESSURE CALCULATION PROGRAM ****
40 REM ** FOR THE SCHMIDT-WENZEL EQUATION OF STATE ****
50 REM **
60 REM *****
70 DIM N$(20),MW(20),TC(20),PC(20),W(20)
80 DIM PEXP(100),XEXP(10,100),YEXP(10,100)
90 CLS : COLOR 0,2
100 LOCATE 10,26 : INPUT "Name of data file to be opened : ",D$
110 OPEN "I",#1,D$
120 INPUT #1,N,T,NDATA
130 T = T + 273.16
140 FOR II=1 TO N
150 INPUT #1,N$(II),MW(II),TC(II),PC(II),W(II)
160 NEXT II
170 FOR I=1 TO NDATA
180 INPUT #1,PEXP(I)
190 FOR II=1 TO N
200 INPUT #1,YEXP(II,I),XEXP(II,I)
210 IF EOF(1) THEN CLOSE #1 : I=0 : GOTO 240
220 NEXT II
230 NEXT I
240 CLS
250 DIM A$(20),TR(20),WA(20),WB(20),AI(20),BI(20),AIJ(20,20)
260 DIM PHIV(20),PHIL(20),YCAL(20),A(20),B(20),PHILN(20),Z(20)
270 DIM WC(20),CC(20),FF(20),CI(20),PHI(20),AA(20),BB(20)
280 DIM DP(100),DPP(100),DY(100)
290 REM *****
300 REM ***** SUBROUTINE BUBL FUNC(X,Y) *****
310 REM *****
320 LOCATE 10,26 : INPUT "THE OPTIMUM VALUE OF Kij = ",FK
330 LPRINT TAB(10) "SCHMIDT-WENZEL EQUATION OF STATE"
340 LPRINT TAB(10) "MIXTURE : ";N$(1);"(1) - ";N$(2);"(2)"
350 LPRINT TAB(10) "TEMP. =";T;"K"
360 LPRINT TAB(10) "Kij = 0"
370 LPRINT : LPRINT TAB(10) "REF. REAMER ET AL. (1960)"
380 LPRINT TAB(6) -----
390 LPRINT TAB(16)"EXPERIMENTAL" TAB(43)"CALCULATED" TAB(63)"DEVIATIONS"
400 LPRINT TAB(8)----- TAB(39)----- TAB(59)----- TAB(51)
410 LPRINT TAB(10)"P(atm)" TAB(21)"X(1)" TAB(31)"Y(1)" TAB(40)"P(atm)" TAB(51)"Y
(1)" TAB(61)"DP;" TAB(69)"DY(1);"
420 LPRINT TAB(6) -----
430 R = 82.057
440 FOR I = 1 TO N
450 TR(I) = T/TC(I)
460 NEXT I
470 REM ***** Schmidt - Wenzel EOS *****
480 FOR I = 1 TO N
490 BETA = .25989 - .0217*W(I) + .00375*W(I)*W(I)
500 CC = 1/(3*(1+BETA*W(I)))
510 WB(I) = BETA*CC
520 WAA = (1-CC*(1-BETA))^3
530 IF W(I) > .3671 THEN GOTO 560
540 MD = .465 + 1.347*W(I) - .528*W(I)*W(I)
550 GOTO 570

```

```
560 MO = .5361 + .9593*W(I)
570 MONE = MO + ((5*TR(I)-3*MO-1)^2)/70
580 MTWO = MO + .71*((TR(I)-.779)^2)
590 IF W(I) <= .4 THEN MM = MONE
600 GOTO 640
610 IF W(I) >= .55 THEN MM = MTWO
620 GOTO 640
630 MM = MTWO*(W(I)-.4)/.15 + MONE*(.55-W(I))/.15
640 IF TR(I) > 1 THEN GOTO 670
650 ALF = 1 + MM*(1-SQR(TR(I)))
660 GOTO 680
670 ALF = 1-(.4774+1.328*W(I))*LOG(TR(I))
680 ALF2 = ALF*ALF
690 WA(I) = WAA*ALF2
700 NEXT I
710 REM ***** CALCULATE A AND B FOR PURE COMPONENTS *****
720 FOR I =1 TO N
730 CI(I) = WC(I)*R*TC(I)/PC(I)
740 BI(I) = WB(I)*R*TC(I)/PC(I)
750 AIJ(I,I) = WA(I)*R*R*TC(I)*TC(I)/PC(I)
760 NEXT I
770 REM ***** BUBL CALCULATION *****
780 FOR III=1 TO NDATA
790 P = PEXP(III)
800 REM ***** INITIALIZE PHIV TO ONE *****
810 FOR K = 1 TO N
820 PHIV(K) = 1!
830 NEXT K
840 NLAP = 0
850 REM ***** CALCULATE VAPOR PHASE MOLE FRACTIONS AND TOTAL PRESSURE
860 YSUM = 0!
870 GOSUB 1240
880 REM ***** PHIMIX XEXP(I,III) *****
890 FOR K = 1 TO N
900 YCAL(K) = PHIL(K)*XEXP(K,III)/PHIV(K)
910 YSUM = YSUM + YCAL(K)
920 NEXT K
930 REM ***** CHECK CONVERGENCE OF Y *****
940 IF ABS(YSUM-1!) < .0001 THEN GOTO 1070
950 P = P*YSUM
960 REM ***** NORMALIZE Y *****
970 FOR K = 1 TO N
980 YCAL(K) = YCAL(K)/YSUM
990 NEXT K
1000 GOSUB 1520
1010 REM PHIMIX Y(I)
1020 NLAP = NLAP + 1
1030 IF NLAP > 35 THEN GOTO 1060
1040 GOTO 860
1050 CLS : LOCATE 12,25
1060 PRINT "OVER 35 NLAP IN BULBP"
1070 CLS
1080 LOCATE 10,26 :PRINT "PCAL = ";P
1090 FOR I=1 TO N
1100 LOCATE ,26 :PRINT "YCAL(";I;") =";YCAL(I)
```

```

1110 NEXT I
1120 LOCATE ,26 :PRINT "VVCAL      :" ;VV
1130 LOCATE ,26 :PRINT "VLCAL      :" ;VL
1140 DPP(III) = ABS(PEXP(III)-P)
1150 DP(III) = DPP(III)/PEXP(III)
1160 DY(III) = ABS(YEXP(1,III) - YCAL(1))
1170 DPR = DPR+DP(III)
1180 LPRINT TAB(8) USING "###.###" ;PEXP(III),XEXP(1,III),YEXP(1,III),P,YCAL(1),
),DPP(III),DY(III)
1190 NEXT III
1200 DPR = DPR/NDATA*100
1210 LPRINT TAB(6) -----
-----
1220 LPRINT TAB(10) "WITH MIN. AAD. :" ;DPR
1230 END
1240 REM ***** SUBROUTINE PHIMIX(P,XEXP,IEQ,FK,IPH,PHI,V,Z)
1250 REM ....CALCULATE A AND B FOR BINARY MIXTURE
1260 IPH = 0
1270 AM = 0 : BM = 0
1280 WM = 0 : WNUM = 0 : WDEN = 0
1290 FOR I = 1 TO N
1300 AI(I) = 0!
1310 BM = BM + XEXP(I,III)*BI(I)
1320 WNUM = WNUM + W(I)*XEXP(I,III)*BI(I)^.7
1330 WDEN = WDEN + XEXP(I,III)*BI(I)^.7
1340 FOR J = 1 TO N
1350 IF J = I THEN GOTO 1380
1360 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1370 GOTO 1390
1380 AIJ(I,J) = AIJ(I,I)
1390 AI(I) = AI(I) + XEXP(J,III)*AIJ(I,J)
1400 AM = AM + XEXP(I,III)*XEXP(J,III)*AIJ(I,J)
1410 NEXT J
1420 NEXT I
1430 WM = WNUM/WDEN
1440 UBAR = WM*3+1
1450 WBAR = -3*WM
1460 GOSUB 1800
1470 FOR I = 1 TO N
1480 PHI(I) = PHI(I)
1490 NEXT I
1500 VL=V : ZL=Z
1510 RETURN
1520 REM ***** SUBROUTINE PHIMIX(P,Y,IEQ,FK,IPH,PHI,V,Z)
1530 REM ....CALCULATE A AND B FOR BINARY MIXTURE
1540 IPH = 1
1550 AM = 0 : BM = 0
1560 WM = 0 : WNUM = 0 : WDEN = 0
1570 FOR I = 1 TO N
1580 AI(I) = 0!
1590 BM = BM + YCAL(I)*BI(I)
1600 WNUM = WNUM + W(I)*YCAL(I)*BI(I)^.7
1610 WDEN = WDEN + YCAL(I)*BI(I)^.7
1620 FOR J = 1 TO N
1630 IF J = I THEN GOTO 1660
1640 AIJ(I,J) = SQR(AIJ(I,I)*AIJ(J,J))*(1! - FK)
1650 GOTO 1670

```

```

1660 AIJ(I,J) = AIJ(I,I)
1670 AI(I) = AI(I) + YCAL(J)*AIJ(I,J)
1680 AM = AM + YCAL(I)*YCAL(J)*AIJ(I,J)
1690 NEXT J
1700 NEXT I
1710 WM = WNUM/WDEN
1720 UBAR = WM^3+1
1730 WBAR = -3*WM
1740 GOSUB 1800
1750 FOR I = 1 TO N
1760 PHIV(I) = PHI(I)
1770 NEXT I
1780 VV=V :ZV=Z
1790 RETURN
1800 REM ***** FOR SCHMIDT AND WENZEL EQUATION OF STATE *****
1810 PBRT = P*BM/R/T
1820 PBRT2 = PBRT*PBRT
1830 PBRT3 = PBRT2*PBRT
1840 ABRT = P*AM/R/T/R/T
1850 PP = -(UBAR*PBRT-PBRT-1)
1860 QQ = WBAR*PBRT2-UBAR*PBRT2-UBAR*PERT+ABRT
1870 RR = WBAR*PBRT3+WBAR*PBRT2+ABRT*PBRT
1880 GOSUB 2170
1890 REM CALL ANAL(PP,QQ,RR,IPH,Z)
1900 V = Z*R*T/P
1910 PRINT " MOLAR VOLUMN V = "; V
1920 KBAR = (UBAR^2+4*UBAR-4)^.5
1930 ZB = (Z - 1!)/BM
1940 ZPB = Z - PBRT
1950 ZPZ = (Z + (UBAR+KBAR)/2*PBRT)/(Z + (UBAR-KBAR)/2*PBRT)
1960 IF ZPB <= 0! OR ZPZ <= 0! THEN GOTO 2090
1970 LZB = LOG(ZPB)
1980 LZAB = LOG(ZPZ)*(ABRT/(KBAR*PBRT))
1990 FOR I = 1 TO N
2000 PHILN(I) = BI(I)*ZB - LZB - (2!*AI(I))/AM - BI(I)/BM*LZAB
2010 IF PHILN(I) < -174! THEN PHILN(I) = -170!
2020 IF PHILN(I) < 174! THEN GOTO 2050
2030 PRINT "LOG OF PHI .GT. 174 IN PHIMIX, PHI SET TO 1"
2040 PHILN(I) = 0!
2050 PHI(I) = EXP(PHILN(I))
2060 PRINT " FUGACITY COEFF. PHI(";I,") =";PHI(I)
2070 NEXT I
2080 RETURN
2090 REM *****...ERROR ADJUSTMENT...
2100 FOR I = 1 TO N
2110 IF IPH = 1 THEN PHI(I) = 1!
2120 IF IPH = 0 THEN PHI(I) = .2
2130 PRINT "NEGATIVE VALUE FOR MOLAR VOLUMN CALC. IN PHIMIX"
2140 PRINT "SO LET ASSUME PHI(";I,") =";PHI(I)
2150 NEXT I
2160 RETURN
2170 REM *****
2180 REM ....SOLVE CUBIC EQUATION BY NEWTON RAPHSON METHOD
2190 REM INITIAL VALUE : Z = 0.0 , FOR IPH = 0
2200 REM Z = 1.0 , FOR IPH = 1

```

```
2210 IF IPH = 1 GOTO 2250
2220 Z      = 0!
2230 NLOOP = 0
2240 GOTO 2270
2250 Z      = 1!
2260 NLOOP = 0
2270 NLOOP = NLOOP + 1
2280 IF NLOOP > 25 THEN GOTO 2360
2290 FZ      = Z*Z*Z - Z*Z*PP + Z*QQ - RR
2300 SLOPE   = (3!*Z*Z - 2!*Z*PP + QQ)
2310 ZN      = Z-(FZ/SLOPE)
2320 EROR   = ABS((ZN-Z)/ZN)
2330 Z      = ZN
2340 IF EROR < .0001 THEN GOTO 2380
2350 GOTO 2270
2360 PRINT "OVER 25 LOOPS OF NEWRAP. CALCULATIONS"
2370 CLS
2380 LOCATE 10,26 :PRINT "    ROOTS OF CUBIC EQUATION WITH"
2390 LOCATE ,26 :PRINT "    IPH      = ";IPH
*2400 LOCATE ,26 :PRINT "    P      = ";PP
2410 LOCATE ,26 :PRINT "    Q      = ";QQ
2420 LOCATE ,26 :PRINT "    R      = ";RR
2430 LOCATE ,26 :PRINT "    Z      = ";Z
2440 RETURN
```

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Appendix B

Results of the Calculations

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จุฬาลงกรณ์มหาวิทยาลัย

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : ETHANE(1) - CO₂(2)

TEMP. = 250 K

K_{ij} = .1346

REF. DAVALOS ET AL. (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
14.2300	0.0444	0.1115	14.2123	0.1044	0.0177	0.0071
15.6800	0.1035	0.2226	15.6166	0.2128	0.0634	0.0098
16.9300	0.1680	0.3009	16.9296	0.3043	0.0004	0.0034
18.0400	0.2245	0.3697	17.9053	0.3688	0.1347	0.0009
19.2300	0.3083	0.4474	19.0792	0.4463	0.1508	0.0011
20.0300	0.3980	0.5056	20.0124	0.5133	0.0176	0.0077
20.5600	0.4692	0.5522	20.5419	0.5587	0.0181	0.0065
20.9900	0.5990	0.6265	21.0814	0.6315	0.0914	0.0050
21.0700	0.6900	0.6802	21.1503	0.6804	0.0803	0.0002
20.8000	0.7908	0.7467	20.8848	0.7405	0.0848	0.0062
19.9900	0.8829	0.8217	20.1466	0.8149	0.1566	0.0068
19.4000	0.9260	0.8696	19.5146	0.8646	0.1146	0.0050
18.5100	0.9701	0.9378	18.5536	0.9346	0.0436	0.0032

WITH MIN. AAD. = .390151

PENG-ROBINSON EQUATION OF STATE

MIXTURE : ETHANE(1) - CO₂(2)

TEMP. = 250 K

K_{ij} = .1084

REF. DAVALOS ET AL. (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
14.2300	0.0444	0.1115	14.5382	0.0941	0.3082	0.0174
15.6800	0.1035	0.2226	15.7759	0.1958	0.0959	0.0268
16.9300	0.1680	0.3009	16.9556	0.2852	0.0256	0.0157
18.0400	0.2245	0.3697	17.8500	0.3502	0.1900	0.0195
19.2300	0.3083	0.4474	18.9550	0.4307	0.2750	0.0167
20.0300	0.3980	0.5056	19.8626	0.5023	0.1674	0.0033
20.5600	0.4692	0.5522	20.3972	0.5519	0.1628	0.0003
20.9900	0.5990	0.6265	20.9796	0.6331	0.0104	0.0066
21.0700	0.6900	0.6802	21.0922	0.6879	0.0222	0.0077
20.8000	0.7908	0.7467	20.8899	0.7542	0.0899	0.0075
19.9900	0.8829	0.8217	20.2711	0.8314	0.2811	0.0097
19.4000	0.9260	0.8696	19.7502	0.8796	0.3502	0.0100
18.5100	0.9701	0.9378	18.9792	0.9435	0.4692	0.0057

WITH MIN. AAD. = 1.028727

PATEL-TEJA EQUATION OF STATE
 MIXTURE : ETHANE(1) - CO₂(2)
 TEMP. = 250 K
 K_{ij} = .1439

REF. DAVALOS ET AL. (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
14.2300	0.0444	0.1115	14.1423	0.1093	0.0877	0.0022
15.6800	0.1035	0.2226	15.6377	0.2204	0.0424	0.0022
16.9300	0.1680	0.3009	17.0174	0.3121	0.0874	0.0112
18.0400	0.2245	0.3697	18.0276	0.3758	0.0124	0.0061
19.2300	0.3083	0.4474	19.2201	0.4510	0.0099	0.0036
20.0300	0.3980	0.5056	20.1430	0.5148	0.1130	0.0092
20.5600	0.4692	0.5522	20.6470	0.5575	0.0870	0.0053
20.9900	0.5990	0.6265	21.1204	0.6252	0.1304	0.0013
21.0700	0.6900	0.6802	21.1343	0.6703	0.0643	0.0099
20.8000	0.7908	0.7467	20.8004	0.7265	0.0004	0.0202
19.9900	0.8829	0.8217	19.9490	0.7994	0.0410	0.0223
19.4000	0.9260	0.8696	19.2153	0.8507	0.1847	0.0189
18.5100	0.9701	0.9378	18.0834	0.9261	0.4266	0.0117

WITH MIN. AAD. = .5307925

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : ETHANE(1) - CO₂(2)
 TEMP. = 250 K
 K_{ij} = .1431

REF. DAVALOS ET AL. (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
14.2300	0.0444	0.1115	13.9820	0.1005	0.2480	0.0110
15.6800	0.1035	0.2226	15.3820	0.2044	0.2980	0.0182
16.9300	0.1680	0.3009	16.7027	0.2917	0.2273	0.0092
18.0400	0.2245	0.3697	17.6969	0.3529	0.3432	0.0168
19.2300	0.3083	0.4474	18.9205	0.4258	0.3095	0.0216
20.0300	0.3980	0.5056	19.9399	0.4881	0.0901	0.0175
20.5600	0.4692	0.5522	20.5600	0.5299	0.0000	0.0223
20.9900	0.5990	0.6265	21.3175	0.5959	0.3275	0.0306
21.0700	0.6900	0.6802	21.5734	0.6399	0.5034	0.0403
20.8000	0.7908	0.7467	21.5064	0.6954	0.7064	0.0513
19.9900	0.8829	0.8217	20.7940	0.7708	0.8040	0.0509
19.4000	0.9260	0.8696	20.0194	0.8263	0.6194	0.0433
18.5100	0.9701	0.9378	18.7027	0.9119	0.1927	0.0259

WITH MIN. AAD. = 1.888433

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : PROPANE(1) - CO₂(2)

TEMP. = 266.49 K

K_{ij} = .134

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.9607	0.0886	0.5207	7.6460	0.5021	0.3147	0.0186
10.5462	0.1620	0.6399	10.5476	0.6446	0.0014	0.0047
11.4647	0.1798	0.6707	11.2125	0.6672	0.2522	0.0035
13.4379	0.2515	0.7253	13.7359	0.7345	0.2980	0.0092
16.3976	0.3464	0.7882	16.6916	0.7901	0.2940	0.0019
17.8265	0.3996	0.8079	18.1633	0.8123	0.3368	0.0044
20.0038	0.4428	0.8318	19.2678	0.8274	0.7360	0.0044
21.3646	0.5266	0.8523	21.1917	0.8519	0.1729	0.0004
23.8820	0.6470	0.8751	23.5416	0.8809	0.3404	0.0058
25.2428	0.7750	0.9157	25.6780	0.9104	0.4352	0.0053
25.7872	0.8189	0.9265	26.3574	0.9217	0.5702	0.0048

WITH MIN. AAD. = 1.992308

PENG-ROBINSON EQUATION OF STATE

MIXTURE : PROPANE(1) - CO₂(2)

TEMP. = 266.49 K

K_{ij} = .118

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.9607	0.0886	0.5207	7.7190	0.4791	0.2417	0.0416
10.5462	0.1620	0.6399	10.5469	0.6242	0.0007	0.0157
11.4647	0.1798	0.6707	11.1995	0.6477	0.2652	0.0230
13.4379	0.2515	0.7253	13.6956	0.7182	0.2577	0.0071
16.3976	0.3464	0.7882	16.6656	0.7774	0.2680	0.0108
17.8265	0.3996	0.8079	18.1700	0.8012	0.3435	0.0067
20.0038	0.4428	0.8318	19.3088	0.8176	0.6950	0.0142
21.3646	0.5266	0.8523	21.3247	0.8444	0.0399	0.0079
23.8820	0.6470	0.8751	23.8472	0.8762	0.0348	0.0011
25.2428	0.7750	0.9157	26.1861	0.9085	0.9433	0.0072
25.7872	0.8189	0.9265	26.9364	0.9207	1.1492	0.0058

WITH MIN. AAD. = 2.075852

PATEL-TEJA EQUATION OF STATE
 MIXTURE : PROPANE(1) - CO₂(2)
 TEMP. = 266.49 K
 K_{ij} = .1366

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.9607	0.0886	0.5207	7.6128	0.5116	0.3479	0.0091
10.5462	0.1620	0.6399	10.5451	0.6521	0.0011	0.0122
11.4647	0.1798	0.6707	11.2141	0.6743	0.2506	0.0036
13.4379	0.2515	0.7253	13.7415	0.7398	0.3036	0.0145
16.3976	0.3464	0.7882	16.6717	0.7934	0.2741	0.0052
17.8265	0.3996	0.8079	18.1149	0.8148	0.2884	0.0069
20.0038	0.4428	0.8318	19.1900	0.8292	0.8138	0.0026
21.3646	0.5266	0.8523	21.0423	0.8526	0.3223	0.0003
23.8820	0.6470	0.8751	23.2655	0.8803	0.6165	0.0052
25.2428	0.7750	0.9157	25.2474	0.9086	0.0046	0.0071
25.7872	0.8189	0.9265	25.8701	0.9196	0.0829	0.0069

WITH MIN. AAD. = 1.873924

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : PROPANE(1) - CO₂(2)
 TEMP. = 266.49 K
 K_{ij} = .1447

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.9607	0.0886	0.5207	7.6484	0.5013	0.3123	0.0194
10.5462	0.1620	0.6399	10.5475	0.6415	0.0013	0.0016
11.4647	0.1798	0.6707	11.2087	0.6637	0.2560	0.0070
13.4379	0.2515	0.7253	13.7076	0.7292	0.2697	0.0039
16.3976	0.3464	0.7882	16.6108	0.7829	0.2132	0.0053
17.8265	0.3996	0.8079	18.0470	0.8041	0.2205	0.0038
20.0038	0.4428	0.8318	19.1220	0.8185	0.8818	0.0133
21.3646	0.5266	0.8523	20.9912	0.8416	0.3734	0.0107
23.8820	0.6470	0.8751	23.2850	0.8689	0.5970	0.0062
25.2428	0.7750	0.9157	25.4064	0.8971	0.1636	0.0186
25.7872	0.8189	0.9265	26.0895	0.9084	0.3023	0.0181

WITH MIN. AAD. = 1.926214

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : PROPANE(1) - CO₂(2)

TEMP. = 244.27 K

K_{ij} = .1322

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.9669	0.1134	0.6589	4.7978	0.6527	0.1691	0.0062
5.7834	0.1453	0.7133	5.5664	0.7048	0.2170	0.0085
7.4164	0.2245	0.7820	7.2918	0.7832	0.1246	0.0012
7.7566	0.2495	0.7945	7.7838	0.7995	0.0272	0.0050
9.0833	0.3229	0.8295	9.0826	0.8352	0.0007	0.0057
10.4986	0.4226	0.8580	10.5238	0.8666	0.0252	0.0086
11.4307	0.5329	0.8828	11.7399	0.8897	0.3091	0.0069
12.5534	0.6672	0.9067	12.8109	0.9103	0.2575	0.0036
12.9616	0.7464	0.9196	13.3027	0.9214	0.3411	0.0018
13.4039	0.8067	0.9316	13.6415	0.9307	0.2376	0.0009

WITH MIN. AAD. = 1.859458

PENG-ROBINSON EQUATION OF STATE

MIXTURE : PROPANE(1) - CO₂(2)

TEMP. = 244.27 K

K_{ij} = .1172

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.9669	0.1134	0.6589	4.8235	0.6279	0.1434	0.0310
5.7834	0.1453	0.7133	5.5746	0.6823	0.2088	0.0310
7.4164	0.2245	0.7820	7.2797	0.7658	0.1367	0.0162
7.7566	0.2495	0.7945	7.7705	0.7835	0.0139	0.0110
9.0833	0.3229	0.8295	9.0833	0.8225	0.0000	0.0070
10.4986	0.4226	0.8580	10.5747	0.8573	0.0761	0.0007
11.4307	0.5329	0.8828	11.8758	0.8834	0.4451	0.0006
12.5534	0.6672	0.9067	13.0712	0.9070	0.5178	0.0003
12.9616	0.7464	0.9196	13.6372	0.9198	0.6756	0.0002
13.4039	0.8067	0.9316	14.0296	0.9303	0.6257	0.0013

WITH MIN. AAD. = 2.714205

PATEL-TEJA EQUATION OF STATE
 MIXTURE : PROPANE(1) - CO₂(2)
 TEMP. = 244.27 K
 K_{ij} = .1373

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.9669	0.1134	0.6589	4.8283	0.6633	0.1386	0.0044
5.7834	0.1453	0.7133	5.6082	0.7139	0.1752	0.0006
7.4164	0.2245	0.7820	7.3435	0.7893	0.0729	0.0073
7.7566	0.2495	0.7945	7.8324	0.8049	0.0758	0.0104
9.0833	0.3229	0.8295	9.1108	0.8388	0.0275	0.0093
10.4986	0.4226	0.8580	10.4974	0.8684	0.0012	0.0104
11.4307	0.5329	0.8828	11.6277	0.8898	0.1970	0.0070
12.5534	0.6672	0.9067	12.5770	0.9085	0.0236	0.0018
12.9616	0.7464	0.9196	12.9952	0.9185	0.0336	0.0011
13.4039	0.8067	0.9316	13.2792	0.9271	0.1247	0.0045

WITH MIN. AAD. = 1.119571

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : PROPANE(1) - CO₂(2)
 TEMP. = 244.27 K
 K_{ij} = .1436

REF. HAMAN & LU (1976)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.9669	0.1134	0.6589	4.8404	0.6499	0.1265	0.0090
5.7834	0.1453	0.7133	5.6105	0.7011	0.1729	0.0122
7.4164	0.2245	0.7820	7.3275	0.7776	0.0889	0.0044
7.7566	0.2495	0.7945	7.8126	0.7935	0.0560	0.0010
9.0833	0.3229	0.8295	9.0861	0.8279	0.0028	0.0016
10.4986	0.4226	0.8580	10.4826	0.8577	0.0160	0.0003
11.4307	0.5329	0.8828	11.6484	0.8789	0.2177	0.0039
12.5534	0.6672	0.9067	12.6788	0.8970	0.1254	0.0097
12.9616	0.7464	0.9196	13.1662	0.9065	0.2046	0.0131
13.4039	0.8067	0.9316	13.5142	0.9148	0.1103	0.0168

WITH MIN. AAD. = 1.294513

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : i-Butane(1) - CO₂(2)
 TEMP. = 310.94 K
 K_{ij} = .1291

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.1442	0.0251	0.2657	7.0067	0.2638	0.1375	0.0019
12.1792	0.0881	0.5668	11.9433	0.5500	0.2359	0.0168
21.0244	0.2056	0.7297	21.0076	0.7295	0.0168	0.0002
27.2840	0.2891	0.7872	27.2800	0.7845	0.0040	0.0027
34.9726	0.3991	0.8267	35.2492	0.8263	0.2766	0.0004
43.0013	0.5195	0.8480	43.5204	0.8540	0.5191	0.0060
49.8733	0.6205	0.8690	50.1362	0.8705	0.2629	0.0015
55.1804	0.7073	0.8822	55.7604	0.8826	0.5800	0.0004

WITH MIN. AAD. = .9415751

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : i-Butane(1) - CO₂(2)
 TEMP. = 310.94 K
 K_{ij} = .1153

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.1442	0.0251	0.2657	7.2060	0.2508	0.0618	0.0149
12.1792	0.0881	0.5668	12.0840	0.5325	0.0952	0.0343
21.0244	0.2056	0.7297	21.0818	0.7143	0.0574	0.0154
27.2840	0.2891	0.7872	27.3463	0.7707	0.0623	0.0165
34.9726	0.3991	0.8267	35.3595	0.8138	0.3869	0.0129
43.0013	0.5195	0.8480	43.7636	0.8423	0.7623	0.0057
49.8733	0.6205	0.8690	50.5616	0.8589	0.6883	0.0101
55.1804	0.7073	0.8822	56.3762	0.8706	1.1958	0.0116

WITH MIN. AAD. = 1.071763

PATEL-TEJA EQUATION OF STATE
 MIXTURE : i-Butane(1) - CO₂(2)
 TEMP. = 310.94 K
 K_{ij} = .125

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.1442	0.0251	0.2657	6.8639	0.2707	0.2803	0.0050
12.1792	0.0881	0.5668	11.8279	0.5579	0.3513	0.0089
21.0244	0.2056	0.7297	20.9426	0.7347	0.0818	0.0050
27.2840	0.2891	0.7872	27.2475	0.7882	0.0365	0.0010
34.9726	0.3991	0.8267	35.2511	0.8287	0.2785	0.0020
43.0013	0.5195	0.8480	43.5441	0.8554	0.5428	0.0074
49.8733	0.6205	0.8690	50.1652	0.8712	0.2919	0.0022
55.1804	0.7073	0.8822	55.7905	0.8829	0.6101	0.0007

WITH MIN. AAD. = 1.38507

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : i-Butane(1) - CO₂(2)
 TEMP. = 310.94 K
 K_{ij} = .1236

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
7.1442	0.0251	0.2657	6.9443	0.2646	0.1999	0.0011
12.1792	0.0881	0.5668	11.8776	0.5502	0.3016	0.0166
21.0244	0.2056	0.7297	20.9708	0.7284	0.0536	0.0013
27.2840	0.2891	0.7872	27.2958	0.7827	0.0118	0.0045
34.9726	0.3991	0.8267	35.3830	0.8236	0.4104	0.0031
43.0013	0.5195	0.8480	43.8597	0.8504	0.8584	0.0024
49.8733	0.6205	0.8690	50.7268	0.8658	0.8535	0.0032
55.1804	0.7073	0.8822	56.6202	0.8767	1.4398	0.0055

WITH MIN. AAD. = 1.632935

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : n-PENTANE(1) - CO₂(2)

TEMP. = 277.66 K

K_{ij} = .1426

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
2.2453	0.0290	0.8528	2.0160	0.8517	0.2293	0.0011
5.5793	0.0856	0.9449	5.3375	0.9418	0.2418	0.0031
10.8864	0.1834	0.9709	10.8823	0.9697	0.0041	0.0012
16.8059	0.3179	0.9803	17.8983	0.9801	1.0924	0.0002
22.1130	0.4858	0.9846	25.1326	0.9848	3.0196	0.0002
27.0119	0.6255	0.9872	29.4575	0.9869	2.4456	0.0003
32.0468	0.8229	0.9894	33.4550	0.9894	1.4082	0.0000
34.0880	0.8998	0.9862	35.1448	0.9913	1.0568	0.0051
36.6055	0.9623	0.9870	37.1726	0.9951	0.5671	0.0081
37.0138	0.9791	0.9900	37.8955	0.9969	0.8817	0.0069

WITH MIN. AAD. = 5.52188

PENG-ROBINSON EQUATION OF STATE

MIXTURE : n-PENTANE(1) - CO₂(2)

TEMP. = 277.66 K

K_{ij} = .1179

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
2.2453	0.0290	0.8528	1.9098	0.8243	0.3355	0.0285
5.5793	0.0856	0.9449	4.9717	0.9300	0.6076	0.0149
10.8864	0.1834	0.9709	10.1349	0.9636	0.7515	0.0073
16.8059	0.3179	0.9803	16.8103	0.9765	0.0044	0.0038
22.1130	0.4858	0.9846	24.0236	0.9824	1.9106	0.0022
27.0119	0.6255	0.9872	28.7258	0.9851	1.7139	0.0021
32.0468	0.8229	0.9894	33.6903	0.9885	1.6435	0.0009
34.0880	0.8998	0.9862	35.7832	0.9910	1.6952	0.0048
36.6055	0.9623	0.9870	38.1351	0.9950	1.5296	0.0080
37.0138	0.9791	0.9900	38.9426	0.9969	1.9287	0.0069

WITH MIN. AAD. = 6.723994

PATEL-TEJA EQUATION OF STATE
 MIXTURE : n-PENTANE(1) - CO₂(2)
 TEMP. = 277.66 K
 K_{ij} = .1359

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
2.2453	0.0290	0.8528	1.9946	0.8640	0.2507	0.0112
5.5793	0.0856	0.9449	5.3263	0.9469	0.2530	0.0020
10.8864	0.1834	0.9709	10.8808	0.9722	0.0056	0.0013
16.8059	0.3179	0.9803	17.8851	0.9815	1.0792	0.0012
22.1130	0.4858	0.9846	25.0309	0.9858	2.9179	0.0012
27.0119	0.6255	0.9872	29.2099	0.9876	2.1980	0.0004
32.0468	0.8229	0.9894	32.9209	0.9899	0.8741	0.0005
34.0880	0.8998	0.9862	34.4908	0.9916	0.4028	0.0054
36.6055	0.9623	0.9870	36.4201	0.9952	0.1854	0.0082
37.0138	0.9791	0.9900	37.1171	0.9969	0.1033	0.0069

WITH MIN. AAD. = 4.820153

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-PENTANE(1) - CO₂(2)
 TEMP. = 277.66 K
 K_{ij} = .1335

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
2.2453	0.0290	0.8528	2.0202	0.8490	0.2251	0.0038
5.5793	0.0856	0.9449	5.3404	0.9406	0.2389	0.0043
10.8864	0.1834	0.9709	10.8863	0.9690	0.0001	0.0019
16.8059	0.3179	0.9803	17.9092	0.9796	1.1033	0.0007
22.1130	0.4858	0.9846	25.1381	0.9845	3.0251	0.0001
27.0119	0.6255	0.9872	29.4298	0.9867	2.4179	0.0005
32.0468	0.8229	0.9894	33.2863	0.9894	1.2395	0.0000
34.0880	0.8998	0.9862	34.8570	0.9915	0.7690	0.0053
36.6055	0.9623	0.9870	36.7374	0.9952	0.1319	0.0082
37.0138	0.9791	0.9900	37.4120	0.9970	0.3982	0.0070

WITH MIN. AAD. = 5.106436

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : n-PENTANE(1) - CO₂(2)

TEMP. = 344.16 K

K_{ij} = .1368

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.0824	0.0072	0.2708	3.7352	0.2100	0.3472	0.0608
6.2597	0.0268	0.5195	6.0213	0.4925	0.2384	0.0270
6.4638	0.0283	0.5367	6.1967	0.5057	0.2671	0.0310
8.6411	0.0444	0.6420	8.0831	0.6123	0.5580	0.0297
14.5606	0.0979	0.7763	14.4003	0.7670	0.1603	0.0093
22.1810	0.1631	0.8427	22.1830	0.8359	0.0020	0.0068
29.7335	0.2249	0.8728	29.6176	0.8670	0.1159	0.0058
38.8508	0.3026	0.8936	39.0004	0.8878	0.1496	0.0058
48.9888	0.3897	0.9040	49.4511	0.8996	0.4623	0.0044
58.1062	0.4698	0.9105	58.8687	0.9043	0.7625	0.0062
68.2441	0.5623	0.9127	69.2878	0.9044	1.0437	0.0083
73.8234	0.6111	0.9125	74.4728	0.9023	0.6494	0.0102
81.7841	0.6830	0.9045	81.5758	0.8957	0.2083	0.0088
88.4520	0.7425	0.8914	86.6931	0.8863	1.7589	0.0051
90.9695	0.7796	0.8694	87.1952	0.8930	3.7743	0.0236

WITH MIN. AAD. = 2.389595

PENG-ROBINSON EQUATION OF STATE

MIXTURE : n-PENTANE(1) - CO₂(2)

TEMP. = 344.16 K

K_{ij} = .1291

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.0824	0.0072	0.2708	3.8974	0.2017	0.1850	0.0691
6.2597	0.0268	0.5195	6.2063	0.4791	0.0534	0.0404
6.4638	0.0283	0.5367	6.3835	0.4923	0.0803	0.0444
8.6411	0.0444	0.6420	8.2890	0.5990	0.3521	0.0430
14.5606	0.0979	0.7763	14.6730	0.7555	0.1124	0.0208
22.1810	0.1631	0.8427	22.5418	0.8257	0.3608	0.0170
29.7335	0.2249	0.8728	30.0635	0.8572	0.3300	0.0156
38.8508	0.3026	0.8936	39.5500	0.8780	0.6992	0.0156
48.9888	0.3897	0.9040	50.1142	0.8892	1.1254	0.0148
58.1062	0.4698	0.9105	59.6085	0.8929	1.5023	0.0176
68.2441	0.5623	0.9127	70.0511	0.8911	1.8070	0.0216
73.8234	0.6111	0.9125	75.2107	0.8874	1.3873	0.0251
81.7841	0.6830	0.9045	82.1367	0.8774	0.3526	0.0271
88.4520	0.7425	0.8914	86.2925	0.8707	2.1595	0.0207
90.9695	0.7796	0.8694	84.0056	0.8812	6.9639	0.0118

WITH MIN. AAD. = 2.396467

PATEL-TEJA EQUATION OF STATE
 MIXTURE : n-PENTANE(1) - CO₂(2)
 TEMP. = 344.16 K
 K_{ij} = .1214

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.0824	0.0072	0.2708	3.5565	0.2211	0.5259	0.0497
6.2597	0.0268	0.5195	5.8450	0.5085	0.4147	0.0110
6.4638	0.0283	0.5367	6.0206	0.5217	0.4432	0.0150
8.6411	0.0444	0.6420	7.9098	0.6270	0.7313	0.0150
14.5606	0.0979	0.7763	14.2408	0.7771	0.3198	0.0008
22.1810	0.1631	0.8427	22.0509	0.8428	0.1301	0.0001
29.7335	0.2249	0.8728	29.5229	0.8722	0.2106	0.0006
38.8508	0.3026	0.8936	38.9702	0.8915	0.1194	0.0021
48.9888	0.3897	0.9040	49.5169	0.9022	0.5281	0.0018
58.1062	0.4698	0.9105	59.0458	0.9061	0.9396	0.0044
68.2441	0.5623	0.9127	69.6179	0.9054	1.3738	0.0073
73.8234	0.6111	0.9125	74.8978	0.9029	1.0744	0.0096
81.7841	0.6830	0.9045	82.1202	0.8957	0.3361	0.0088
88.4520	0.7425	0.8914	87.3068	0.8858	1.1452	0.0056
90.9695	0.7796	0.8694	83.6198	0.9041	7.3497	0.0347

WITH MIN. AAD. = 3.638368

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-PENTANE(1) - CO₂(2)
 TEMP. = 344.16 K
 K_{ij} = .1077

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.0824	0.0072	0.2708	3.8136	0.2287	0.2688	0.0421
6.2597	0.0268	0.5195	6.3672	0.5186	0.1075	0.0009
6.4638	0.0283	0.5367	6.5633	0.5317	0.0995	0.0050
8.6411	0.0444	0.6420	8.6754	0.6358	0.0343	0.0062
14.5606	0.0979	0.7763	15.7802	0.7820	1.2196	0.0057
22.1810	0.1631	0.8427	24.6055	0.8450	2.4245	0.0023
29.7335	0.2249	0.8728	33.1208	0.8725	3.3873	0.0003
38.8508	0.3026	0.8936	43.9881	0.8899	5.1373	0.0037
48.9888	0.3897	0.9040	56.2876	0.8982	7.2988	0.0058
58.1062	0.4698	0.9105	67.5593	0.8992	9.4531	0.0113
68.2441	0.5623	0.9127	80.2316	0.8933	11.9875	0.0194
73.8234	0.6111	0.9125	86.6056	0.8864	12.7822	0.0261
81.7841	0.6830	0.9045	95.3456	0.8663	13.5615	0.0382
88.4520	0.7425	0.8914	99.5431	0.8648	11.0911	0.0266
90.9695	0.7796	0.8694	90.5928	0.6598	0.3767	0.2096

WITH MIN. AAD. = 9.982879

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 352.61 K
 K_{ij} = .1129

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.1845	0.0310	0.8600	4.1835	0.8601	0.0010	0.0001
15.6492	0.1260	0.9560	15.7269	0.9556	0.0777	0.0004
15.8533	0.1270	0.9570	15.8516	0.9558	0.0017	0.0012
30.9582	0.2400	0.9660	30.3840	0.9709	0.5742	0.0049
32.9314	0.2560	0.9680	32.5146	0.9718	0.4168	0.0038
33.8839	0.2630	0.9680	33.4508	0.9721	0.4331	0.0041
49.4651	0.3790	0.9740	49.4188	0.9751	0.0463	0.0011
49.9414	0.3810	0.9720	49.7010	0.9751	0.2404	0.0031
65.0462	0.4900	0.9720	65.3819	0.9743	0.3357	0.0023
65.3184	0.4980	0.9740	66.5484	0.9741	1.2300	0.0001
84.3016	0.6240	0.9720	84.9383	0.9690	0.6367	0.0030
84.6418	0.6250	0.9710	85.0820	0.9690	0.4402	0.0020
97.0250	0.7150	0.9630	97.6384	0.9610	0.6134	0.0020
97.1611	0.7190	0.9630	98.1646	0.9606	1.0035	0.0024
104.5775	0.7690	0.9540	104.4605	0.9531	0.1170	0.0009
105.1218	0.7750	0.9520	105.1636	0.9520	0.0418	0.0000
114.5794	0.8470	0.9050	111.2219	0.9416	3.3575	0.0366

WITH MIN. AAD. = .8191268

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 352.61 K
 K_{ij} = .1013

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.1845	0.0310	0.8600	4.2190	0.8475	0.0345	0.0125
15.6492	0.1260	0.9560	15.7253	0.9504	0.0761	0.0056
15.8533	0.1270	0.9570	15.8497	0.9507	0.0036	0.0063
30.9582	0.2400	0.9660	30.3649	0.9669	0.5933	0.0009
32.9314	0.2560	0.9680	32.4917	0.9678	0.4397	0.0002
33.8839	0.2630	0.9680	33.4277	0.9682	0.4562	0.0002
49.4651	0.3790	0.9740	49.4133	0.9710	0.0518	0.0030
49.9414	0.3810	0.9720	49.6962	0.9710	0.2452	0.0010
65.0462	0.4900	0.9720	65.4057	0.9696	0.3595	0.0024
65.3184	0.4980	0.9740	66.5746	0.9694	1.2562	0.0046
84.3016	0.6240	0.9720	85.0071	0.9627	0.7055	0.0093
84.6418	0.6250	0.9710	85.1507	0.9626	0.5089	0.0084
97.0250	0.7150	0.9630	97.6724	0.9524	0.6474	0.0106
97.1611	0.7190	0.9630	98.1926	0.9518	1.0315	0.0112
104.5775	0.7690	0.9540	104.3985	0.9421	0.1790	0.0119
105.1218	0.7750	0.9520	105.0782	0.9407	0.0436	0.0113
114.5794	0.8470	0.9050	108.9972	0.9363	5.5822	0.0313

WITH MIN. AAD. = 1.014926

PATEL-TEJA EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 352.61 K
 K_{ij} = .0838

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.1845	0.0310	0.8600	4.0987	0.8787	0.0858	0.0187
15.6492	0.1260	0.9560	15.6497	0.9613	0.0005	0.0053
15.8533	0.1270	0.9570	15.7745	0.9615	0.0788	0.0045
30.9582	0.2400	0.9660	30.3444	0.9740	0.6138	0.0080
32.9314	0.2560	0.9680	32.4797	0.9748	0.4517	0.0068
33.8839	0.2630	0.9680	33.4194	0.9751	0.4645	0.0071
49.4651	0.3790	0.9740	49.4734	0.9772	0.0083	0.0032
49.9414	0.3810	0.9720	49.7576	0.9772	0.1838	0.0052
65.0462	0.4900	0.9720	65.5793	0.9758	0.5331	0.0038
65.3184	0.4980	0.9740	66.7590	0.9756	1.4406	0.0016
84.3016	0.6240	0.9720	85.4256	0.9701	1.1240	0.0019
84.6418	0.6250	0.9710	85.5719	0.9701	0.9301	0.0009
97.0250	0.7150	0.9630	98.4118	0.9618	1.3868	0.0012
97.1611	0.7190	0.9630	98.9629	0.9613	1.8018	0.0017
104.5775	0.7690	0.9540	105.4574	0.9536	0.8799	0.0004
105.1218	0.7750	0.9520	106.1855	0.9524	1.0637	0.0004
114.5794	0.8470	0.9050	112.4668	0.9418	2.1126	0.0368

WITH MIN. AAD. = 1.182261

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 352.61 K
 K_{ij} = -.0002

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
4.1845	0.0310	0.8600	4.0224	0.8521	0.1621	0.0079
15.6492	0.1260	0.9560	15.1675	0.9527	0.4817	0.0033
15.8533	0.1270	0.9570	15.2892	0.9530	0.5641	0.0040
30.9582	0.2400	0.9660	29.6975	0.9690	1.2607	0.0030
32.9314	0.2560	0.9680	31.8489	0.9700	1.0825	0.0020
33.8839	0.2630	0.9680	32.7995	0.9704	1.0844	0.0024
49.4651	0.3790	0.9740	49.4577	0.9734	0.0074	0.0006
49.9414	0.3810	0.9720	49.7606	0.9734	0.1808	0.0014
65.0462	0.4900	0.9720	67.1957	0.9723	2.1495	0.0003
65.3184	0.4980	0.9740	68.5499	0.9721	3.2315	0.0019
84.3016	0.6240	0.9720	91.4856	0.9647	7.1840	0.0073
84.6418	0.6250	0.9710	91.6800	0.9646	7.0382	0.0064
97.0250	0.7150	0.9630	110.2454	0.9470	13.2204	0.0160
97.1611	0.7190	0.9630	111.1212	0.9453	13.9601	0.0177
104.5775	0.7690	0.9540	126.3113	0.7695	21.7338	0.1845
105.1218	0.7750	0.9520	127.7705	0.7753	22.6487	0.1767
114.5794	0.8470	0.9050	138.7970	0.8578	24.2176	0.0472

WITH MIN. AAD. = 8.117238

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 394.27 K
 K_{ij} = .1027

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
11.1586	0.0730	0.8190	12.5213	0.8245	1.3627	0.0055
30.6180	0.1930	0.9210	31.1018	0.9108	0.4838	0.0102
30.8902	0.1950	0.9150	31.4229	0.9113	0.5327	0.0037
47.6960	0.2960	0.9360	48.1338	0.9280	0.4378	0.0080
47.9682	0.2960	0.9360	48.1338	0.9280	0.1656	0.0080
56.9495	0.3450	0.9390	56.5853	0.9313	0.3642	0.0077
61.6442	0.3760	0.9420	62.0428	0.9323	0.3986	0.0097
62.3927	0.3780	0.9420	62.3974	0.9324	0.0047	0.0096
63.6174	0.3840	0.9410	63.4631	0.9325	0.1543	0.0085
85.0500	0.5000	0.9390	84.5596	0.9303	0.4904	0.0087
85.7984	0.5030	0.9390	85.1132	0.9302	0.6852	0.0088
102.4002	0.5890	0.9340	101.0264	0.9225	1.3738	0.0115
103.0126	0.5940	0.9340	101.9499	0.9218	1.0627	0.0122
118.7978	0.6860	0.9140	118.1641	0.9048	0.6337	0.0092
130.6368	0.7610	0.8780	127.3338	0.8927	3.3030	0.0147
131.3852	0.7680	0.8820	127.4305	0.8936	3.9547	0.0116

WITH MIN. AAD. = 1.758537

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 394.27 K
 K_{ij} = .0912

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
11.1586	0.0730	0.8190	12.6428	0.8132	1.4842	0.0058
30.6180	0.1930	0.9210	31.2267	0.9023	0.6087	0.0187
30.8902	0.1950	0.9150	31.5475	0.9029	0.6573	0.0121
47.6960	0.2960	0.9360	48.2201	0.9195	0.5241	0.0165
47.9682	0.2960	0.9360	48.2202	0.9195	0.2520	0.0165
56.9495	0.3450	0.9390	56.6297	0.9224	0.3198	0.0166
61.6442	0.3760	0.9420	62.0496	0.9231	0.4054	0.0189
62.3927	0.3780	0.9420	62.4012	0.9231	0.0085	0.0189
63.6174	0.3840	0.9410	63.4576	0.9232	0.1598	0.0178
85.0500	0.5000	0.9390	84.2744	0.9188	0.7756	0.0202
85.7984	0.5030	0.9390	84.8251	0.9185	0.9733	0.0205
102.4002	0.5890	0.9340	100.2832	0.9082	2.1170	0.0258
103.0126	0.5940	0.9340	101.1704	0.9073	1.8422	0.0267
118.7978	0.6860	0.9140	116.4204	0.8856	2.3774	0.0284
130.6368	0.7610	0.8780	121.4314	0.8837	9.2054	0.0057
131.3852	0.7680	0.8820	120.5436	0.8860	10.8416	0.0040

WITH MIN. AAD. = 2.732916

PATEL-TEJA EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 394.27 K
 K_{ij} = 6.490001E-02

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
11.1586	0.0730	0.8190	12.3422	0.8404	1.1836	0.0214
30.6180	0.1930	0.9210	30.9867	0.9175	0.3687	0.0035
30.8902	0.1950	0.9150	31.3089	0.9180	0.4187	0.0030
47.6960	0.2960	0.9360	48.0805	0.9321	0.3845	0.0039
47.9682	0.2960	0.9360	48.0805	0.9321	0.1123	0.0039
56.9495	0.3450	0.9390	56.5636	0.9345	0.3859	0.0045
61.6442	0.3760	0.9420	62.0417	0.9350	0.3975	0.0070
62.3927	0.3780	0.9420	62.3976	0.9351	0.1500	0.0059
63.6174	0.3840	0.9410	63.4674	0.9314	0.4049	0.0076
85.0500	0.5000	0.9390	84.6451	0.9312	0.5976	0.0078
85.7984	0.5030	0.9390	85.2008	0.9312	0.4699	0.0107
102.4002	0.5890	0.9340	101.1685	0.9224	1.2317	0.0116
103.0126	0.5940	0.9340	102.0943	0.9216	0.9183	0.0124
118.7978	0.6860	0.9140	118.3279	0.9033	3.3768	0.0133
130.6368	0.7610	0.8780	127.2600	0.8913	4.1237	0.0105
131.3852	0.7680	0.8820	127.2615	0.8925		

WITH MIN. AAD. = 1.572444

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-Heptane(1) - CO₂(2)
 TEMP. = 394.27 K
 K_{ij} = -0.0824

REF. KALRA & KUBOTA (1978)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
11.1586	0.0730	0.8190	11.9720	0.8153	0.8134	0.0037
30.6180	0.1930	0.9210	30.0073	0.9052	0.6107	0.0158
30.8902	0.1950	0.9150	30.3242	0.9058	0.5660	0.0092
47.6960	0.2960	0.9360	47.1309	0.9230	0.5651	0.0130
47.9682	0.2960	0.9360	47.1309	0.9230	0.8373	0.0130
56.9495	0.3450	0.9390	55.8857	0.9263	1.0638	0.0127
61.6442	0.3760	0.9420	61.6535	0.9272	0.0093	0.0148
62.3927	0.3780	0.9420	62.0315	0.9272	0.3612	0.0148
63.6174	0.3840	0.9410	63.1699	0.9273	0.4475	0.0137
85.0500	0.5000	0.9390	86.6284	0.9234	1.5784	0.0156
85.7984	0.5030	0.9390	87.2722	0.9231	1.4738	0.0159
102.4002	0.5890	0.9340	106.6538	0.9104	4.2536	0.0236
103.0126	0.5940	0.9340	107.8310	0.9093	4.8184	0.0247
118.7978	0.6860	0.9140	133.2434	0.6975	14.4456	0.2165
130.6368	0.7610	0.8780	150.1457	0.7800	19.5089	0.0980
131.3852	0.7680	0.8820	150.6174	0.7965	19.2322	0.0855

WITH MIN. AAD. = 4.459265

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : n-DECANE(1) - CO₂(2)

TEMP. = 462.56 K

K_{ij} = .1489

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3600	0.0913	0.9075	19.6035	0.8837	0.2435	0.0238
30.3800	0.1472	0.9306	31.1981	0.9161	0.8181	0.0145
40.1000	0.1883	0.9410	40.0671	0.9274	0.0329	0.0136
50.7000	0.2358	0.9478	50.6919	0.9350	0.0081	0.0128

WITH MIN. AAD. = 1.01215

PENG-ROBINSON EQUATION OF STATE

MIXTURE : n-DECANE(1) - CO₂(2)

TEMP. = 462.56 K

K_{ij} = .128

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3600	0.0913	0.9075	19.7349	0.8744	0.3749	0.0331
30.3800	0.1472	0.9306	31.2919	0.9078	0.9119	0.0228
40.1000	0.1883	0.9410	40.1000	0.9191	0.0000	0.0219
50.7000	0.2358	0.9478	50.6128	0.9263	0.0872	0.0215

WITH MIN. AAD. = 1.277532

PATEL-TEJA EQUATION OF STATE

MIXTURE : n-DECANE(1) - CO₂(2)

TEMP. = 462.56 K

K_{ij} = .0731

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3600	0.0913	0.9075	19.5778	0.8959	0.2178	0.0116
30.3800	0.1472	0.9306	31.2300	0.9233	0.8500	0.0073
40.1000	0.1883	0.9410	40.0979	0.9325	0.0021	0.0085
50.7000	0.2358	0.9478	50.6669	0.9382	0.0331	0.0096

WITH MIN. AAD. = .9984673

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-DECANE(1) - CO₂(2)
 TEMP. = 462.56 K
 K_{ij} = .1433

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3600	0.0913	0.9075	19.6211	0.8793	0.2611	0.0282
30.3800	0.1472	0.9306	31.2114	0.9106	0.8314	0.0200
40.1000	0.1883	0.9410	40.0696	0.9213	0.0304	0.0197
50.7000	0.2358	0.9478	50.6927	0.9278	0.0073	0.0200

WITH MIN. AAD. = 1.043821

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : n-DECANE(1) - CO₂(2)
 TEMP. = 542.96 K
 K_{ij} = .1968

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3800	0.0656	0.5700	20.1518	0.5164	0.7718	0.0536
29.6300	0.1147	0.6818	29.7825	0.6350	0.1525	0.0468
39.5000	0.1628	0.7357	39.4985	0.6963	0.0015	0.0394
51.0000	0.2145	0.7655	50.2442	0.7349	0.7558	0.0306

WITH MIN. AAD. = 1.495811

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : n-DECANE(1) - CO₂(2)
 TEMP. = 542.96 K
 K_{ij} = .1672

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3800	0.0656	0.5700	20.4272	0.4980	1.0472	0.0720
29.6300	0.1147	0.6818	29.9747	0.6131	0.3447	0.0687
39.5000	0.1628	0.7357	39.4989	0.6719	0.0011	0.0638
51.0000	0.2145	0.7655	49.8939	0.7080	1.1061	0.0575

WITH MIN. AAD. = 2.184591

PATEL-TEJA EQUATION OF STATE
 MIXTURE : n-DECANE(1) - CO₂(2)
 TEMP. = 542.96 K
 K_{ij} = .0857

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3800	0.0656	0.5700	19.9913	0.5354	0.6113	0.0346
29.6300	0.1147	0.6818	29.7616	0.6465	0.1316	0.0353
39.5000	0.1628	0.7357	39.4974	0.7014	0.0026	0.0343
51.0000	0.2145	0.7655	50.1124	0.7343	0.8876	0.0312

WITH MIN. AAD. = 1.336291

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : n-DECANE(1) - CO₂(2)
 TEMP. = 542.96 K
 K_{ij} = .2581

REF. SEBASTIAN ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
19.3800	0.0656	0.5700	20.1474	0.5131	0.7674	0.0569
29.6300	0.1147	0.6818	29.8052	0.6251	0.1752	0.0567
39.5000	0.1628	0.7357	39.4987	0.6808	0.0014	0.0549
51.0000	0.2145	0.7655	50.1720	0.7135	0.8280	0.0520

WITH MIN. AAD. = 1.54454

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Methane(1) - Ethane(2)

TEMP. = 199.93 K

K_{ij} = 0

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.6200	0.0214	0.3005	3.1620	0.3221	0.4580	0.0216
4.4200	0.0512	0.5098	4.5990	0.5315	0.1790	0.0217
6.8000	0.1039	0.6800	7.1454	0.6965	0.3454	0.0165
10.9000	0.1875	0.7957	11.1973	0.8048	0.2973	0.0091
17.0000	0.3100	0.8679	17.1534	0.8716	0.1534	0.0037
23.8000	0.4526	0.9052	24.1104	0.9084	0.3104	0.0032
34.0000	0.6601	0.9337	34.3728	0.9368	0.3728	0.0031
40.8000	0.7852	0.9461	40.8846	0.9488	0.0846	0.0027
47.6500	0.8942	0.9562	47.2603	0.9586	0.3897	0.0024
48.9000	0.9126	0.9584	48.4563	0.9602	0.4437	0.0018
49.4000	0.9175	0.9578	48.7767	0.9605	0.6233	0.0027

WITH MIN. AAD. = 2.818702

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Methane(1) - Ethane(2)

TEMP. = 199.93 K

K_{ij} = 0

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.6200	0.0214	0.3005	3.3076	0.3003	0.3124	0.0002
4.4200	0.0512	0.5098	4.7146	0.5063	0.2946	0.0035
6.8000	0.1039	0.6800	7.2174	0.6750	0.4174	0.0050
10.9000	0.1875	0.7957	11.2227	0.7890	0.3227	0.0067
17.0000	0.3100	0.8679	17.1690	0.8605	0.1690	0.0074
23.8000	0.4526	0.9052	24.2102	0.9002	0.4102	0.0050
34.0000	0.6601	0.9337	34.7786	0.9307	0.7786	0.0030
40.8000	0.7852	0.9461	41.5678	0.9430	0.7678	0.0031
47.6500	0.8942	0.9562	46.6013	0.9543	1.0487	0.0019
48.9000	0.9126	0.9584	48.7620	0.9551	0.1380	0.0033
49.4000	0.9175	0.9578	49.1023	0.9550	0.2977	0.0028

WITH MIN. AAD. = 3.124452

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 199.93 K
 $K_{ij} = 0$

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.6200	0.0214	0.3005	3.1489	0.3254	0.4711	0.0249
4.4200	0.0512	0.5098	4.5943	0.5350	0.1743	0.0252
6.8000	0.1039	0.6800	7.1520	0.6992	0.3520	0.0192
10.9000	0.1875	0.7957	11.2127	0.8064	0.3127	0.0107
17.0000	0.3100	0.8679	17.1603	0.8723	0.1603	0.0044
23.8000	0.4526	0.9052	24.0770	0.9087	0.2770	0.0035
34.0000	0.6601	0.9337	34.2388	0.9369	0.2388	0.0032
40.8000	0.7852	0.9461	40.6899	0.9490	0.1101	0.0029
47.6500	0.8942	0.9562	47.0459	0.9593	0.6041	0.0031
48.9000	0.9126	0.9584	48.2545	0.9610	0.6455	0.0026
49.4000	0.9175	0.9578	48.6346	0.9611	0.7654	0.0033

WITH MIN. AAD. = 2.929054

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 199.93 K
 $K_{ij} = 0$

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.6200	0.0214	0.3005	3.2011	0.3264	0.4189	0.0259
4.4200	0.0512	0.5098	4.5551	0.5367	0.1351	0.0269
6.8000	0.1039	0.6800	7.2315	0.7010	0.4315	0.0210
10.9000	0.1875	0.7957	11.1054	0.8085	0.2054	0.0128
17.0000	0.3100	0.8679	17.9494	0.8734	0.9494	0.0055
23.8000	0.4526	0.9052	24.0214	0.9085	0.2214	0.0033
34.0000	0.6601	0.9337	35.0576	0.9375	1.0576	0.0038
40.8000	0.7852	0.9461	39.9840	0.9498	0.8160	0.0037
47.6500	0.8942	0.9562	46.5102	0.9610	1.1398	0.0048
48.9000	0.9126	0.9584	48.8205	0.9626	0.0795	0.0042
49.4000	0.9175	0.9578	49.0165	0.9615	0.3835	0.0037

WITH MIN. AAD. = 3.437713

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 260 K
 $K_{ij} = .0103$

REF. GUPTA ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
17.8000	0.0088	0.0467	18.1148	0.0453	0.3148	0.0014
19.4200	0.0239	0.1150	19.7547	0.1130	0.3347	0.0020
21.6000	0.0445	0.1922	21.9918	0.1896	0.3918	0.0026
23.2200	0.0592	0.2387	23.5877	0.2355	0.3677	0.0032
25.2600	0.0788	0.2924	25.7169	0.2878	0.4569	0.0046
29.9800	0.1220	0.3810	30.3965	0.3770	0.4165	0.0040
34.6900	0.1652	0.4483	35.0583	0.4413	0.3683	0.0070
40.5900	0.2189	0.5052	40.8058	0.4986	0.2158	0.0066
50.3000	0.3087	0.5664	50.1826	0.5586	0.1174	0.0078
55.1800	0.3545	0.5823	54.7700	0.5768	0.4100	0.0055
59.4000	0.3952	0.5896	58.6571	0.5870	0.7429	0.0026

WITH MIN. AAD. = 1.264398

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 260 K
 $K_{ij} = .0215$

REF. GUPTA ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
17.8000	0.9912	0.9533	18.7244	0.9560	0.9244	0.0027
19.4200	0.9761	0.8850	20.4154	0.8900	0.9954	0.0050
21.6000	0.9555	0.8078	22.7224	0.8155	1.1224	0.0077
23.2200	0.9408	0.7613	24.3656	0.7709	1.1456	0.0096
25.2600	0.9212	0.7076	26.5530	0.7202	1.2930	0.0126
29.9800	0.8780	0.6190	31.3580	0.6341	1.3780	0.0151
34.6900	0.8348	0.5517	36.1246	0.5725	1.4346	0.0208
40.5900	0.7811	0.4948	41.9690	0.5183	1.3789	0.0235
50.3000	0.6913	0.4336	51.3888	0.4640	1.0887	0.0304
55.1800	0.6455	0.4177	55.8975	0.4495	0.7175	0.0318
59.4000	0.6048	0.4104	59.6295	0.4433	0.2295	0.0329

WITH MIN. AAD. = 3.777113

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 260 K
 $K_{ij} = .0031$

REF. GUPTA ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
17.8000	0.0088	0.0467	17.9030	0.0453	0.1030	0.0014
19.4200	0.0239	0.1150	19.5234	0.1132	0.1034	0.0018
21.6000	0.0445	0.1922	21.7355	0.1899	0.1355	0.0023
23.2200	0.0592	0.2387	23.3145	0.2359	0.0945	0.0028
25.2600	0.0788	0.2924	25.4197	0.2884	0.1597	0.0040
29.9800	0.1220	0.3810	30.0608	0.3779	0.0808	0.0031
34.6900	0.1652	0.4483	34.6897	0.4425	0.0003	0.0058
40.5900	0.2189	0.5052	40.4089	0.5002	0.1811	0.0050
50.3000	0.3087	0.5664	49.7762	0.5610	0.5238	0.0054
55.1800	0.3545	0.5823	54.3812	0.5796	0.7988	0.0027
59.4000	0.3952	0.5896	58.2985	0.5904	1.1015	0.0008

WITH MIN. AAD. = .712533

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - Ethane(2)
 TEMP. = 260 K
 $K_{ij} = .0203$

REF. GUPTA ET AL. (1980)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
17.8000	0.0088	0.0467	18.0054	0.0402	0.2054	0.0065
19.4200	0.0239	0.1150	19.5487	0.1124	0.1287	0.0026
21.6000	0.0445	0.1922	22.1865	0.1867	0.5865	0.0055
23.2200	0.0592	0.2387	23.8135	0.2310	0.5935	0.0077
25.2600	0.0788	0.2924	26.0756	0.2843	0.8156	0.0081
29.9800	0.1220	0.3810	30.8138	0.3731	0.8338	0.0079
34.6900	0.1652	0.4483	35.4976	0.4403	0.8076	0.0080
40.5900	0.2189	0.5052	39.8540	0.4983	0.7360	0.0069
50.3000	0.3087	0.5664	49.5112	0.5597	0.7888	0.0067
55.1800	0.3545	0.5823	54.1301	0.5780	1.0499	0.0043
59.4000	0.3952	0.5896	58.9802	0.5934	0.4198	0.0038

WITH MIN. AAD. = 1.946985

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Methane(1) - Propane(2)

TEMP. = 273.16 K

K_{ij} = .0215

REF. AKERS ET AL. (1954)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0120	0.2300	6.4057	0.2442	0.3983	0.0142
13.6080	0.0590	0.5660	13.1092	0.5985	0.4988	0.0325
20.4120	0.1060	0.7150	19.8990	0.7145	0.5130	0.0005
27.2160	0.1520	0.7800	26.6165	0.7698	0.5995	0.0102
34.0200	0.2000	0.8080	33.6932	0.8026	0.3268	0.0054
40.8240	0.2480	0.8300	40.8188	0.8225	0.0052	0.0075
47.6280	0.2960	0.8430	47.9694	0.8346	0.3414	0.0084
54.4320	0.3470	0.8520	55.5568	0.8419	1.1248	0.0101
61.2360	0.3990	0.8560	63.2352	0.8448	1.9992	0.0112
68.0400	0.4510	0.8540	70.7776	0.8438	2.7376	0.0102
74.8440	0.5080	0.8500	78.7485	0.8385	3.9045	0.0115

WITH MIN. AAD. = 2.77256

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Methane(1) - Propane(2)

TEMP. = 273.16 K

K_{ij} = .0251

REF. AKERS ET AL. (1954)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
6.8040	0.9880	0.7700	6.6254	0.7686	0.1786	0.0014
13.6080	0.9410	0.4340	13.2628	0.4196	0.3452	0.0144
20.4120	0.8940	0.2850	19.9991	0.3019	0.4129	0.0169
27.2160	0.8480	0.2200	26.6774	0.2453	0.5386	0.0253
34.0200	0.8000	0.1920	33.7191	0.2118	0.3009	0.0198
40.8240	0.7520	0.1700	40.8209	0.1917	0.0031	0.0217
47.6280	0.7040	0.1570	47.9574	0.1796	0.3294	0.0226
54.4320	0.6530	0.1480	55.5262	0.1728	1.0942	0.0248
61.2360	0.6010	0.1440	63.1743	0.1707	1.9383	0.0267
68.0400	0.5490	0.1460	70.6608	0.1729	2.6208	0.0269
74.8440	0.4920	0.1500	78.5193	0.1802	3.6753	0.0302

WITH MIN. AAD. = 2.244067

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - Propane(2)
 TEMP. = 273.16 K
 $K_{ij} = .0132$

REF. AKERS ET AL. (1954)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0120	0.2300	6.2968	0.2499	0.5072	0.0199
13.6080	0.0590	0.5660	13.0343	0.6050	0.5737	0.0390
20.4120	0.1060	0.7150	19.8534	0.7193	0.5586	0.0043
27.2160	0.1520	0.7800	26.5944	0.7734	0.6216	0.0066
34.0200	0.2000	0.8080	33.6898	0.8053	0.3302	0.0027
40.8240	0.2480	0.8300	40.8273	0.8244	0.0033	0.0056
47.6280	0.2960	0.8430	47.9826	0.8361	0.3546	0.0069
54.4320	0.3470	0.8520	55.5664	0.8429	1.1344	0.0091
61.2360	0.3990	0.8560	63.2314	0.8454	1.9954	0.0106
68.0400	0.4510	0.8540	70.7502	0.8441	2.7102	0.0099
74.8440	0.5080	0.8500	78.6837	0.8384	3.8397	0.0116

WITH MIN. AAD. = 2.988168

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - Propane(2)
 TEMP. = 273.16 K
 $K_{ij} = 0.0386$

REF. AKERS ET AL. (1954)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0120	0.2300	6.4546	0.2487	0.3494	0.0187
13.6080	0.0590	0.5660	13.2024	0.5891	0.4056	0.0231
20.4120	0.1060	0.7150	20.0020	0.7200	0.4100	0.0050
27.2160	0.1520	0.7800	26.7871	0.7713	0.4289	0.0087
34.0200	0.2000	0.8080	33.5409	0.8045	0.4791	0.0035
40.8240	0.2480	0.8300	40.2805	0.8254	0.5435	0.0046
47.6280	0.2960	0.8430	47.8617	0.8381	0.2337	0.0049
54.4320	0.3470	0.8520	55.6743	0.8457	1.2423	0.0063
61.2360	0.3990	0.8560	63.1107	0.8468	1.8747	0.0092
68.0400	0.4510	0.8540	70.5998	0.8460	2.5598	0.0080
74.8440	0.5080	0.8500	77.6215	0.8397	2.7775	0.0103

WITH MIN. AAD. = 2.522511

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Methane(1) - Propane(2)

TEMP. = 213.72 K

K_{ij} = .0056

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
1.8700	0.0205	0.7669	1.8632	0.7648	0.0068	0.0021
3.5000	0.0443	0.8706	3.5410	0.8731	0.0410	0.0025
6.8000	0.0899	0.9288	6.7876	0.9306	0.0124	0.0018
10.2000	0.1358	0.9505	10.0958	0.9509	0.1042	0.0004
20.4000	0.2709	0.9698	20.0488	0.9710	0.3512	0.0012
27.2000	0.3656	0.9741	27.1764	0.9757	0.0236	0.0016
34.0000	0.4580	0.9760	34.1945	0.9778	0.1945	0.0018
40.8500	0.5563	0.9767	41.6479	0.9784	0.7979	0.0017
47.6500	0.6555	0.9755	49.0201	0.9775	1.3700	0.0020
54.4500	0.7573	0.9726	56.2339	0.9745	1.7839	0.0019

WITH MIN. AAD. = 1.322089

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Methane(1) - Propane(2)

TEMP. = 213.72 K

K_{ij} = .0087

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
1.8700	0.9795	0.2331	1.8920	0.2608	0.0220	0.0277
3.5000	0.9557	0.1294	3.5430	0.1429	0.0430	0.0135
6.8000	0.9101	0.0712	6.7442	0.0789	0.0558	0.0077
10.2000	0.8642	0.0495	10.0148	0.0560	0.1852	0.0065
20.4000	0.7291	0.0302	19.9121	0.0333	0.4879	0.0031
27.2000	0.6344	0.0259	27.0581	0.0280	0.1419	0.0021
34.0000	0.5420	0.0240	34.1482	0.0257	0.1482	0.0017
40.8500	0.4437	0.0233	41.7456	0.0252	0.8956	0.0019
47.6500	0.3445	0.0245	49.3423	0.0264	1.6923	0.0019
54.4500	0.2427	0.0274	56.8502	0.0304	2.4002	0.0030

WITH MIN. AAD. = 1.854268

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - Propane(2)
 TEMP. = 213.72 K
 $K_{ij} = .001$

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
1.8700	0.0205	0.7669	1.8585	0.7704	0.0115	0.0035
3.5000	0.0443	0.8706	3.5435	0.8764	0.0435	0.0058
6.8000	0.0899	0.9288	6.8017	0.9323	0.0017	0.0035
10.2000	0.1358	0.9505	10.1185	0.9521	0.0815	0.0016
20.4000	0.2709	0.9698	20.0744	0.9715	0.3256	0.0017
27.2000	0.3656	0.9741	27.1808	0.9760	0.0192	0.0019
34.0000	0.4580	0.9760	34.1565	0.9780	0.1565	0.0020
40.8500	0.5563	0.9767	41.5400	0.9785	0.6900	0.0018
47.6500	0.6555	0.9755	48.8183	0.9777	1.1683	0.0022
54.4500	0.7573	0.9726	55.9270	0.9748	1.4770	0.0022

WITH MIN. AAD. = 1.16619

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - Propane(2)
 TEMP. = 213.72 K
 $K_{ij} = 0.0229$

REF. WICHTERLE & KOBAYASHI (1972)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
1.8700	0.0205	0.7669	1.9004	0.7712	0.0304	0.0043
3.5000	0.0443	0.8706	3.6114	0.8772	0.1114	0.0066
6.8000	0.0899	0.9288	6.9192	0.9365	0.1192	0.0077
10.2000	0.1358	0.9505	10.5102	0.9620	0.3102	0.0115
20.4000	0.2709	0.9698	20.8054	0.9716	0.4054	0.0018
27.2000	0.3656	0.9741	27.8547	0.9767	0.6547	0.0026
34.0000	0.4580	0.9760	34.6702	0.9790	0.6702	0.0030
40.8500	0.5563	0.9767	41.4316	0.9792	0.5816	0.0025
47.6500	0.6555	0.9755	48.1813	0.9781	0.5313	0.0026
54.4500	0.7573	0.9726	54.9730	0.9752	0.5230	0.0026

WITH MIN. AAD. = 1.946732

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Methane(1) - n-Butane(2)

TEMP. = 283.16 K

K_{ij} = .0139

REF. KALRA (1974)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.4700	0.0130	0.5660	3.5670	0.5650	0.0970	0.0010
6.8000	0.0350	0.7750	7.1212	0.7701	0.3212	0.0049
13.6800	0.0760	0.8750	13.8628	0.8701	0.1828	0.0049
27.2200	0.1520	0.9250	26.7748	0.9191	0.4452	0.0059
40.8200	0.2320	0.9390	40.9473	0.9346	0.1273	0.0044
54.4300	0.3040	0.9410	54.1966	0.9391	0.2334	0.0019
68.0400	0.3770	0.9410	68.0381	0.9389	0.0019	0.0021
81.6500	0.4420	0.9330	80.6240	0.9355	1.0260	0.0025
95.2600	0.5140	0.9240	94.6600	0.9279	0.6000	0.0039

WITH MIN. AAD. = 1.45785

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Methane(1) - n-Butane(2)

TEMP. = 283.16 K

K_{ij} = .0208

REF. KALRA (1974)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
3.4700	0.9870	0.4340	3.6625	0.4568	0.1925	0.0228
6.8000	0.9650	0.2250	7.1898	0.2463	0.3898	0.0213
13.6800	0.9240	0.1250	13.8897	0.1411	0.2097	0.0161
27.2200	0.8480	0.0750	26.7527	0.0891	0.4673	0.0141
40.8200	0.7680	0.0610	40.9158	0.0729	0.0958	0.0119
54.4300	0.6960	0.0590	54.1758	0.0686	0.2542	0.0096
68.0400	0.6230	0.0590	68.0511	0.0695	0.0111	0.0105
81.6500	0.5580	0.0670	80.6505	0.0740	0.9995	0.0070
95.2600	0.4860	0.0760	94.6460	0.0833	0.6140	0.0073

WITH MIN. AAD. = 1.901851

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - n-Butane(2)
 TEMP. = 283.16 K
 $K_{ij} = 0$

REF. KALRA (1974)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.4700	0.0130	0.5660	3.5161	0.5779	0.0461	0.0119
6.8000	0.0350	0.7750	7.0965	0.7788	0.2965	0.0038
13.6800	0.0760	0.8750	13.8831	0.8750	0.2031	0.0000
27.2200	0.1520	0.9250	26.8628	0.9216	0.3572	0.0034
40.8200	0.2320	0.9390	41.0786	0.9360	0.2586	0.0030
54.4300	0.3040	0.9410	54.3353	0.9399	0.0947	0.0011
68.0400	0.3770	0.9410	68.1445	0.9393	0.1045	0.0017
81.6500	0.4420	0.9330	80.6608	0.9355	0.9892	0.0025
95.2600	0.5140	0.9240	94.5655	0.9275	0.6945	0.0035

WITH MIN. AAD. = 1.265256

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - n-Butane(2)
 TEMP. = 283.16 K
 $K_{ij} = 0.0160$

REF. KALRA (1974)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
3.4700	0.0130	0.5660	3.5867	0.6795	0.1167	0.1135
6.8000	0.0350	0.7750	7.3578	0.7825	0.5578	0.0075
13.6800	0.0760	0.8750	14.3531	0.8912	0.6731	0.0162
27.2200	0.1520	0.9250	28.0154	0.9416	0.7954	0.0166
40.8200	0.2320	0.9390	42.0002	0.9501	1.1802	0.0111
54.4300	0.3040	0.9410	55.1563	0.9564	0.7263	0.0154
68.0400	0.3770	0.9410	68.9864	0.9530	0.9464	0.0120
81.6500	0.4420	0.9330	82.5132	0.9412	0.8632	0.0082
95.2600	0.5140	0.9240	94.4026	0.9327	0.8574	0.0087

WITH MIN. AAD. = 2.998033

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Methane(1) - n-Pentane(2)
 TEMP. = 273.17 K
 $K_{ij} = .0298$

REF. PRODANY & WILLIAMS (1971)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6220	0.0909	0.9758	15.7050	0.9793	2.0830	0.0035
27.2300	0.1653	0.9839	29.2186	0.9853	1.9886	0.0014
40.8260	0.2320	0.9855	42.0565	0.9866	1.2305	0.0011
54.4350	0.2920	0.9856	54.2332	0.9864	0.2018	0.0008
68.0440	0.3481	0.9839	66.1884	0.9854	1.8556	0.0015
81.6520	0.4005	0.9818	77.8690	0.9837	3.7830	0.0019
95.2610	0.4480	0.9782	88.8984	0.9813	6.3626	0.0031
108.8700	0.4980	0.9722	100.9272	0.9777	7.9428	0.0055
122.4780	0.5501	0.9623	113.8614	0.9725	8.6166	0.0102
136.0880	0.6117	0.9450	129.4687	0.9635	6.6193	0.0185

WITH MIN. AAD. = 5.921303

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Methane(1) - n-Pentane(2)
 TEMP. = 273.17 K
 $K_{ij} = .043$

REF. PRODANY & WILLIAMS (1971)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
13.6220	0.9091	0.0242	16.0415	0.0235	2.4195	0.0007
27.2300	0.8347	0.0161	29.8876	0.0170	2.6576	0.0009
40.8260	0.7680	0.0145	43.0951	0.0158	2.2691	0.0013
54.4350	0.7080	0.0144	55.6722	0.0163	1.2372	0.0019
68.0440	0.6519	0.0161	68.0531	0.0178	0.0091	0.0017
81.6520	0.5995	0.0182	80.1750	0.0201	1.4770	0.0019
95.2610	0.5520	0.0218	91.6319	0.0233	3.6291	0.0015
108.8700	0.5020	0.0278	104.1232	0.0279	4.7468	0.0001
122.4780	0.4499	0.0377	117.5316	0.0346	4.9464	0.0031
136.0880	0.3883	0.0550	133.5913	0.0461	2.4967	0.0089

WITH MIN. AAD. = 5.12169

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - n-Pentane(2)
 TEMP. = 273.17 K
 $K_{ij} = .0142$

REF. PRODANY & WILLIAMS (1971)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6220	0.0909	0.9758	16.1933	0.9814	2.5713	0.0056
27.2300	0.1653	0.9839	30.1228	0.9865	2.8928	0.0026
40.8260	0.2320	0.9855	43.3245	0.9874	2.4985	0.0019
54.4350	0.2920	0.9856	55.8136	0.9869	1.3786	0.0013
68.0440	0.3481	0.9839	68.0390	0.9856	0.0050	0.0017
81.6520	0.4005	0.9818	79.9521	0.9836	1.6999	0.0018
95.2610	0.4480	0.9782	91.1406	0.9810	4.1204	0.0028
108.8700	0.4980	0.9722	103.2957	0.9771	5.5743	0.0049
122.4780	0.5501	0.9623	116.2857	0.9713	6.1923	0.0090
136.0880	0.6117	0.9450	131.8182	0.9615	4.2698	0.0165

WITH MIN. AAD. = 5.788049

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - n-Pentane(2)
 TEMP. = 273.17 K
 $K_{ij} = .0142$

REF. PRODANY & WILLIAMS (1971)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6220	0.0909	0.9758	15.2046	0.9823	1.5826	0.0065
27.2300	0.1653	0.9839	31.0002	0.9866	3.7702	0.0027
40.8260	0.2320	0.9855	42.8006	0.9879	1.9746	0.0024
54.4350	0.2920	0.9856	56.4321	0.9861	1.9971	0.0005
68.0440	0.3481	0.9839	70.1325	0.9850	2.0885	0.0011
81.6520	0.4005	0.9818	79.0009	0.9843	2.6511	0.0025
95.2610	0.4480	0.9782	92.0120	0.9820	3.2490	0.0038
108.8700	0.4980	0.9722	105.0302	0.9786	3.8398	0.0064
122.4780	0.5501	0.9623	119.2051	0.9700	3.2729	0.0077
136.0880	0.6117	0.9450	129.2013	0.9626	6.8867	0.0176

WITH MIN. AAD. = 5.495560

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 423.16 K
 $K_{ij} = .1172$

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0110	0.4420	10.3194	0.2321	0.3194	0.2099
20.0000	0.0464	0.5625	19.6726	0.5422	0.3274	0.0203
30.0000	0.0826	0.6695	29.4058	0.6611	0.5942	0.0084
40.0000	0.1187	0.7220	39.2801	0.7210	0.7199	0.0010
50.0000	0.1553	0.7520	49.4491	0.7564	0.5509	0.0044
60.0000	0.1915	0.7675	59.6500	0.7783	0.3500	0.0108
70.0000	0.2278	0.7780	70.0020	0.7922	0.0020	0.0142
80.0000	0.2645	0.7800	80.5656	0.8009	0.5656	0.0209
90.0000	0.3040	0.7600	92.0112	0.8059	2.0112	0.0459
100.0000	0.3440	0.7380	103.6224	0.8073	3.6224	0.0693

WITH MIN. AAD. = 1.686372

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 423.16 K
 $K_{ij} = .1191$

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
10.0000	0.9890	0.5580	10.6012	0.7759	0.6012	0.2179
20.0000	0.9536	0.4375	20.0278	0.4723	0.0278	0.0348
30.0000	0.9174	0.3305	29.7997	0.3553	0.2003	0.0248
40.0000	0.8813	0.2780	39.6633	0.2964	0.3367	0.0184
50.0000	0.8447	0.2480	49.7672	0.2621	0.2328	0.0141
60.0000	0.8085	0.2325	59.8410	0.2415	0.1590	0.0090
70.0000	0.7722	0.2220	69.9929	0.2289	0.0071	0.0069
80.0000	0.7355	0.2200	80.2766	0.2217	0.2766	0.0017
90.0000	0.6960	0.2400	91.3011	0.2186	1.3011	0.0214
100.0000	0.6560	0.2620	102.3572	0.2193	2.3572	0.0427

WITH MIN. AAD. = 1.255001

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 423.16 K
 κ_{ij} = .0521

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0110	0.4420	10.0003	0.2473	0.0003	0.1947
20.0000	0.0464	0.5625	19.5757	0.5592	0.4243	0.0033
30.0000	0.0826	0.6695	29.4827	0.6731	0.5173	0.0036
40.0000	0.1187	0.7220	39.4703	0.7290	0.5297	0.0070
50.0000	0.1553	0.7520	49.6863	0.7611	0.3137	0.0091
60.0000	0.1915	0.7675	59.8584	0.7803	0.1416	0.0128
70.0000	0.2278	0.7780	70.0987	0.7919	0.0987	0.0139
80.0000	0.2645	0.7800	80.4557	0.7985	0.4557	0.0185
90.0000	0.3040	0.7600	91.5634	0.8014	1.5634	0.0414
100.0000	0.3440	0.7380	102.6979	0.8006	2.6979	0.0626

WITH MIN. AAD. = 1.118232

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 423.16 K
 κ_{ij} = 0.1246

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0110	0.4420	10.1856	0.3567	0.1856	0.0853
20.0000	0.0464	0.5625	18.7587	0.5748	1.2413	0.0123
30.0000	0.0826	0.6695	28.6875	0.6459	1.3125	0.0236
40.0000	0.1187	0.7220	39.1687	0.7103	0.8313	0.0117
50.0000	0.1553	0.7520	51.2136	0.7325	1.2136	0.0195
60.0000	0.1915	0.7675	61.8754	0.7896	1.8754	0.0221
70.0000	0.2278	0.7780	69.1769	0.7963	0.8231	0.0183
80.0000	0.2645	0.7800	77.2365	0.8016	2.7635	0.0216
90.0000	0.3040	0.7600	93.4521	0.7935	3.4521	0.0335
100.0000	0.3440	0.7380	103.5624	0.7567	3.5624	0.0187

WITH MIN. AAD. = 3.209692

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Methane(1) - n-Hexane(2)

TEMP. = 348.16 K

K_{ij} = .0478

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0364	0.8460	9.9324	0.8601	0.0676	0.0141
20.0000	0.0767	0.9028	19.8905	0.9200	0.1095	0.0172
30.0000	0.1165	0.9267	30.0381	0.9393	0.0381	0.0126
40.0000	0.1543	0.9385	39.9715	0.9479	0.0285	0.0094
50.0000	0.1920	0.9457	50.1786	0.9524	0.1786	0.0067
60.0000	0.2280	0.9492	60.2035	0.9546	0.2035	0.0054
70.0000	0.2625	0.9524	70.0792	0.9554	0.0792	0.0030
80.0000	0.2963	0.9555	80.0043	0.9553	0.0043	0.0002
90.0000	0.3295	0.9580	89.9835	0.9546	0.0165	0.0034
100.0000	0.3600	0.9605	99.3630	0.9532	0.6370	0.0073

WITH MIN. AAD. = .2892117

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Methane(1) - n-Hexane(2)

TEMP. = 348.16 K

K_{ij} = .0536

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(2)	Y(2)	P(atm)	Y(2)	DP	DY(2)
10.0000	0.9636	0.1540	10.0025	0.1508	0.0025	0.0032
20.0000	0.9233	0.0972	19.9437	0.0874	0.0563	0.0098
30.0000	0.8835	0.0733	30.0777	0.0671	0.0777	0.0062
40.0000	0.8457	0.0615	39.9962	0.0582	0.0038	0.0033
50.0000	0.8080	0.0543	50.1865	0.0537	0.1865	0.0006
60.0000	0.7720	0.0508	60.1936	0.0517	0.1936	0.0009
70.0000	0.7375	0.0476	70.0305	0.0512	0.0305	0.0036
80.0000	0.7037	0.0445	79.9113	0.0516	0.0887	0.0071
90.0000	0.6705	0.0420	89.8369	0.0529	0.1631	0.0109
100.0000	0.6400	0.0395	99.1382	0.0548	0.8618	0.0153

WITH MIN. AAD. = .2468151

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 348.16 K
 $K_{ij} = .0016$

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0364	0.8460	9.9081	0.8723	0.0919	0.0263
20.0000	0.0767	0.9028	19.9456	0.9264	0.0544	0.0236
30.0000	0.1165	0.9267	30.1411	0.9435	0.1411	0.0168
40.0000	0.1543	0.9385	40.0872	0.9509	0.0872	0.0124
50.0000	0.1920	0.9457	50.2697	0.9546	0.2697	0.0089
60.0000	0.2280	0.9492	60.2316	0.9562	0.2316	0.0070
70.0000	0.2625	0.9524	70.0045	0.9565	0.0045	0.0041
80.0000	0.2963	0.9555	79.7832	0.9560	0.2168	0.0005
90.0000	0.3295	0.9580	89.5702	0.9548	0.4298	0.0032
100.0000	0.3600	0.9605	98.7243	0.9531	1.2757	0.0074

WITH MIN. AAD. = .4835586

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Methane(1) - n-Hexane(2)
 TEMP. = 348.16 K
 $K_{ij} = 0.0502$

REF. SHIM & KOHN (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.0000	0.0364	0.8460	10.0254	0.8810	0.0254	0.0350
20.0000	0.0767	0.9028	19.8754	0.9302	0.1246	0.0274
30.0000	0.1165	0.9267	29.5416	0.9467	0.4584	0.0200
40.0000	0.1543	0.9385	39.1350	0.9531	0.8650	0.0146
50.0000	0.1920	0.9457	50.0679	0.9578	0.0679	0.0121
60.0000	0.2280	0.9492	58.8776	0.9594	1.1224	0.0102
70.0000	0.2625	0.9524	71.0325	0.9615	1.0325	0.0091
80.0000	0.2963	0.9555	79.6784	0.9689	0.3216	0.0134
90.0000	0.3295	0.9580	90.1254	0.9676	0.1254	0.0096
100.0000	0.3600	0.9605	99.3657	0.9684	0.6343	0.0079

WITH MIN. AAD. = 0.922460

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Ethane(1) - Propane(2)
 TEMP. = 333.16 K
 $K_{ij} = 0$

REF. MATSCHKE & THODOS (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
23.8140	0.0711	0.1400	24.0313	0.1346	0.2173	0.0054
30.6180	0.2300	0.3670	30.6404	0.3570	0.0224	0.0100
37.4220	0.3780	0.5150	37.1909	0.5032	0.2311	0.0118
44.2260	0.5150	0.6180	43.5966	0.6051	0.6294	0.0129

WITH MIN. AAD. = .7565909

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Ethane(1) - Propane(2)
 TEMP. = 333.16 K
 $K_{ij} = 0$

REF. MATSCHKE & THODOS (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
23.8140	0.0711	0.1400	24.4157	0.1306	0.6017	0.0094
30.6180	0.2300	0.3670	31.4295	0.3474	0.8115	0.0196
37.4220	0.3780	0.5150	37.9887	0.4897	0.5667	0.0253
44.2260	0.5150	0.6180	44.7958	0.6002	0.5698	0.0178

WITH MIN. AAD. = 1.994950

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Ethane(1) - Propane(2)
 TEMP. = 333.16 K
 $K_{ij} = 0$

REF. MATSCHKE & THODOS (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
23.8140	0.0711	0.1400	23.7566	0.1365	0.0574	0.0035
30.6180	0.2300	0.3670	30.4370	0.3600	0.1810	0.0070
37.4220	0.3780	0.5150	37.2010	0.5106	0.2210	0.0044
44.2260	0.5150	0.6180	43.6217	0.6111	0.6043	0.0069

WITH MIN. AAD. = 0.697286

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - Propane(2)
 TEMP. = 333.16 K
 $K_{ij} = 0$

REF. MATSCHKE & THODOS (1962)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
23.8140	0.0711	0.1400	24.2354	0.1337	0.4214	0.0063
30.6180	0.2300	0.3670	31.2106	0.3620	0.5926	0.0050
37.4220	0.3780	0.5150	38.0024	0.5067	0.5804	0.0083
44.2260	0.5150	0.6180	43.5204	0.6089	0.7056	0.0091

WITH MIN. AAD. = 1.712853

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 344.49 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
12.9956	0.0367	0.1771	13.0635	0.1339	0.0679	0.0432
19.6636	0.1697	0.4513	19.8940	0.4266	0.2305	0.0247
28.4407	0.3285	0.6201	28.6868	0.6023	0.2461	0.0178
34.9045	0.4333	0.6962	34.9152	0.6735	0.0107	0.0227
41.3683	0.5366	0.7382	41.3899	0.7240	0.0215	0.0142

WITH MIN. AAD. = .528426

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 344.49 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
12.9956	0.0367	0.1771	13.4493	0.1294	0.4537	0.0477
19.6636	0.1697	0.4513	20.3451	0.4152	0.6815	0.0361
28.4407	0.3285	0.6201	29.2357	0.5882	0.7950	0.0319
34.9045	0.4333	0.6962	35.5316	0.6581	0.6271	0.0381
41.3683	0.5366	0.7382	42.1024	0.7230	0.7341	0.0152

WITH MIN. AAD. = 2.664686

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 344.49 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
12.9956	0.0367	0.1771	12.8360	0.1378	0.1596	0.0393
19.6636	0.1697	0.4513	19.7761	0.4332	0.1125	0.0181
28.4407	0.3285	0.6201	28.6759	0.6068	0.2352	0.0133
34.9045	0.4333	0.6962	34.9600	0.6766	0.0555	0.0196
41.3683	0.5366	0.7382	41.4784	0.7257	0.1101	0.0125

WITH MIN. AAD. = .610405

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 344.49 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
12.9956	0.0367	0.1771	12.6751	0.1279	0.3206	0.0492
19.6636	0.1697	0.4513	19.1007	0.4258	0.5628	0.0255
28.4407	0.3285	0.6201	28.1650	0.6141	0.2757	0.0060
34.9045	0.4333	0.6962	35.1009	0.6901	0.1964	0.0061
41.3683	0.5366	0.7382	42.7257	0.7412	1.3574	0.0030

WITH MIN. AAD. = 2.028487

จุฬาลงกรณ์มหาวิทยาลัย

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 311.27 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.5462	0.1782	0.5524	11.2105	0.5627	0.6643	0.0103
22.1810	0.4841	0.8277	23.1654	0.8142	0.9843	0.0135
30.5500	0.6648	0.8879	31.4249	0.8817	0.8749	0.0062
39.7354	0.8314	0.9267	40.3813	0.9299	0.6459	0.0032
45.1786	0.9135	0.9588	45.6917	0.9539	0.5132	0.0049

WITH MIN. AAD. = 3.272332

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 311.27 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.5462	0.1782	0.5524	11.4907	0.5508	0.9445	0.0016
22.1810	0.4841	0.8277	23.6191	0.8047	1.4381	0.0230
30.5500	0.6648	0.8879	32.0593	0.8736	1.5093	0.0143
39.7354	0.8314	0.9267	41.2843	0.9227	1.5489	0.0040
45.1786	0.9135	0.9588	45.5316	0.9533	0.3530	0.0055

WITH MIN. AAD. = 5.011823

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 311.27 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.5462	0.1782	0.5524	11.1183	0.5706	0.5721	0.0182
22.1810	0.4841	0.8277	23.1030	0.8170	0.9220	0.0107
30.5500	0.6648	0.8879	31.3330	0.8829	0.7830	0.0050
39.7354	0.8314	0.9267	40.3564	0.9286	0.6210	0.0019
45.1786	0.9135	0.9588	45.5883	0.9501	0.4097	0.0087

WITH MIN. AAD. = 2.922822

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - i-Butane(2)
 TEMP. = 311.27 K
 $K_{ij} = 0$

REF. BESSERER & ROBINSON (1973)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
10.5462	0.1782	0.5524	10.3057	0.5465	0.2405	0.0059
22.1810	0.4841	0.8277	22.0556	0.8255	0.1254	0.0022
30.5500	0.6648	0.8879	31.0719	0.8973	0.5220	0.0094
39.7354	0.8314	0.9267	41.1099	0.9417	1.3745	0.0150
45.1786	0.9135	0.9588	46.8646	0.9603	1.6860	0.0015

WITH MIN. AAD. = 2.349154

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Ethane(1) - n-Pentane(2)

TEMP. = 277.6 K

K_{ij} = .0069

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.2891	0.9504	6.8372	0.9603	0.0332	0.0099
10.2060	0.4316	0.9659	10.2649	0.9752	0.0589	0.0093
17.0100	0.6950	0.9838	17.0073	0.9882	0.0027	0.0044
23.8140	0.9235	0.9960	23.6940	0.9962	0.1200	0.0002

WITH MIN. AAD. = .396215

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Ethane(1) - n-Pentane(2)

TEMP. = 277.6 K

K_{ij} = 0

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.2891	0.9504	6.7294	0.9546	0.0746	0.0042
10.2060	0.4316	0.9659	10.1756	0.9718	0.0304	0.0059
17.0100	0.6950	0.9838	17.1695	0.9868	0.1595	0.0030
23.8140	0.9235	0.9960	24.3103	0.9959	0.4963	0.0001

WITH MIN. AAD. = 1.103913

PATEL-TEJA EQUATION OF STATE

MIXTURE : Ethane(1) - n-Pentane(2)

TEMP. = 277.6 K

K_{ij} = 0

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.2891	0.9504	6.7476	0.9634	0.0564	0.0130
10.2060	0.4316	0.9659	10.1448	0.9770	0.0612	0.0111
17.0100	0.6950	0.9838	16.8310	0.9890	0.1790	0.0052
23.8140	0.9235	0.9960	23.4603	0.9965	0.3537	0.0005

WITH MIN. AAD. = .99142

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 277.6 K
 $K_{ij} = 0$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.2891	0.9504	6.8316	0.9622	0.0276	0.0118
10.2060	0.4316	0.9659	10.4077	0.9778	0.2017	0.0119
17.0100	0.6950	0.9838	17.5690	0.9909	0.5590	0.0071
23.8140	0.9235	0.9960	23.9257	0.9976	0.1117	0.0016

WITH MIN. AAD. = 1.534444

SOAVE-REDLICH-KWONG EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 344.27 K
 $K_{ij} = .0055$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0755	0.5855	7.1335	0.5752	0.3295	0.0103
13.6080	0.1900	0.7692	13.8569	0.7710	0.2489	0.0018
20.4120	0.2982	0.8391	20.5929	0.8388	0.1809	0.0003
27.2160	0.3991	0.8722	27.2465	0.8722	0.0305	0.0000
34.0200	0.4940	0.8909	33.8584	0.8918	0.1616	0.0009
40.8240	0.5804	0.9032	40.2032	0.9037	0.6208	0.0005
47.6280	0.6579	0.9091	46.1657	0.9108	1.4623	0.0017

WITH MIN. AAD. = 1.819469

PENG-ROBINSON EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 344.27 K
 $K_{ij} = 0$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0755	0.5855	7.1873	0.5550	0.3833	0.0305
13.6080	0.1900	0.7692	13.7957	0.7559	0.1877	0.0133
20.4120	0.2982	0.8391	20.4725	0.8270	0.0605	0.0121
27.2160	0.3991	0.8722	27.1226	0.8623	0.0934	0.0099
34.0200	0.4940	0.8909	33.7890	0.8829	0.2310	0.0080
40.8240	0.5804	0.9032	40.2393	0.8951	0.5847	0.0081
47.6280	0.6579	0.9091	46.3289	0.9020	1.2991	0.0071

WITH MIN. AAD. = 1.784492

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 344.27 K
 $K_{ij} = 0$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0755	0.5855	7.0205	0.5932	0.2165	0.0077
13.6080	0.1900	0.7692	13.8350	0.7822	0.2270	0.0130
20.4120	0.2982	0.8391	20.6429	0.8462	0.2309	0.0071
27.2160	0.3991	0.8722	27.3478	0.8774	0.1318	0.0052
34.0200	0.4940	0.8909	33.9917	0.8955	0.0283	0.0046
40.8240	0.5804	0.9032	40.3511	0.9064	0.4729	0.0032
47.6280	0.6579	0.9091	46.3158	0.9127	1.3122	0.0036

WITH MIN. AAD. = 1.49466

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 344.27 K
 $K_{ij} = 0$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
6.8040	0.0755	0.5855	6.7057	0.5584	0.0983	0.0271
13.6080	0.1900	0.7692	13.1468	0.7683	0.4612	0.0009
20.4120	0.2982	0.8391	20.0931	0.8432	0.3189	0.0041
27.2160	0.3991	0.8722	27.4728	0.8803	0.2568	0.0081
34.0200	0.4940	0.8909	35.3508	0.9013	1.3308	0.0104
40.8240	0.5804	0.9032	43.4171	0.9128	2.5931	0.0096
47.6280	0.6579	0.9091	51.4374	0.9175	3.8094	0.0084

WITH MIN. AAD. = 3.657385

SOAVE-REDLICH-KWONG EQUATION OF STATE

MIXTURE : Ethane(1) - n-Pentane(2)

TEMP. = 410.94 K

K_{ij} = .0278

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6080	0.0084	0.0481	13.6604	0.0477	0.0524	0.0004
20.4120	0.0821	0.3257	20.6897	0.3175	0.2777	0.0082
27.2160	0.1520	0.4612	27.4684	0.4489	0.2524	0.0123
34.0200	0.2197	0.5402	34.1022	0.5251	0.0822	0.0151
40.8240	0.2842	0.5874	40.4249	0.5714	0.3991	0.0160
47.6280	0.3426	0.6107	46.0798	0.5982	1.5482	0.0125

WITH MIN. AAD. = 1.190366

PENG-ROBINSON EQUATION OF STATE

MIXTURE : Ethane(1) - n-Pentane(2)

TEMP. = 410.94 K

K_{ij} = .0139

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6080	0.0084	0.0481	14.0242	0.0442	0.4162	0.0039
20.4120	0.0821	0.3257	20.8362	0.3000	0.4242	0.0257
27.2160	0.1520	0.4612	27.4303	0.4279	0.2143	0.0333
34.0200	0.2197	0.5402	33.8957	0.5027	0.1243	0.0375
40.8240	0.2842	0.5874	40.0605	0.5477	0.7635	0.0397
47.6280	0.3426	0.6107	45.5505	0.5730	2.0775	0.0377

WITH MIN. AAD. = 2.087002

PATEL-TEJA EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 410.94 K
 $K_{ij} = .0173$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6080	0.0084	0.0481	13.2625	0.0500	0.3455	0.0019
20.4120	0.0821	0.3257	20.4430	0.3270	0.0310	0.0013
27.2160	0.1520	0.4612	27.3592	0.4581	0.1432	0.0031
34.0200	0.2197	0.5402	34.1177	0.5326	0.0977	0.0076
40.8240	0.2842	0.5874	40.5484	0.5771	0.2756	0.0103
47.6280	0.3426	0.6107	46.2876	0.6023	1.3404	0.0084

WITH MIN. AAD. = 1.165621

SCHMIDT-WENZEL EQUATION OF STATE
 MIXTURE : Ethane(1) - n-Pentane(2)
 TEMP. = 410.94 K
 $K_{ij} = .0125$

REF. REAMER ET AL. (1960)

EXPERIMENTAL			CALCULATED		DEVIATIONS	
P(atm)	X(1)	Y(1)	P(atm)	Y(1)	DP	DY(1)
13.6080	0.0084	0.0481	13.4362	0.0483	0.1718	0.0002
20.4120	0.0821	0.3257	20.4977	0.3228	0.0857	0.0029
27.2160	0.1520	0.4612	27.5625	0.4569	0.3465	0.0043
34.0200	0.2197	0.5402	34.7452	0.5338	0.7252	0.0064
40.8240	0.2842	0.5874	41.8792	0.5788	1.0552	0.0086
47.6280	0.3426	0.6107	48.5612	0.6014	0.9332	0.0093

WITH MIN. AAD. = 1.605173

Vita

Mr.Pipat Mahawattanangul was born on September 17, 1965 in Bangkok. he recieved a Bechelor's Degree in Mechanical Engineering from Chulalongkorn University in 1985.

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